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

Bias-Variance Tradeoff

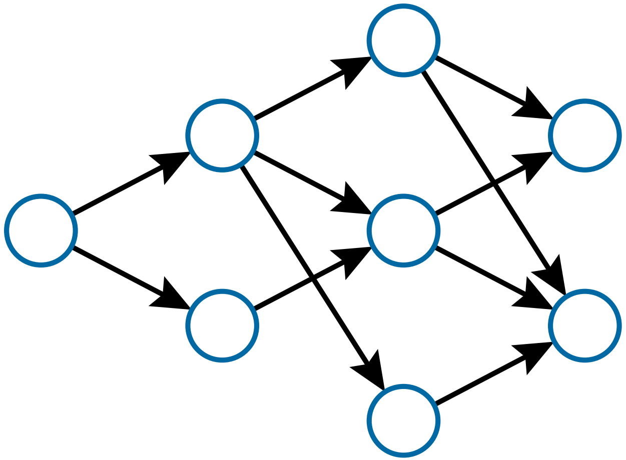
Data Mining 06 (データマイニング)

Mahito Sugiyama (杉山麿人)

Today's Outline

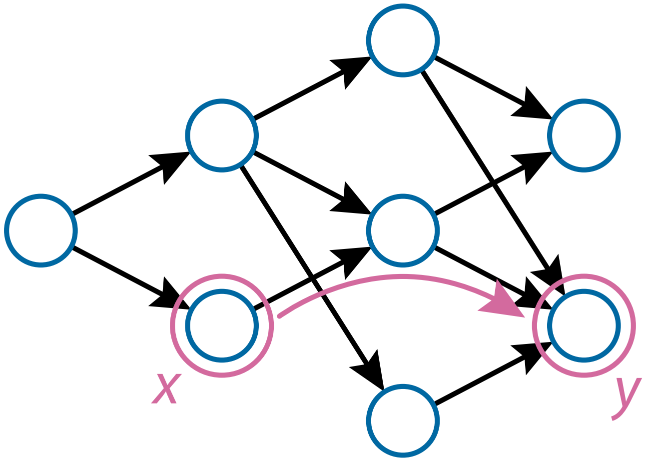
- Log-linear models on posets
  - A generalized formulation of Boltzmann machines
- Bias-variance tradeoff
- Fisher information & Cramér-Rao inequality

Partially Ordered Set (Poset)



- Partially ordered set (poset) $(S, \leq)$
  (i) $x \leq x$ (reflexivity)
  (ii) $x \leq y, y \leq x \Rightarrow x = y$ (antisymmetry)
  (iii) $x \leq y, y \leq z \Rightarrow x \leq z$ (transitivity)
  – We assume that S is finite and includes the least element (bottom) $\perp \in S$

Partially Ordered Set



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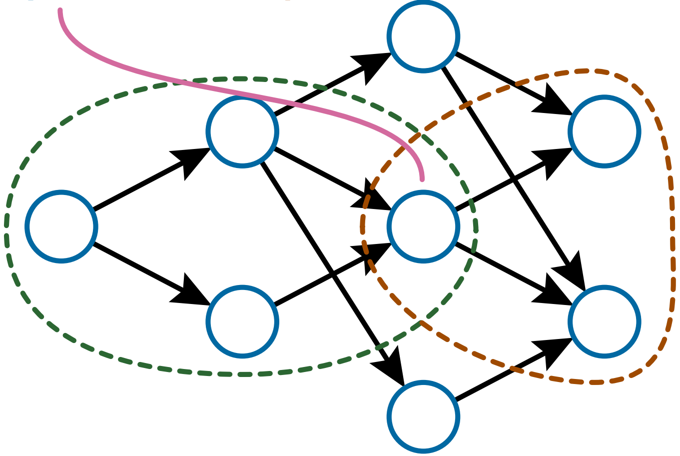
- Equivalent to a DAG
  - Each $x \in S$ is a node
  - $x \leq y \iff y$ is reachable from x

Log-Linear Model on Poset

Each $x \in S$ has a triple:
$(p(x), \theta(x), \eta(x))$



- A probability distribution $p: S \to (0, 1)$ s.t. $\sum_{x \in S} p(x) = 1$
- We introduce $\theta: S \to \mathbb{R}$ and $\eta: S \to \mathbb{R}$ as

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

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

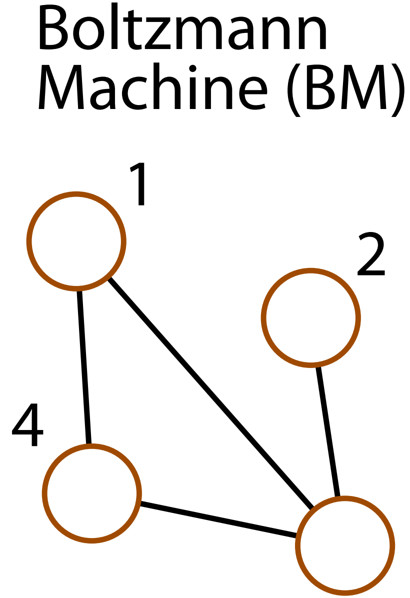
  - Parameter set $B \subseteq S$
  - $\theta(s) = 0$ if $s \notin B$

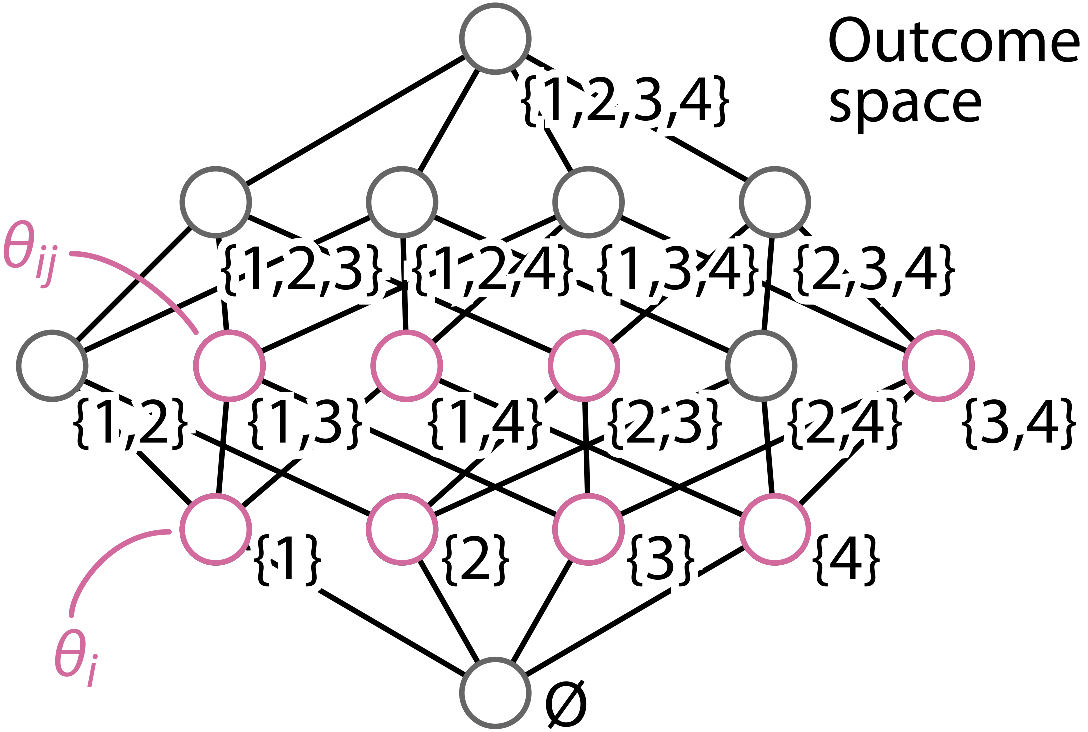
Log-Linear Model on Powerset

- Probability distribution over the power set 2^V with $V = \{1, 2, \dots, n\}$
  - $x \leq y \iff x \subseteq y$, $S = 2^V$
- Probability $p(x)$ for each $x \in 2^V$ is given as $\log p(x) = \sum_{s \subseteq x} \theta(s)$
  - Parameter set $B \subseteq 2^V$
  - $\theta(s) = 0$ if $s \notin B$
- MLE: Find $\theta(s)$ from a dataset $D \subseteq 2^V$ for all $s \in B$ s.t. $\eta(s) = \hat{\eta}(s)$

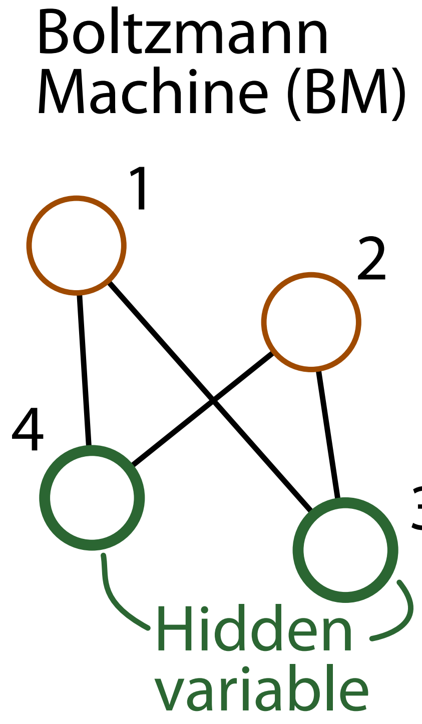
$$\eta(s) = \sum_{x \supseteq s} p(x), \quad \hat{\eta}(s) = \frac{1}{|D|} \sum_{x \in D} \mathbf{1}[x \supseteq s] = |\{x \in D \mid x \supseteq s\}| \,/\, |D|$$

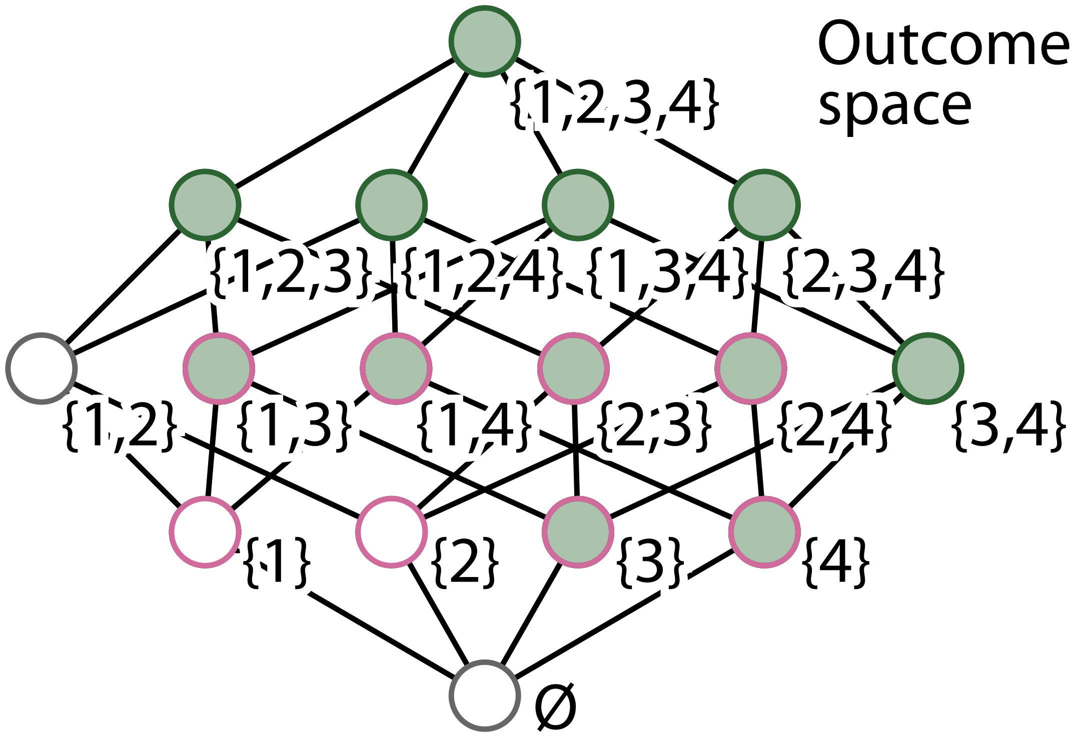
Boltzmann Machines



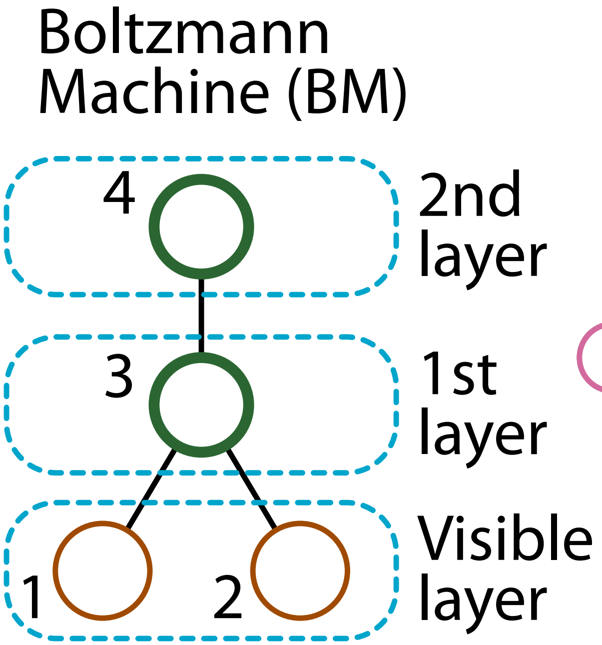


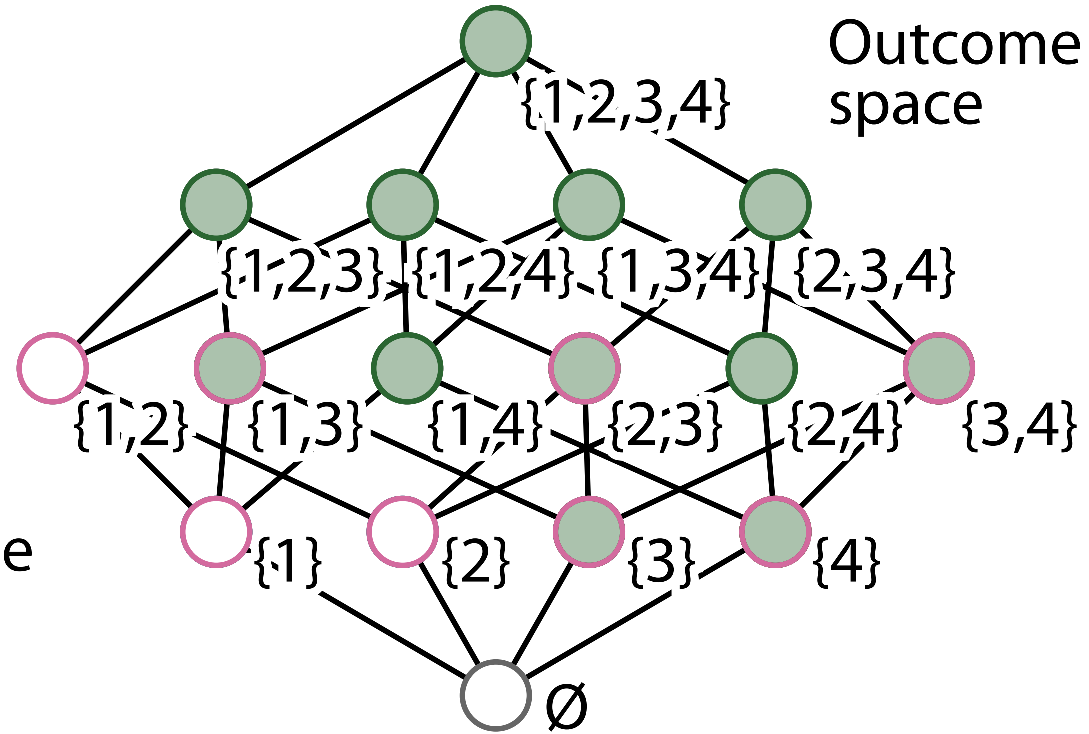
Restricted Boltzmann Machines (RBMs)



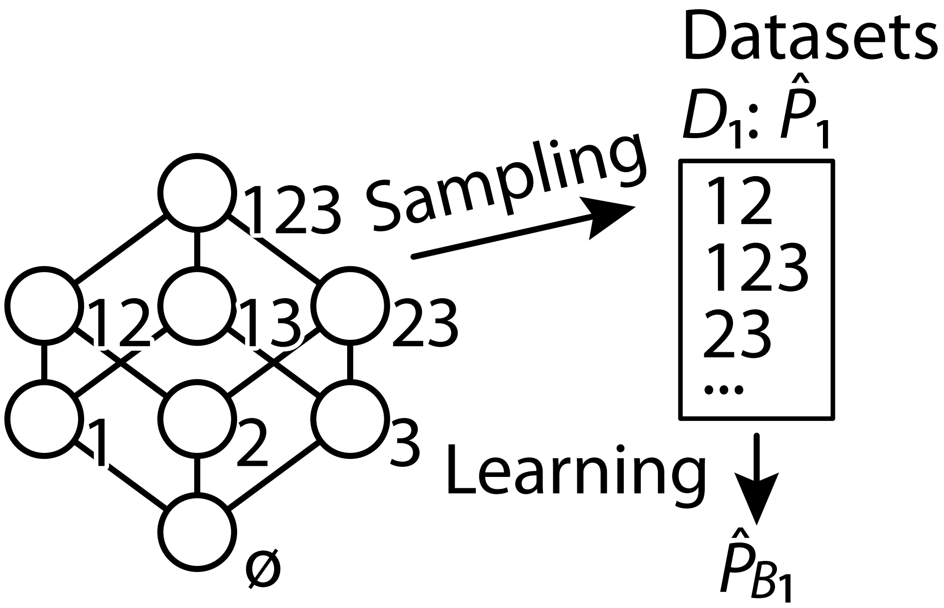


Deep Boltzmann Machines (DBMs)





Learning from Data



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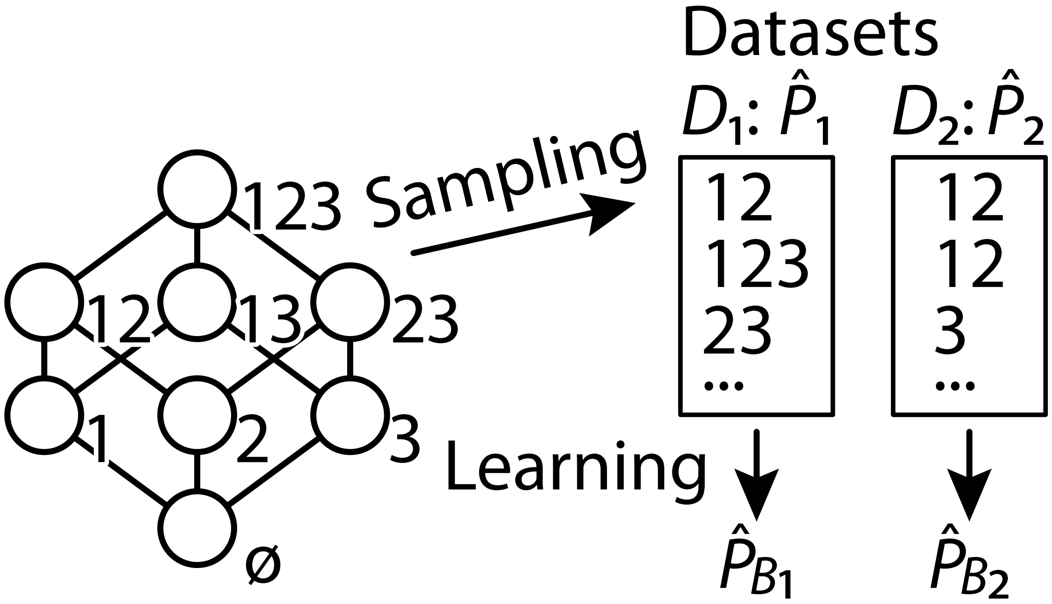

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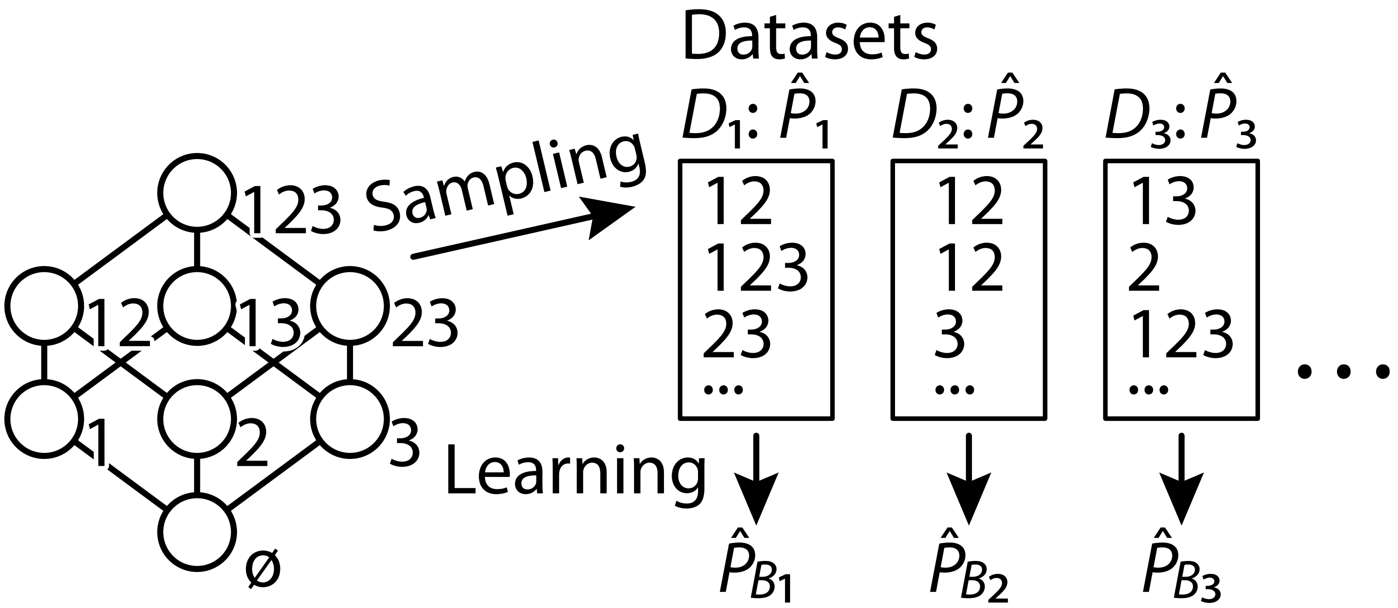

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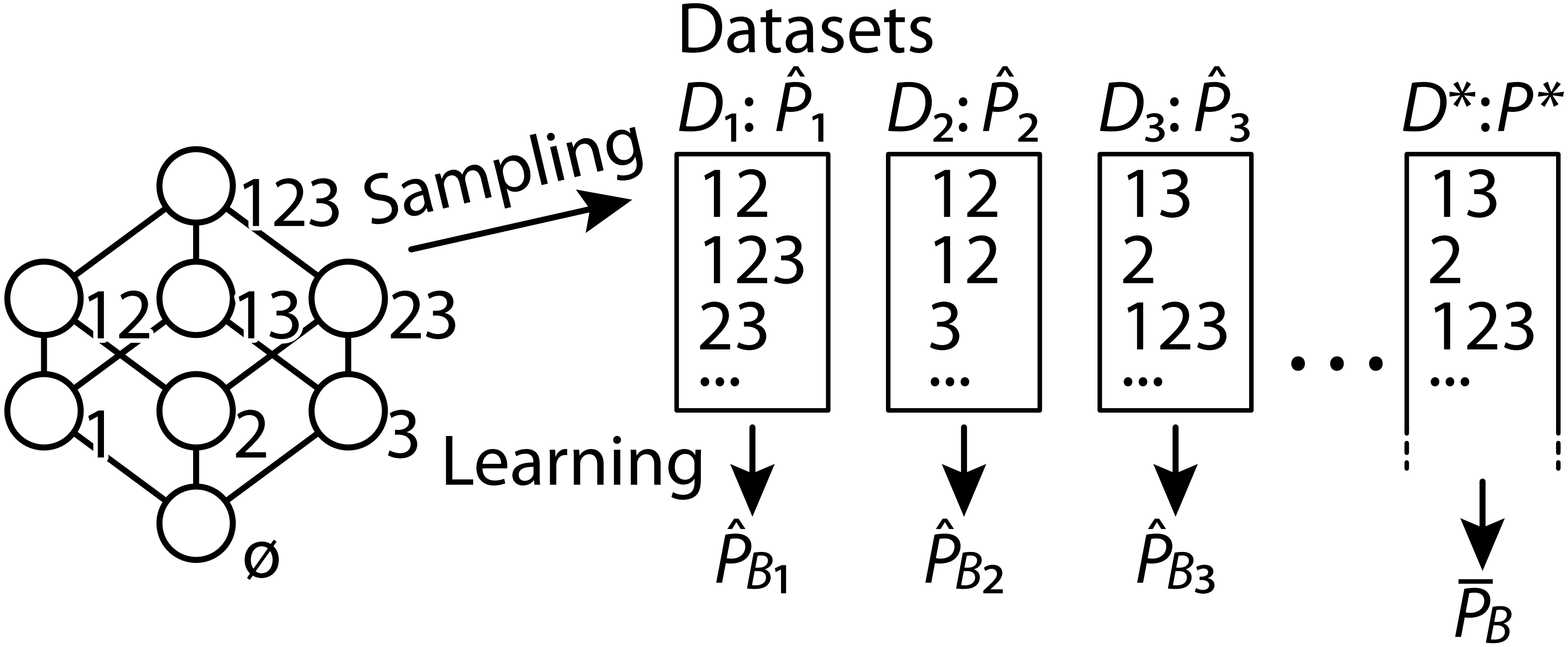

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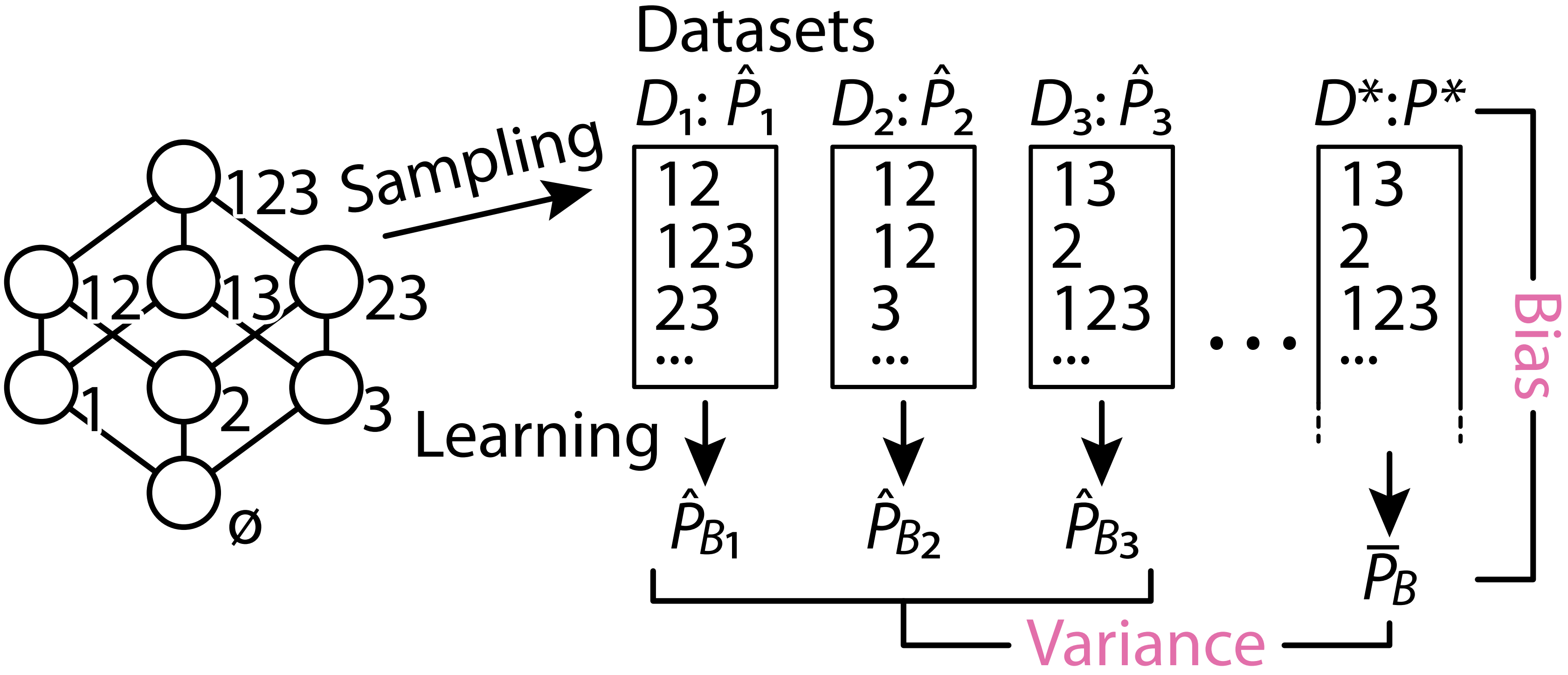


Bias-Variance Tradeoff

- Bias = $D_{\mathrm{KL}}(P^*, \bar{P}_B)$
- Variance = $\mathbf{E}[D_{\mathrm{KL}}(\bar{P}_B, \hat{P}_B)]$
- If we include more parameters in B:
  → Bias will decrease
  → Variance will increase
- Two extreme cases:
  - If $B = 2^V$, then $\hat{P}_B = \hat{P}$, thus bias = 0 but variance will be large
  - If $B = \varnothing$, $\hat{P}_B$ is always the uniform distribution U,
    thus bias = $D_{\mathrm{KL}}(U, P^*)$ and variance = 0

Bias-Variance Decomposition

- Decomposition of MSE (Mean Squared Error)

$$\mathbf{E}\left[(\hat{\theta} - \theta^*)^2\right] = (\bar{\theta} - \theta^*)^2 + \mathbf{E}\left[(\hat{\theta} - \bar{\theta})^2\right]$$

$$= \text{bias}^2(\hat{\theta}) + \text{var}\left[\hat{\theta}\right]$$

$$\text{MSE} = \text{bias}^2 + \text{variance}$$

  - θ^*: the true parameter
  - $\hat{\theta}$: the estimate
  - $\bar{\theta}$: the expected value of the estimate, $\bar{\theta} = \mathbf{E}[\hat{\theta}]$
    (the estimate obtained from infinitely many data points)
  - The expectation $\mathbf{E}$ is about the true distribution $p(D; \theta^*)$

Example: Gaussian Mean Estimation

- Estimate the mean from N data points $x_1, x_2, \ldots, x_N$ sampled from a Gaussian distribution $N(\theta^* = 1, \sigma^2)$

- Strategy 1: MLE

$$\text{bias} = \mathbf{E}[\hat{\theta}] - \theta^* = \mathbf{E}\left[\frac{1}{N}\sum_{i=1}^{N} x_i\right] - \theta^* = N\theta^*/N - \theta^* = 0$$

  variance $= \sigma^2/N$

- Strategy 2: MAP estimate with a prior $N(\theta_0, \sigma^2/\kappa_0)$

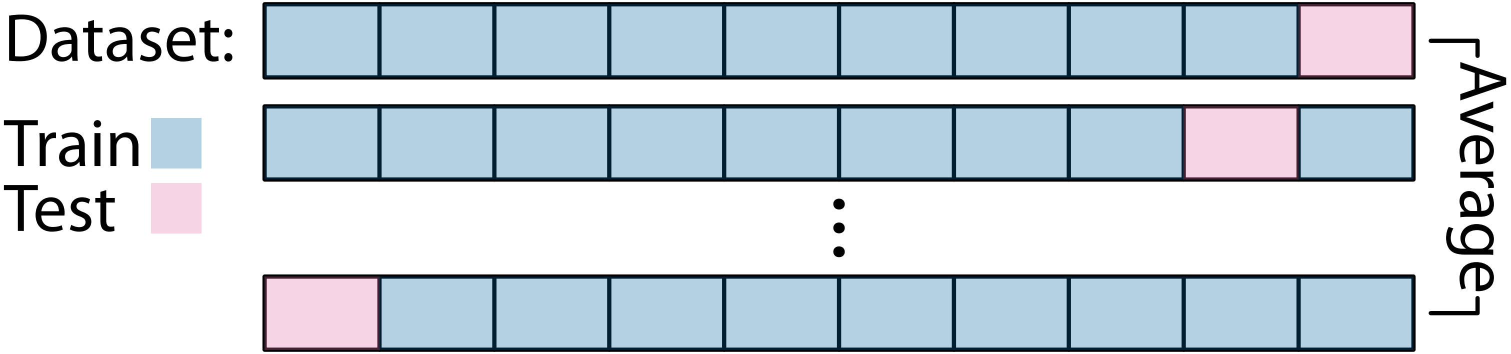
$$\text{bias} = \left(w\mathbf{E}[\hat{\theta}] + (1-w)\theta_0\right) - \theta^* = (1-w)(\theta_0 - \theta^*), \quad w = N/(N+\kappa_0),$$

  variance $= w^2\sigma^2/N$

Practical Solution: Cross-Validation

- CV (Cross Validation) is the most convenient way to find the best parameter from data without seeing the true parameter

- K-fold cross-validation is typically used



Fisher Information

- Let $p(x;\xi)$ be a distribution with a parameter ξ

- The Fisher information $g(\xi)$ of ξ is

$$g(\xi) = \mathbf{E}\left[\left(\frac{\partial}{\partial\xi}\log p(x;\xi)\right)^2\right] = \sum_{x\in S} p(x;\xi)\left(\frac{\partial}{\partial\xi}\log p(x;\xi)\right)^2$$

- If there are multiple parameters $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_m)$, the Fisher information matrix is a $m \times m$ matrix $G(\xi)$ given as

$$g(\boldsymbol{\xi})_{ij} = \mathbf{E}\left[\frac{\partial}{\partial\xi_i}\log p(x;\xi)\frac{\partial}{\partial\xi_j}\log p(x;\xi)\right]$$

Cramér-Rao Lower Bound

- Let $\boldsymbol{\xi}$ be unbiased: $\mathbf{E}[\hat{\boldsymbol{\xi}}] = \boldsymbol{\xi}^*$

- Cramér-Rao inequality:

  $$E \geq \frac{1}{N} G(\boldsymbol{\xi})^{-1}$$

  where $E = (e_{ij})$, each $e_{ij} = \mathbf{E}\left[\left(\hat{\xi}_i - \xi_i^*\right)\left(\hat{\xi}_j - \xi_j^*\right)\right]$

  - E coincides with the covariance matrix, $e_{ii} = \mathbf{E}[\,(\hat{\xi}_i - \xi_i^*)^2\,] = \mathrm{var}(\hat{\xi}_i)$
  - $A > B$ if $A - B$ is positive definite
    - C is positive definite if $\boldsymbol{x}^T C \boldsymbol{x} > 0$ for any non-zero $\boldsymbol{x} \in \mathbb{R}^n$

- In MLE, $E \to (1/N) G(\boldsymbol{\xi})^{-1}$ when $N \to \infty$

Example in Gaussian Mean Estimation

- Estimate the mean from N data points $x_1, x_2, \ldots, x_N$ sampled from a Gaussian distribution $N(\theta^*, \sigma^2)$

- Fisher information:
$$g(\theta) = \frac{1}{\sigma^2}$$

- Cramér-Rao bound:
$$\mathrm{var}[\hat{\theta}] \geq \frac{\sigma^2}{N}$$
  - In this case, $\mathrm{var}[\hat{\theta}] = \sigma^2/N$ always holds

Model Selection by AIC

- The AIC (Akaike information criterion) is one of the most famous measure of the quality of statistical models

  $$\mathrm{AIC} = -2l(D) + 2k$$

  – $l(D)$ is the maximized log-likelihood
  – k is the number of parameters

- This cannot be directly used for log-linear models on posets as it is a hierarchical model with including higher-order associations
  – It is still under development...