Learning the structure of probabilistic graphical model with infinite directed acyclic graphs

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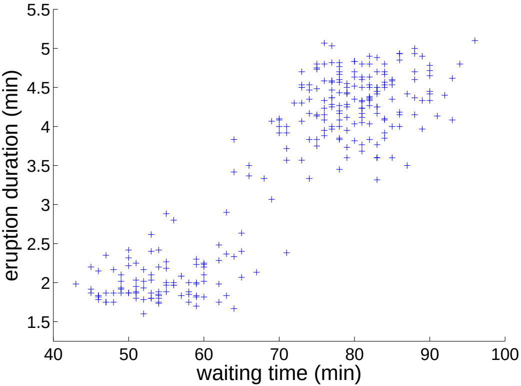
Introduction

Task: Discovering structure in data

Motivation: Predictions, reproduce data, knowledge discovery, etc.

Approach: Bayesian learning considering all possible structures

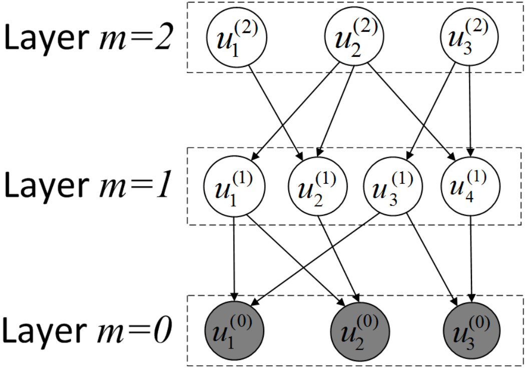


Outline of the talk

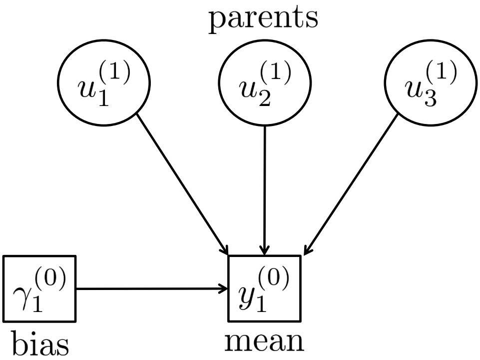
- The belief network
- Learning the structure
- Infinite dimensional layers (IBP)
- Infinitely deep networks (CIBP)
- Jumping-connections (eCIBP)
- Results on learning belief networks

Belief networks

Structure of the belief network

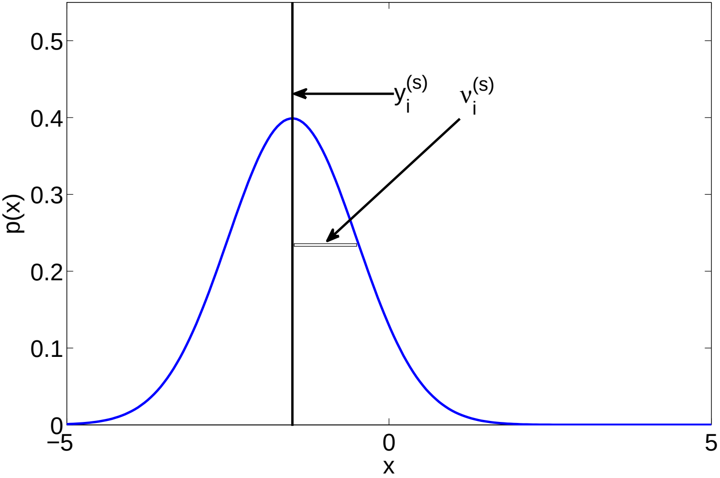


Unit activations - weighted sum

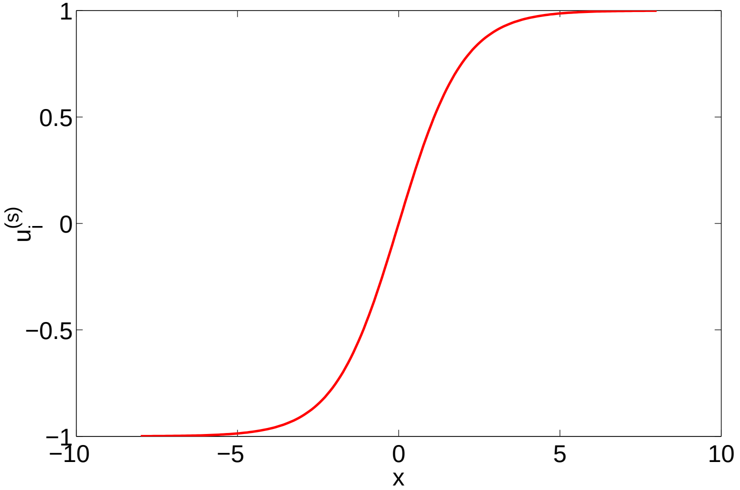


$$y_i^{(s)} = \gamma_i^{(s)} + \sum_k Z_{i,k}^{(s,m)} W_{i,k}^{(s,m)} u_k^{(m)}$$

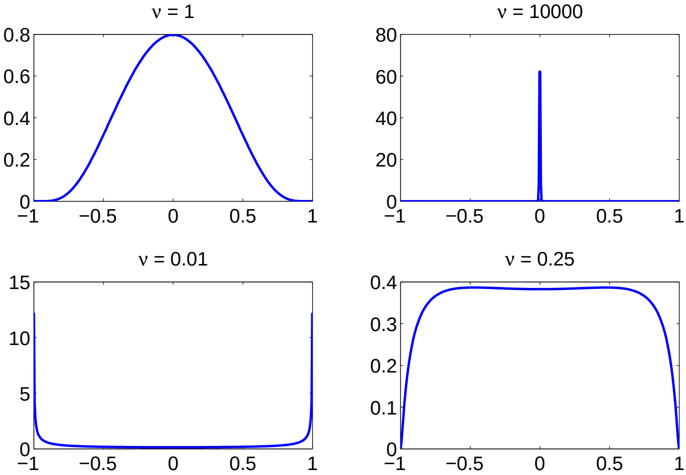
Unit activations - Gaussian random variable



Unit activations - sigmoid transformation



Conditional activation probabilities



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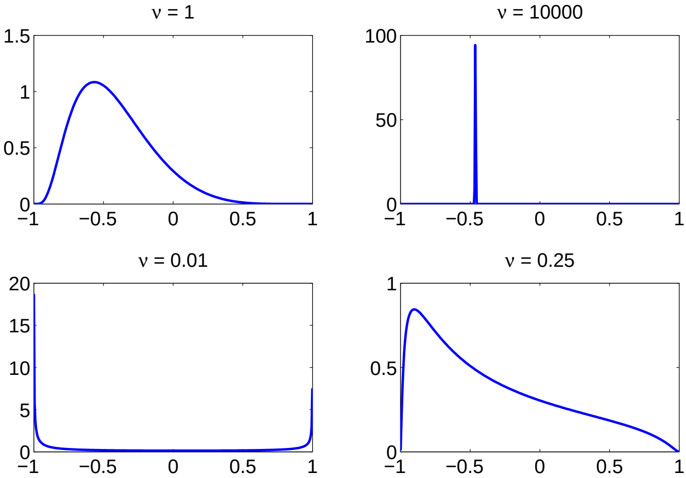
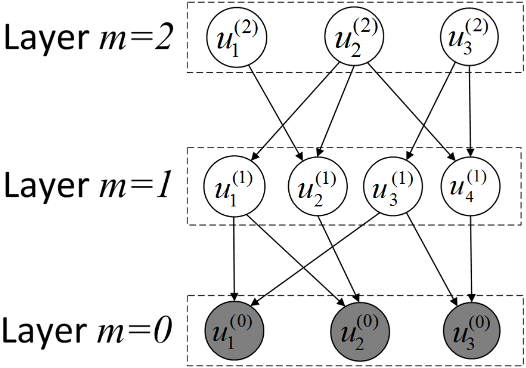
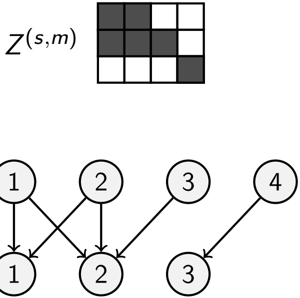


Learning the structure

Structure of the belief network

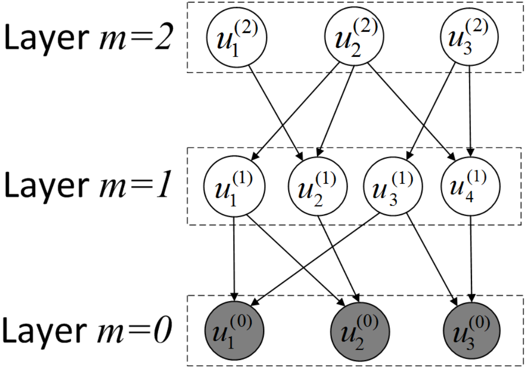


Structure as binary matrix



Infinite dimensional layer

Structure of the belief network



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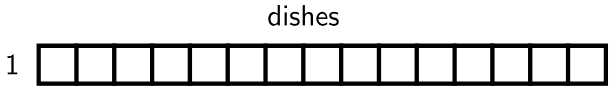

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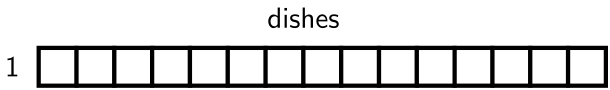

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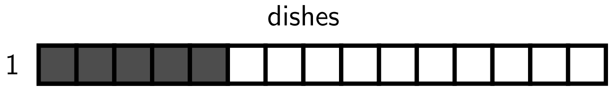

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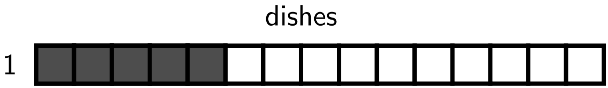

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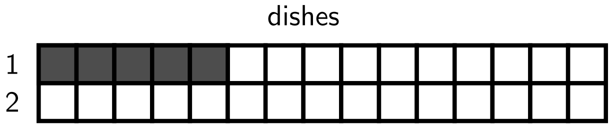

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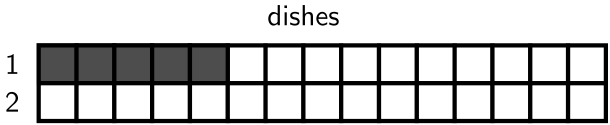

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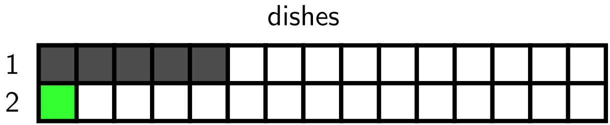

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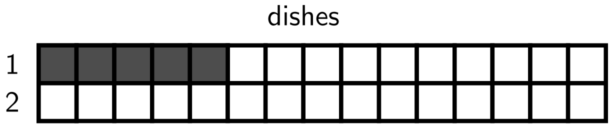

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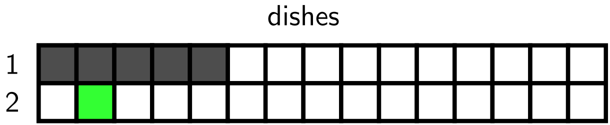

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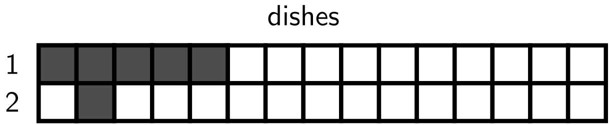

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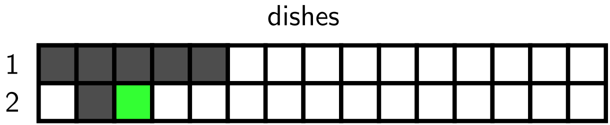

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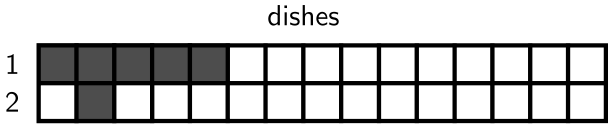

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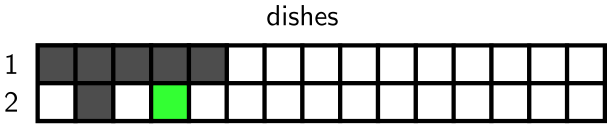

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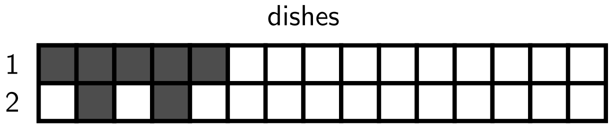

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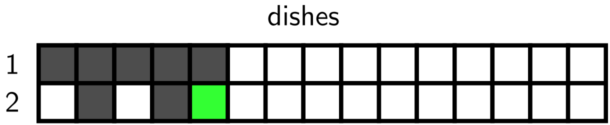

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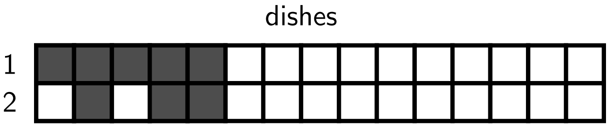

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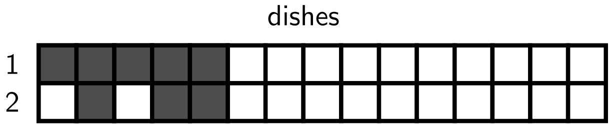

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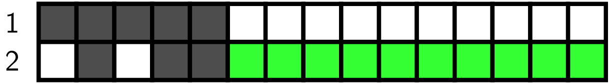

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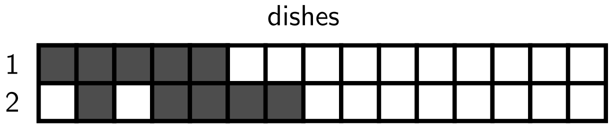

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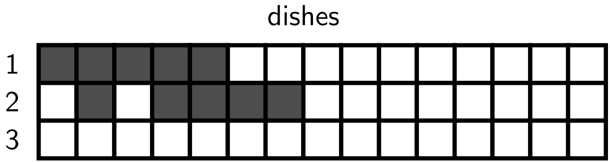

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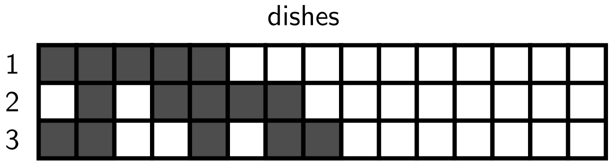

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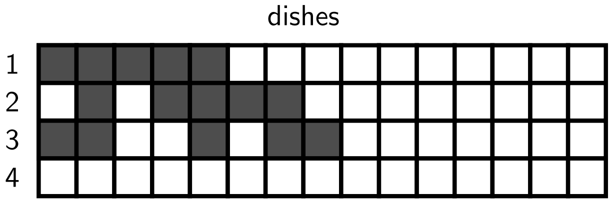

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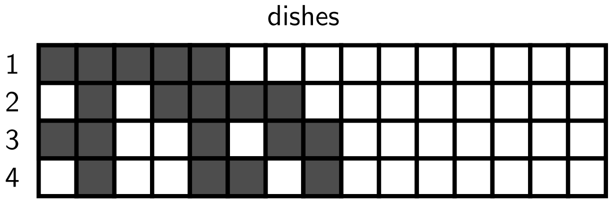

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We can generate a $K^{(m-1)} \times \infty$ binary matrix $Z^{(m-1,m)}$ by

- sampling an infinite discrete measure $B^{(m)} \sim \mathrm{BP}(\beta, B_0^{(m)})$
- draw samples from a Bernoulli process $Z_{i,\cdot}^{(m-1,m)} \sim \mathrm{BeP}(B^{(m)})$

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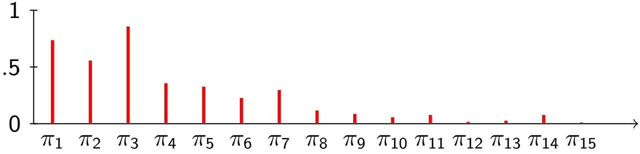

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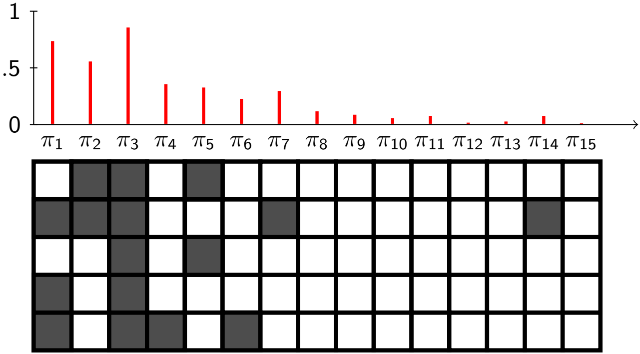
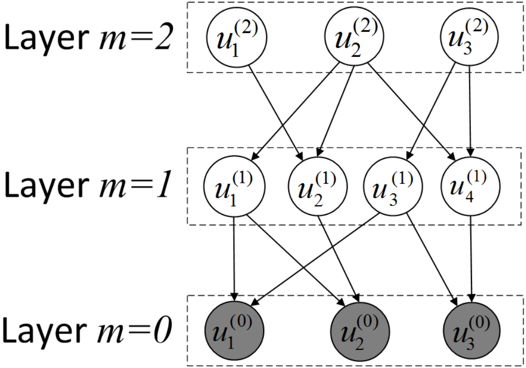


Infinitely deep network

Structure of the belief network



The cascading indian buffet process

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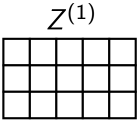
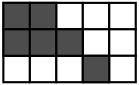


The cascading indian buffet process

Assume infinitely many layer $M \to \infty$ and apply IBP recursively

- N customers enter the first restaurant and apply the IBP
- The $K^{(m)}$ unique dishes sampled in a restaurant corresponds to the number of customers entering the next

$Z^{(1)}$



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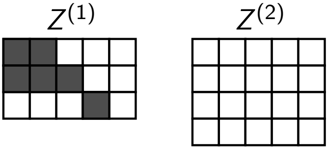

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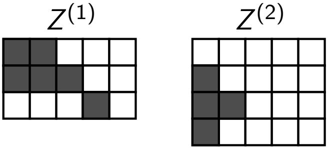

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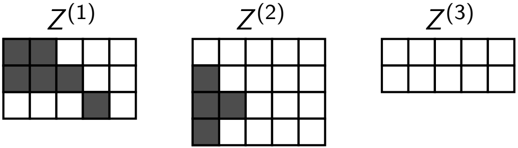

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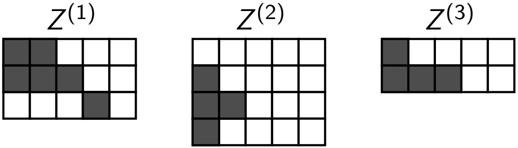

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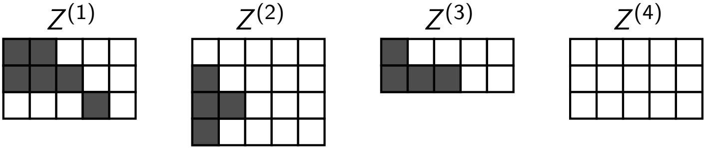

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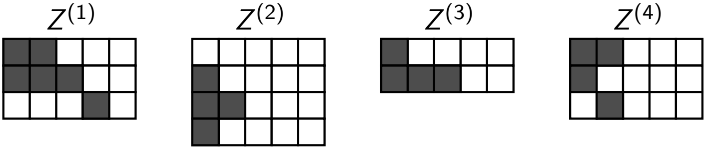

Directed acyclic graph with CIBP

The binary value $Z_{i,k}^{(s,m)}$ indicates whether an edge is leaving the k^{th} nodes in layer m to connect to the i^{th} nodes in layer s.

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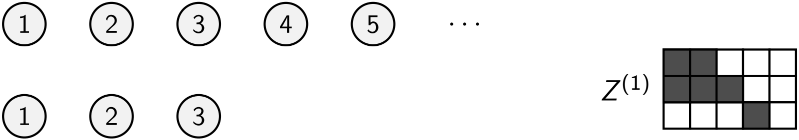

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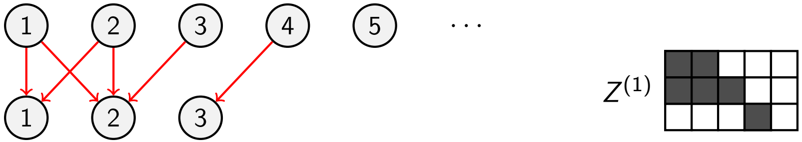

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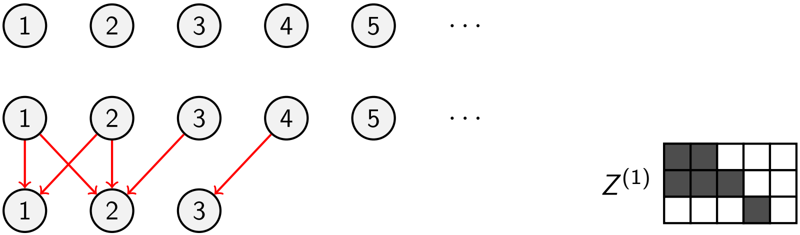

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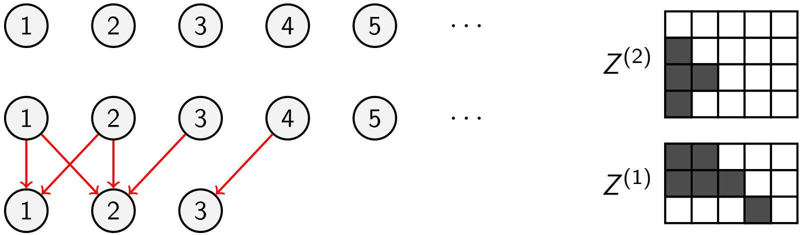

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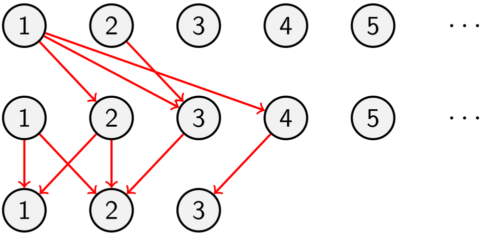

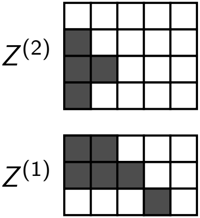

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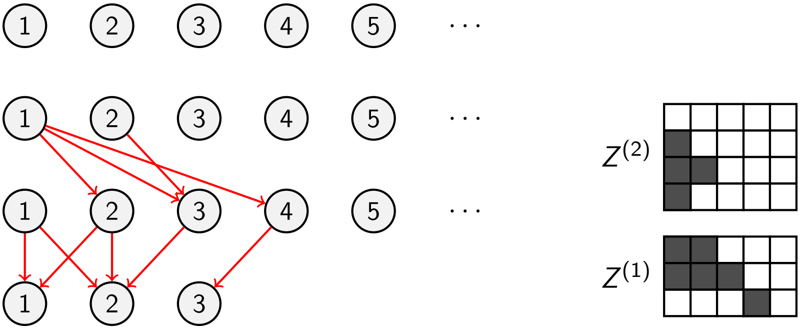

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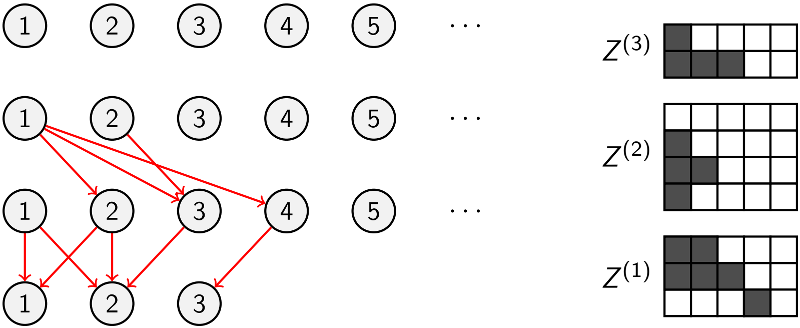

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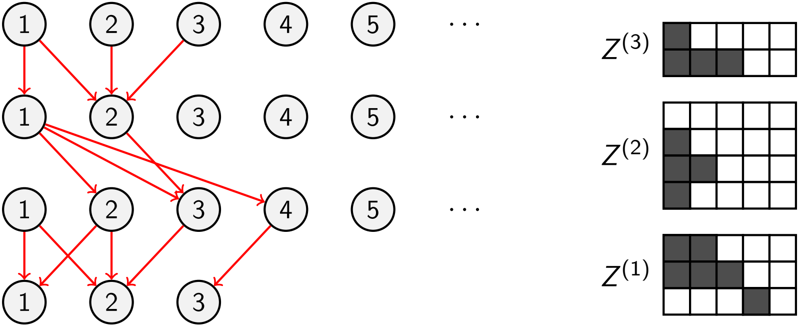

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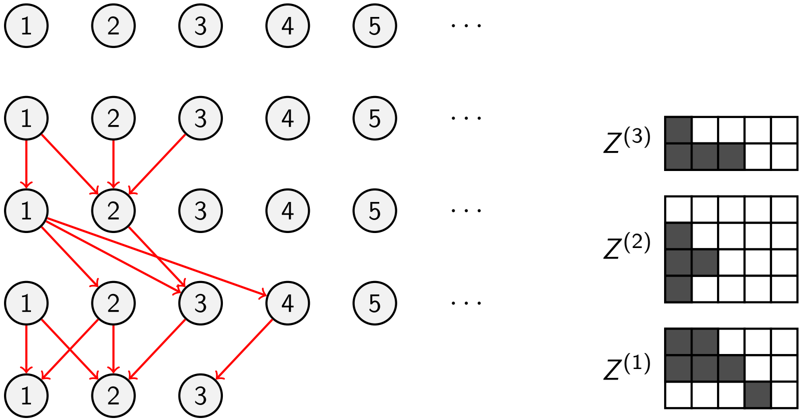

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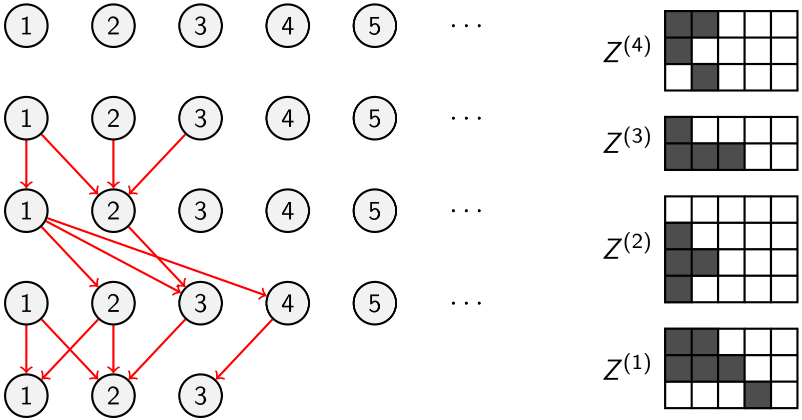

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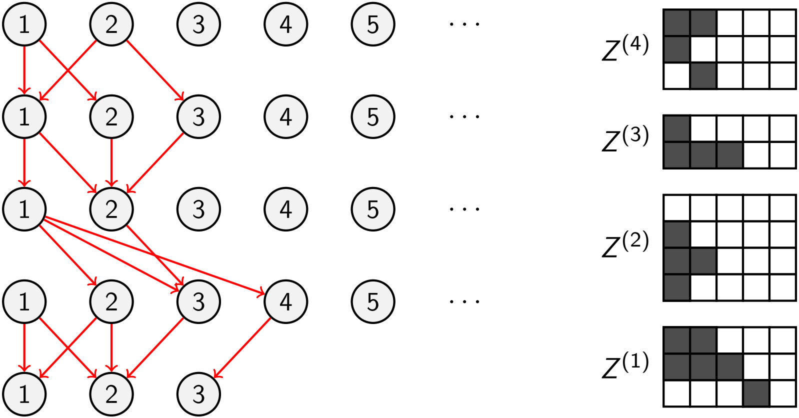
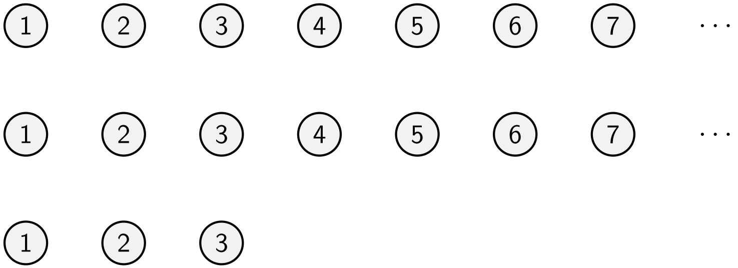


Beta process representation for CIBP

To generate sequence of binary matrices, we can recursively:

- draw a measure $B^{(m)}$ where $\pi_k^{(m)}$ is the popularity of dish $\theta_k^{(m)}$.
- construct $Z^{(m-1,m)}$ by sampling $Z_{i,\cdot}^{(m-1,m)} \sim \text{BeP}(B^{(m)})$ for the $K^{(m-1)}$ customers entering this restaurant.



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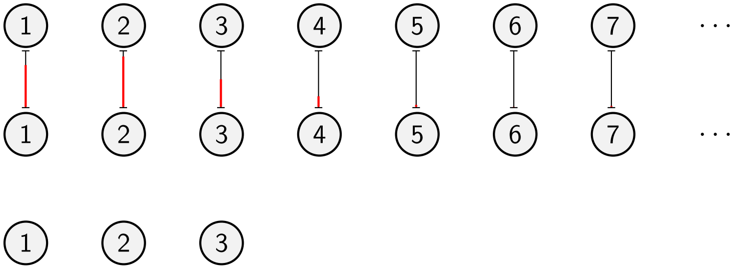

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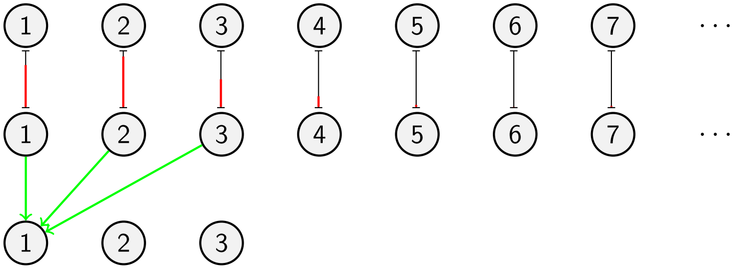

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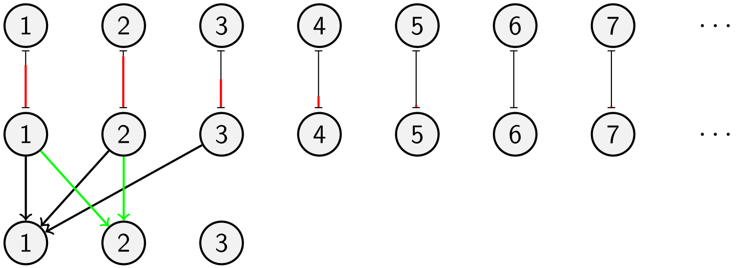

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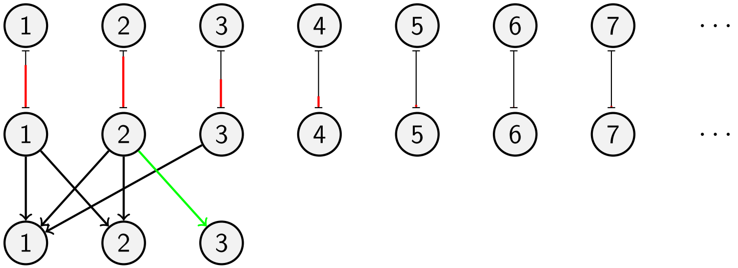

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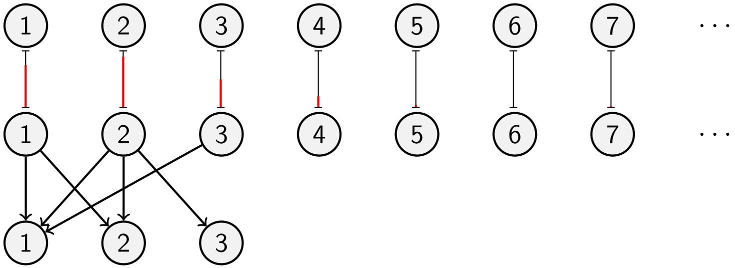

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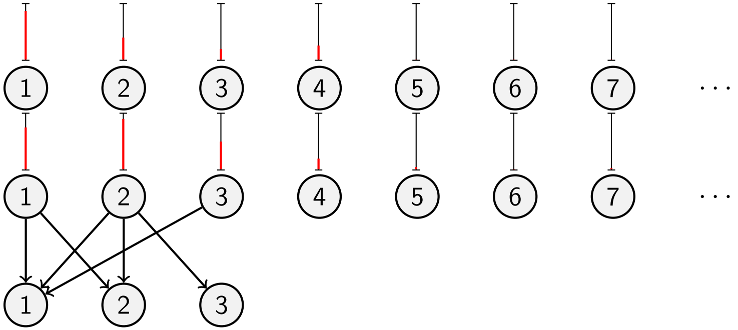

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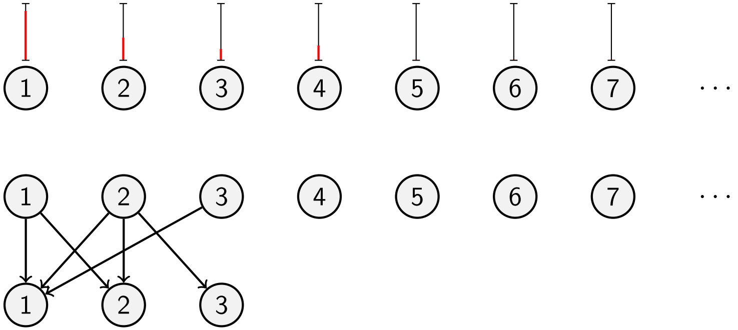

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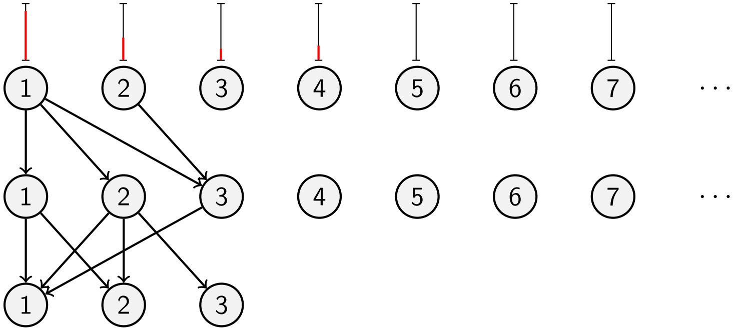
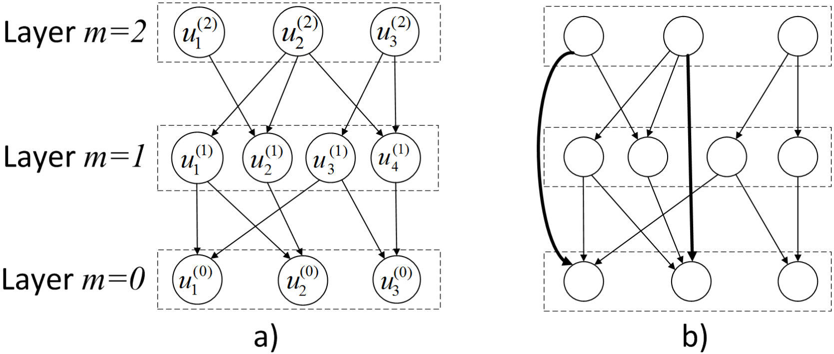


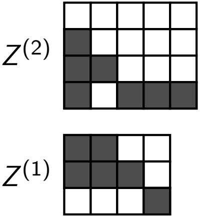
Extending the CIBP

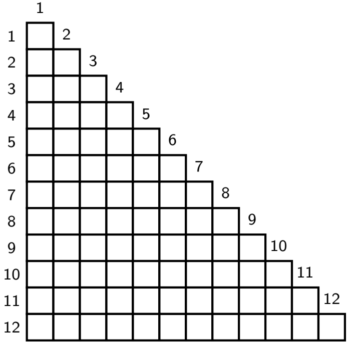
Structure of the belief network

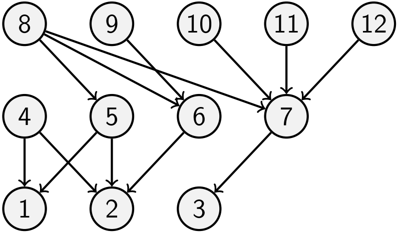


Triangular binary matrix representation

- Layer exchangeability is ensured by crosses.
- Adjacency matrix is IBP subdiagonal by blocks.
- Hierarchical BP allows jumping connections.







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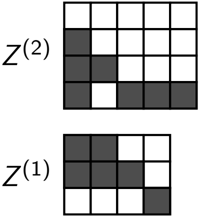

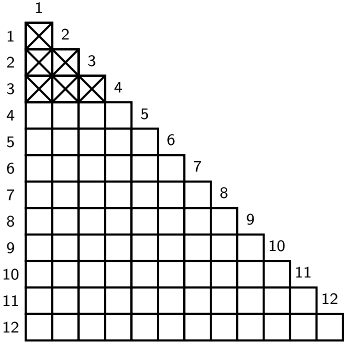

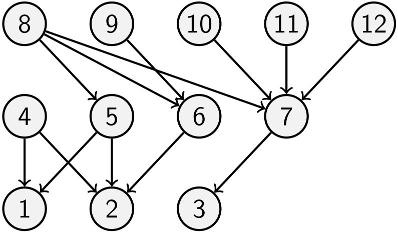

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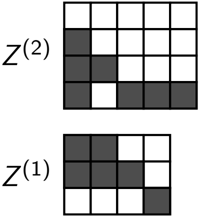

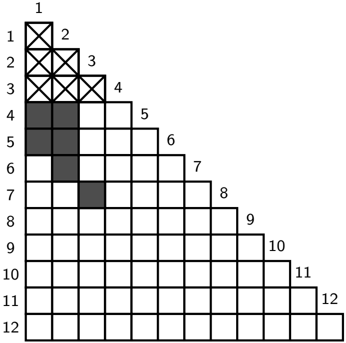

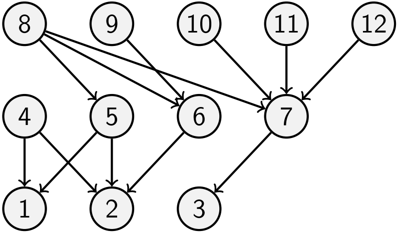

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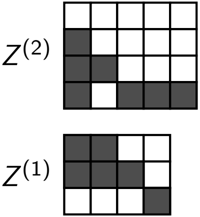

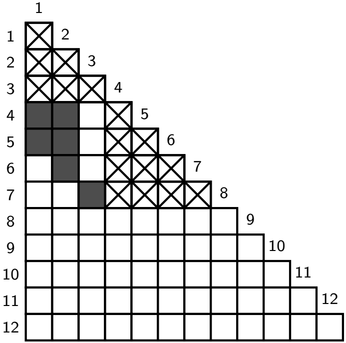

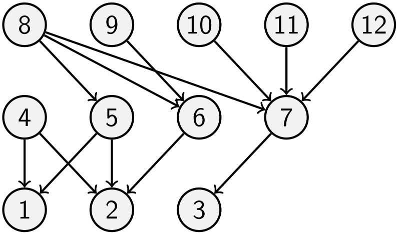

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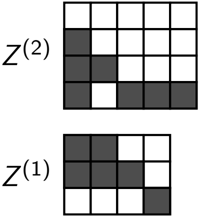

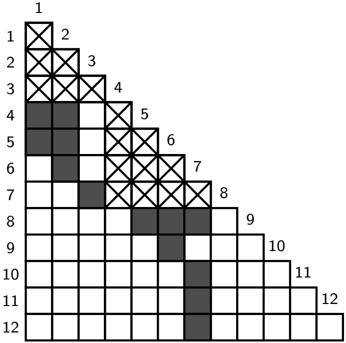

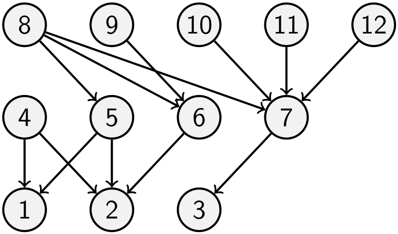

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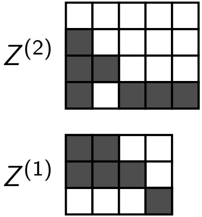

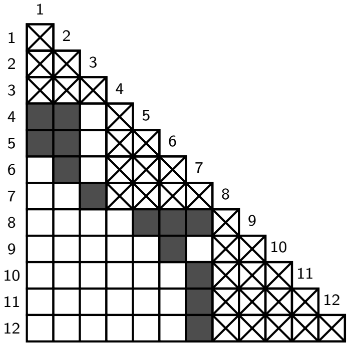

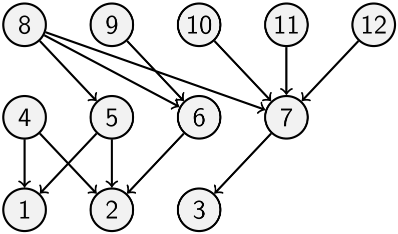

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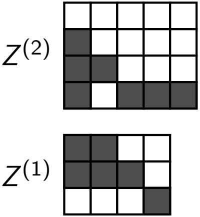

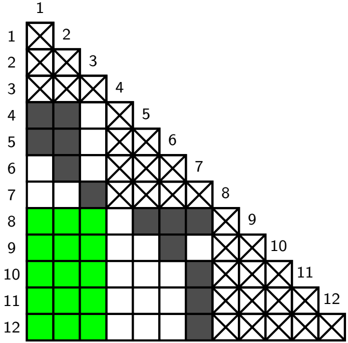

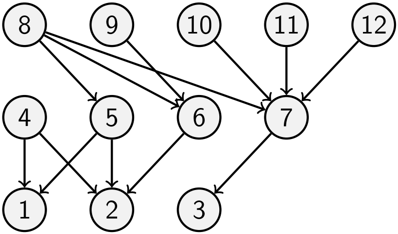

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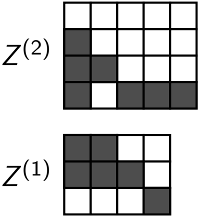
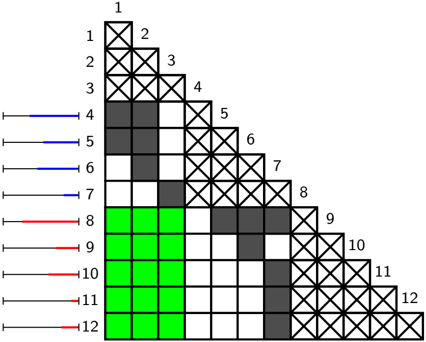
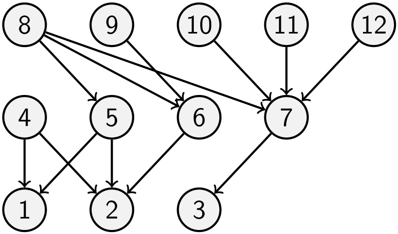






Extended cascading Indian buffet process metaphor

Every customers are associated to an Indian buffet restaurant

- The $K^{(m-1)}$ **customers** from restaurant $m-1$ enter restaurant m and select dishes according to the usual IBP.
- Next, the $K^{(s)}$ **visitors** from previous restaurants $s < m-1$ enters and select dishes according to probability:

$$\frac{\beta'}{\beta' + K(s)} \frac{n_k^{(m)}}{\beta + K(m)} + \frac{n_k^{(s,m)}}{\beta' + K(s)}$$

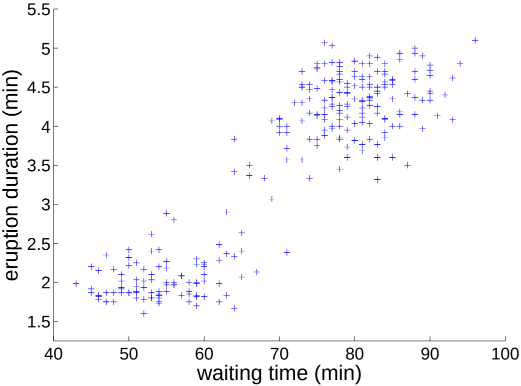
where $n_k^{(s,m)}$ denote the number of times dish k has been selected by preceding members of its visiting group s.

Results

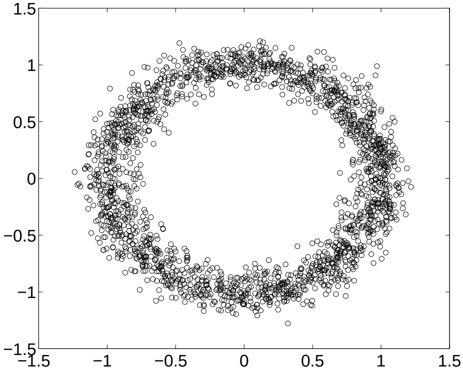
Experiments

- Learn the generative process of the data
- Produce fantasy data with posterior models
- Measure the testset/fantasy divergence
- Evaluate the structural complexity

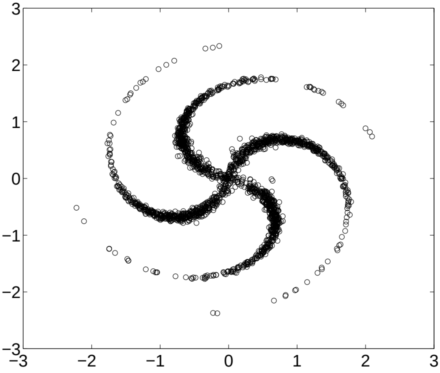
Dataset - Geyser



Dataset - Ring



Dataset - Pinwheel



More datasets

- Iris : 4 continuous dimensions
- Abalone : 7 continuous + 2 discretes dimensions

Results - Divergence

Table: Kullback-Leibler divergence estimations

Dataset	CIBP	eCIBP	DPMoG	KDE
Ring	0.049 ± 0.055	$\mathbf{0.030} \pm \mathbf{0.034}$	0.051 ± 0.029	0.085 ± 0.034
Pinwheel	0.162 ± 0.049	0.161 ± 0.041	$\mathbf{0.154} \pm \mathbf{0.080}$	0.216 ± 0.043
Geyser	0.078 ± 0.150	$\mathbf{0.075} \pm \mathbf{0.145}$	0.077 ± 0.120	0.143 ± 0.099
Iris	0.207 ± 0.333	$\mathbf{0.177} \pm \mathbf{0.280}$	0.231 ± 0.269	0.305 ± 0.227
Abalone	0.074 ± 0.080	$\mathbf{0.070} \pm \mathbf{0.108}$	4.760 ± 0.220	2.934 ± 0.134

Results - Structure complexity

Table: Total number of units

Dataset	CIBP	eCIBP
Ring	11.6 ± 4.1	$\mathbf{9.3} \pm \mathbf{3.2}$
Pinwheel	22.4 ± 3.0	$\mathbf{19.7} \pm \mathbf{1.6}$
Geyser	9.1 ± 4.3	$\mathbf{8.7} \pm \mathbf{3.9}$
Iris	14.2 ± 4.4	$\mathbf{10.3} \pm \mathbf{3.4}$
Abalone	54.2 ± 12.3	$\mathbf{45.2} \pm \mathbf{11.2}$

Results - Structure complexity

Table: Total number of edges

Dataset	CIBP	eCIBP
Ring	$\mathbf{20.3 \pm 8.4}$	20.6 ± 7.3
Pinwheel	105.4 ± 11.1	$\mathbf{104.1 \pm 9.3}$
Geyser	$\mathbf{13.1 \pm 9.9}$	$\mathbf{13.1 \pm 9.5}$
Iris	28.4 ± 11.4	$\mathbf{20.5 \pm 7.2}$
Abalone	233.8 ± 23.0	$\mathbf{210.4 \pm 23.8}$

End