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Inter-University Research Institute Corporation /
Research Organization of Information and Systems
National Institute of Informatics

Machine Learning and Information Geometry

Introduction to Intelligent Systems Science II

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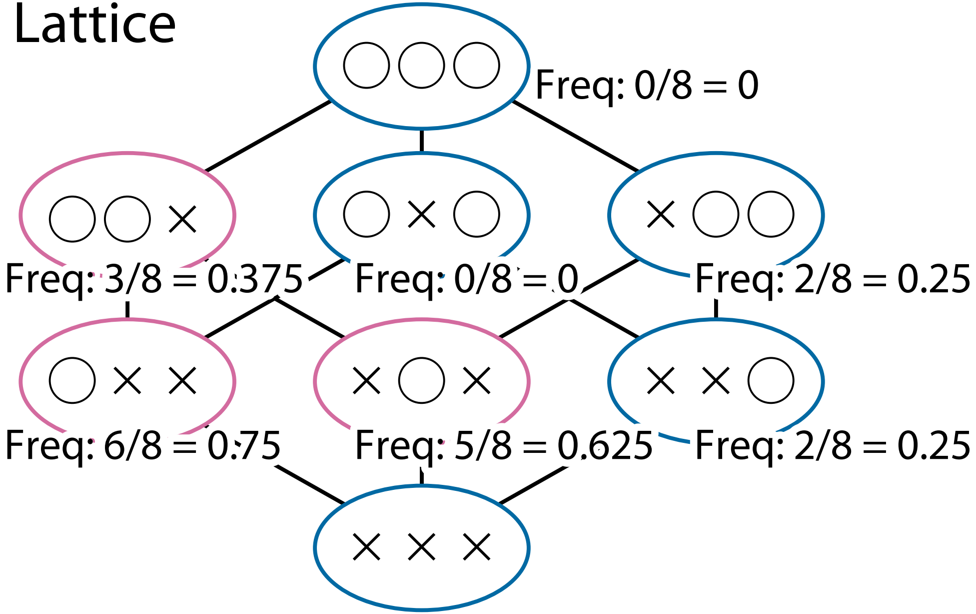
Learning Hierarchical Distribution (1/2)

Dataset

	Bread	Milk	Apple
ID 1	○	×	×
ID 2	○	○	×
ID 3	○	×	×
ID 4	×	○	○
ID 5	×	○	○
ID 6	○	○	×
ID 7	○	×	×
ID 8	○	○	×

Lattice

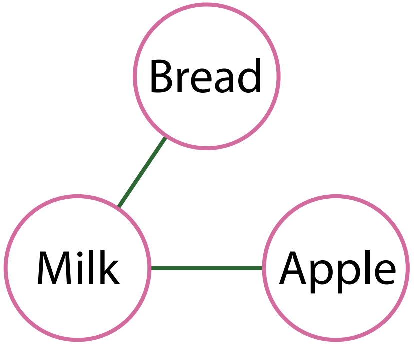


Learning Hierarchical Distribution (2/2)

$$\log(\text{prob.}) = -10.41 + 9.43[\text{Bread}] + 8.52[\text{Milk}] - 9.84[\text{Apple}] - 9.03[\text{Bread\&Milk}] + 9.43[\text{Milk\&Apple}]$$

MLE

Boltzmann machine



Bread	Milk	Apple	Prob. from data	Learned prob.
×	×	×	?	0.0000300109
◯	×	×	0.375	0.3749599867
×	◯	×	?	0.1499903954
×	×	◯	?	0.0000000016
◯	◯	×	0.375	0.2250096042
◯	×	◯	?	0.0000200043
×	◯	◯	0.25	0.0999895960
◯	◯	◯	?	0.1500004008

Matrix Balancing

$$\begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix}$$

Matrix Balancing

Find r and s:

(Make doubly stochastic matrix)

$$\begin{bmatrix} r_1 & 0 \\ 0 & r_2 \end{bmatrix} \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix} \begin{bmatrix} s_1 & 0 \\ 0 & s_2 \end{bmatrix}$$

$$= \begin{bmatrix} r_1 s_1 p_{11} & r_1 s_2 p_{12} \\ r_2 s_1 p_{21} & r_2 s_2 p_{22} \end{bmatrix} \begin{array}{l} \rightarrow \sum_j r_1 s_j p_{1j} = 1 \\ \rightarrow \sum_j r_2 s_j p_{2j} = 1 \end{array}$$

$$\downarrow \qquad \downarrow$$

$$\sum_i r_i s_1 p_{i1} = 1 \quad \sum_i r_i s_2 p_{i2} = 1$$

Sinkhorn-Knopp Algorithm

- Alternately rescale all rows and columns of a matrix P to sum to 1
- Commonly used to compute entropy-regularized Optimal transport (Wasserstein distance)
  - [Cuturi, 2013]

Revisit Matrix Balancing

$$\begin{array}{ccc} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{array}$$

[Sugiyama, Nakahara, Tsuda, ICML2017]

Introduce η

η_{11} η_{12} η_{13}

p_{11} p_{12} p_{13}

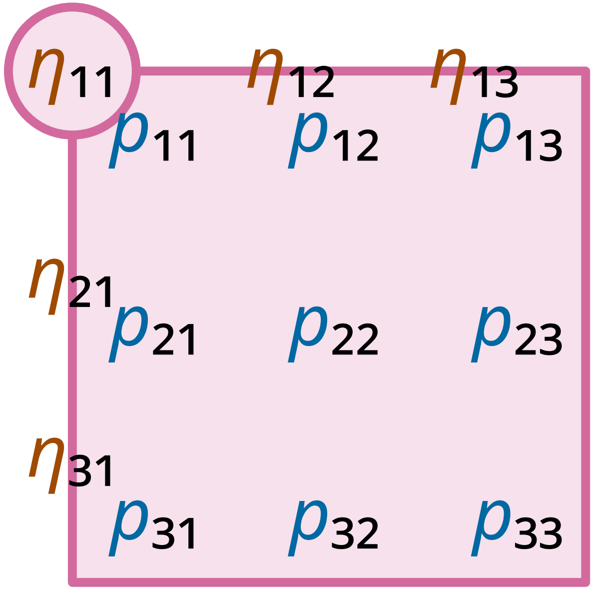
η_{21}

p_{21} p_{22} p_{23}

η_{31}

p_{31} p_{32} p_{33}

Introduce η



Introduce η

$$
\begin{array}{llllll}
\eta_{11} & & \eta_{12} & & \eta_{13} & \\
& p_{11} & & p_{12} & & p_{13} \\
\eta_{21} & & & & & \\
& p_{21} & & p_{22} & & p_{23} \\
\eta_{31} & & & & & \\
& p_{31} & & p_{32} & & p_{33}
\end{array}
$$

Introduce η

$$
\begin{array}{cccccc}
\eta_{11} & & \eta_{12} & & \eta_{13} & \\
 & p_{11} & & p_{12} & & p_{13} \\
\eta_{21} & & & & & \\
 & p_{21} & & p_{22} & & p_{23} \\
\eta_{31} & & & & & \\
 & p_{31} & & p_{32} & & p_{33}
\end{array}
$$

Introduce η

$$
\begin{array}{cccccc}
3 & \eta_{11} & 2 & \eta_{12} & 1 & \eta_{13} \\
 & p_{11} & & p_{12} & & p_{13} \\
2 & \eta_{21} & & & & \\
 & p_{21} & & p_{22} & & p_{23} \\
1 & \eta_{31} & & & & \\
 & p_{31} & & p_{32} & & p_{33}
\end{array}
$$

Introduce θ

$$
\begin{array}{ccccc}
p_{11} & & p_{12} & & p_{13} & \\
p_{21} & & p_{22} & & p_{23} & \\
& & & \theta_{22} & & \theta_{23} \\
p_{31} & & p_{32} & & p_{33} & \\
& & & \theta_{32} & & \theta_{33}
\end{array}
$$

$$
\begin{aligned}
\theta_{ij} = \quad & \log p_{ij} \\
& - \log p_{i-1j} - \log p_{ij-1} \\
& + \log p_{i-1j-1}
\end{aligned}
$$

Introduce θ

$$\begin{array}{cccccc}
p_{11} & & p_{12} & & p_{13} & \\
p_{21} & & p_{22} & & p_{23} & \\
 & & & \theta_{22} & & \theta_{23} \\
p_{31} & & p_{32} & & p_{33} & \\
 & & & \theta_{32} & & \theta_{33}
\end{array}$$

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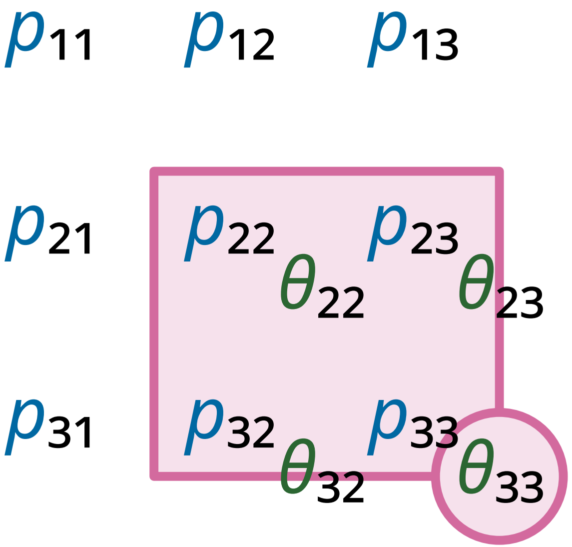
& + \log p_{i-1j-1}
\end{aligned}$$

Introduce θ

$$\begin{array}{ccc} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22}\;\theta_{22} & p_{23}\;\theta_{23} \\ p_{31} & p_{32}\;\theta_{32} & p_{33}\;\theta_{33} \end{array}$$

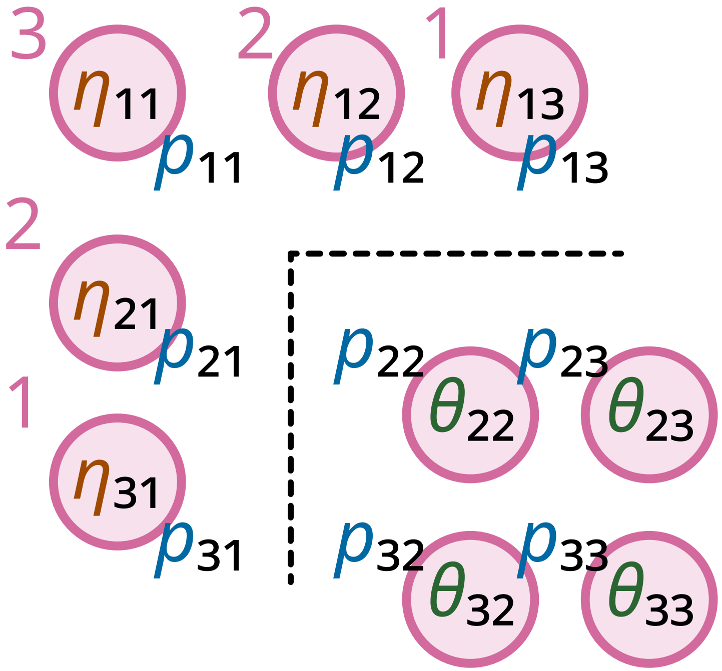
$$\begin{aligned} \theta_{ij} = \quad & \log p_{ij} \\ & - \log p_{i-1j} - \log p_{ij-1} \\ & + \log p_{i-1j-1} \end{aligned}$$

Introduce θ



$$\begin{aligned}\theta_{ij} = &\quad \log p_{ij} \\ &- \log p_{i-1j} - \log p_{ij-1} \\ &+ \log p_{i-1j-1}\end{aligned}$$

Balancing as Constraints on η and θ

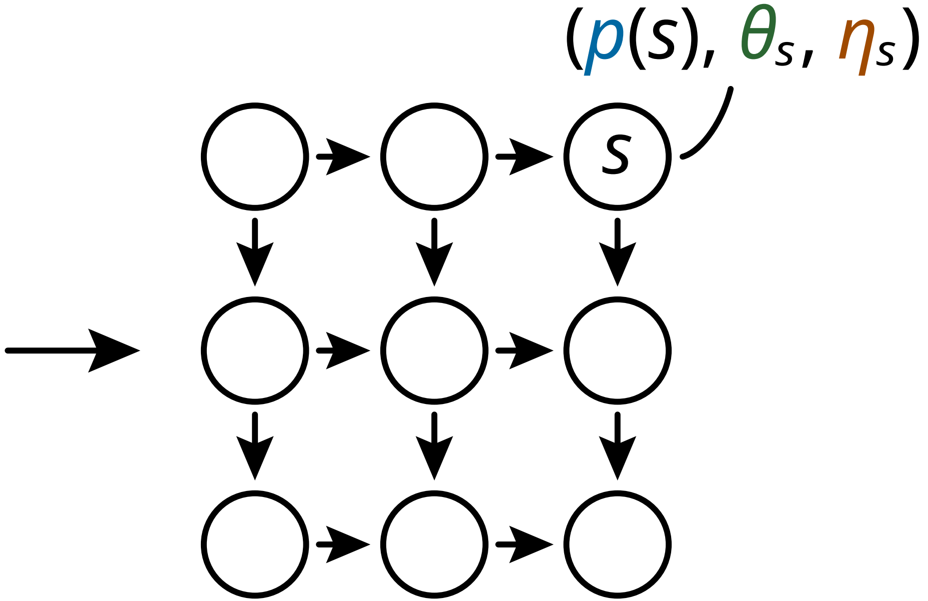


$$\theta_{ij} = \log p_{ij} - \log p_{i-1j} - \log p_{ij-1} + \log p_{i-1j-1}$$

Matrix balancing $\Leftrightarrow$
Satisfy $\eta_{i1} = \eta_{1i} = 3 - i + 1$
with keeping all θ_{ij}

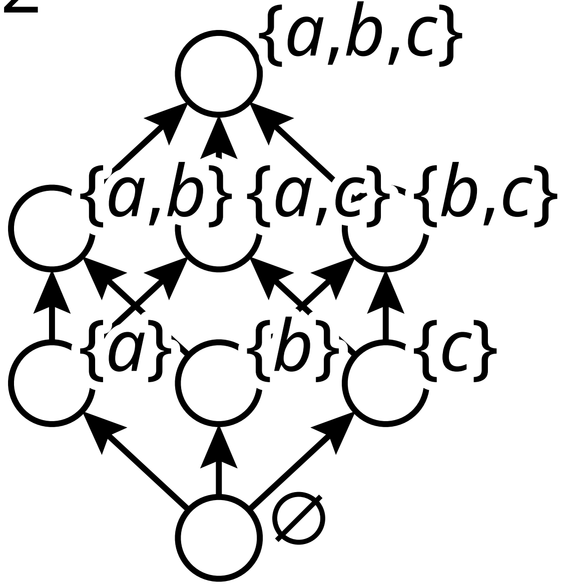
Introduce Partial Order Structure

$$\begin{bmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{bmatrix}$$

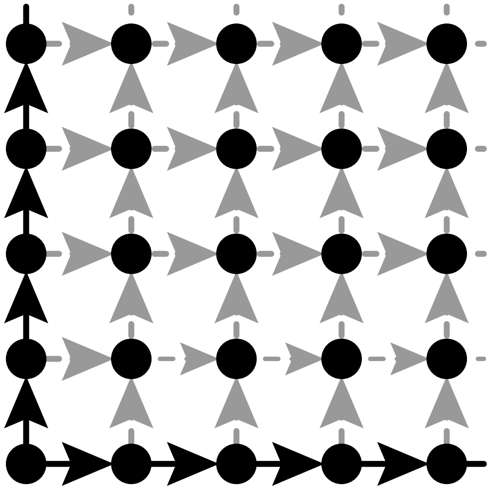


Partially Ordered Sets (Posets)

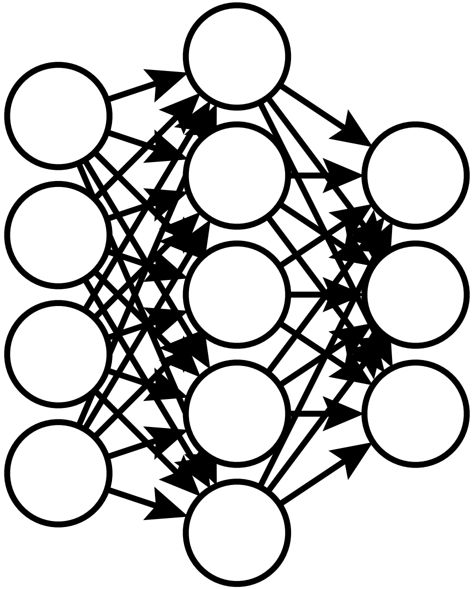
$2^{\{a,b,c\}}$



$\mathbb{N}^2$



Network



Incidence Algebra

- Incidence algebra is defined over a poset $(S, \leq)$
  - (Closed) Interval $[a, b] = \{s \in S \mid a \leq s \leq b\}$
- Members of the incidence algebra are functions $\alpha(a, b)$ from intervals $[a, b]$ to a scalar with

$$(\alpha + \beta)(a, b) = \alpha(a, b) + \beta(a, b)$$

$$(\alpha\beta)(a, b) = \sum_{a \leq x \leq b} \alpha(a, x)\beta(x, b) \quad \text{(convolution)}$$

Special Elements

- Delta function δ:

$$\delta(a,b) = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{otherwise} \end{cases}$$

- Zeta function ζ: (integral)

$$\zeta(a,b) = \begin{cases} 1 & \text{if } a \leq b \\ 0 & \text{otherwise} \end{cases}$$

- Möbius function $\mu = \zeta^{-1}$: $\zeta\mu = \delta$ (differential)

(ζ, μ) Leads to Non-Singularity

- For a poset $(S, \leq)$, let $S = \{s_1, s_2, \dots, s_n\}$
- Let us define the zeta matrix $\mathbf{Z} \in \{0,1\}^{n \times n}$ as

  $$z_{ij} = \zeta(s_i, s_j)$$

- Relationship between ζ and μ guarantees that $\mathbf{Z}$ is always regular:

  $$\mathbf{Z}^{-1} = \mathbf{M} \quad \text{such that} \quad m_{ij} = \mu(s_i, s_j)$$

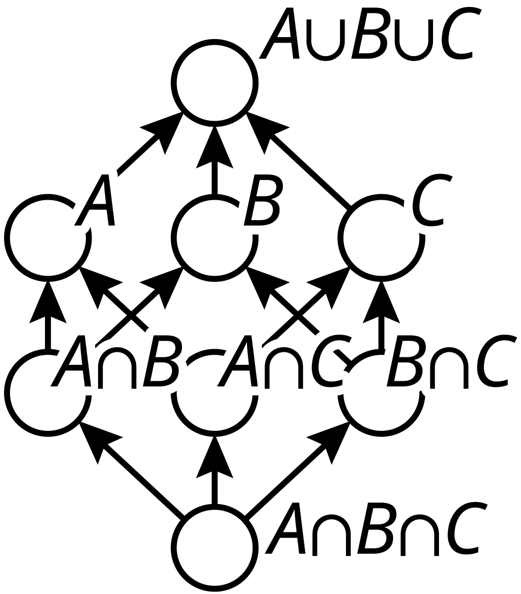
  - $\mathbf{M} \in \mathbb{Z}^{n \times n}$

Möbius Inversion Formula

- Given a poset S, for any functions $f, g : S \to \mathbb{R}$, the Möbius inversion formula is given as

$$\begin{cases} g(x) = \sum_{s \in S} \zeta(s,x) f(s) = \sum_{s \leq S} \zeta(s,x) f(s) = \sum_{s \leq x} f(s) \\ f(x) = \sum_{s \in S} \mu(s,x) g(s) = \sum_{s \leq S} \mu(s,x) g(s) \end{cases}$$

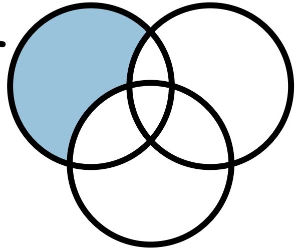
E.g.1: Inclusion-Exclusion Principle



$$|A\cup B\cup C| = |A| + |B| + |C| - |A\cap B| - |A\cap C| - |B\cap C| + |A\cap B\cap C|$$

$$f(X) = |X| \quad g(X) = |X \setminus \bigcup_{Y \subset X} Y|$$

$$\begin{cases} f(X) = \sum_{Y \le X} g(Y) \\ g(X) = \sum_{Y \le X} \mu(Y,X) f(Y) \end{cases}$$



Log-Linear Model on Poset [ICML2017]

- For probability $p : S \to (0, 1)$ with $\sum_{x \in S} p(x) = 1$, introduce θ and η as

  $\theta_x = \sum_{s \in S} \mu(s, x) \log p(s)$,

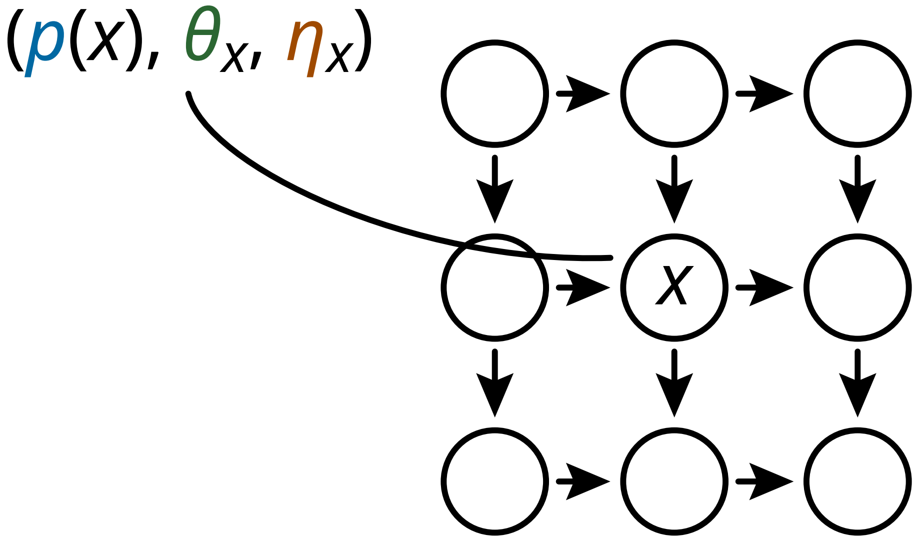
  $\eta_x = \sum_{s \in S} \zeta(x, s) p(s) = \sum_{s \geq x} p(s)$

- From the Möbius inversion formula, log-linear model is:

  $\log p(x) = \sum_{s \in S} \zeta(s, x) \theta_s = \sum_{s \leq x} \theta_s$

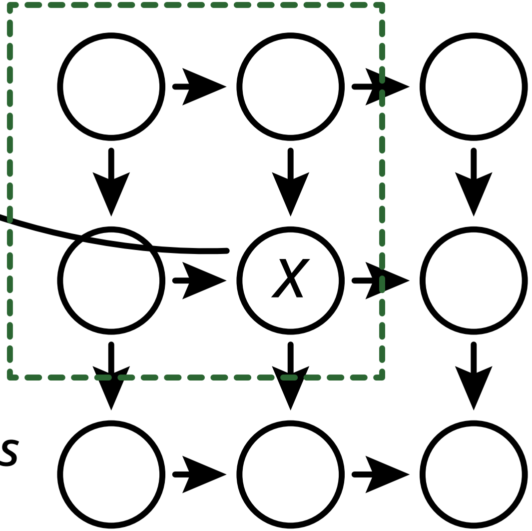
  - In the matrix form: $\log \boldsymbol{p} = \mathbf{Z}\theta$

Log-Linear Model on Poset



Log-Linear Model on Poset

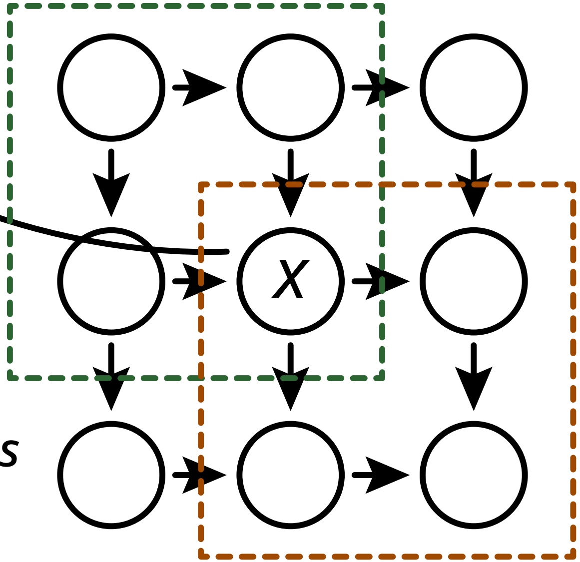
$(p(x), \theta_x, \eta_x)$



$\log p(x) = \sum_{s \leq x} \theta_s$

Log-Linear Model on Poset

$(p(x), \theta_x, \eta_x)$



$$\eta_x = \sum_{s \geq x} p(s)$$

$$\log p(x) = \sum_{s \leq x} \theta_s$$

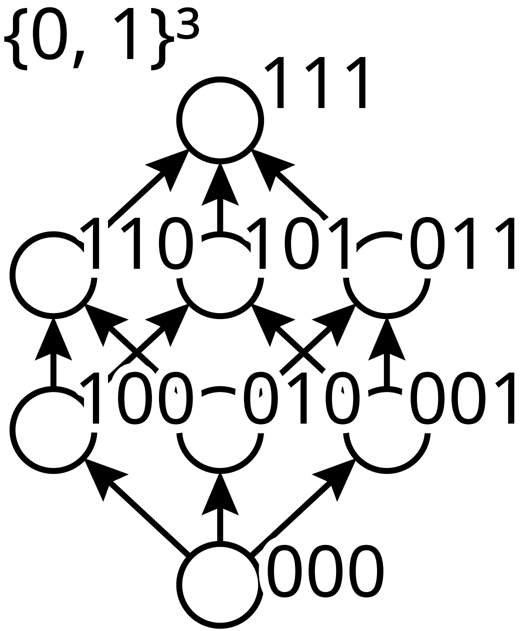
Exponential Family

- The log-linear model on posets belongs to the exponential family

- θ : Natural parameter
- η : Expectation parameter

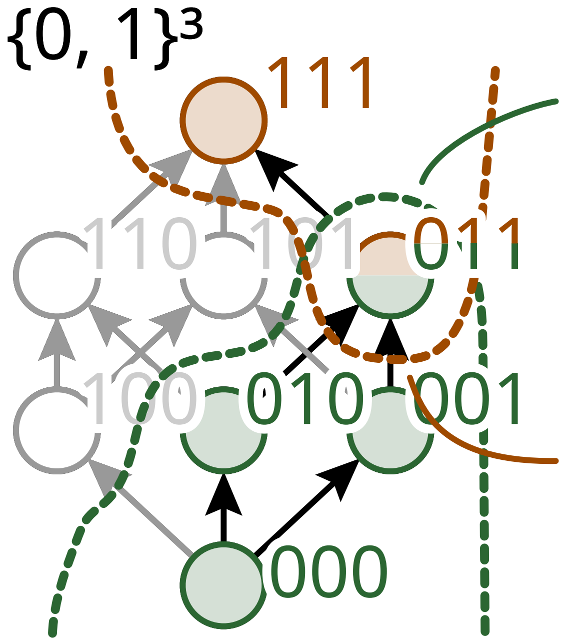
Binary Log-Linear Model

(= Boltzmann machine)



[Luo & Sugiyama, AAAI2019]

Binary Log-Linear Model



(= Boltzmann machine)

$$\log p(x) = -\psi + \textstyle\sum_i \theta_i x_i + \sum_{i,j} \theta_{ij} x_i x_j + \cdots$$
$$= \textstyle\sum_{s \le x} \theta_s$$

For $\boldsymbol{x}$ with $x_{i_1} = \cdots = x_{i_k} = 1$,

$$\eta_x = \mathbb{E}[x_{i_1} \cdots x_{i_k}] = \Pr(x_{i_1} = \cdots = x_{i_k} = 1)$$
$$= \textstyle\sum_{s \ge x} p(s)$$

[Luo & Sugiyama, AAAI2019]

Dually Flat Structure

- Let $\psi(\theta) = -\theta(\bot)$ (convex, partition function)

$$\psi(\theta) \xrightarrow{\text{Legendre transformation}} \phi(\eta) = \sum_{x \in S} p(x) \log p(x)$$

- $(\psi(\theta), \phi(\eta))$ leads to dually flat coordinate system (θ, η):

$$\nabla \psi(\theta) = \eta, \quad \frac{\partial}{\partial \theta_x} \psi(\theta) = \eta_x$$

$$\nabla \phi(\eta) = \theta, \quad \frac{\partial}{\partial \eta_x} \phi(\eta) = \theta_x$$

Riemannian Metric (Fisher Information)

$$\frac{\partial}{\partial \theta_x}\frac{\partial}{\partial \theta_y}\psi(\theta) = \frac{\partial}{\partial \theta_x}\eta_y = \sum_{s\in S}\zeta(x,s)\zeta(y,s)p(s) - \eta_x\eta_y$$

$$\frac{\partial}{\partial \eta_x}\frac{\partial}{\partial \eta_y}\phi(\eta) = \frac{\partial}{\partial \eta_x}\theta_y = \sum_{s\in S}\mu(s,x)\mu(s,y)p(s)^{-1}$$

$$\mathbb{E}_s\left[\frac{\partial}{\partial \theta_x}\log p(s)\frac{\partial}{\partial \eta_y}\log p(s)\right] = \delta(x,y)$$

Riemannian Metric (Fisher Information)

$$\mathbb{E}_s\left[\frac{\partial}{\partial \theta_x}\log p(s)\frac{\partial}{\partial \theta_y}\log p(s)\right] = \sum_{s\in S}\zeta(x,s)\zeta(y,s)p(s) - \eta_x\eta_y$$

$$\mathbb{E}_s\left[\frac{\partial}{\partial \eta_x}\log p(s)\frac{\partial}{\partial \eta_y}\log p(s)\right] = \sum_{s\in S}\mu(s,x)\mu(s,y)p(s)^{-1}$$

$$\mathbb{E}_s\left[\frac{\partial}{\partial \theta_x}\log p(s)\frac{\partial}{\partial \eta_y}\log p(s)\right] = \delta(x,y)$$

Mixed Coordinate System

- Many problems are formulated as coordinate mixing

$$P = (\theta_1, \theta_2, \ldots, \theta_{i-1}, \theta_i, \theta_{i+1}, \ldots, \theta_n)$$

e-projection (MLE)

$$Q = (\eta_1, \eta_2, \ldots, \eta_{i-1}, \theta_i, \theta_{i+1}, \ldots, \theta_n)$$

m-projection

$$R = (\eta_1, \eta_2, \ldots, \eta_{i-1}, \eta_i, \eta_{i+1}, \ldots, \eta_n)$$

Pythagorean theorem: (Q is always unique)

$$\mathrm{KL}(P, R) = \mathrm{KL}(P, Q) + \mathrm{KL}(Q, R)$$

Mixed Coordinate System (Example)

- Many problems are formulated as coordinate mixing

$$P = (\,0\,,\,0\,,\,\dots,\,0\,,\,\boxed{0,\,0\,,\,\dots,\,0}\,) \rightarrow \text{Uniform dist.}$$

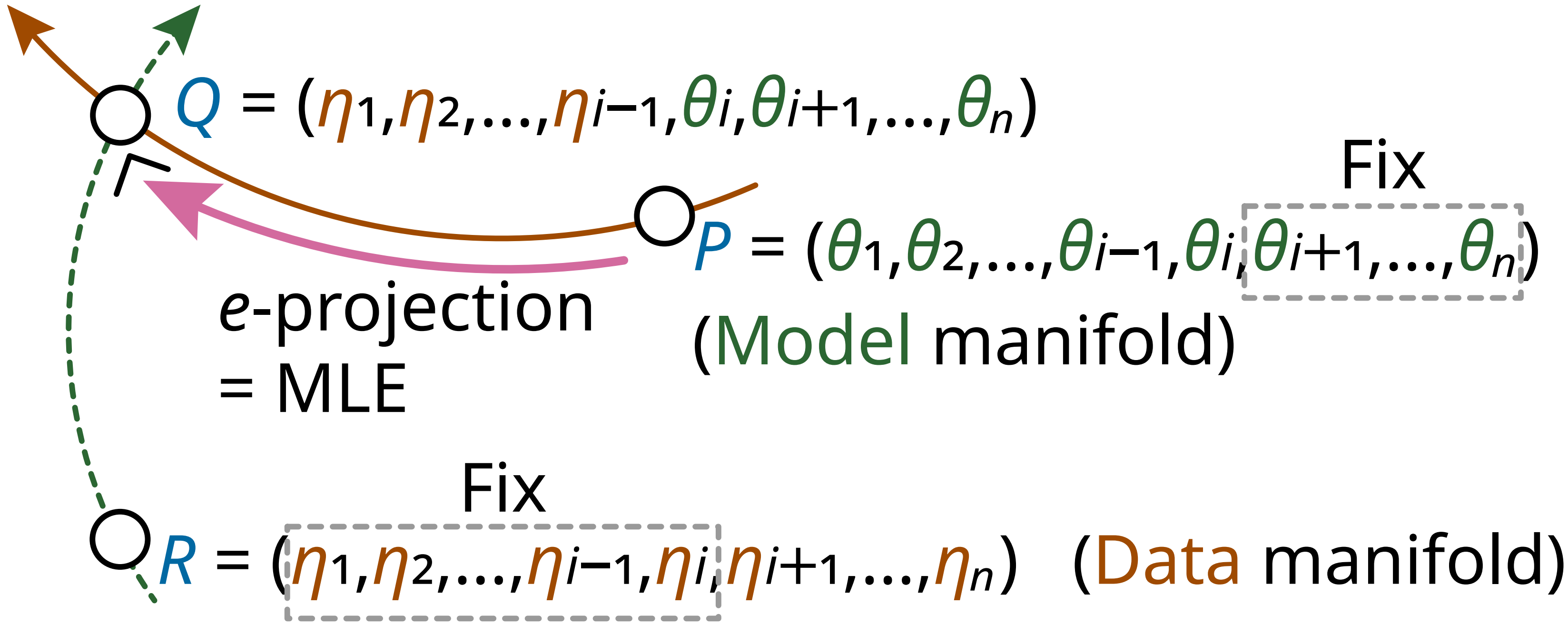
$$Q = (\,\boxed{\hat{\eta}_1,\,\hat{\eta}_2,\,\dots,\,\hat{\eta}_{i-1}},\,\boxed{0\,,\,0\,,\,\dots,\,0}\,)$$

$$R = (\,\boxed{\hat{\eta}_1,\,\hat{\eta}_2,\,\dots,\,\hat{\eta}_{i-1}},\,\hat{\eta}_i,\,\hat{\eta}_{i+1},\,\dots,\,\hat{\eta}_n\,) \rightarrow \text{Empirical dist.}$$

Pythagorean theorem: (Q is always unique)

$$\mathrm{KL}(P, R) = \mathrm{KL}(P, Q) + \mathrm{KL}(Q, R)$$

Two Submanifolds



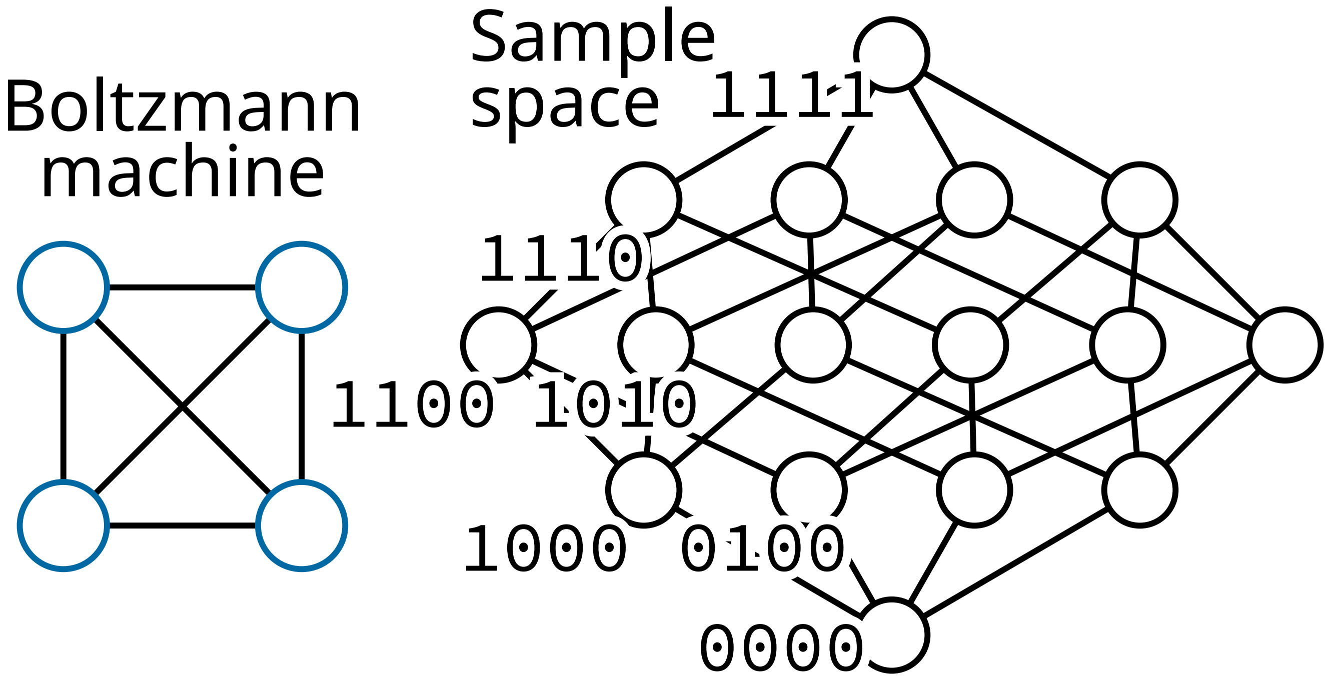
Gradient methods for *e*-projection

- *e*-projection is convex optimization
- Gradient descent (first-order):

  $\theta_{\text{next}} \leftarrow \theta - \varepsilon(\eta - \hat{\eta}_{\text{target}})$
- Natural gradient (second-order)

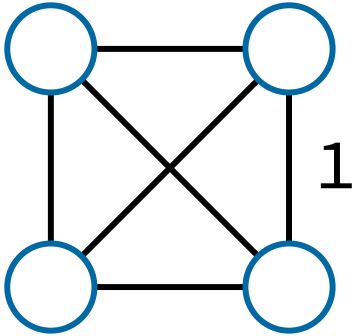
  $\theta_{\text{next}} \leftarrow \theta - G^{-1}(\eta - \hat{\eta}_{\text{target}})$
  - G is Fisher information matrix w.r.t. θ
- Coordinate descent [Hayashi, Sugiyama, Matsushima, DSAA2020]

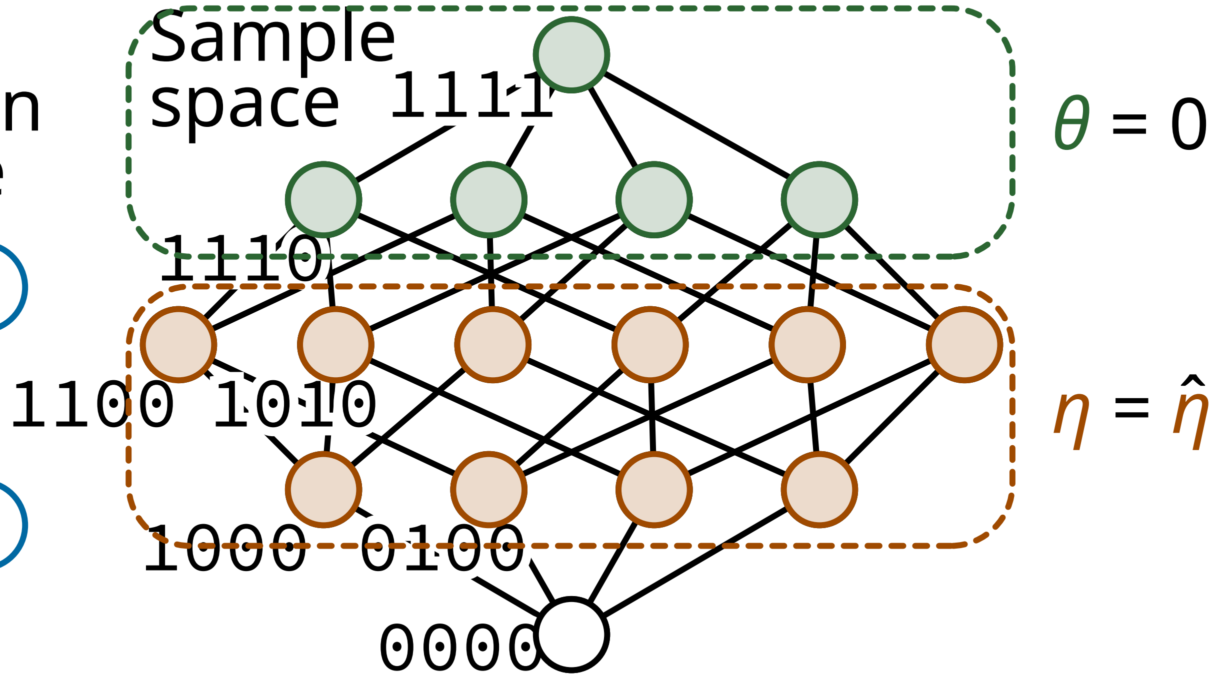
Boltzmann Machine Training



Boltzmann Machine Training

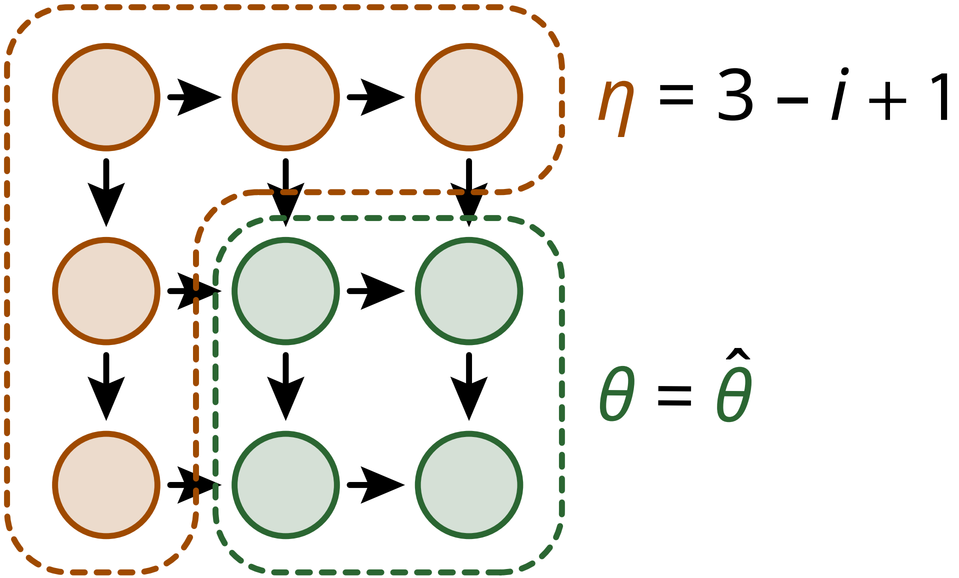
Boltzmann
machine





Matrix Balancing

3x3 matrix
as poset:



Summary

- Information geometric formulation for partial order structures
  - Learning process can be achieved as a projection in the parameter space (dually flat manifold)
- Several applications
  - Boltzmann machines
  - Matrix (Tensor) balancing