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IBIS2016

Partial Order Structure and Information Geometry
(順序構造と情報幾何)

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Today's Model on Poset $(S, \leq)$

$$\boxed{\begin{aligned} \log p(x) &= \sum_{s \in S} \zeta(s, x)\theta(s) \\ p(x) &= \sum_{s \in S} \mu(x, s)\eta(s) \end{aligned}}$$

Today's Model on Poset $(S, \leq)$

Coefficient of log-linear model
(Bias/weight in Boltzmann machines)
(Natural parameter of exponential family)

Probability

Zeta function

$$\boxed{\begin{aligned} \log p(x) &= \sum_{s \in S} \zeta(s, x)\theta(s) \\ p(x) &= \sum_{s \in S} \mu(x, s)\eta(s) \end{aligned}}$$

Möbius function

Expectation
(Frequency in pattern mining)
(Sufficient statistics in exponential family)

Outcome

- Given a poset $(S, \leq)$ and consider distributions on S

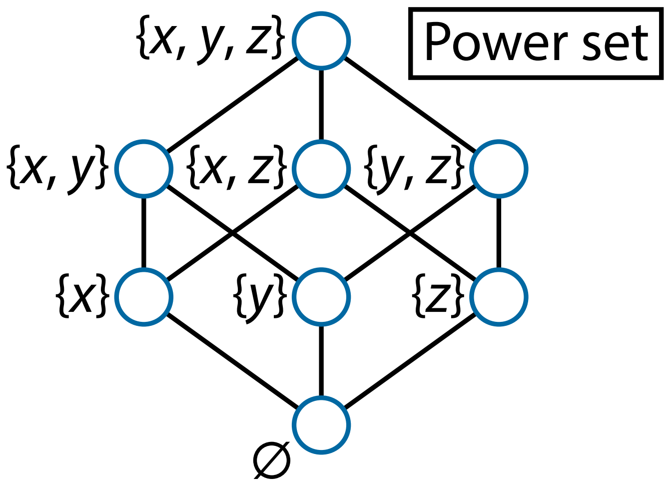
1. KL divergence decomposition:

   $D_{\mathrm{KL}}[P, R] = D_{\mathrm{KL}}[P, Q] + D_{\mathrm{KL}}[Q, R]$

   with Q s.t. $\theta_Q(x) = \theta_R(x)$ or $\eta_Q(x) = \eta_P(x)$ for all $x \in S$

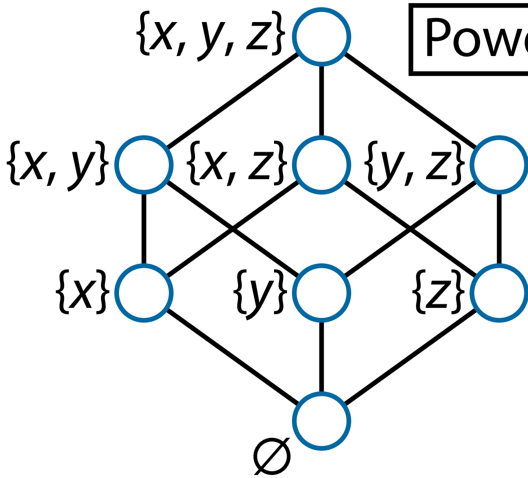
2. The set of probability distributions on $(S, \leq)$ is a dually flat manifold w.r.t. θ and η
   - p, θ, and η are coordinate systems
   - θ and η are orthogonal
   - θ introduces the structure of exponential family
   - η introduces the structure of mixture family

Partially Ordered Sets

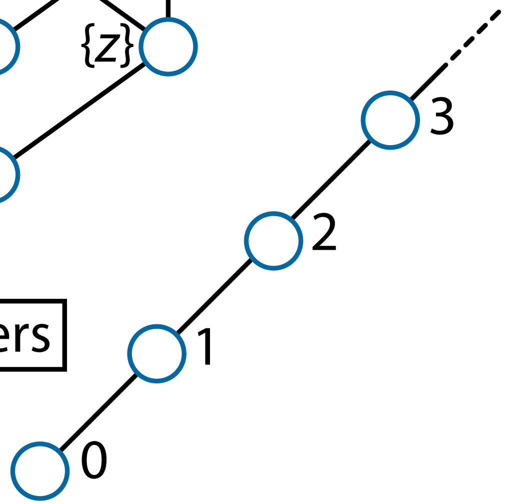


Partially Ordered Sets

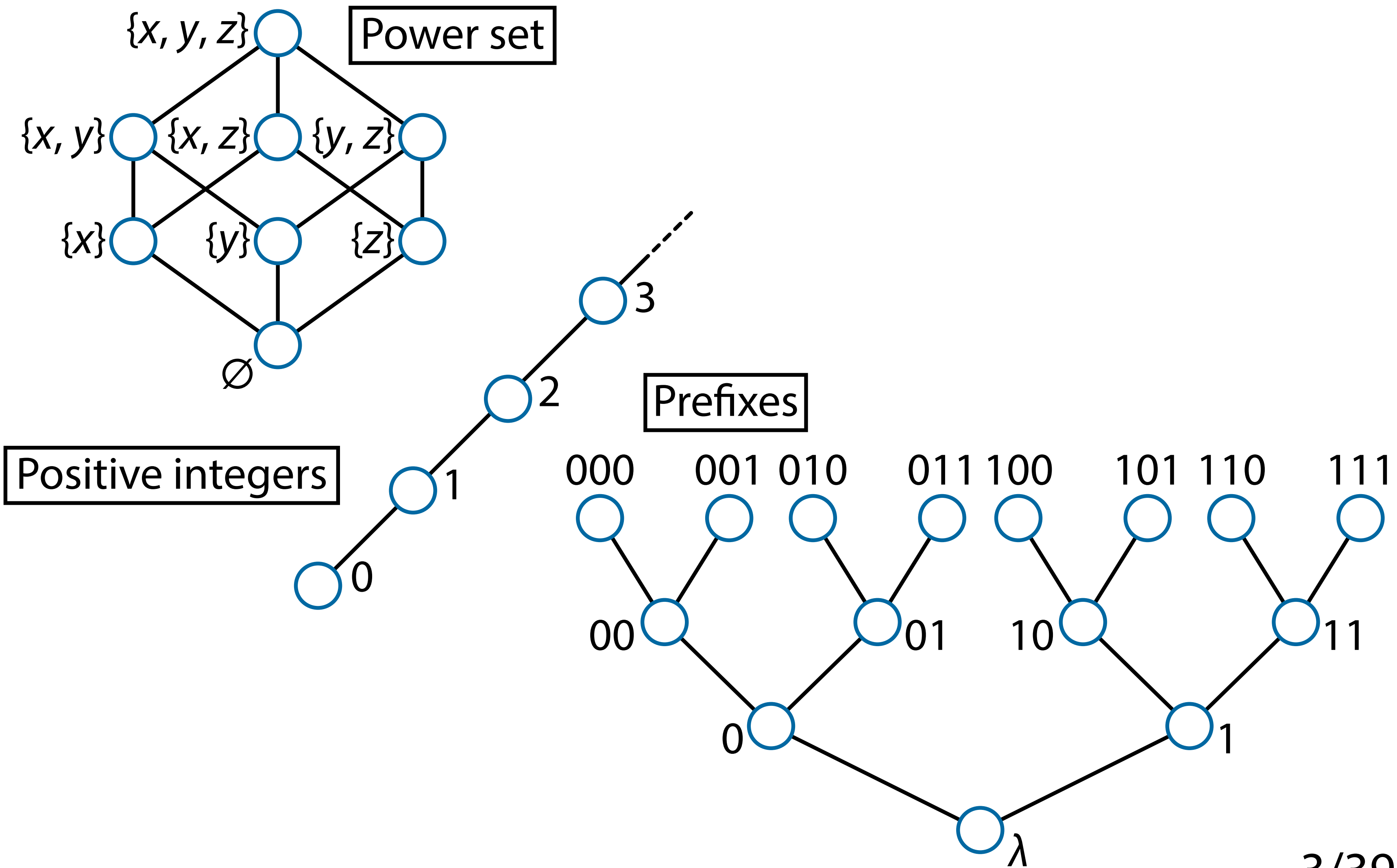
Power set



Positive integers

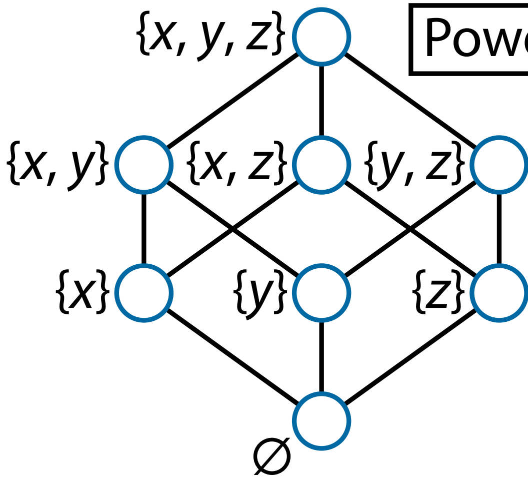


Partially Ordered Sets

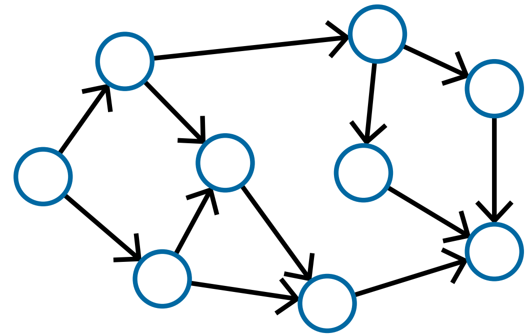


Partially Ordered Sets

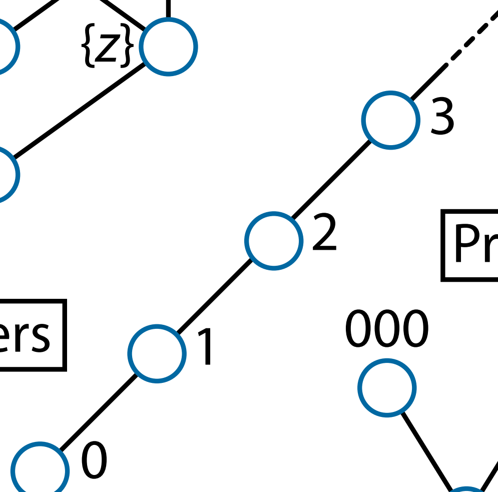
Power set



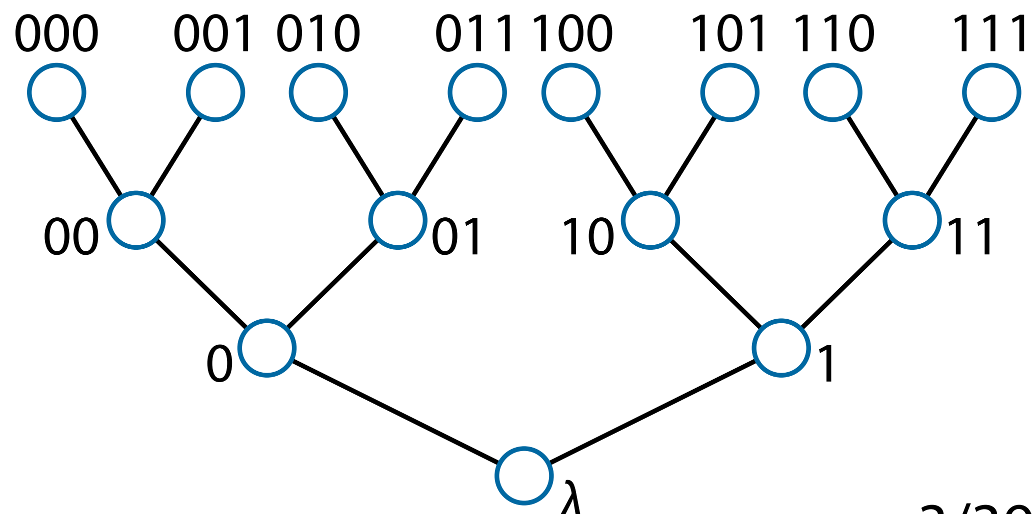
Directed Acyclic Graph



Positive integers

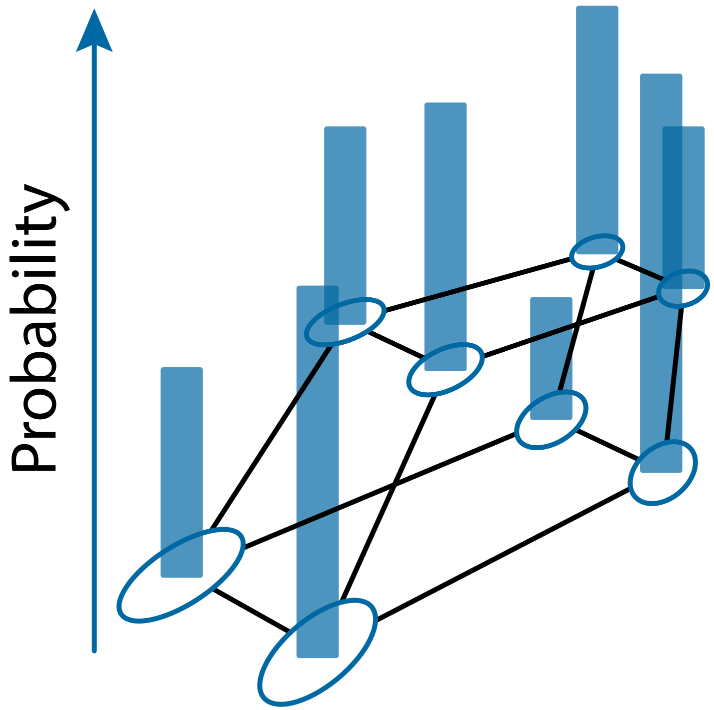


Prefixes



Posets with Probability Distribution

Probability distribution
on posets (partially ordered sets)



Posets with Probability Distribution

Probability distribution
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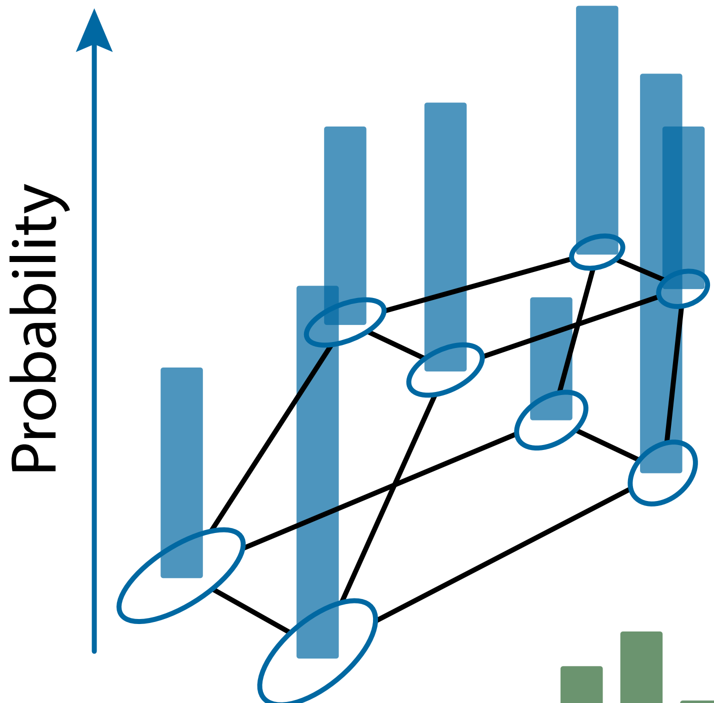
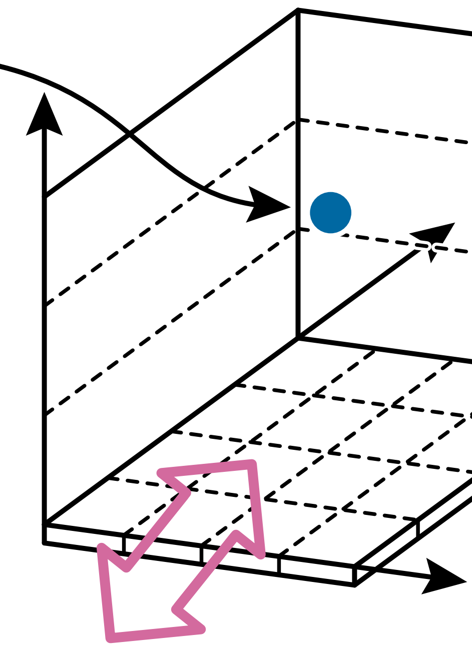
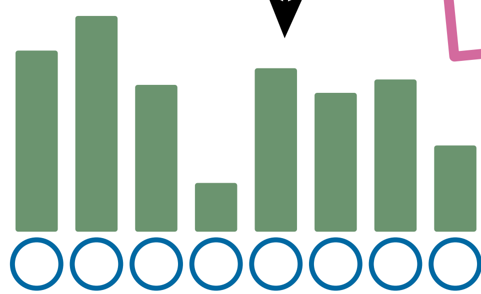


Information
geometry





Decomposition in
the log-linear model

$$\log p(x) = \sum \zeta(s, x)\theta(s)$$

Posets with Probability Distribution

Probability distribution
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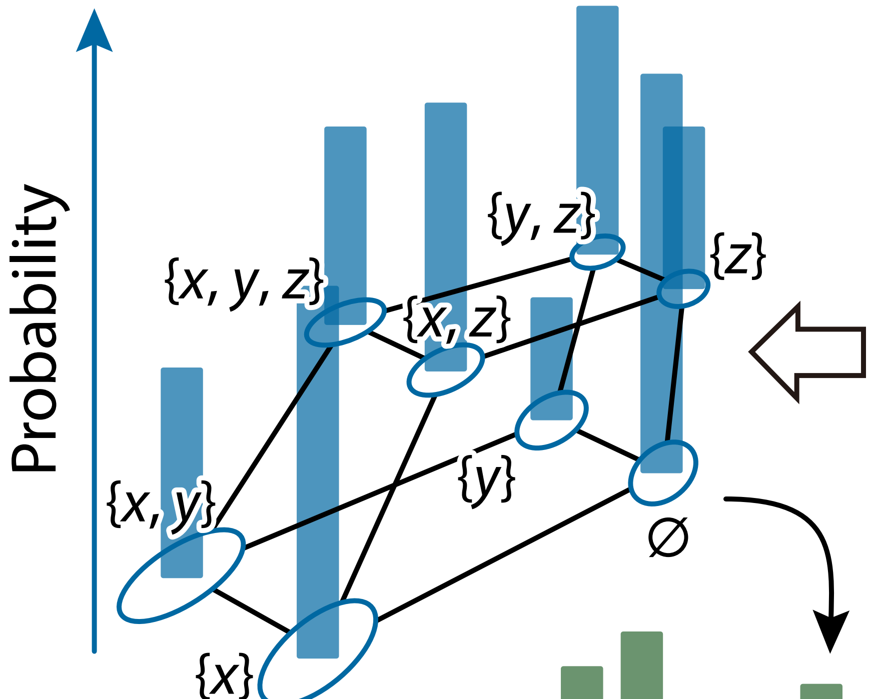
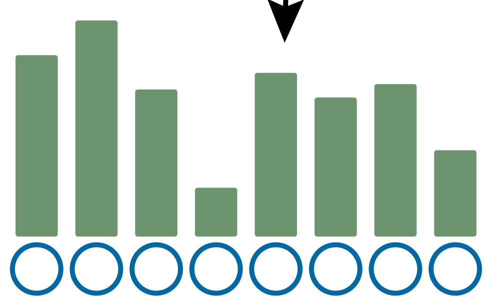


x	y	z (e.g. Neurons, SNPs, ...)
0	0	1 ···
1	0	0 ···
1	1	1 ···
0	0	0 ···
1	1	0 ···
0	1	1 ···
1	0	1 ···
1	0	1 ···
1	0	1 ···
1	1	0 ···

Numerical score (KL divergence) and the p-value for higher-order intractions

Decomposition in the log-linear model

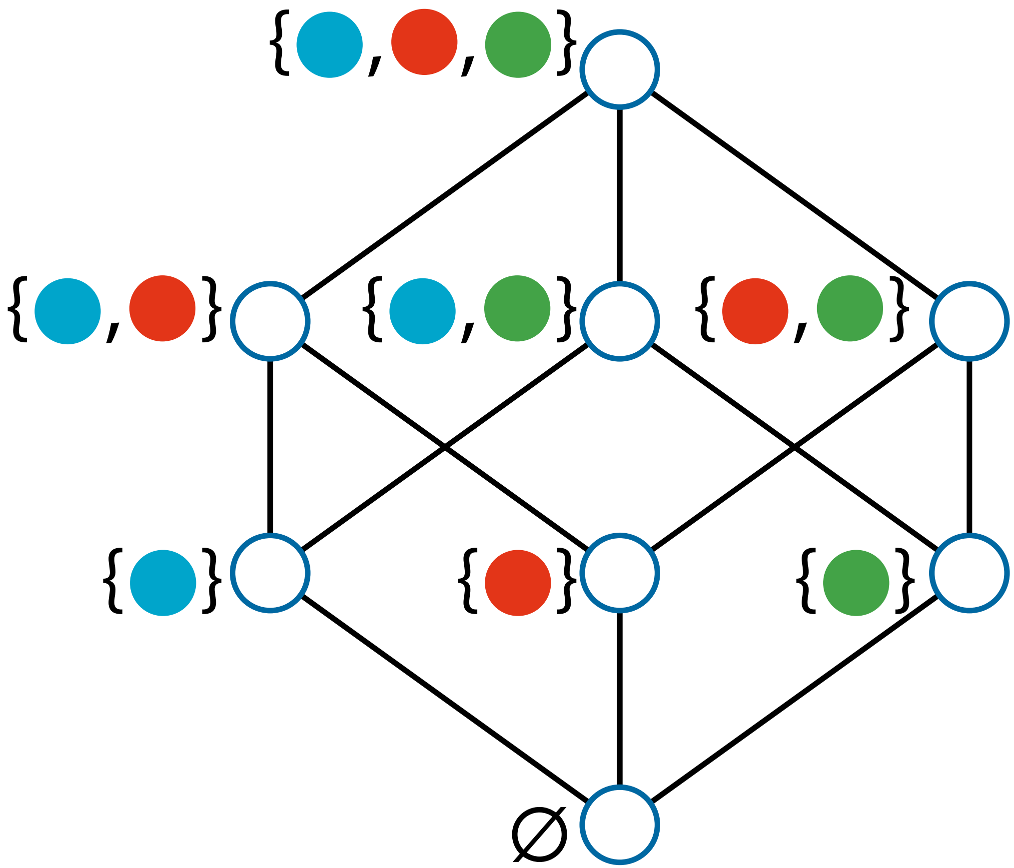


$$\log p(x) = \sum \zeta(s, x)\theta(s)$$

Binary vectors (Transaction database)

ID 1:	1	1	0
ID 2:	1	1	1
ID 3:	1	1	0
ID 4:	1	1	1
ID 5:	1	1	0
ID 6:	1	0	1
ID 7:	1	0	1
ID 8:	1	1	1
ID 9:	1	0	0
ID10:	0	1	0

Poset (itemset lattice)



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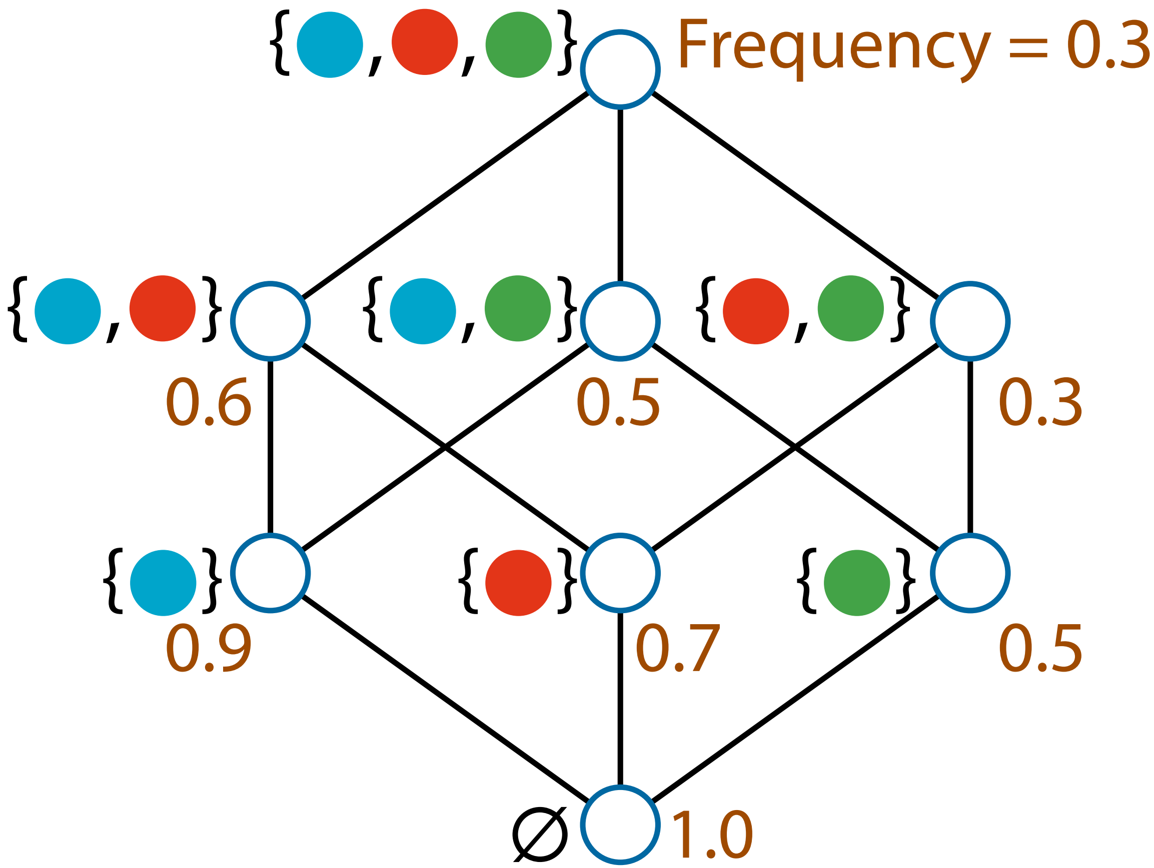
Poset (itemset lattice)



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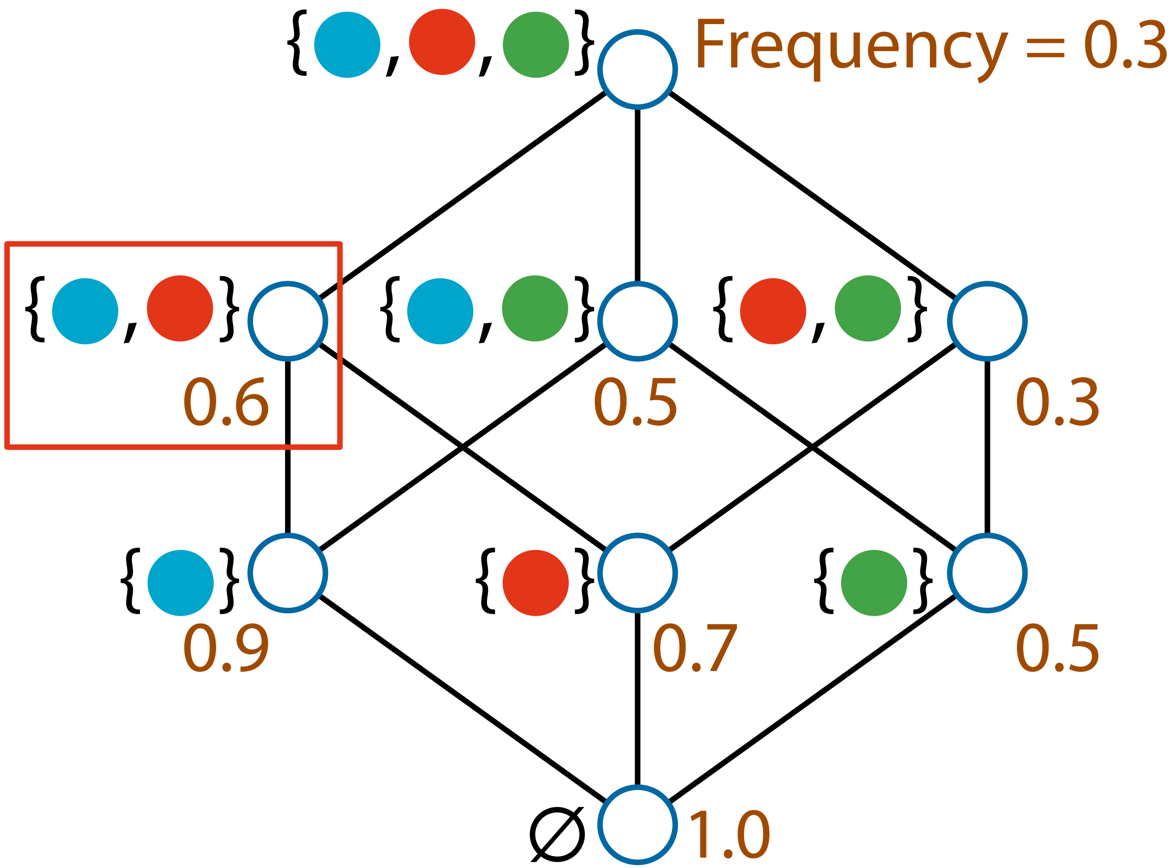

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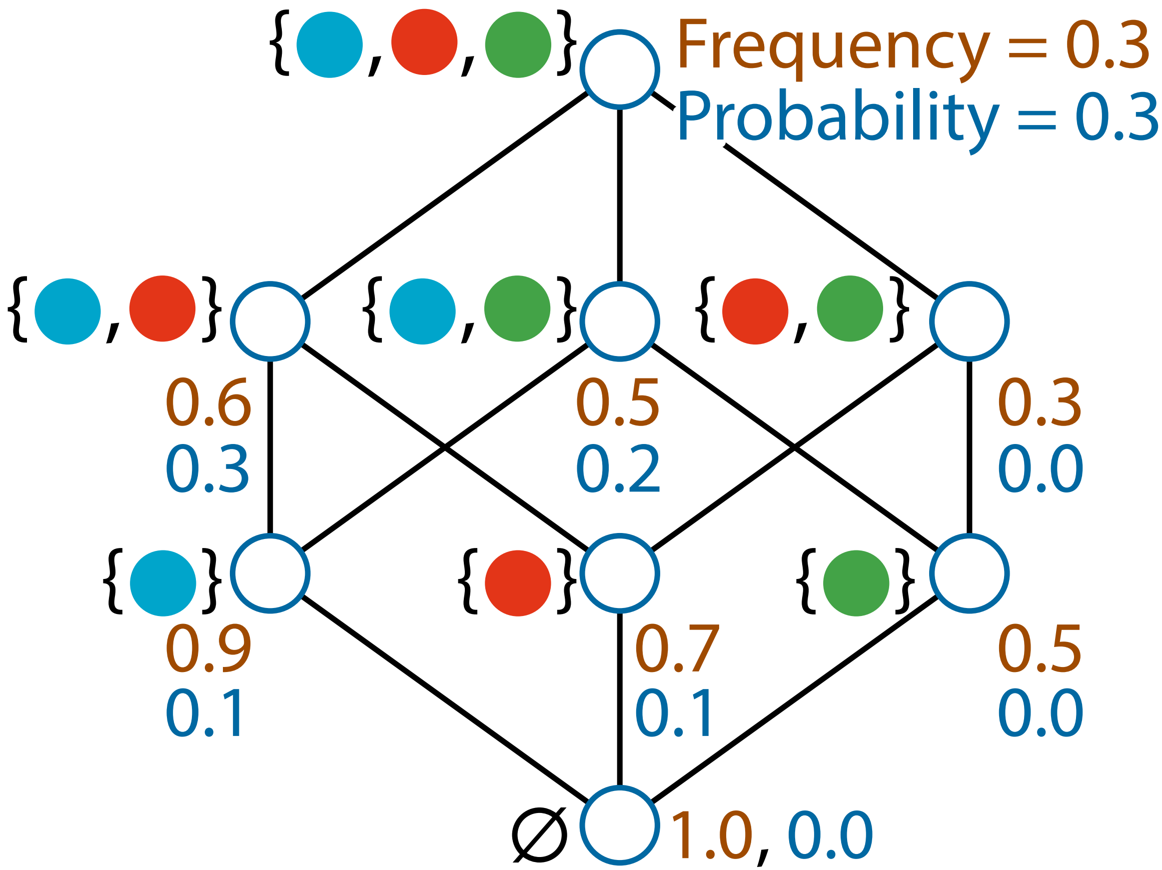
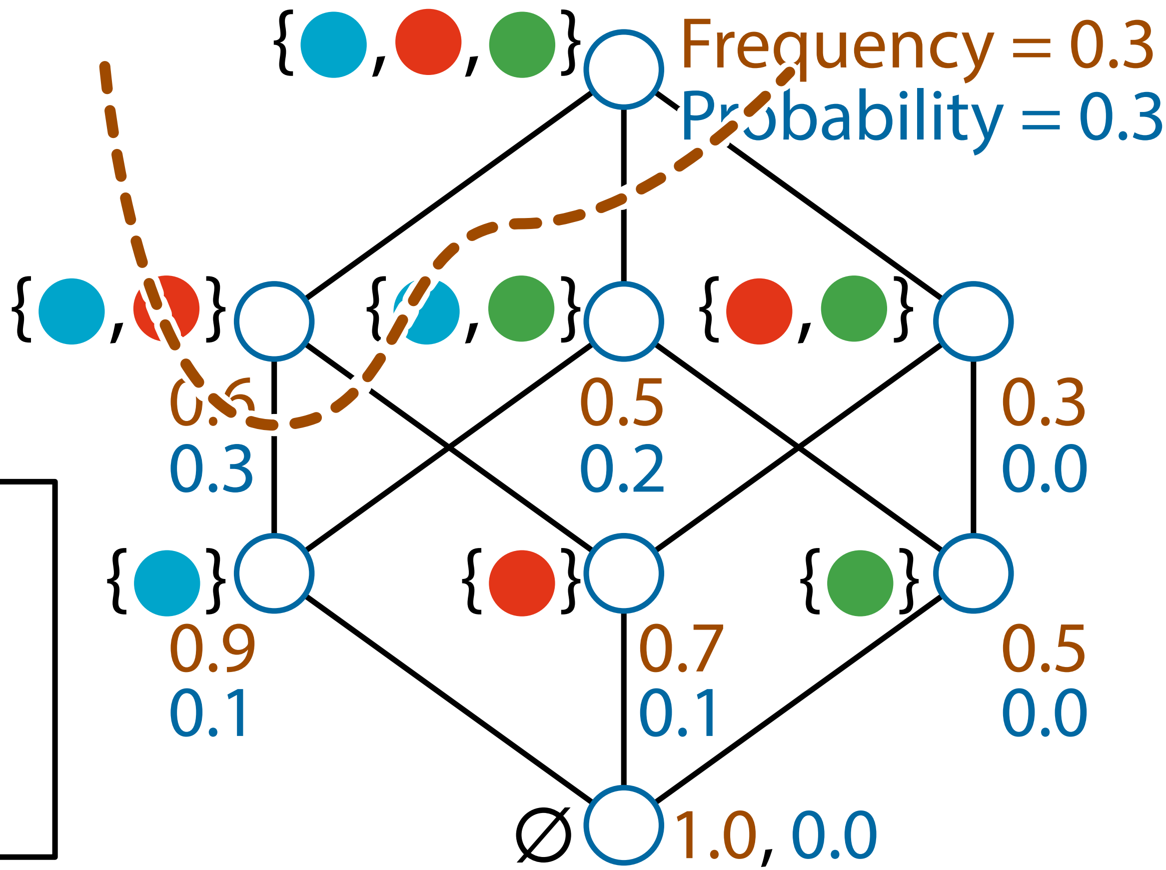
Poset (itemset lattice)



Upward = Pattern mining

Poset (itemset lattice)



η: Frequency

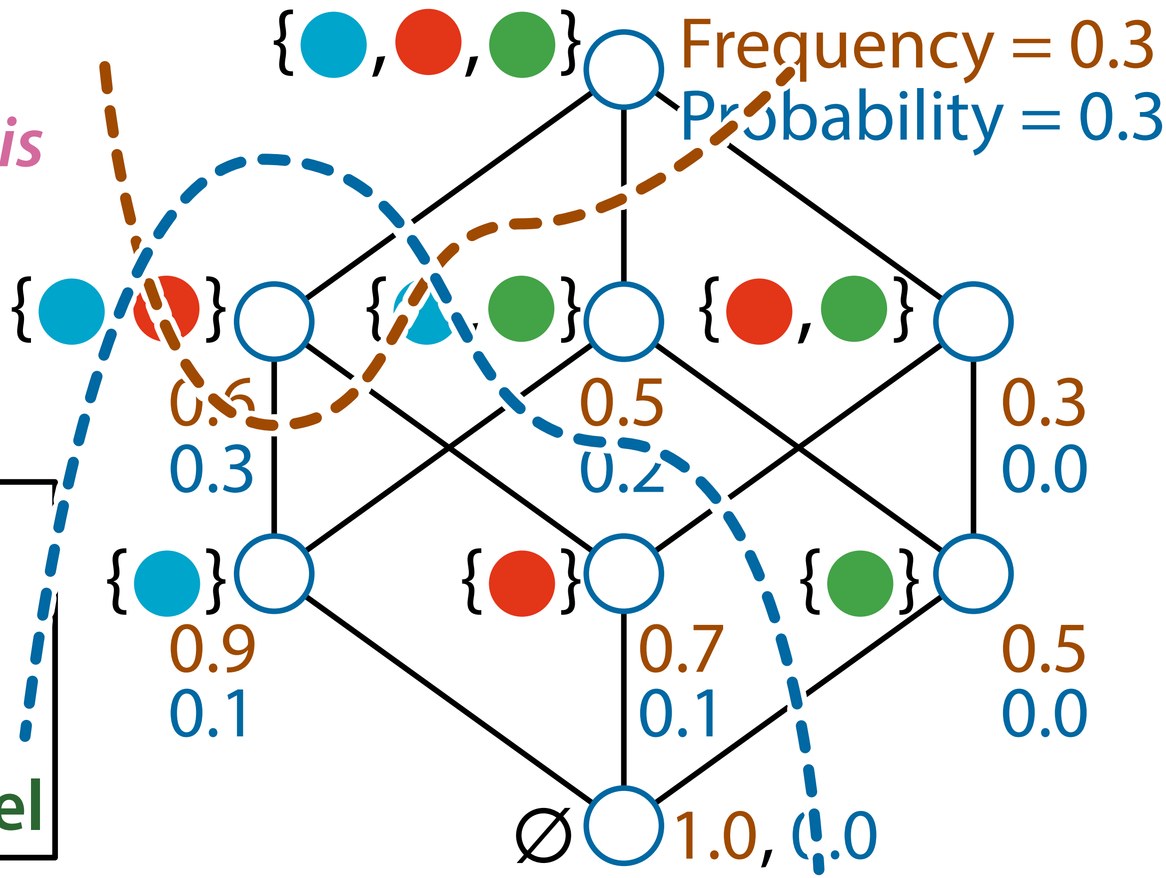
p: Probability

$$\eta(\{\bullet,\bullet\}) = p(\{\bullet,\bullet\}) + p(\{\bullet,\bullet,\bullet\})$$

Upward = Pattern mining

Downward = Log-linear analysis

Poset (itemset lattice)



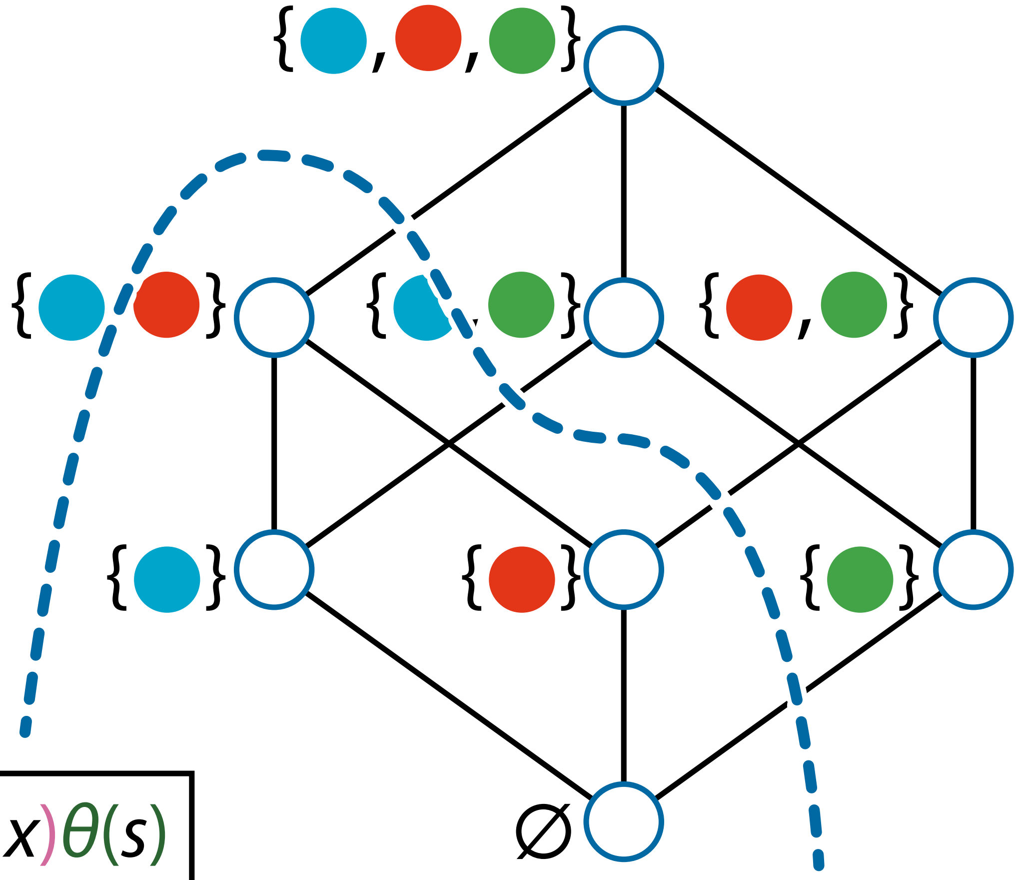
η: Frequency

p: Probability

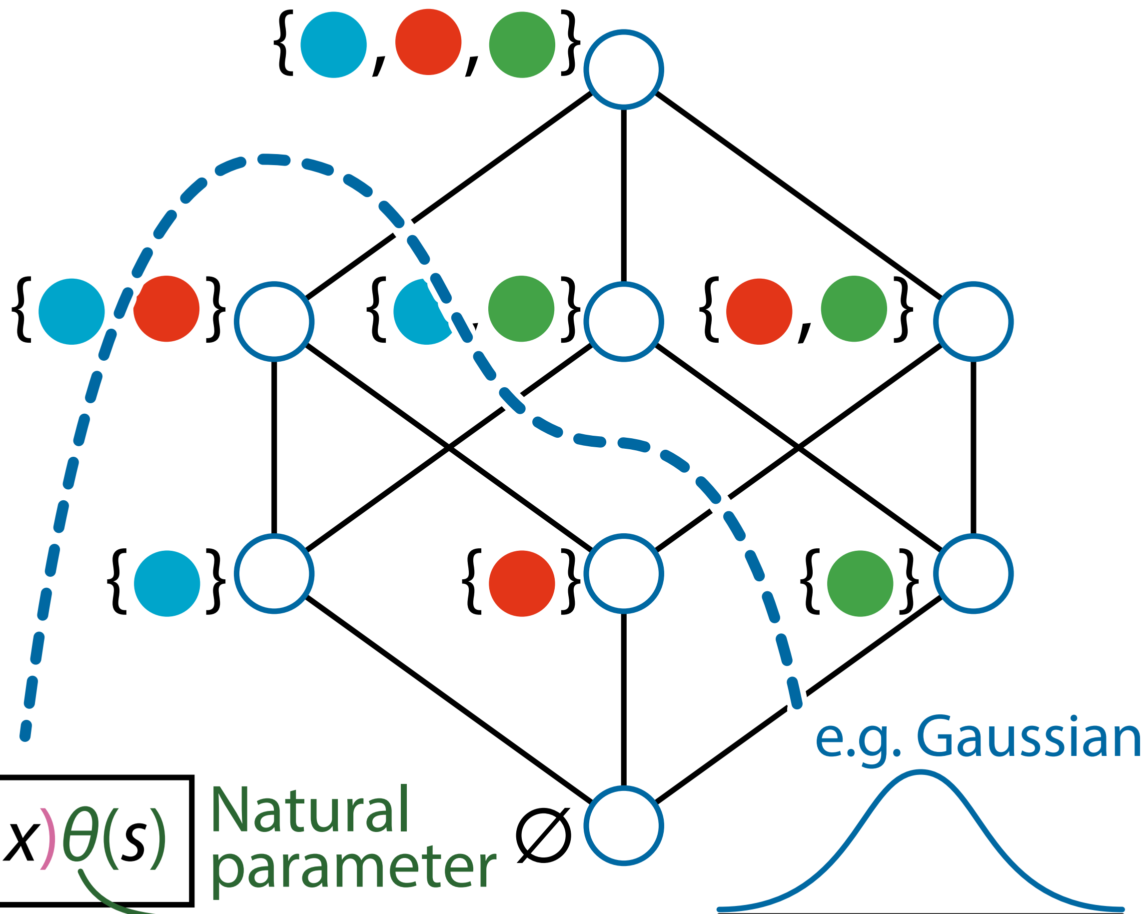
θ: Coefficient of **log-linear model**

$$\eta(\{\color{cyan}\bullet\color{black},\color{red}\bullet\color{black}\}) = p(\{\color{cyan}\bullet\color{black},\color{red}\bullet\color{black}\}) + p(\{\color{cyan}\bullet\color{black},\color{red}\bullet\color{black},\color{green}\bullet\color{black}\})$$

$$\log p(\{\color{cyan}\bullet\color{black},\color{red}\bullet\color{black}\}) = \theta(\{\color{cyan}\bullet\color{black},\color{red}\bullet\color{black}\}) + \theta(\{\color{cyan}\bullet\color{black}\}) + \theta(\{\color{red}\bullet\color{black}\}) + \theta(\varnothing)$$



$$\log p(x) = \sum \zeta(s, x)\theta(s)$$



$$\log p(x) = \sum \zeta(s, x)\theta(s)$$

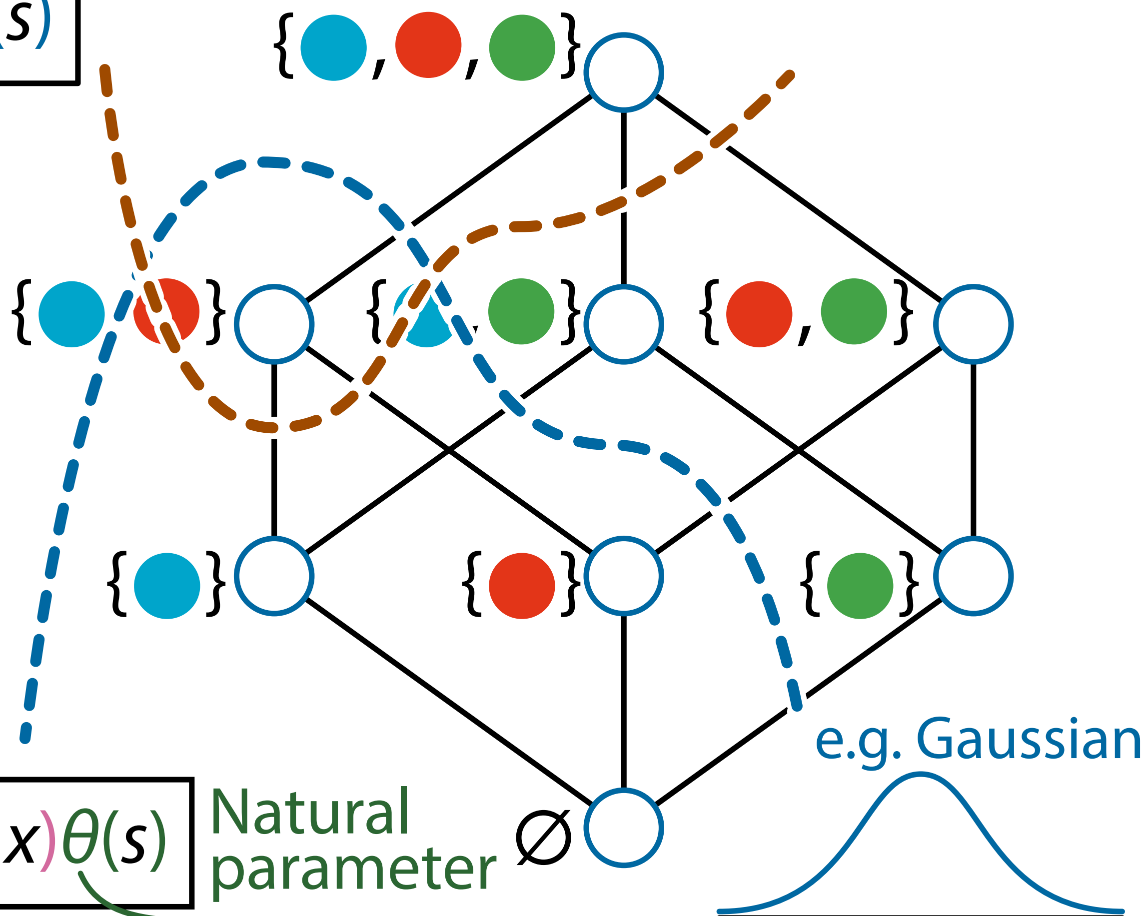
Natural parameter

Exponential family: $p(x) = \exp\left(\sum \theta(s) F_s(x) - \psi(\theta) \right)$

$$\eta(x) = \sum \zeta(x, s)p(s)$$

$$\eta(x) = \mathbb{E}[\, F_x(s) \,]$$

Sufficient statistics of exponential family



$$\log p(x) = \sum \zeta(s, x)\theta(s)$$

Natural parameter

Exponential family: $p(x) = \exp\left(\sum \theta(s)F_s(x) - \psi(\theta) \right)$

Möbius Inversion on Posets

- Zeta function $\zeta : S \times S \to \{0, 1\}$:

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

- Möbius function $\mu : S \times S \to \mathbb{Z}$, defined as $\mu = \zeta^{-1}$:

$$\mu(x, y) = \begin{cases} 1, & \text{if } x = y, \\ -\sum_{x \leq s < y} \mu(x, s) & \text{if } x < y, \\ 0 & \text{otherwise} \end{cases}$$

- The Möbius inversion formula [Rota (1964)]:

$$g(x) = \sum_{s \in S} \zeta(s, x) f(s) \iff f(x) = \sum_{s \in S} \mu(s, x) g(s)$$

Möbius Function Is Generalization of Inclusion-Exclusion Principle

- For sets A, B, C,

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

- In general, for $A_1, A_2, \ldots, A_n$,

$$\left|\bigcup_i A_i\right| = \sum_{J \subseteq \{1,\ldots,n\}, J \neq \emptyset} (-1)^{|J|-1} \left|\bigcap_{j \in J} A_j\right|$$

- The Möbius function μ is the generalization of "$(-1)^{|J|-1}$"

Mathematical Formulation

- Log-linear model and its sufficient statistics:

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

$$\eta(x) = \sum_{s \in S} \zeta(x, s)p(s) = \sum_{s \ge x} p(s)$$

  - Generalization of the log-linear model on binary vectors:

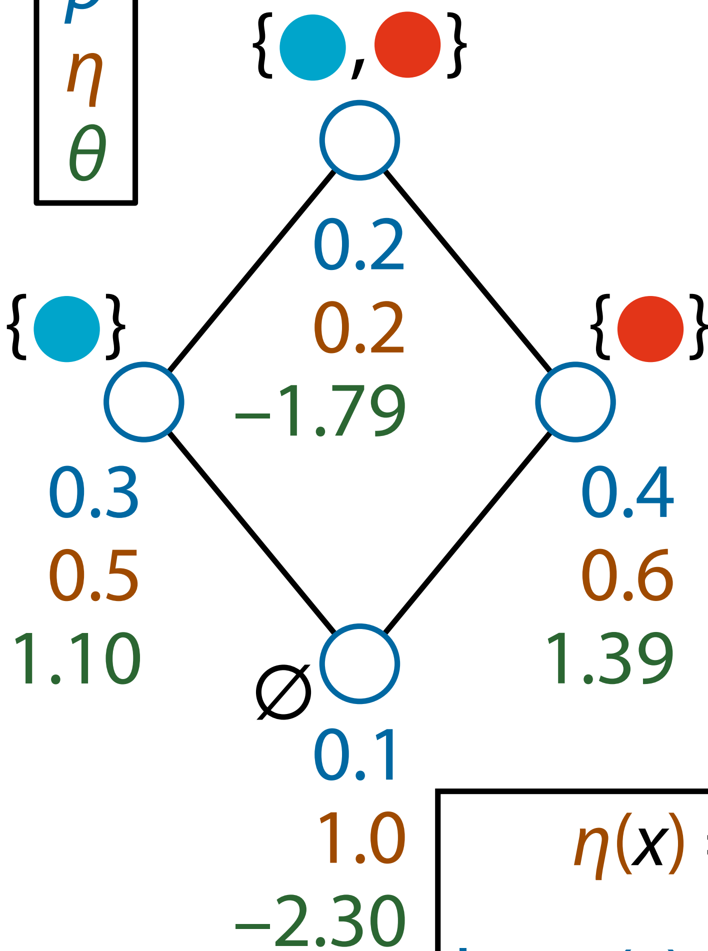
$$\log p(\boldsymbol{x}) = \sum_{i} \theta^{i} x^{i} + \sum_{i<j} \theta^{ij} x^{i} x^{j} + \cdots + \theta^{1\ldots n} x^{1} x^{2} \ldots x^{n},$$

- From the Möbius inversion formula,

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

Triple for each node

$$\boxed{\begin{array}{c} p \\ \eta \\ \theta \end{array}}$$

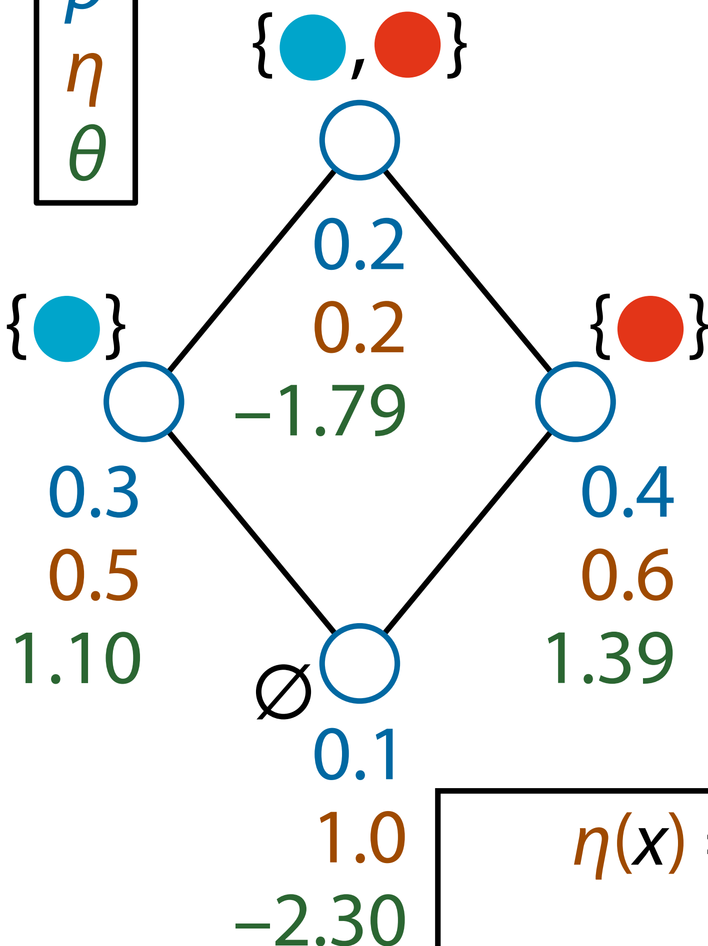


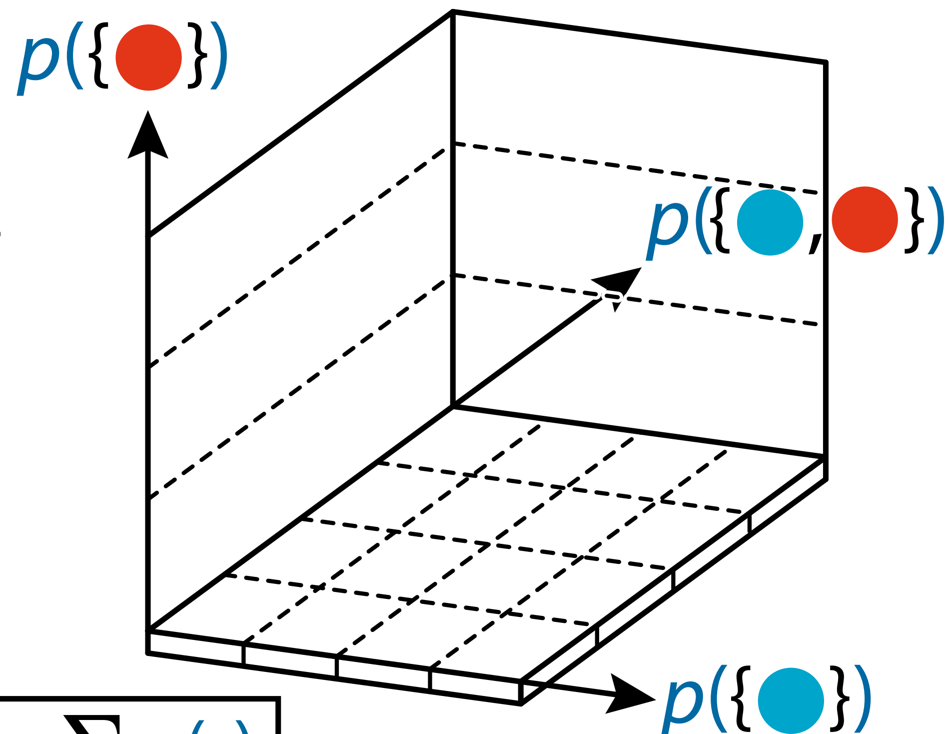
$$\eta(x) = \sum_{s \geq x} p(s)$$

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

Triple for each node

p
η
θ





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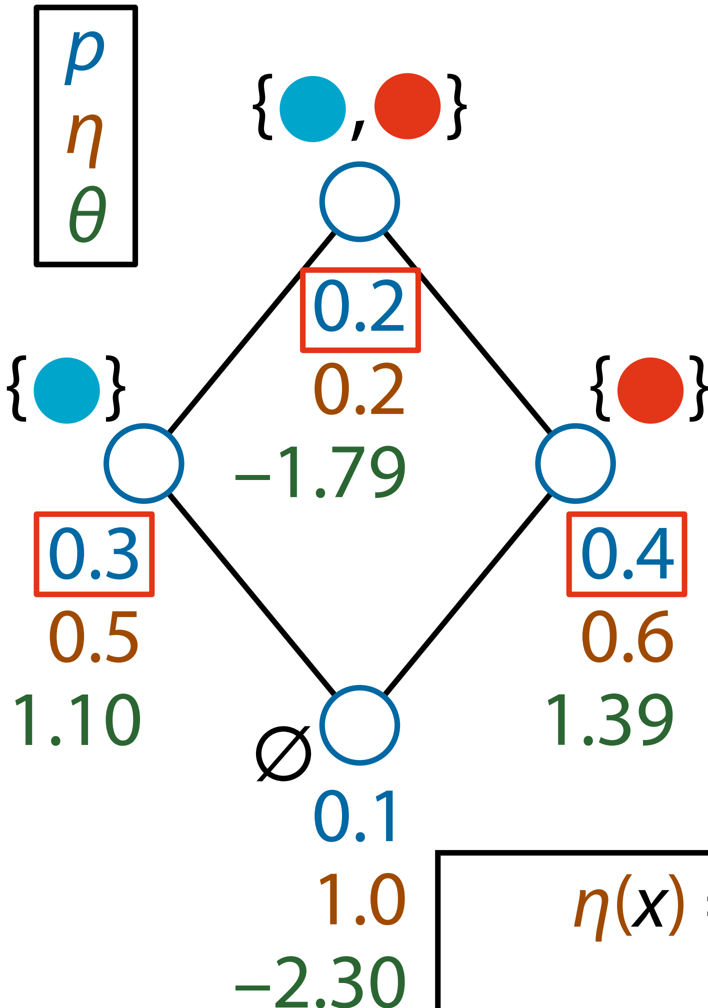
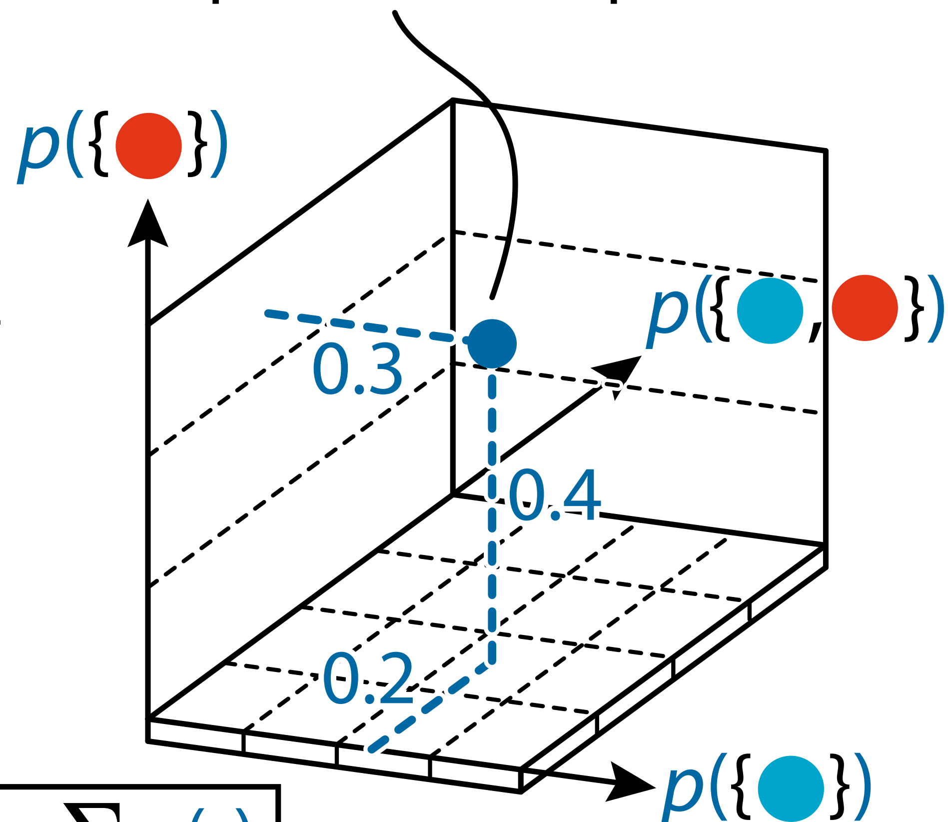
Triple for each node



Probability distribution is a “point” in 3D space



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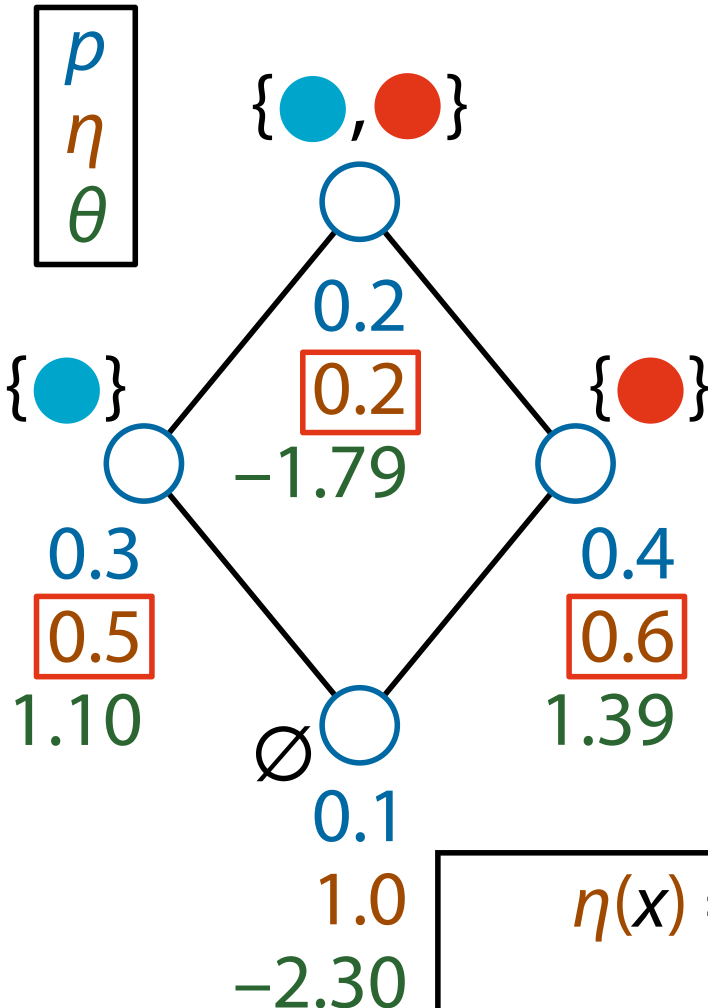
Triple for each node



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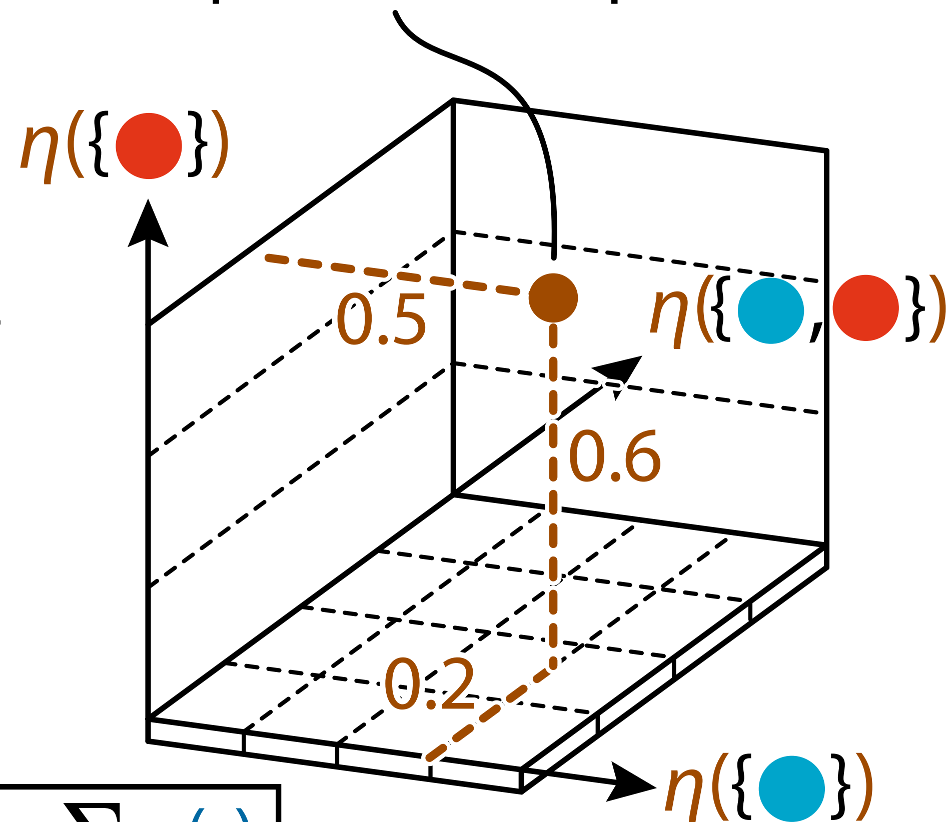

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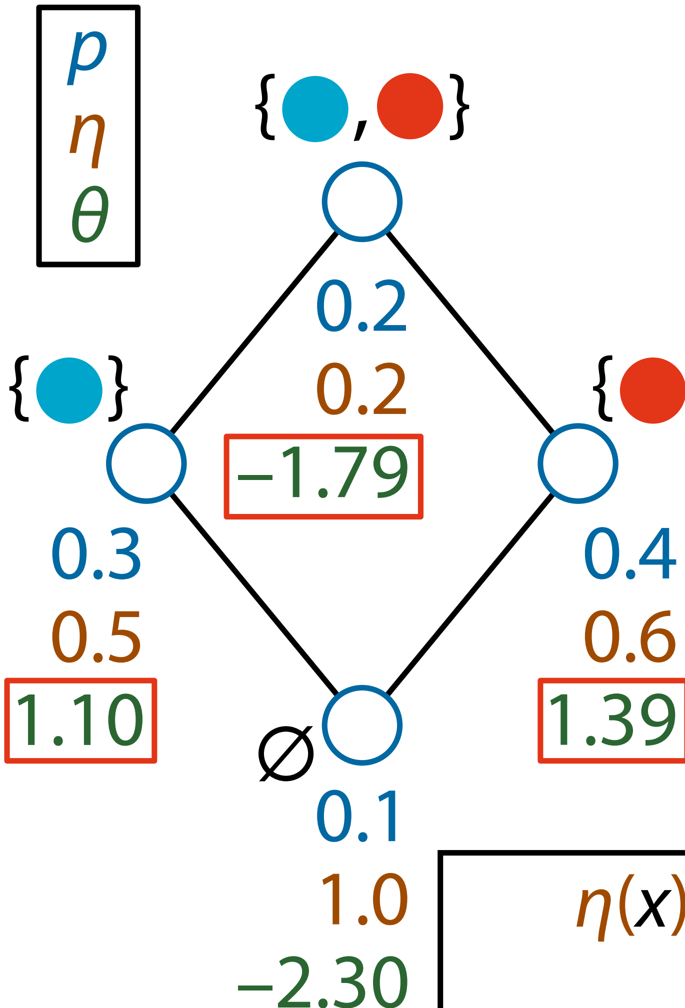
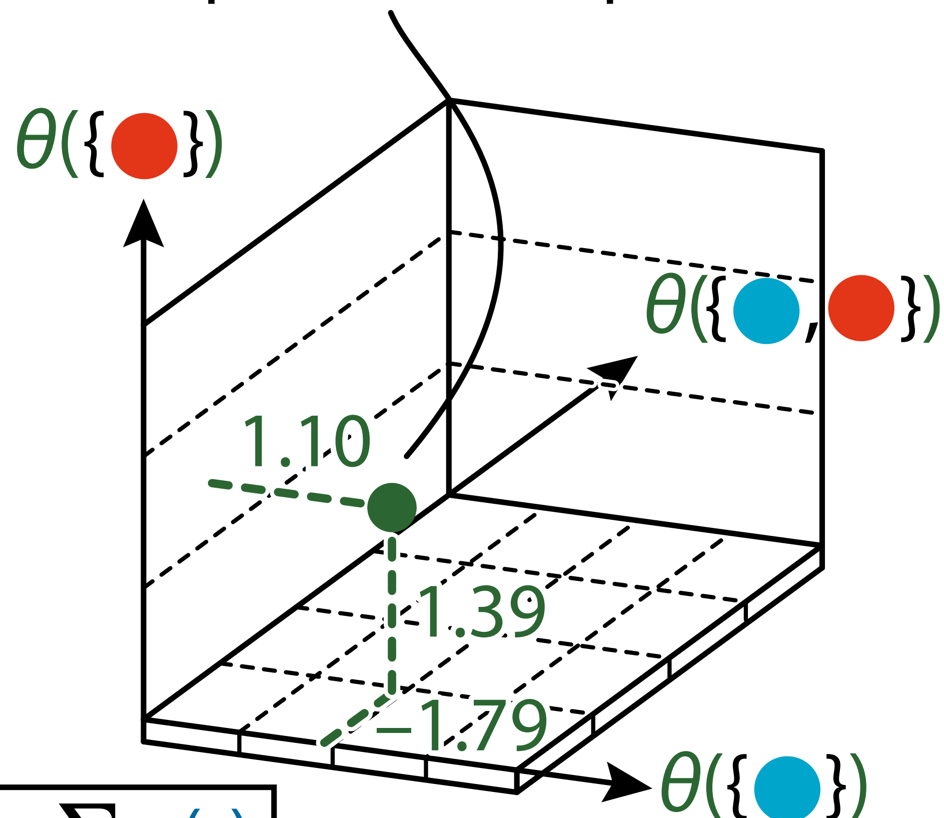
Triple for each node



Probability distribution is a "point" in 3D space



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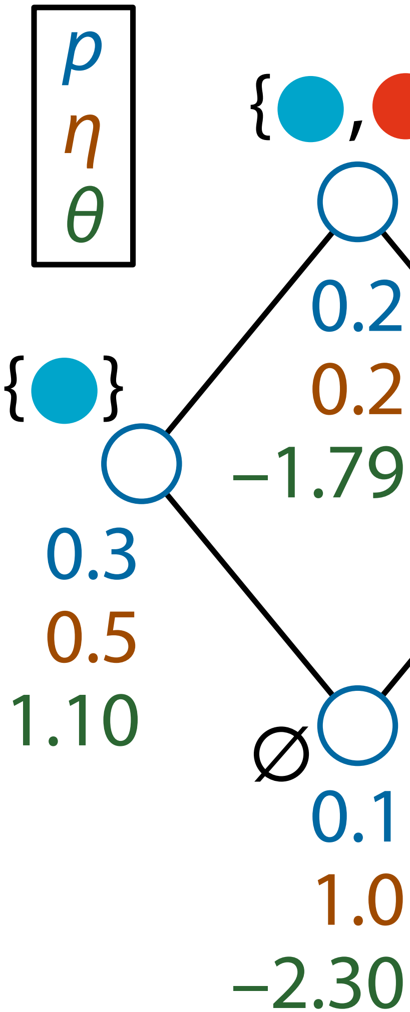
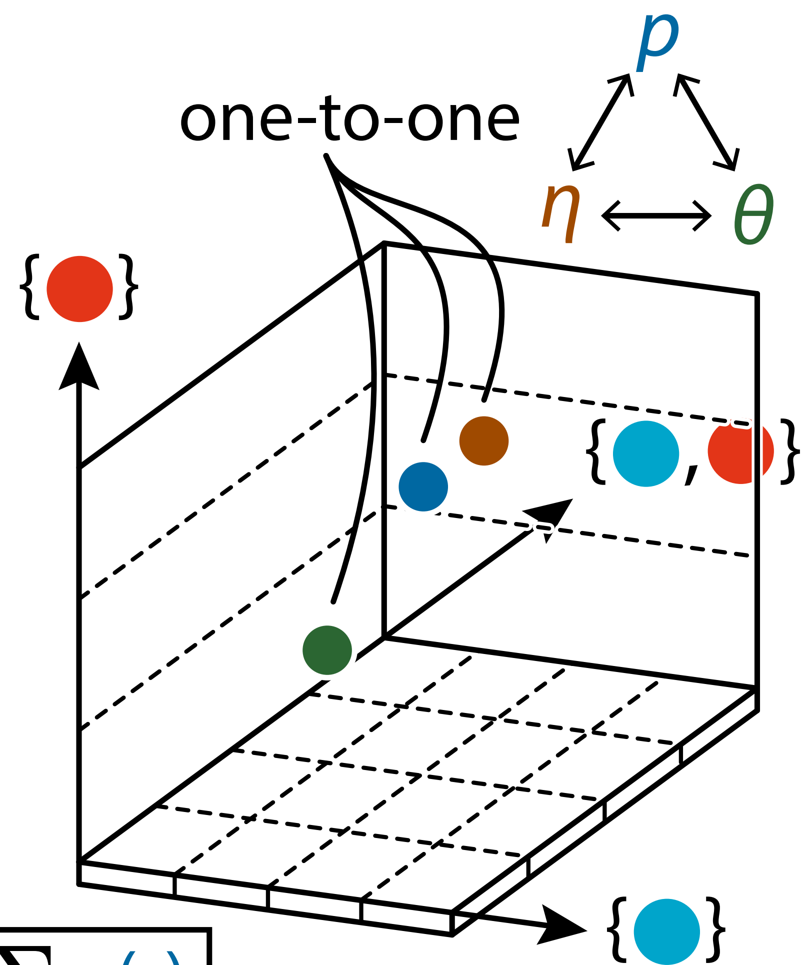
Triple for each node





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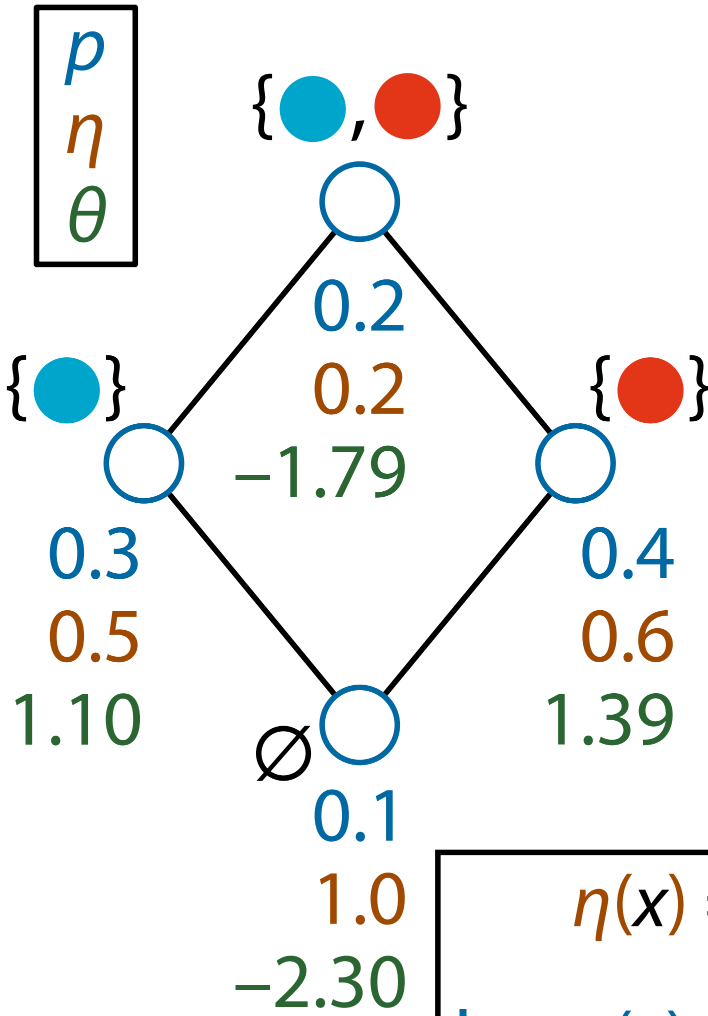
Triple for each node



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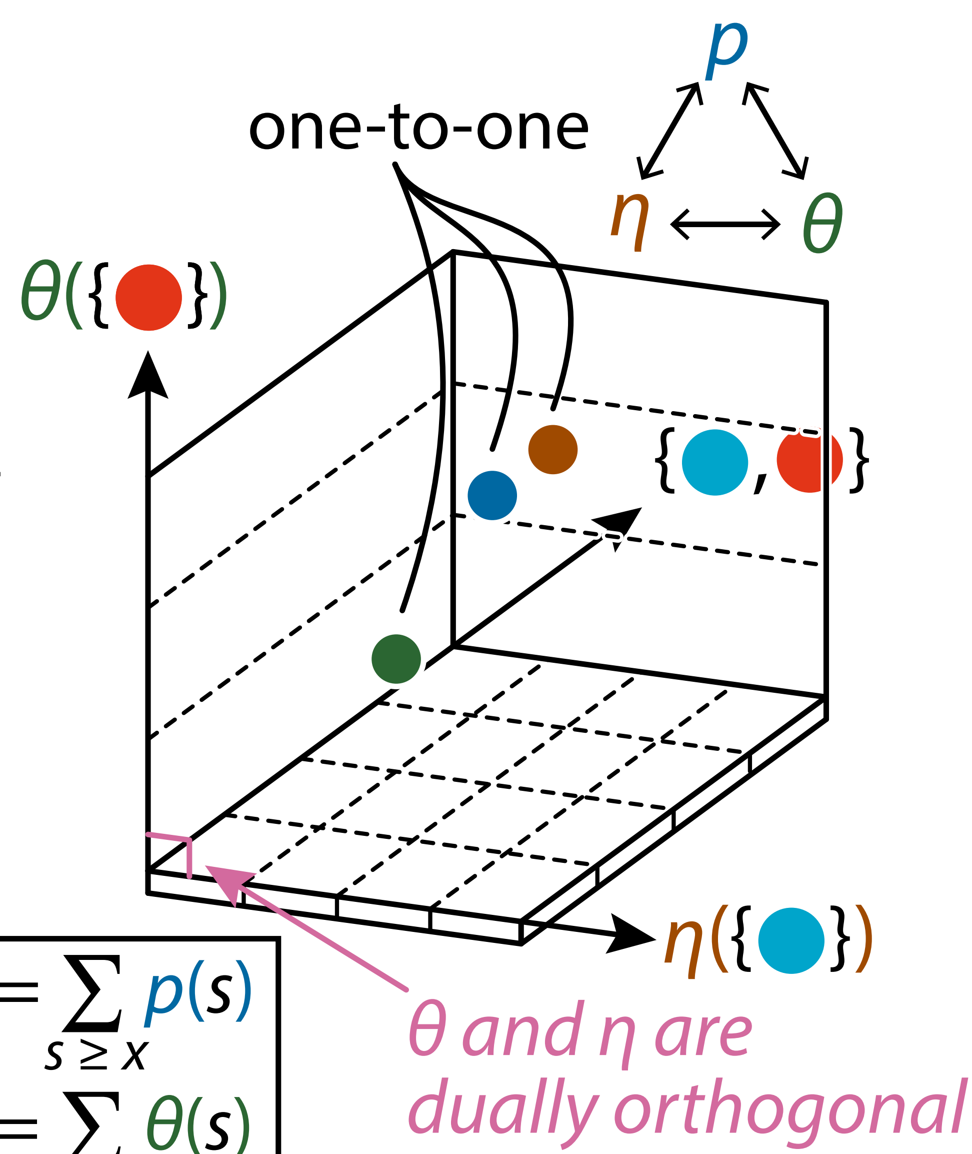


Orthogonality of $\boldsymbol{\theta}$ and $\boldsymbol{\eta}$

- From Möbius inversion,

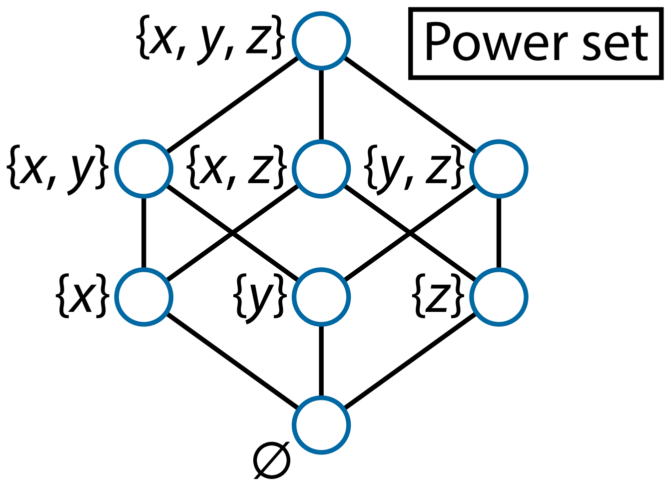
$$\sum_{s \in S} \zeta(x, s)\mu(s, y) = \delta_{x,y}, \quad \delta_{x,y} = \begin{cases} 1 & \text{if } x = y, \\ 0 & \text{otherwise} \end{cases}$$

- θ and η are dually orthogonal:

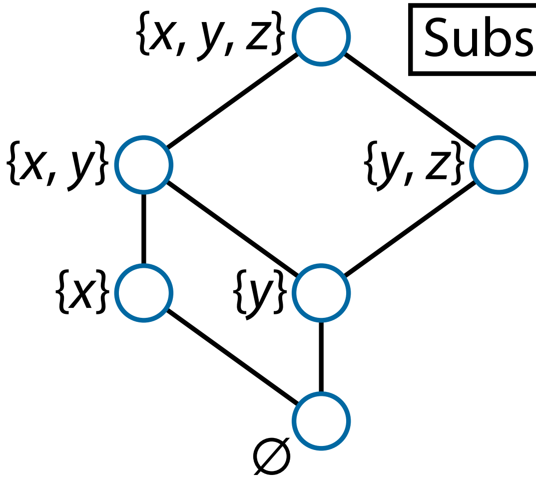
$$\mathrm{E}\left[\frac{\partial}{\partial\theta(x)} \log p(s) \frac{\partial}{\partial\eta(y)} \log p(s)\right] = \sum_{s \in S} \zeta(x, s)\mu(s, y) = \delta_{x,y}$$

- Partial order structure leads to the same dually flat structure with the exponential family

Existing Approach Limited To Power Set

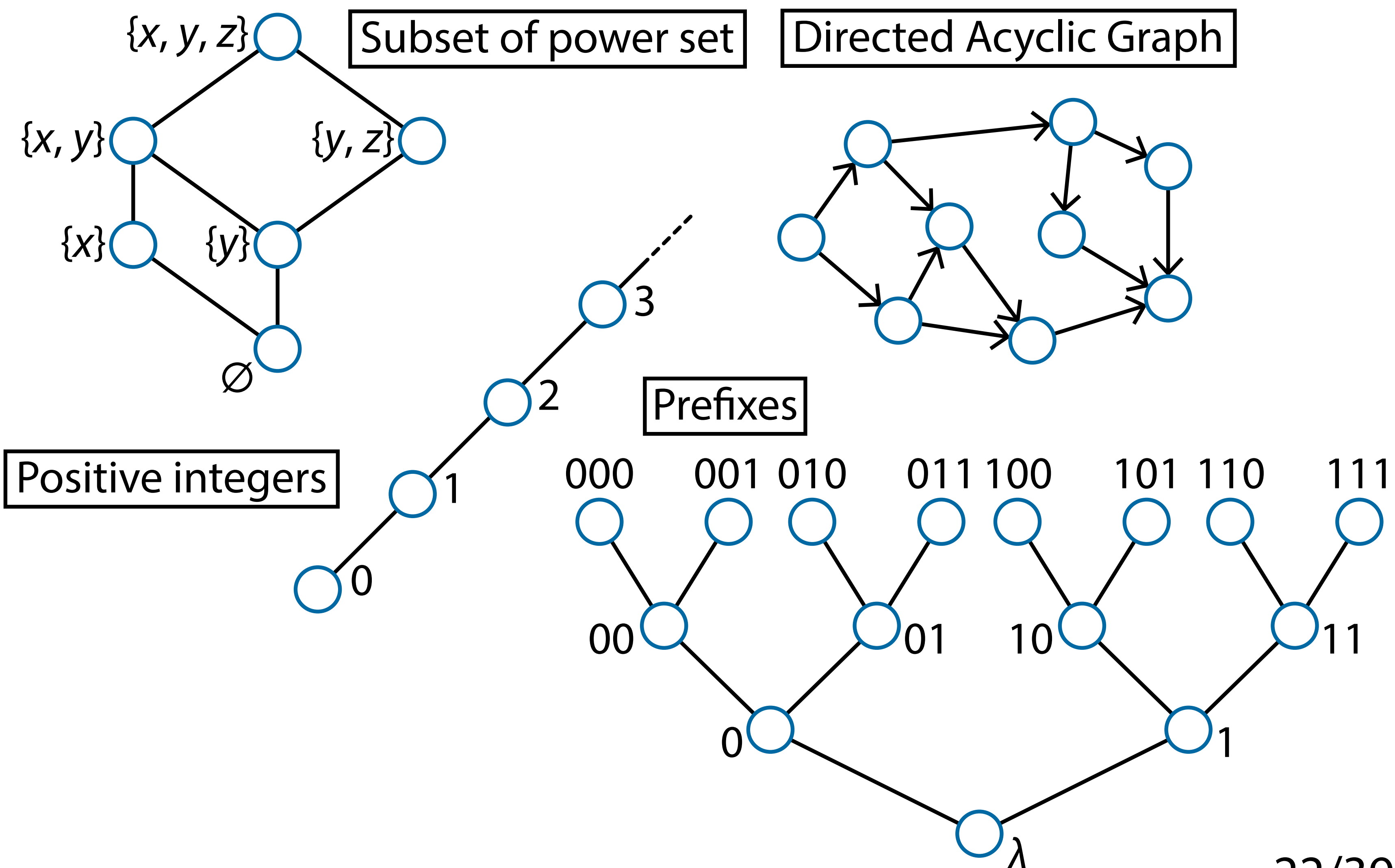


Our Approach Applies Any Posets



Subset of power set

Our Approach Applies Any Posets



KL Divergence Decomposition

- KL divergence decomposition:

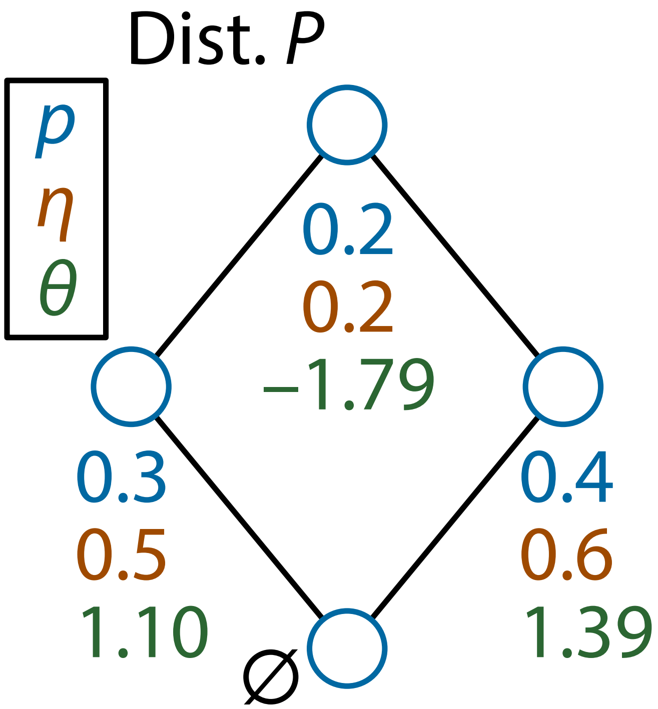
  $D_{\mathrm{KL}}[P,R] = D_{\mathrm{KL}}[P,Q] + D_{\mathrm{KL}}[Q,R]$

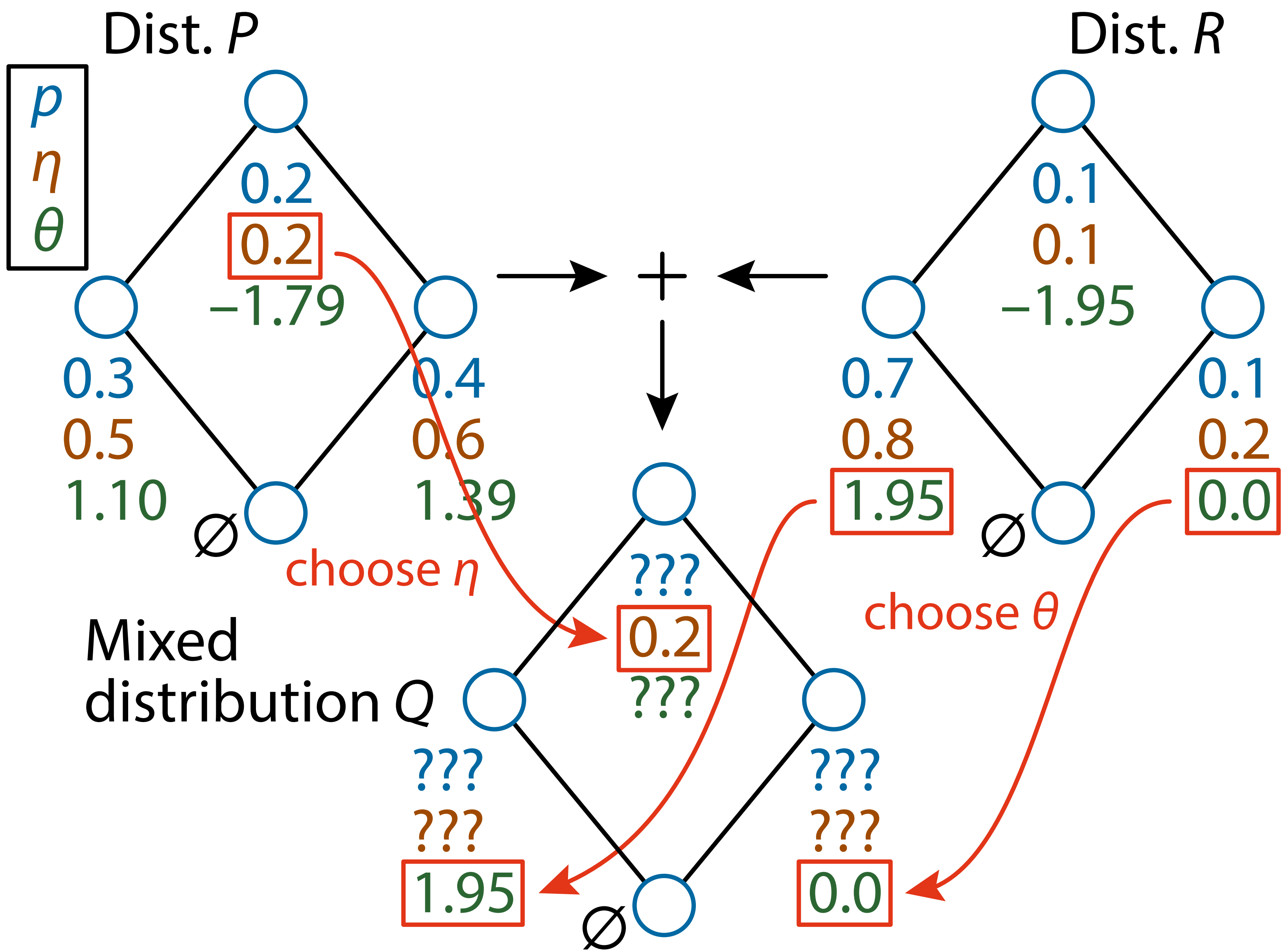
  with Q s.t. $\theta_Q(x) = \theta_R(x)$ or $\eta_Q(x) = \eta_P(x)$ for all $x \in S$
  - Q is called the mixed distribution of (P,R)
  - It is known as the (generalized) Pythagoras theorem in Information Geometry

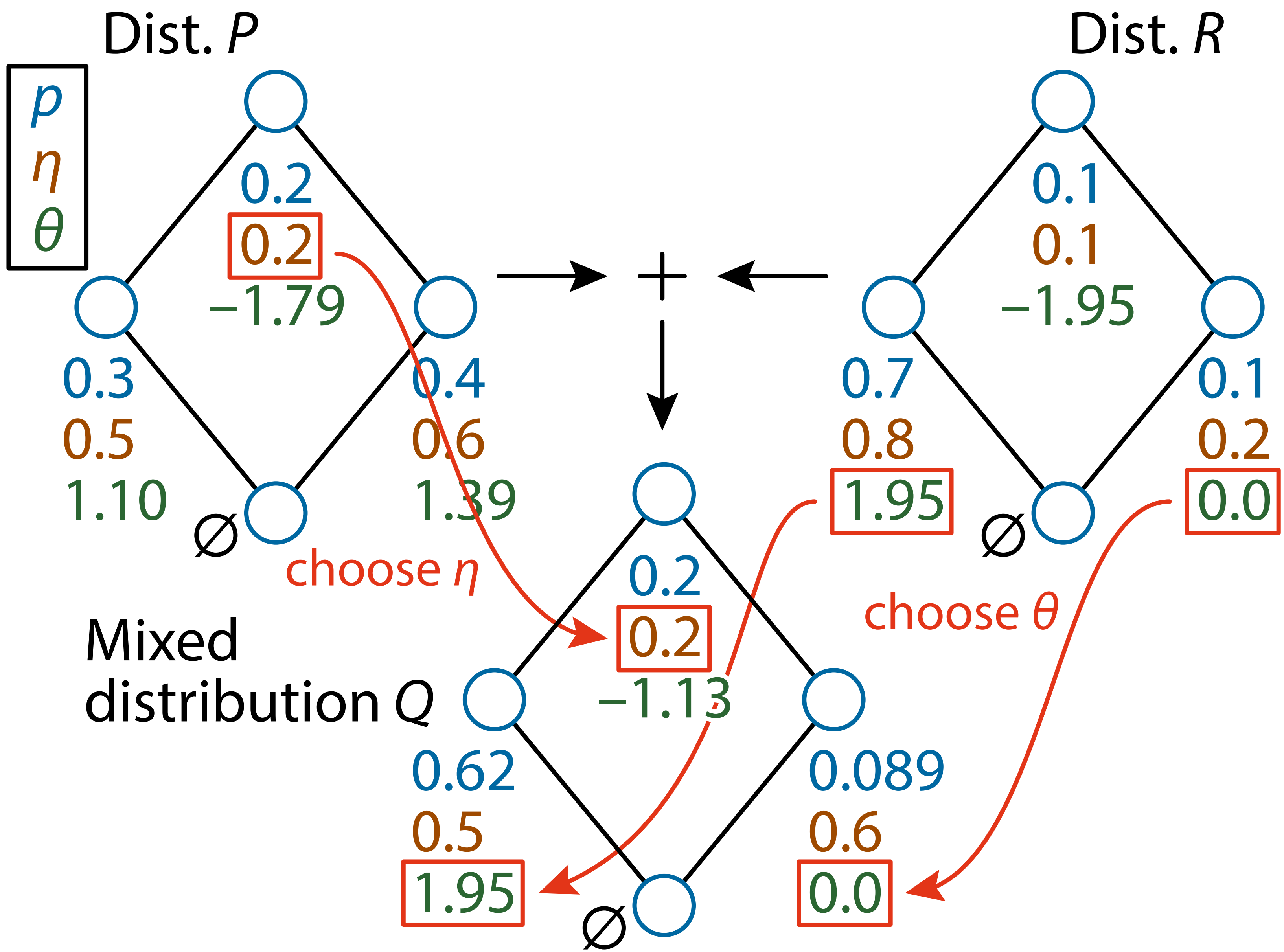
- We can derive from Möbius inversion:

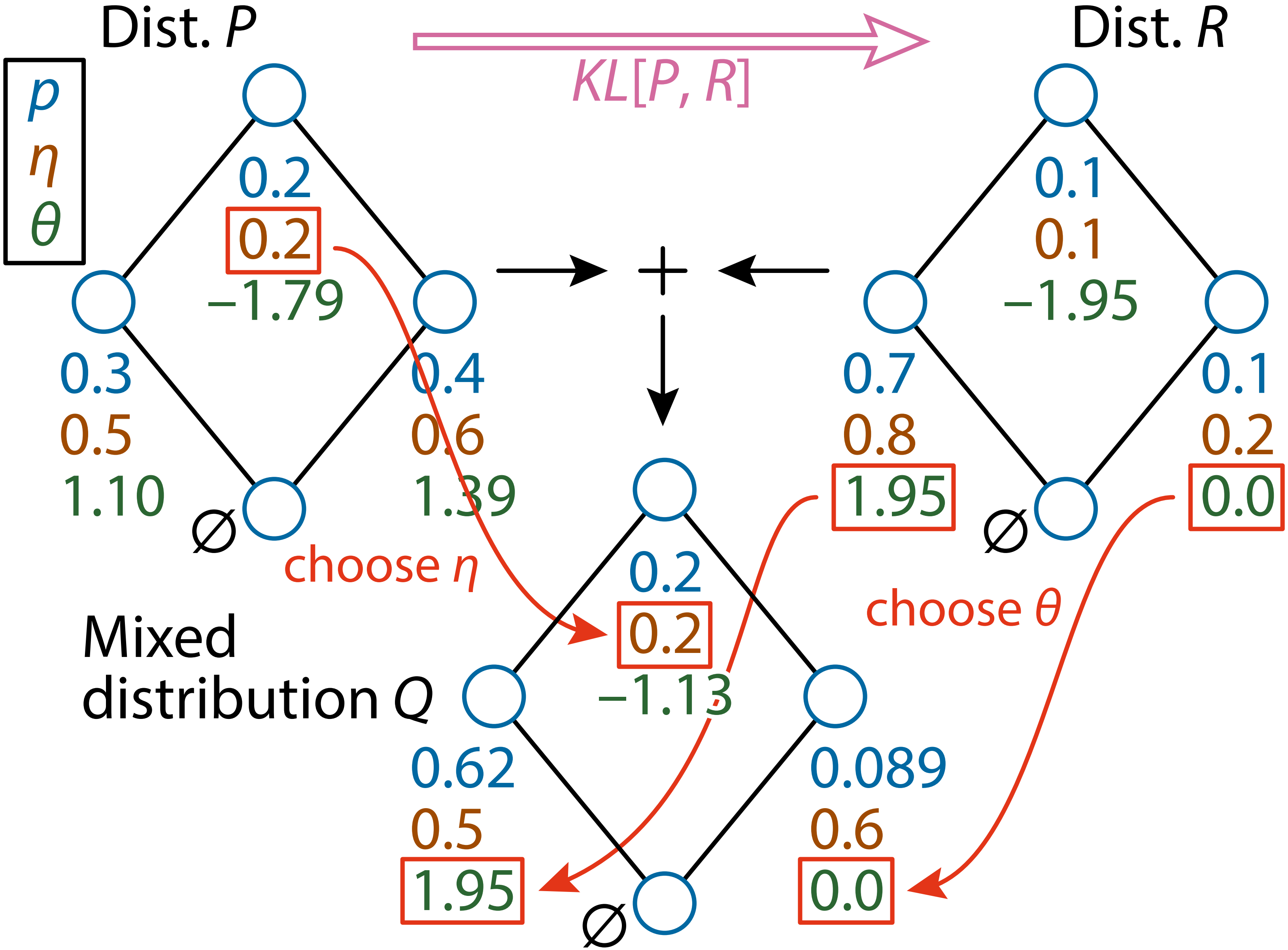
$$D_{\mathrm{KL}}[P,Q] + D_{\mathrm{KL}}[Q,R] - D_{\mathrm{KL}}[P,R]$$

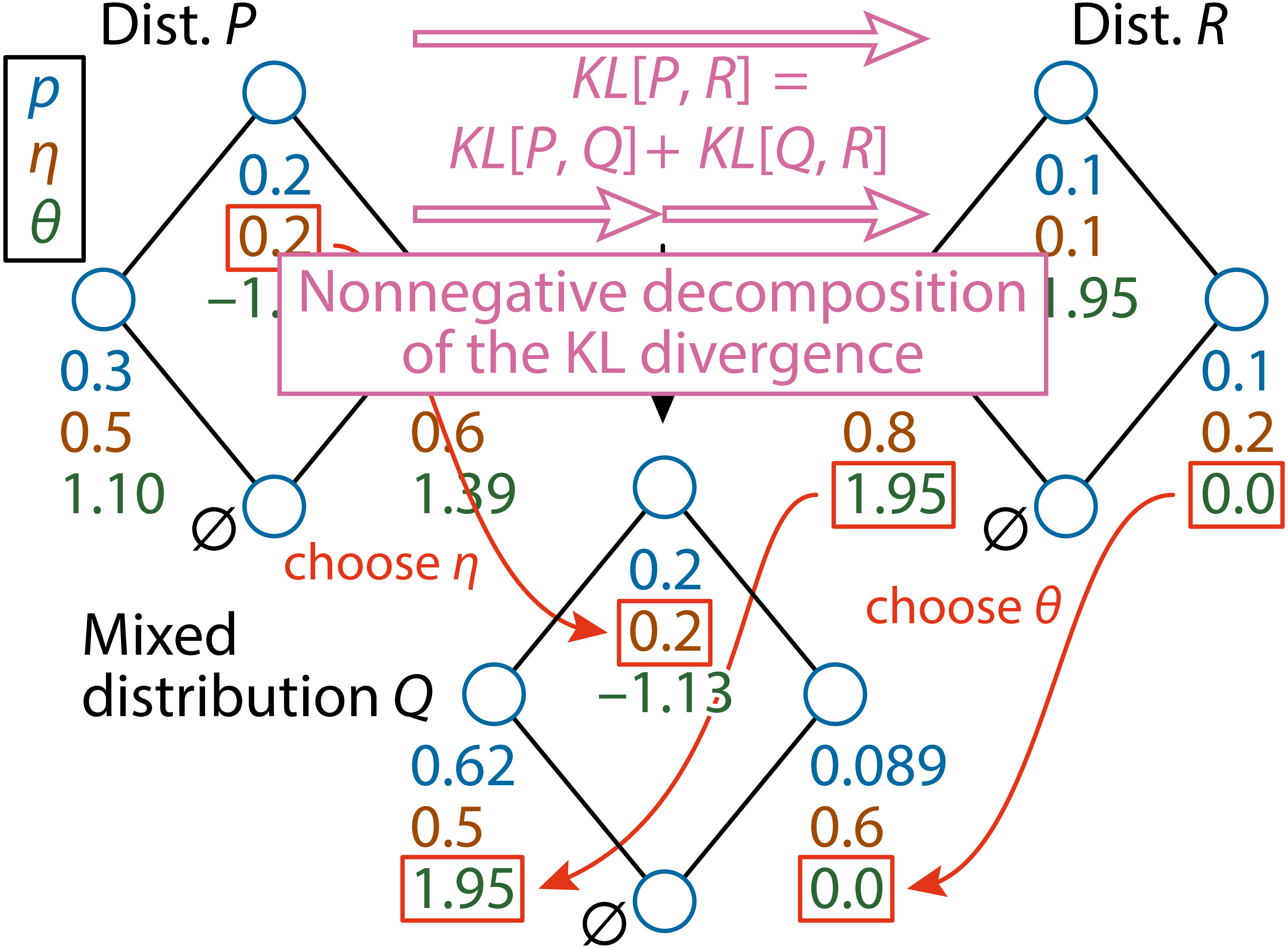
$$= \sum_{s \in S} (\eta_Q(s) - \eta_P(s))(\theta_Q(s) - \theta_R(s))$$

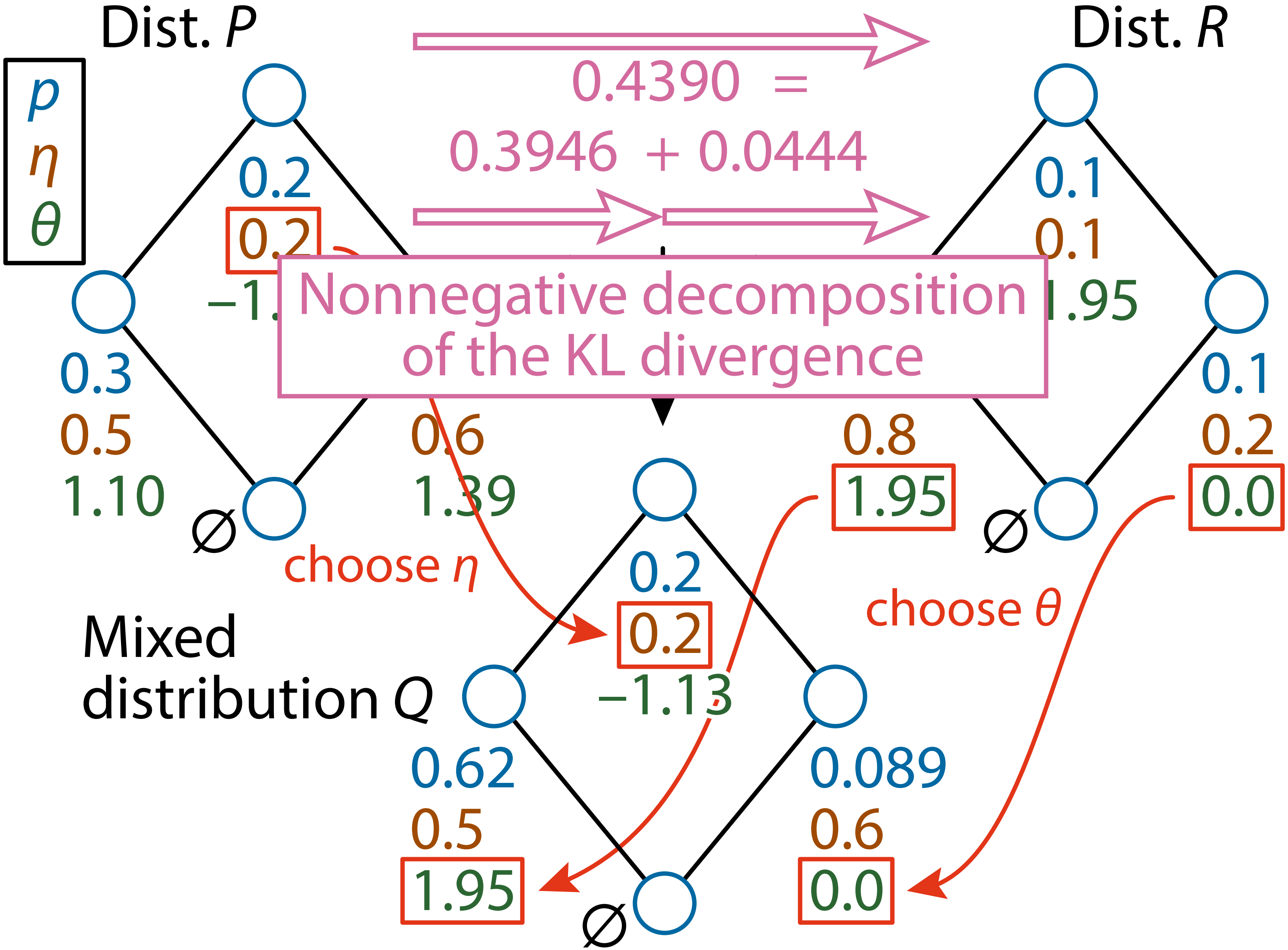

Dist. P
p
η
θ
0.2
0.2
−1.79
0.3
0.5
1.10
0.4
0.6
1.39
∅
Dist. R
0.1
0.1
−1.95
0.7
0.8
1.95
0.1
0.2
0.0
∅


Dist. P
Dist. R
p
η
θ
0.2
0.2
−1.79
0.3
0.5
1.10
0.4
0.6
1.39
∅
0.1
0.1
−1.95
0.7
0.8
1.95
0.1
0.2
0.0
∅
+
choose η
choose θ
Mixed distribution Q
???
0.2
???
???
???
1.95
???
???
0.0
∅


Dist. P
p
η
θ
0.2
0.2
−1.79
0.3
0.5
1.10
0.4
0.6
1.39
∅
choose η
Dist. R
0.1
0.1
−1.95
0.7
0.8
1.95
0.1
0.2
0.0
∅
choose θ
Mixed distribution Q
0.2
0.2
−1.13
0.62
0.5
1.95
0.089
0.6
0.0
∅

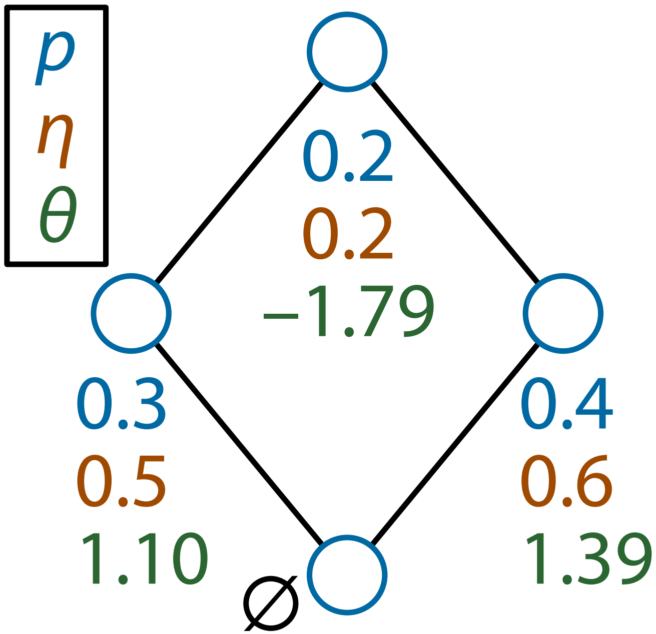

Dist. P
p
η
θ
0.2
0.2
−1.79
0.3
0.5
1.10
0.4
0.6
1.39
∅
$KL[P, R]$
Dist. R
0.1
0.1
−1.95
0.7
0.8
1.95
0.1
0.2
0.0
∅
choose η
choose θ
Mixed distribution Q
0.2
0.2
−1.13
0.62
0.5
1.95
0.089
0.6
0.0
∅


Dist. P
Dist. R
p
η
θ
KL[P, R] =
KL[P, Q] + KL[Q, R]
Nonnegative decomposition of the KL divergence
0.2
0.2
0.3
0.5
1.10
0.6
1.39
0.1
0.1
1.95
0.8
1.95
0.1
0.2
0.0
choose η
choose θ
Mixed distribution Q
0.2
0.2
−1.13
0.62
0.5
1.95
0.089
0.6
0.0
∅

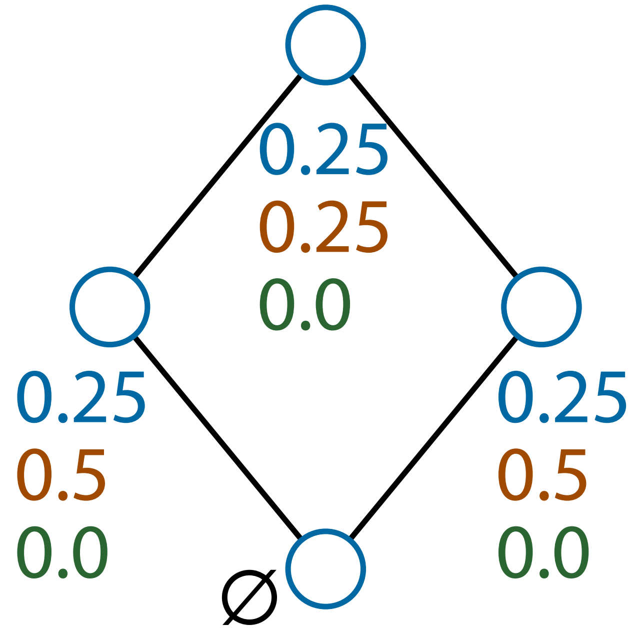


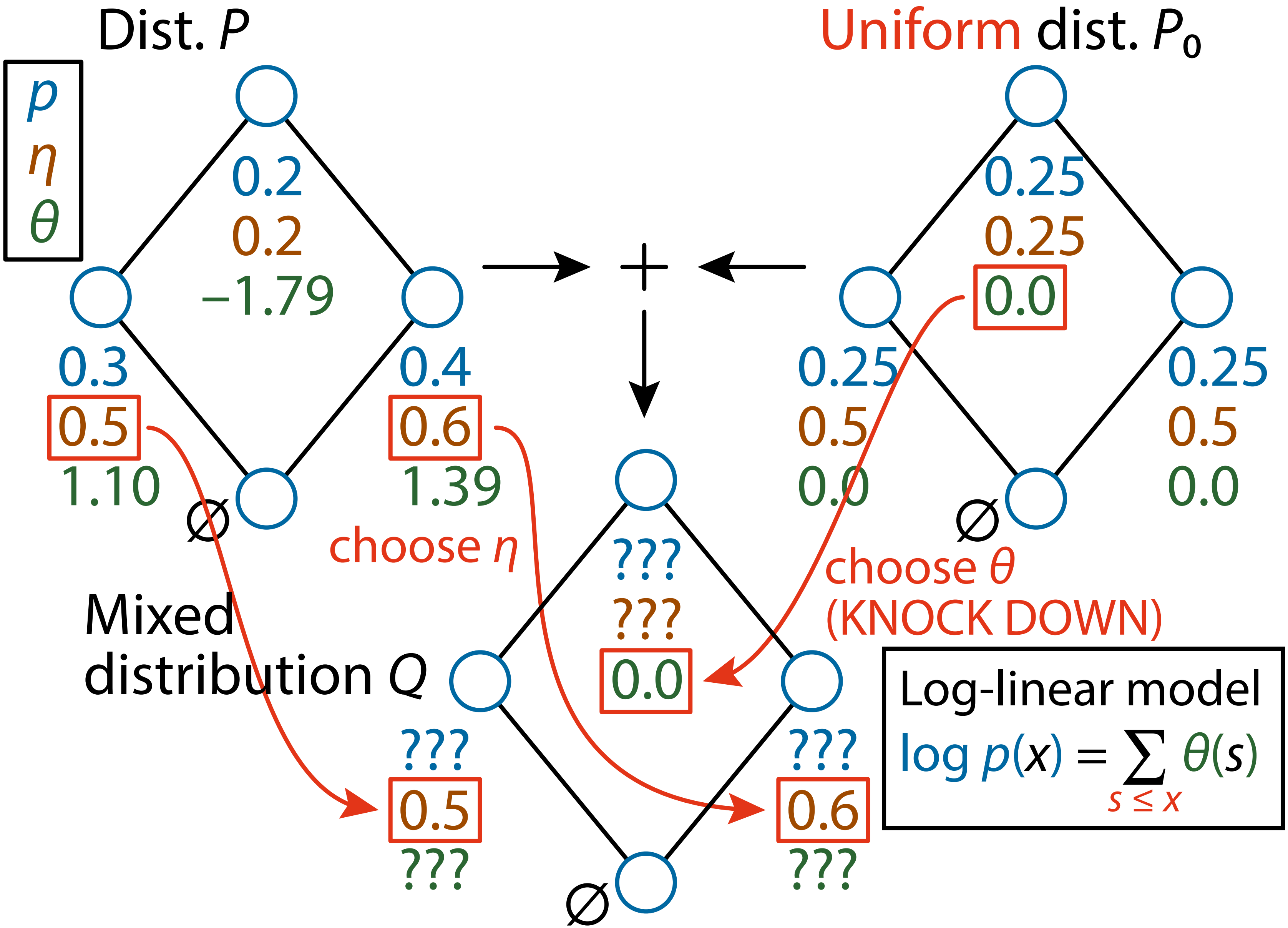
Dist. P
Dist. R
p
η
θ
0.4390 =
0.3946 + 0.0444
Nonnegative decomposition of the KL divergence
0.2
0.2
0.3
0.5
1.10
0.6
1.39
0.1
0.1
1.95
0.1
0.2
0.0
0.8
1.95
choose η
choose θ
Mixed distribution Q
0.2
0.2
−1.13
0.62
0.5
1.95
0.089
0.6
0.0

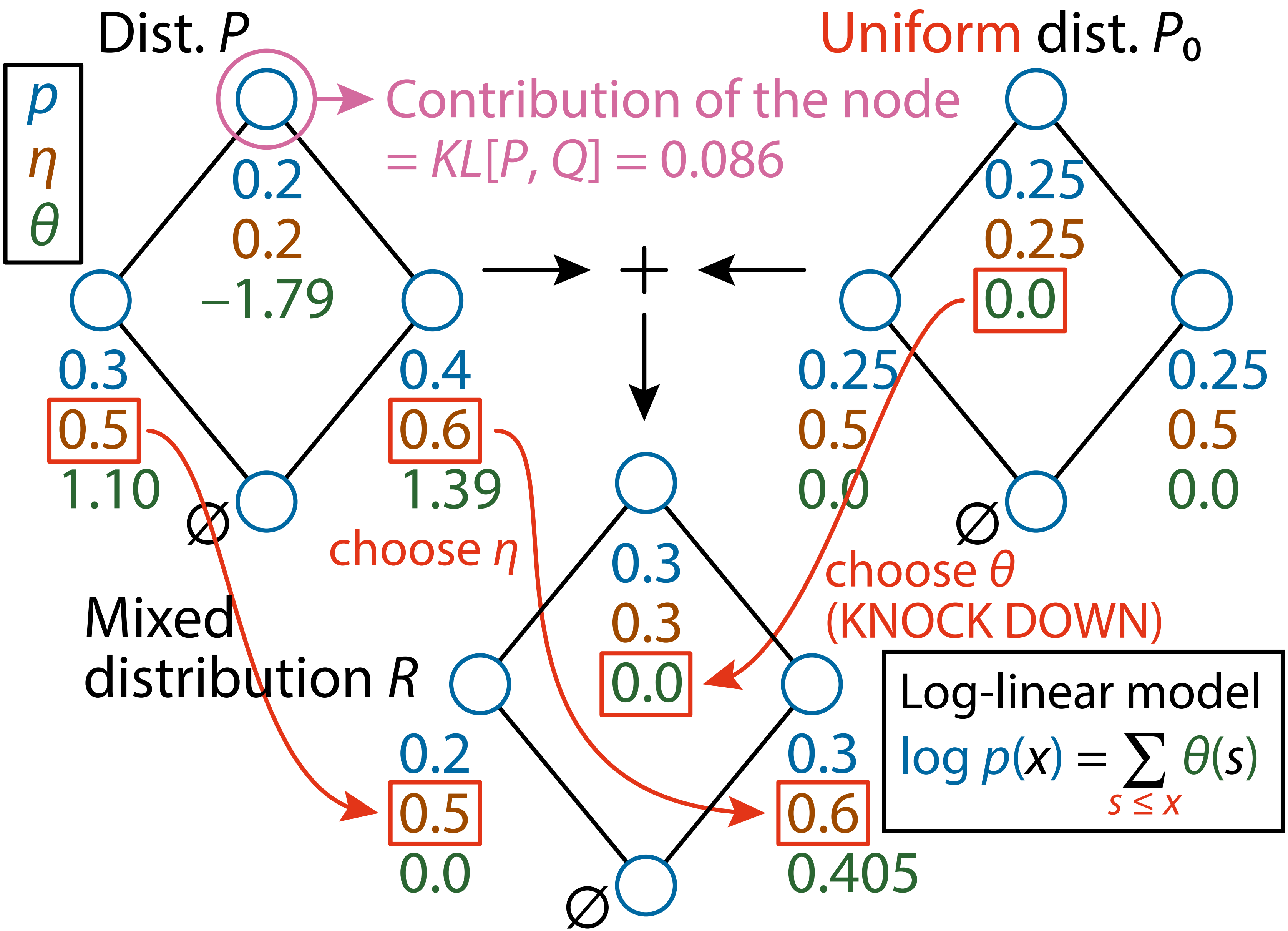
Dist. P

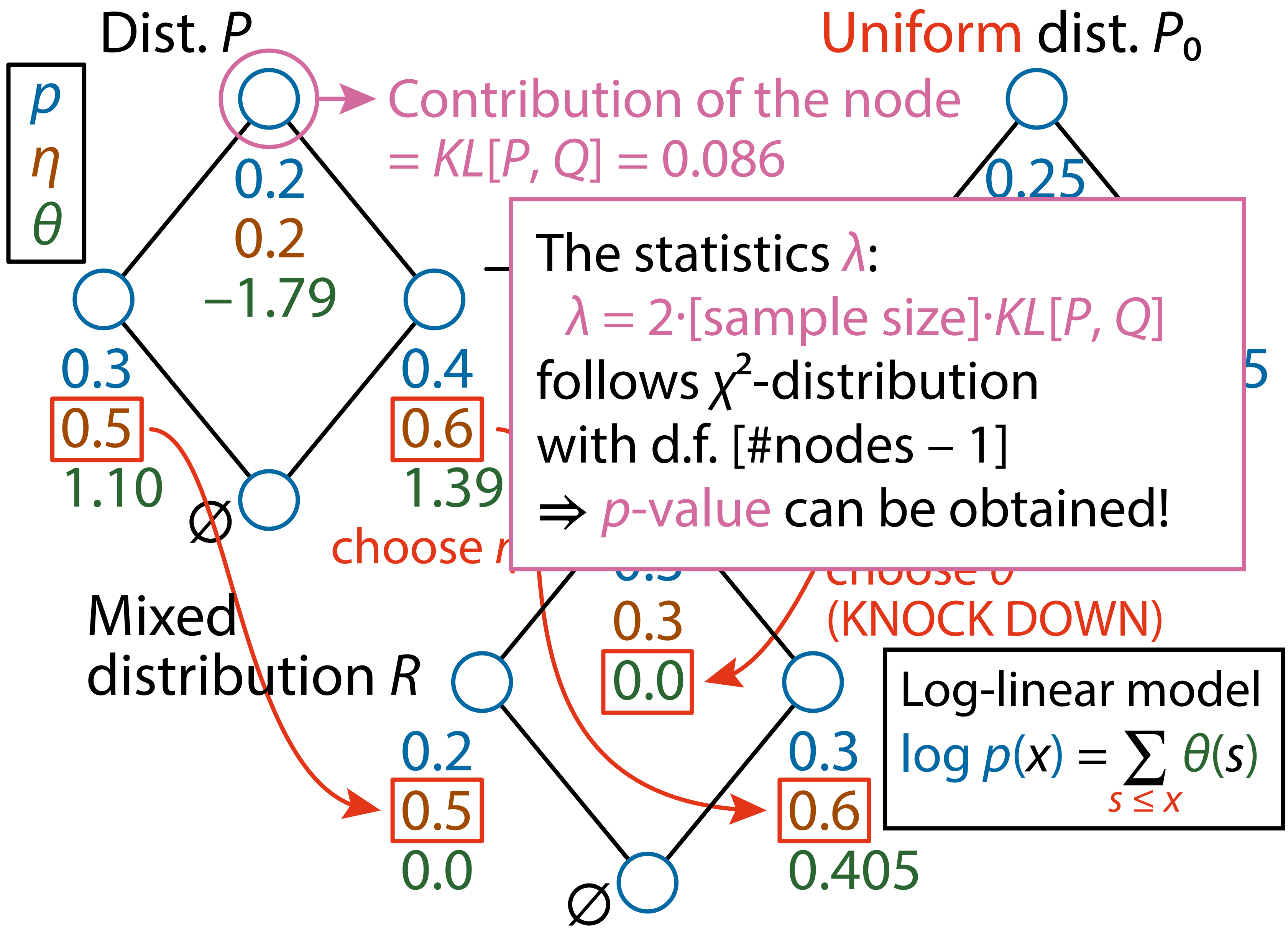


Uniform dist. P_0

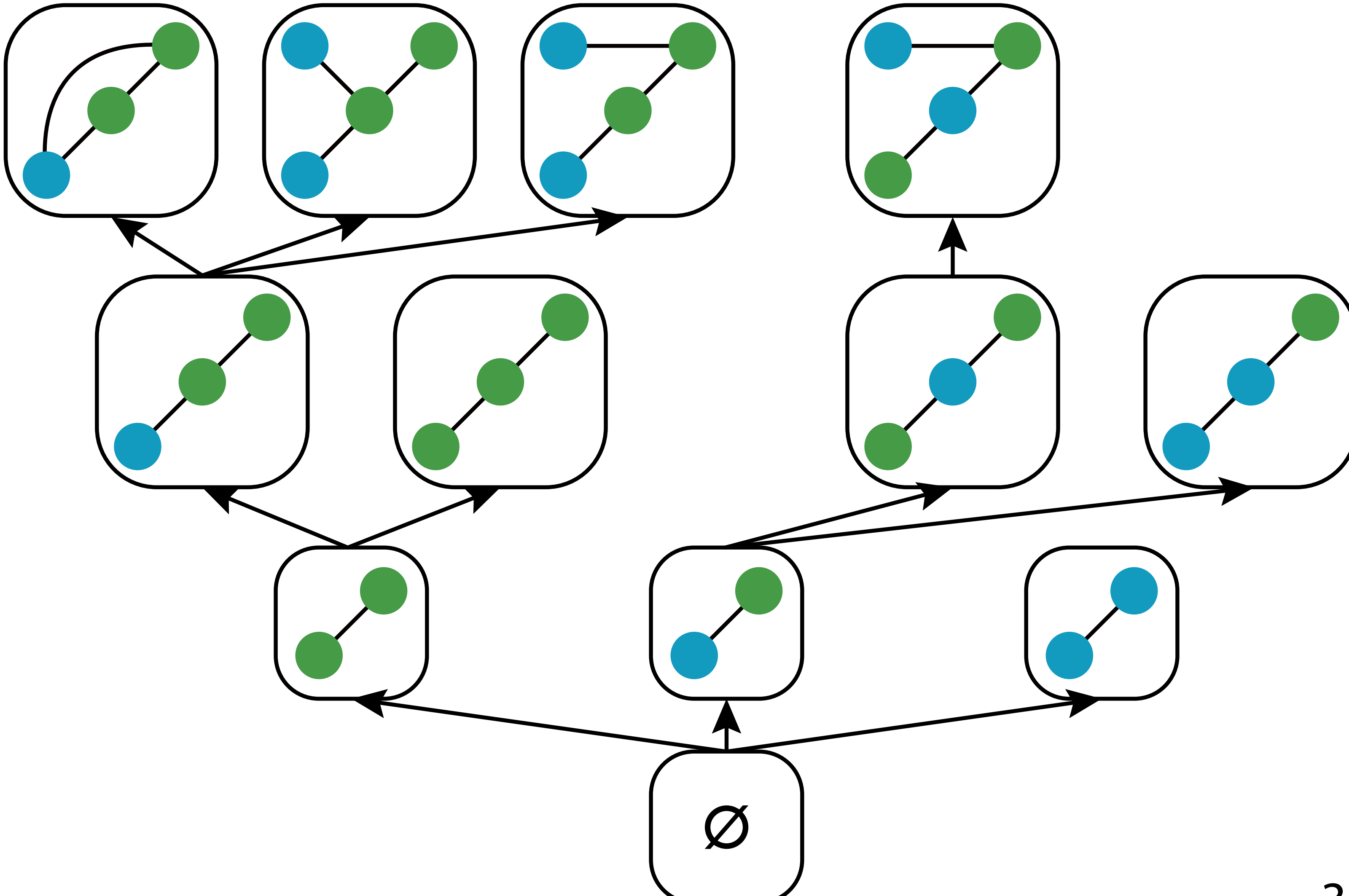



Dist. P
p
η
θ
0.2
0.2
−1.79
0.3
0.5
1.10
0.4
0.6
1.39
$\varnothing$
choose η
Uniform dist. P_0
0.25
0.25
0.0
0.25
0.5
0.0
0.25
0.5
0.0
$\varnothing$
choose θ
(KNOCK DOWN)
Mixed distribution Q
???
???
0.0
???
0.5
???
???
0.6
???
$\varnothing$
Log-linear model
$\log p(x) = \sum_{s \le x} \theta(s)$

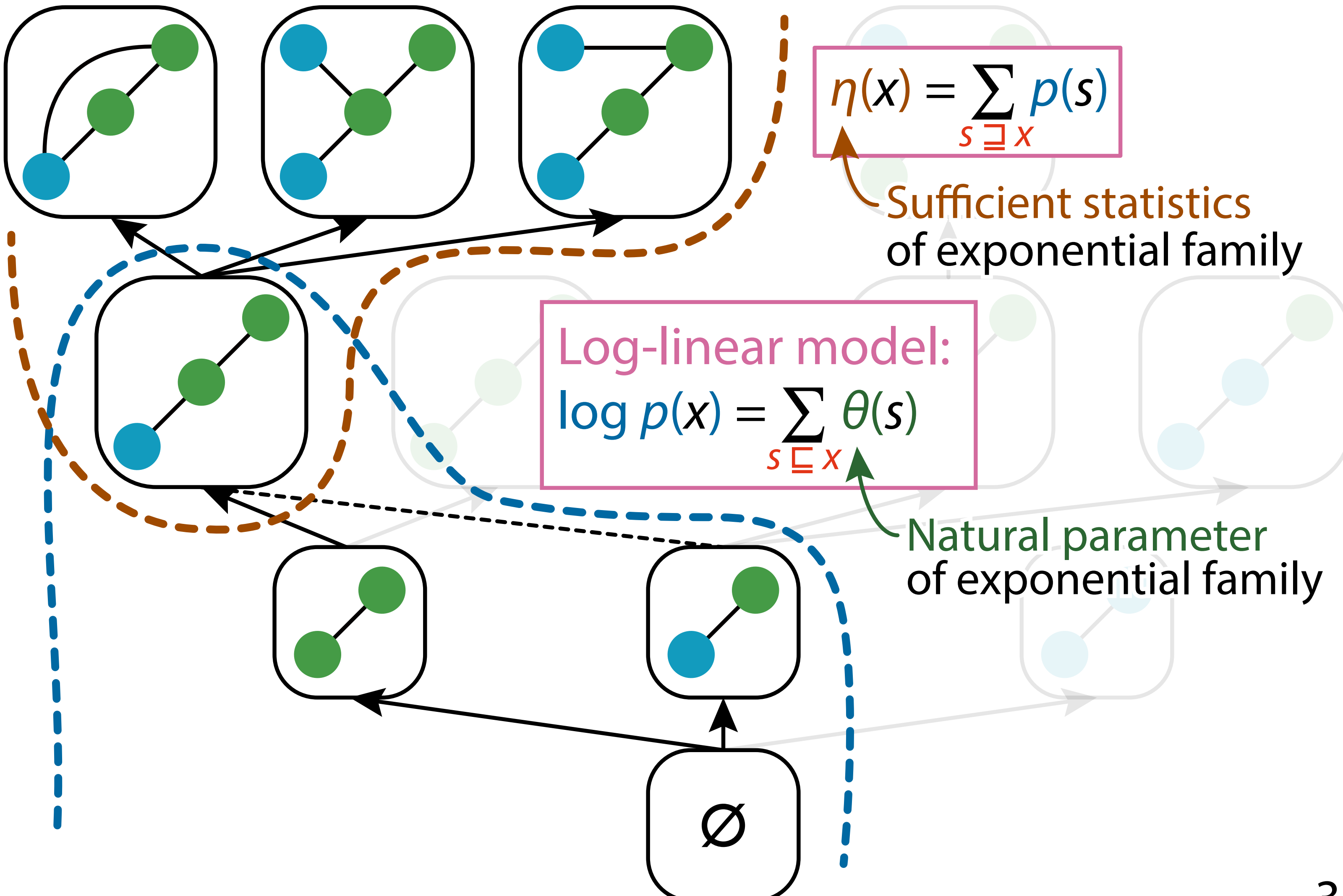

Dist. P
p
η
θ
0.2
0.2
−1.79
0.3
0.5
1.10
0.4
0.6
1.39
∅
Contribution of the node
= KL[P, Q] = 0.086
Uniform dist. P0
0.25
0.25
0.0
0.25
0.5
0.0
0.25
0.5
0.0
∅
+
choose η
choose θ
(KNOCK DOWN)
Mixed
distribution R
0.3
0.3
0.0
0.2
0.5
0.0
0.3
0.6
0.405
∅
Log-linear model
log p(x) = ∑ θ(s)
s ≤ x


Dist. P
p
η
θ
0.2
0.2
−1.79
0.3
0.5
1.10
0.4
0.6
1.39
∅
Contribution of the node
$= KL[P, Q] = 0.086$
Uniform dist. P_0
0.25
The statistics λ:
$\lambda = 2 \cdot [\text{sample size}] \cdot KL[P, Q]$
follows χ^2-distribution
with d.f. [#nodes – 1]
⇒ p-value can be obtained!
(KNOCK DOWN)
Mixed
distribution R
0.3
0.0
0.2
0.5
0.0
0.3
0.6
0.405
∅
Log-linear model
$\log p(x) = \sum_{s \leq x} \theta(s)$

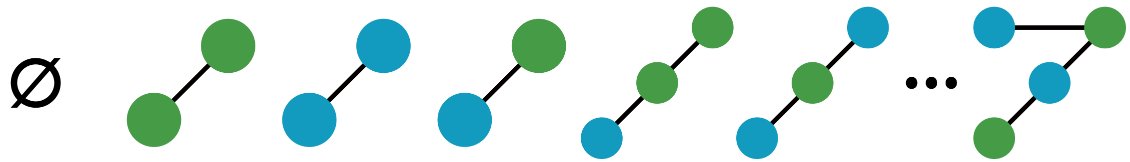
Poset of Subgraphs

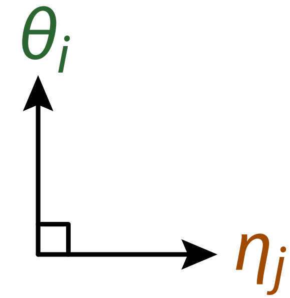


Log-Linear Model on Subgraphs



Information of Each Subgraph

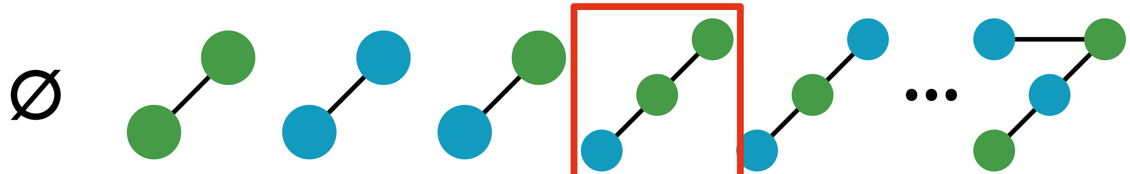


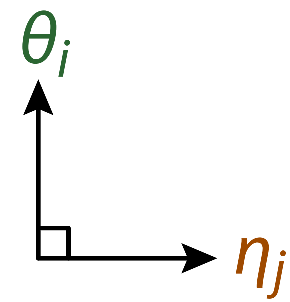


P: Empirical distribution

$$\begin{array}{l} \text{Freq.} \\ \text{Coef.} \end{array} \begin{bmatrix} \eta_0 & \eta_1 & \eta_2 & \eta_3 & \eta_4 & \eta_5 & \cdots & \eta_k \\ \theta_0 & \theta_1 & \theta_2 & \theta_3 & \theta_4 & \theta_5 & \cdots & \theta_k \end{bmatrix}$$

Information of Each Subgraph





P: Empirical distribution

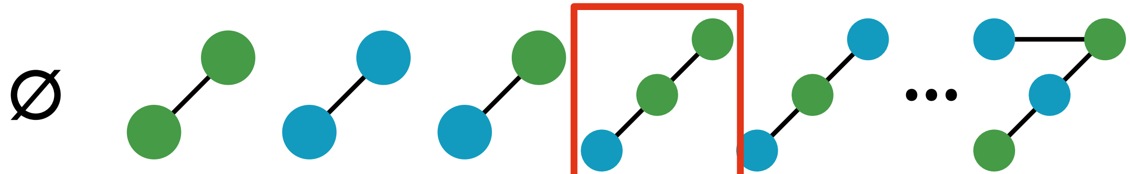
$$\begin{array}{l} \text{Freq.} \\ \text{Coef.} \end{array} \begin{bmatrix} \eta_0 & \eta_1 & \eta_2 & \eta_3 & \eta_4 & \eta_5 & \cdots & \eta_k \\ \theta_0 & \theta_1 & \theta_2 & \theta_3 & \theta_4 & \theta_5 & \cdots & \theta_k \end{bmatrix}$$

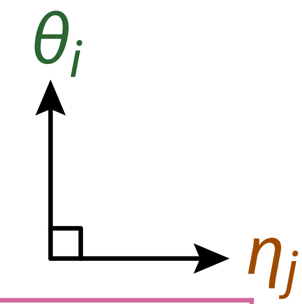
Q: Null distribution

$$\begin{array}{l} \text{Freq.} \\ \text{Coef.} \end{array} \begin{bmatrix} \eta_0 & \eta_1 & \eta_2 & \eta_3 & ? & \eta_5 & \cdots & \eta_k \\ ? & ? & ? & ? & 0 & ? & \cdots & ? \end{bmatrix}$$

$\mathrm{KL}(P, Q)$

Information of Each Subgraph





P: Empirical distribution

$$\begin{array}{l} \text{Freq.} \\ \text{Coef.} \end{array} \begin{bmatrix} \eta_0 & \eta_1 & \eta_2 & \eta_3 & \eta_4 & \eta_5 & \cdots & \eta_k \\ \theta_0 & \theta_1 & \theta_2 & \theta_3 & \theta_4 & \theta_5 & & \theta_k \end{bmatrix}$$

Q: Null distribution

$$\begin{array}{l} \text{Freq.} \\ \text{Coef.} \end{array} \begin{bmatrix} \eta_0 & \eta_1 & \eta_2 & \eta_3 & ? & \eta_5 & \cdots & \eta_k \\ ? & ? & ? & ? & 0 & ? & & ? \end{bmatrix}$$

R: Uniform distribution

$$\begin{array}{l} \text{Freq.} \\ \text{Coef.} \end{array} \begin{bmatrix} 1.0 & ? & ? & ? & ? & ? & \cdots & ? \\ \theta'_0 & 0 & 0 & 0 & 0 & 0 & & 0 \end{bmatrix}$$

$\mathrm{KL}(P, Q)$

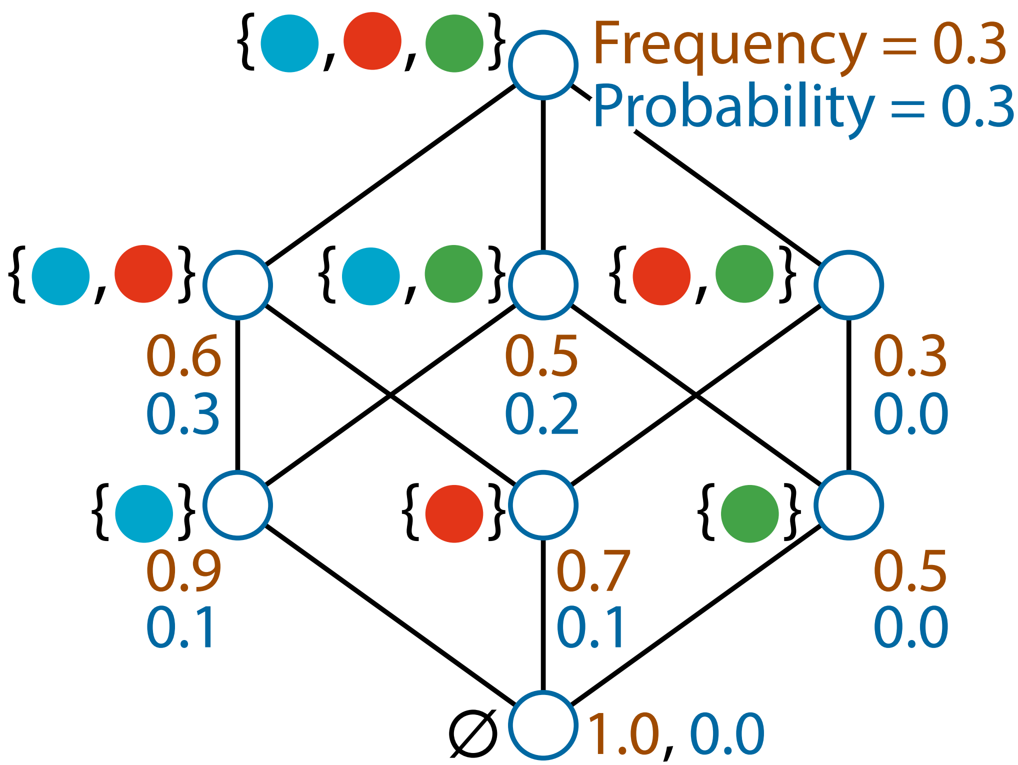
$\mathrm{KL}(Q, R)$

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

Make a Poset from Data

Dataset

ID 1:	1	1	0
ID 2:	1	1	1
ID 3:	1	1	0
ID 4:	1	1	1
ID 5:	1	1	0
ID 6:	1	0	1
ID 7:	1	0	1
ID 8:	1	1	1
ID 9:	1	0	0
ID10:	0	1	0

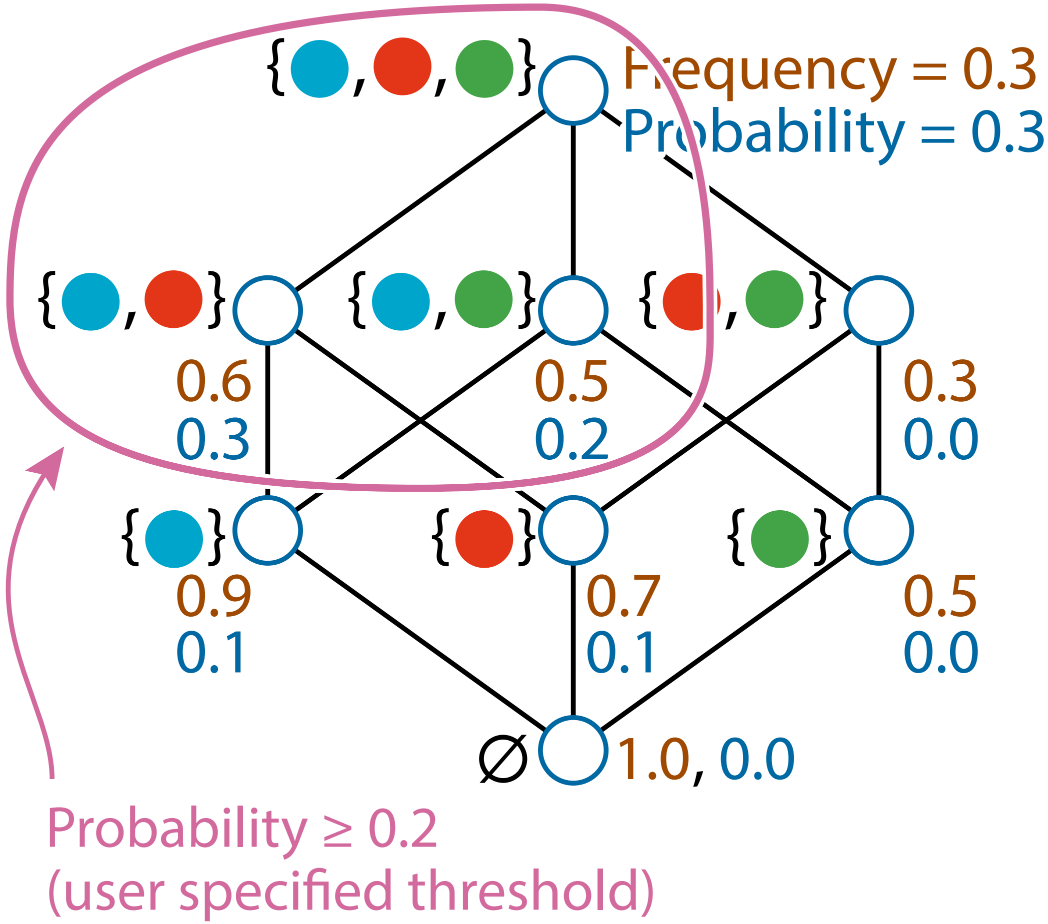


Number of nodes = $2^{\#features}$
⇒combinatorial explosion!

Make a Poset from Data

Dataset

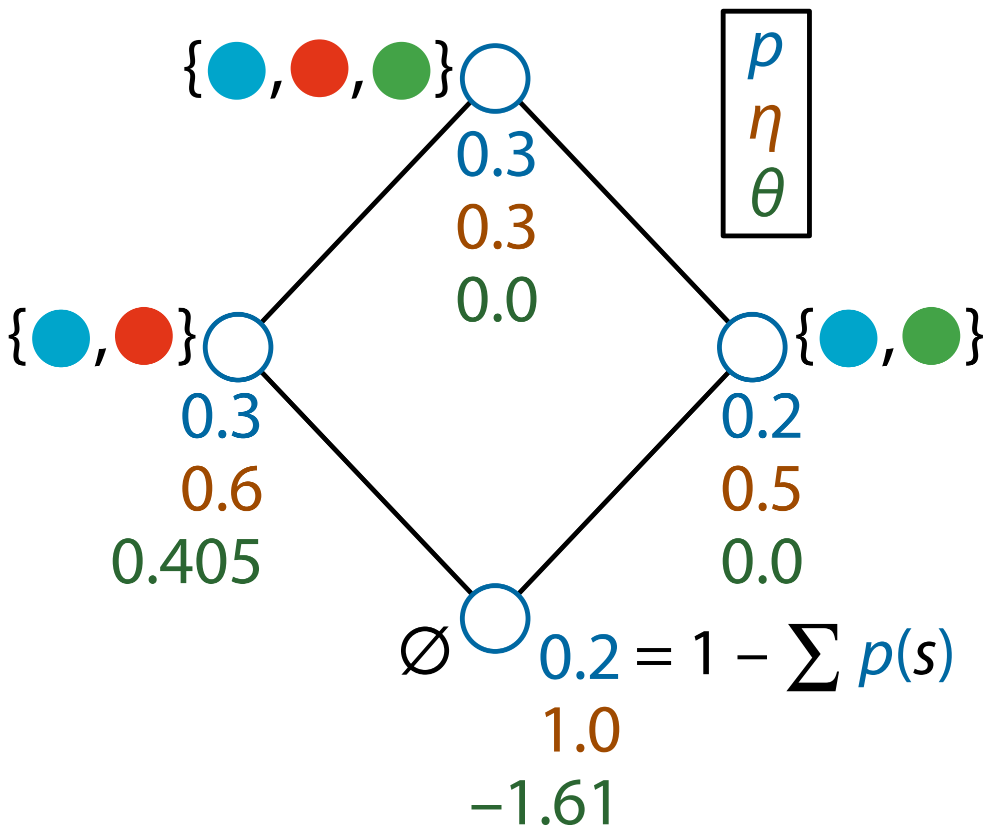
ID 1:	1	1	0
ID 2:	1	1	1
ID 3:	1	1	0
ID 4:	1	1	1
ID 5:	1	1	0
ID 6:	1	0	1
ID 7:	1	0	1
ID 8:	1	1	1
ID 9:	1	0	0
ID10:	0	1	0



Remove Nodes with Probability 0

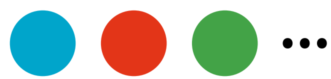
Dataset

ID 1:	1	1	0
ID 2:	1	1	1
ID 3:	1	1	0
ID 4:	1	1	1
ID 5:	1	1	0
ID 6:	1	0	1
ID 7:	1	0	1
ID 8:	1	1	1
ID 9:	1	0	0
ID10:	0	1	0



Example on Real Data (kosarak)

\# features: 41,270

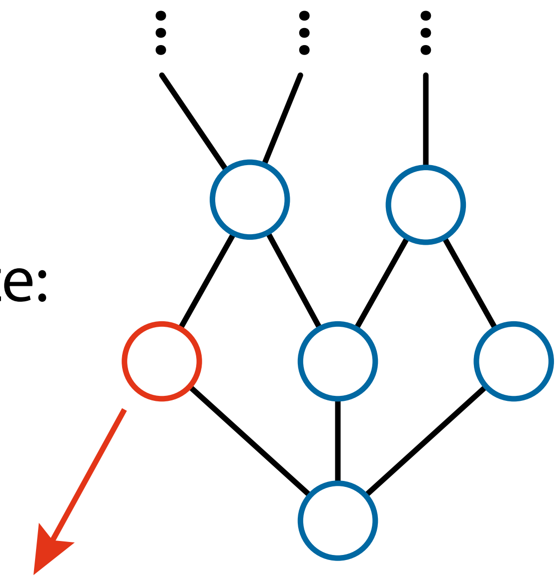


ID 1:	1	1	0	
ID 2:	1	1	1	
ID 3:	1	1	0	...
ID 4:	1	1	1	
ID 5:	1	1	0	
⋮		⋮		

Sample size:
990,002

Total runtime:
4.95 seconds

\# nodes: 3,253
(Threshold: 10^{-5})



\# significant interactions: 583

Single feature: 537

Pairwise interactions: 41

Triple interactions: 5

Example on Real Data (accidents)

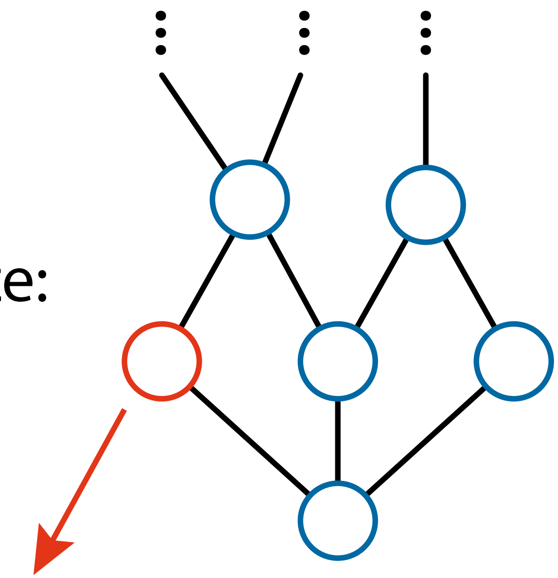
features: 468

ID 1:	1	1	0	
ID 2:	1	1	1	
ID 3:	1	1	0	...
ID 4:	1	1	1	
ID 5:	1	1	0	
⋮		⋮		

Sample size: 340,183

Total runtime: 4.95 seconds

nodes: 281
(Threshold: 5×10^{-6})



significant interactions: 280
features in each interaction is between 26 to 41

Conclusion

- A close connection between the partial order structure and information geometry
  - Möbius inversion leads to the dually flat manifolds
    - M. Sugiyama, H. Nakahara, K. Tsuda, *Information Decomposition on Structured Space*, IEEE ISIT (2016)
    - S. Amari, *Information geometry on hierarchy of probability distributions*, IEEE Trans. Info. Theory (2001)
    - H. Nakahara, S. Amari, *Information-geometric measure for neural spikes*, Neural Computation (2002)

- We can decompose the KL divergence and asses the significance on any posets