

Probabilistic Graphical Models

Lectures 22

Introduction to Learning
Learning Bayesian Networks

Sampling vs. Learning



$$P_{\theta}(X) = P(X; \theta) = P(X | \theta)$$

Sampling $P_{\theta}(X) = \checkmark$ ^{given} \Rightarrow generate data X^1, X^2, \dots, X^m
i.i.d samples

Learning data $X^1, X^2, \dots, X^m = \checkmark$ ^{given} \Rightarrow find $P_{\theta}(X)$

find $P_{\theta}(X)$ $\left\{ \begin{array}{l} \text{find parameters } \theta \\ \text{find structure (connections in BN/MRF) graph} \end{array} \right.$

Likelihood function



given data X^1, X^2, \dots, X^m what is the probability of occurrence of X^1, \dots, X^m ?

$$\Pr(X^1, X^2, \dots, X^m) \underset{\text{independent samples}}{=} \prod_{i=1}^m \Pr(X^i) = \prod_{i=1}^m P_{\theta}(X^i)$$

all are samples of $P_{\theta}(X)$

$$l(\theta) = \prod_{i=1}^m P_{\theta}(X^i) \quad \text{likelihood}$$

Maximum Likelihood Solution



$i=1$
One Solution: choose θ that maximized the likelihood
 $\theta^* = \operatorname{argmax}_{\theta} \ell(\theta) = \operatorname{argmax}_{\theta} \prod_{i=1}^m P_{\theta}(X^i)$
maximum-likelihood solution

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maximum-likelihood solution

Example: tossing a coin



(unfair) coin

$$P_{\theta}(X) \quad X \in \{H, T\}$$

$$\theta = \Pr(X=H) = P_{\theta}(H)$$

$$\Pr(X=T) = 1 - \theta = P_{\theta}(T)$$

X^1, X^2, \dots, X^m

H H T H T T ..

Example: tossing a coin



$$l(\theta) = \prod_{i=1}^m P_{\theta}(X^i)$$

$$P_{\theta}(X^i) = \begin{cases} \theta & X^i = H \\ 1-\theta & X^i = T \end{cases}$$

$n_H = \text{no. of } H$
 $n_T = \text{no. of } T$

$$= \prod_{i=1}^m (\theta \mathbb{1}(X^i = H) + (1-\theta) \mathbb{1}(X^i = T))$$

$$m = n_H + n_T$$

$$\Rightarrow \underline{l(\theta) = \theta^{n_H} (1-\theta)^{n_T}}$$

Example: tossing a coin



$$\begin{aligned}l\left(\theta = \frac{n_H}{m}\right) &= \left(\frac{n_H}{m}\right)^{n_H} \left(1 - \frac{n_H}{m}\right)^{n_T} \\ &= \left(\frac{n_H}{m}\right)^{n_H} \left(\frac{n_T}{m}\right)^{n_T} \quad (> 0 \text{ if } n_H, n_T > 0)\end{aligned}$$

$$l(\theta) = l(\theta = 0) = l(\theta = 1) = 0 \quad (\text{if } n_H, n_T > 0)$$

$$\theta^* = \frac{n_H}{n_H + n_T} = \frac{n_H}{m}$$

maximum-likelihood solution
log-likelihood = $l(\theta)$

Example: tossing a coin - log-likelihood



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$$\begin{aligned} \theta^* &= \operatorname{argmax}_{\theta} l(\theta) = \operatorname{argmax}_{\theta} \log \ell(\theta) = \operatorname{argmax}_{\theta} \log \prod_{i=1}^m P_{\theta}(X^i) \\ &= \operatorname{argmax}_{\theta} \sum_{i=1}^m \log P_{\theta}(X^i) \\ &= \operatorname{argmax}_{\theta} n_H \log \theta + n_T \log(1-\theta) \end{aligned}$$

$\log\text{-likelihood} = \ell(\theta)$

$$\begin{aligned} \max_{\theta} \ell(\theta) &\Rightarrow \frac{d}{d\theta} \ell(\theta) = \frac{d}{d\theta} (n_H \log \theta + n_T \log(1-\theta)) \Rightarrow \frac{n_H}{\theta} - \frac{n_T}{1-\theta} \\ &= \frac{n_H(1-\theta) - n_T \theta}{\theta(1-\theta)} = 0 \Rightarrow \boxed{\theta^* = \frac{n_H}{n_H + n_T}} \end{aligned}$$

Sufficient statistics



data $X^1, X^2, \dots, X^m \Rightarrow \ell(\theta) = \theta^{n_H} (1-\theta)^{n_T}$ 27

$$n_H = \sum \mathbb{1}(X^i = H)$$

$$n_T = \sum_{i=1}^m \mathbb{1}(X^i = T)$$

$$\ell(\theta) = n_H \log \theta + n_T \log (1-\theta)$$

for calculating the likelihood
we only need n_H, n_T (not the
complete data)

n_H, n_T : sufficient statistics

Example 2: normal distribution

$$P_{\theta}(x) = P_{(\mu, \sigma)}(x) = \frac{1}{\sqrt{2\pi} \sigma} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2}$$

Example 2: Normal Distribution



Example 2: normal distribution

$$P_{\theta}(x) = P_{(\mu, \sigma)}(x) = \frac{1}{\sqrt{2\pi} \sigma} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma}\right)^2}$$

data x^1, x^2, \dots, x^m find maximum-likelihood solution for μ, σ

Example 2: Normal Distribution



$$\ell(\theta) = \sum_{i=1}^m \log P_{\theta}(x^i) = \sum_{i=1}^m \left(-\log \sqrt{2\pi} - \log \sigma - \frac{1}{2} \frac{(x^i - \mu)^2}{\sigma^2} \right)$$

$$\ell(\theta) = C - m \log \sigma - \frac{1}{2} \frac{\sum_{i=1}^m [x^i]^2 + m\mu^2 - 2\mu \sum_{i=1}^m x^i}{\sigma^2}$$

$$= C - m \log \sigma - \frac{1}{2\sigma^2} \left(\sum_{i=1}^m (x^i)^2 - 2\mu \sum_{i=1}^m x^i + m\mu^2 \right)$$

sufficient statistics $\left(\sum (x^i)^2, \sum x^i, m \right)$

Example 2: Normal Distribution



$$\frac{\partial}{\partial \mu} \ell(\theta) = \frac{\partial}{\partial \mu} \ell(\mu, \sigma) = -\frac{1}{2\sigma^2} \left(-2 \sum_{i=1}^m x^i + 2m\mu \right) = 0$$

$$\Rightarrow 2m\mu = 2 \sum_{i=1}^m x^i \Rightarrow \boxed{\mu^* = \frac{1}{m} \sum_{i=1}^m x^i}$$


$$\frac{\partial}{\partial \sigma} \ell(\theta) = \frac{-m}{\sigma} - \frac{1}{2} \times (-2) \frac{\sum (x^i - \mu^*)^2}{\sigma^3} = 0$$

$$m\sigma^2 = \sum_{i=1}^m (x^i - \mu^*)^2$$

$$\Rightarrow \boxed{\sigma^2 = \frac{1}{m} \sum_{i=1}^m (x^i - \mu^*)^2} \quad \sigma = \sqrt{\sigma^2}$$

Example 3: Tossing a dice



 $P_{\theta}(X)$ $X \in \{1, 2, \dots, q\}$ 27 (IV)

$X \in \{1, 2, 3, 4, 5, 6\}$ $\theta = (\theta_1, \theta_2, \dots, \theta_q)$

$\theta_1 = \Pr(X=1)$
 $\theta_2 = \Pr(X=2)$
:
 $\theta_q = \Pr(X=q) = 1 - \theta_1 - \theta_2 - \dots - \theta_{q-1}$

$\sum_{j=1}^q \theta_j = 1$ data = X^1, X^2, \dots, X^m

$l(\theta) = l(\theta_1, \dots, \theta_q) = \prod_{i=1}^m P_{\theta}(X) = \theta_1^{n_1} \theta_2^{n_2} \dots \theta_q^{n_q}$

Example 3: Tossing a dice



$$l(\theta) = l(\theta_1, \dots, \theta_q) = \prod_{i=1}^m p_{\theta}(X^i) = \theta_1^{n_1} \theta_2^{n_2} \dots \theta_q^{n_q}$$

suff. stat: $n_j = \sum_{i=1}^m \mathbb{1}(X^i = j) = \# X^i = j$

$$ll(\theta) = \sum_{i=1}^m n_i \log \theta_i$$

Example 3: Tossing a dice



$$\theta^* = \underset{\theta_1, \theta_2, \dots, \theta_q}{\operatorname{argmax}} \sum_{j=1}^q n_j \log \theta_j \quad \text{subject to} \quad \sum_{j=1}^q \theta_j = 1$$

Lagrange multipliers

$$\text{or } \theta_q = 1 - \sum_{j=1}^{q-1} \theta_j$$

$$\Rightarrow \theta_j^* = \frac{n_j}{\sum_{k=1}^q n_k} = \frac{n_j}{m}$$

PGM problems



PGM $P_{\theta}(X) = P_{\theta}(X_1, X_2, \dots, X_n)$ n : large

data: $X^1 = (X_1^1, X_2^1, X_3^1, \dots, X_n^1)$

$$X^2 = (X_1^2, X_2^2, \dots, X_n^2)$$

⋮

$$X^m = (X_1^m, X_2^m, \dots, X_n^m)$$

Bayes Nets Parameter Learning



pgm 22 (III)

$$P_{\theta}(X) = P_{\theta}(X_1, X_2, \dots, X_n)$$
$$= \prod_{i=1}^n P_{\theta}(X_i | X_{P_i})$$

parents of X_i

Data: $X^1, X^2, \dots, X^m = (X_1^1, X_2^1, \dots, X_n^1), (X_1^2, X_2^2, \dots, X_n^2), \dots, (X_1^m, X_2^m, \dots, X_n^m)$

$$\begin{aligned} \ell(\theta) &= \sum_{k=1}^m \log P_{\theta}(X^k) = \sum_{k=1}^m \log \prod_{i=1}^n P_{\theta}(X_i^k | X_{P_i}^k) \\ &= \sum_{k=1}^m \sum_{i=1}^n \log P_{\theta}(X_i^k | X_{P_i}^k) \end{aligned}$$

No shared parameters



1: Each CPD has its own parameters

$$\theta = (\theta_1, \theta_2, \dots, \theta_n)$$

$$P_{\theta}(X_i | X_{P_i}) = P_{\theta_i}(X_i | X_{P_i})$$

$$\begin{aligned} \Rightarrow \ell(\theta) &= \sum_{k=1}^m \sum_{i=1}^n \log P_{\theta}(X_i^k | X_{P_i}^k) \\ &= \sum_{k=1}^m \sum_{i=1}^n \log P_{\theta_i}(X_i^k | X_{P_i}^k) \\ &= \sum_{i=1}^n \underbrace{\sum_{k=1}^m \log P_{\theta_i}(X_i^k | X_{P_i}^k)}_{\text{local log-likelihood}} \end{aligned}$$

No shared parameters



$$\begin{aligned}\Rightarrow ll(\theta) &= \sum_{k=1}^m \sum_{i=1}^n \log P_{\theta} (X_i^k | X_{P_i}^k) \\ &= \sum_{k=1}^m \sum_{i=1}^n \log P_{\theta_i} (X_i^k | X_{P_i}^k) \\ &= \sum_{i=1}^n \underbrace{\sum_{k=1}^m \log P_{\theta_i} (X_i^k | X_{P_i}^k)}_{\text{local log-likelihood}}\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial \theta_j} ll(\theta) &= \frac{\partial}{\partial \theta_j} ll(\theta_1, \theta_2, \dots, \theta_n) \\ &= \sum_{k=1}^m \frac{\partial}{\partial \theta_j} \log P_{\theta_j} (X_i^k | X_{P_i}^k) \\ &= \sum_{k=1}^m \frac{\frac{\partial}{\partial \theta_j} P_{\theta_j} (X_i^k | X_{P_i}^k)}{P_{\theta_j} (X_i^k | X_{P_i}^k)}\end{aligned}$$

gradient w.r.t. θ_j

each θ_j can be found independently of other θ_{i-1} 's



No shared parameters - table representation

$$\sum_{i=1}^n \sum_{k=1}^m \log P_{\theta_i^k}(X_i^k | X_{P_i^k}^k)$$

local log-likelihood

table representation

Example $P(X_i | Y_i)$ $X_i, X_i \in \{0, 1\}$

X_i	Y_i	$P(X_i Y_i)$
1	0	θ_0
0	0	$1 - \theta_0$
1	1	θ_1
0	1	$1 - \theta_1$

→ local likelihood

$$\sum_{k=1}^m \log P(X_i^k | Y_i^k)$$

$$\frac{\partial}{\partial \theta_0} \sum_{k=1}^m \log P(X_i^k | Y_i^k)$$

$$\frac{\partial}{\partial \theta_0} \sum_{\substack{k=1 \\ Y_i^k=0}}^m \log P(X_i^k | 0) + \sum_{\substack{k=1 \\ Y_i^k=1}}^m \log P(X_i^k | 1)$$

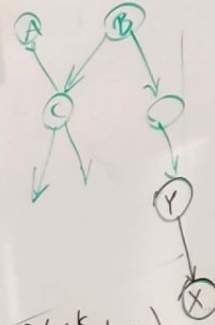
a function of θ_0

a function of θ_1

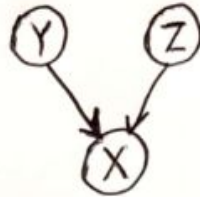
$$= \frac{\partial}{\partial \theta_0} (n_{10} \log \theta_0 + n_{00} \log(1 - \theta_0)) \Rightarrow \theta_0^* = \frac{n_{10}}{n_{10} + n_{00}}$$

$$n_{10} = \#(X_i^k = 1, Y_i^k = 0)$$

$$n_{00} = \#(X_i^k = 0, Y_i^k = 0)$$



No shared parameters - table representation



$$X \in \{1, 2, \dots, C\}$$

$$Y, Z \in \{0, 1\}$$

$$\delta_{00}^i = \checkmark$$

$$\delta_{01}^i = \Pr(X=i \mid Y=0, Z=1)$$

$$\delta_{10}^i = \Pr(X=i \mid Y=1, Z=0)$$

$$\delta_{11}^i = \Pr(X=i \mid Y=1, Z=1)$$

$$\sum_x \delta_{10}^i = 1$$

local likelihood $\sum_{k=1}^m \log P_y(X^k \mid Y^k, Z^k)$

$$\sum_{k=1}^m \log \delta_{Y^k, Z^k}^{X^k}$$

No shared parameters - table representation



$$\text{local likelihood } \sum_{k=1}^m \log P_y(X^k | Y, Z)$$

$$\sum_{k=1}^m \log \gamma_{Y, Z}^{X^k}$$

$$\sum_{y=0}^1 \sum_{z=0}^1 \sum_{x=1}^{2^c} (\log \gamma_{yz}^x) \cdot \underbrace{\left[\#(X^k=x, Y^k=y, Z^k=z) \right]}_{\text{sufficient statistics}}$$

$$\boxed{\sum_x \gamma_{yz}^x = 1}$$

$$\gamma_{yz}^x = \frac{\#(X^k=x, Y^k=y, Z^k=z)}{\#(X^k=y, Z^k=z)}$$

No shared parameters - table representation



$$\sum_{y=0}^1 \sum_{z=0}^1 \sum_{x=1}^{ac} (\log \gamma_{yz}^x) \cdot \# \left[\left(X^k = x, Y^k = y, Z^k = z \right) \right]$$

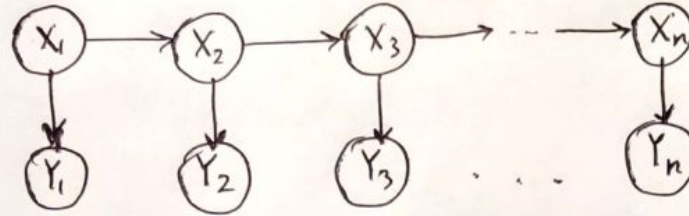
$$\sum_n \gamma_{yz}^n = 1$$

sufficient statistics

$$\gamma_{yz}^x = \frac{\#(X^k = x, Y^k = y, Z^k = z)}{\#(X^k = y, Z^k = z)}$$

$$= \frac{\sum_{k=1}^m \mathbb{1}(X^k = x, Y^k = y, Z^k = z)}{\sum_{k=1}^m \mathbb{1}(Y^k = y, Z^k = z)}$$

shared parameters



$$P_{\theta}(X_1, \dots, X_n, Y_1, \dots, Y_n) = P_{\alpha}(X_1) \prod_{i=2}^n P_{\beta}(X_i | X_{i-1}) \prod_{i=1}^n P_{\gamma}(Y_i | X_i)$$

$$\theta = (\alpha, \beta, \gamma)$$

$$\begin{aligned} \ell(\theta) = & \sum_{k=1}^m \log P_{\alpha}(X_i^k) + \sum_{k=1}^m \sum_{i=2}^n \log P_{\beta}(X_i^k | X_{i-1}^k) \\ & + \sum_{k=1}^m \sum_{i=1}^n \log P_{\gamma}(Y_i^k | X_i^k) \end{aligned}$$

$$\frac{\partial \ell(\theta)}{\partial \beta} = \sum_{k=1}^m \sum_{i=2}^n \frac{\partial}{\partial \beta} \log P_{\beta}(X_i^k | X_{i-1}^k)$$

shared parameters - table representation



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table representation $X_i \in \{0, 1\}$

$$\beta_0 = \beta_{00}, \beta_{10}, \beta_{11}, \beta_{01}$$

$$\beta_{01} = P(X_i = 0 \mid X_{i-1} = 1) \quad \text{independent of } i$$

ML solution

$$\beta_{01}^* = \frac{\#(X_i^k = 0, X_{i-1}^k = 1)}{\#(X_{i-1}^k = 1)}$$

$$= \frac{\sum_{i=2}^n \sum_{k=1}^m \mathbb{1}(X_i^k = 0, X_{i-1}^k = 1)}{\sum_{i=2}^n \sum_{k=1}^m \mathbb{1}(X_{i-1}^k = 1)}$$

shared parameters - table representation

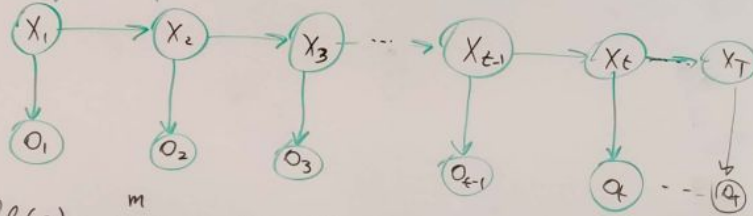


Shared parameters

$$\forall^k X^1, \dots, X^m$$

$$\ell(\theta) = \sum_{k=1}^m \sum_{i=1}^n \log P(X_i^k | X_{P_i}^k)$$

Example X_1



$$\begin{aligned} \ell(\theta) = & \sum_{k=1}^m \log P(X_1^k) + \sum_{k=1}^m \sum_{i=2}^T \log P(X_i^k | X_{i-1}^k) \\ & + \sum_{k=1}^m \sum_{i=1}^T \log P(O_i^k | X_i^k) \end{aligned}$$

$$P(X_t = k | X_{t-1} = l) = f_{\theta}(k, l)$$

$$P(X_t | X_{t-1}) = f_{\theta}(X_t, X_{t-1}) =$$

$$P(O_t | X_t) = g_{\gamma}(O_t, X_t)$$

table representation:

$$P(X_t = j | X_{t-1} = l) = \lambda_{j,l}$$

$$P(O_t = j | X_t = l) = \gamma_{j,l}$$

$$\frac{\partial \ell(\lambda, \gamma)}{\partial \lambda_{l,h}} = \sum_{k=1}^m \sum_{i=2}^T \log P(X_i^k | X_{i-1}^k)$$

shared parameters - table representation



$$P(X_t = k | X_{t-1} = l) = f_{\theta}(k, l)$$

$$P(X_t | X_{t-1}) = f_{\theta}(X_t, X_{t-1}) =$$

$$P(O_t | X_t) = g_{\gamma}(O_t, X_t)$$

table representation:

$$P(X_t = j | X_{t-1} = l) = \lambda_{j,l}$$

$$P(O_t = j | X_t = l) = \gamma_{j,l}$$

$$\frac{\partial \ell(\lambda, \gamma)}{\partial \lambda_{ln}} = \sum_{k=1}^m \sum_{i=2}^T \log P(X_i^k | X_{i-1}^k)$$

$$\rightarrow = \sum_{j=1}^q \sum_{l=1}^q \sum_{\substack{i=2 \\ X_i^k=j \\ X_{i-1}^k=l}}^T \log P(X_i^k | X_{i-1}^k)$$

$$\sum_{j=1}^q \sum_{l=1}^q \sum_{\substack{X_i^k=j, X_{i-1}^k=l \\ X_i^k=j \\ X_{i-1}^k=l}} \log P(j | l)$$

$$\sum_{j=1}^q \sum_{l=1}^q \sum_{\substack{X_i^k=j \\ X_{i-1}^k=l}} \log \lambda_{j,l}$$

$$\lambda_{j,l}^* = \frac{\#(X_i = j, X_{i-1} = l)}{\#(X_{i-1} = l)}$$

Data $X_1^1, X_2^1, \dots, X_T^1, O_1^1, O_2^1, \dots, O_T^1$
 $X_1^2, X_2^2, \dots, X_T^2, O_1^2, O_2^2, \dots, O_T^2$
 \vdots
 $X_1^m, X_2^m, \dots, X_T^m, O_1^m, \dots, O_T^m$

$X_t \in \{1, 2, \dots, q\}$