Big Data Analysis (MA60306)

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Spring 2022-23, IIT Kharagpur

Lecture 20 March 17, 2023

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Some more observations from the last model through an example.

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We call a node y, a descendant of a node x if there is a path from x to y in which each step of the path follows the directions

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D-separation

 \rightarrow Consider a directed graph in which A, B, C are arbitrary nonintersecting sets of nodes, whose union may be smaller than the total set of nodes in the graph

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- \rightarrow Consider a directed graph in which A, B, C are arbitrary nonintersecting sets of nodes, whose union may be smaller than the total set of nodes in the graph
- \rightarrow We wish to ascertain whether a particular conditional independence statement $A \perp \mid B \mid C$ is implied by a given directed acyclic graph!

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Consider all possible paths from any node in A to any node in B. Any such path is called blocked if it includes a node such that either

- (a) the arrows on the path meet either head-to-tail or tail-to-tail at the node which is in C, or
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- If all the paths are blocked, then A is said to be *d*-separated from B by C, and the joint distribution over all the variables in the graph will satisfy $A \perp\!\!\!\perp B \mid C$

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Question Develop an algorithm for D-separation for DAGs.

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Exponential family of distributions - The exponential family of distributions over \mathbf{x} , given parameters $\boldsymbol{\eta}$ is said to be distributions of the form

$$p(\mathbf{x}; \boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\{\boldsymbol{\eta}^{\mathsf{T}}\mathbf{u}(\mathbf{x})\},\$$

where **x** may be scalar or vector, and may be continuous and discrete, $\eta = [\eta_1, \ldots, \eta_K]^T$ is called the vector of natural parameters of the distribution, and $\mathbf{u}(\mathbf{x}) = [u_1(\mathbf{x}), \ldots, u_K(\mathbf{x})]^T$ is the vector of sufficient statistics, each sufficient statistic $u_k(\mathbf{x})$ being a function of **x**, $h(\mathbf{x})$ is the base measure which is a function of **x** independent of η , and $g(\eta)$ is the partition function such that

$$\frac{1}{g(\eta)} = \int \exp(\eta^T \mathbf{u}(\mathbf{x})) h(\mathbf{x}) d\mathbf{x}$$

for continuous rvs and $\frac{1}{g(\eta)} = \sum_{\mathbf{x}} \exp(\eta^T \mathbf{u}(x)) h(\mathbf{x})$ for discrete rv

Sufficient statistic Let $p(\mathbf{x}, \theta)$ be the distribution of a rv **X** that depends on θ . A function $f(\mathbf{x})$ is a sufficient statistic for the estimate of θ if the likelihood $p(\mathbf{x}, \theta)$ of the parameters θ depends on **x** only through the function $f(\mathbf{x})$.

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For example, $X \sim \mathcal{N}(0, \sigma^2)$, the function $f(x) = x^2$ can be easily seen to be sufficient for the estimate of the variance σ^2

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Bernoulli -

$$p(x,\mu) = \mu^{x}(1-\mu)^{1-x} = \exp\{x \ln \mu + (1-x)\ln(1-\mu)\}\$$

= $(1-\mu)\exp\{\ln\left(\frac{\mu}{1-\mu}\right)x\}$

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Set $\eta = \ln\left(\frac{\mu}{1-\mu}\right)$ and $g(\eta) = \frac{1}{1+\exp(-\eta)} \Rightarrow p(x,\mu) = g(-\eta)\exp(\eta x)$, g is called the logistic sigmoid function

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Gaussian -

$$p(x; \mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{-2\sigma^2}(x-\mu)^2\right\}$$

= $\frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{-2\sigma^2}x^2 + \frac{\mu}{\sigma^2}x - \frac{1}{2\sigma^2}\mu^2\right\}$
= $h(\mathbf{x})g(\eta) \exp\{\eta^T u(\mathbf{x})\}$

$$\eta = \begin{bmatrix} \mu/\sigma^2\\ -1/2\sigma^2 \end{bmatrix}, \ u(x) = \begin{bmatrix} x\\ x^2 \end{bmatrix}, \ h(x) = (2\pi)^{-1/2},$$
$$g(\eta) = (-2\eta_2)^{1/2} \exp\left(\frac{\eta_1^2}{4\eta_2}\right)$$

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Examples of Exponential Families

Bernoulli: distribution on (0, 1)Categorical: distribution on $\{1, 2, \ldots, k\}$ Gaussian: distribution on \mathbb{R}^d Beta: distribution on [0, 1] (including uniform) Dirichlet: distribution on discrete probabilities Wishart: distribution on positive-definite matrices Poisson: distribution on non-negative integers. Gamma: distribution on positive real numbers many more....

Maximum likelihood and sufficient statistics How to estimate the values of the parameters from a data which supposedly follows a distribution from the exponential family?

Recall that

→ The gradient of a differentiable function $f(\mathbf{x})$ with $\mathbf{x} = [x_1, \dots, x_d] \in \mathbb{R}^d$ is defined as

$$\nabla f(\mathbf{x}) = [\partial f(\mathbf{x}) / \partial x_1, \dots, \partial f(\mathbf{x}) / \partial x_d]^T$$

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 \rightarrow The Hessian of $f(\mathbf{x})$ is a $d \times d$ matrix with *ij*-th entry $\partial^2 f(\mathbf{x}) / \partial x_i \partial x_j$

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Taking the gradient both sides of $g(\eta) \int h(\mathbf{x}) \exp \{\eta^T \mathbf{u}(\mathbf{x})\} d\mathbf{x} = 1$ we obtain

$$abla g(oldsymbol{\eta})\int h(\mathbf{x})\exp\left\{oldsymbol{\eta}^{ op}\mathbf{u}(\mathbf{x})
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Which implies

$$-\frac{1}{g(\eta)}\nabla g(\eta) = g(\eta)\int h(\mathbf{x})\exp\left\{\eta^{T}\mathbf{u}(\mathbf{x})\right\}\mathbf{u}(\mathbf{x})d\mathbf{x} = \mathbb{E}[\mathbf{u}(\mathbf{x})]$$

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Similarly the covariance matrix of $\mathbf{u}(\mathbf{x})$ can be expressed in terms of the second derivative of $g(\eta)$, and the higher order moments. The covariance matrix is also equal to the Fisher information matrix for natural parameters

Estimation of η_{ML} Consider a set of iid data denoted by $\mathbf{X} = \{X_1, \dots, X_N\}$. Then the likelihood function is

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$$p(\mathbf{X}, \boldsymbol{\eta}) = \left(\prod_{n=1}^{N} h(\mathbf{x}_n)\right) g(\boldsymbol{\eta})^N \exp\left\{\boldsymbol{\eta}^T \sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n)\right\}$$

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Setting the gradient of $\ln p(\mathbf{X}, \eta)$ wrt η to zero, we obtain the following condition to be satisfied by the maximum likelihood estimator η_{ML}

$$-\nabla \ln g(\boldsymbol{\eta}_{ML}) = rac{1}{N} \sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n),$$

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which can in principle be solved to obtain η_{ML} Observation The MLE depends on the data through $\sum_{n} \mathbf{u}(\mathbf{x}_{n})$, which is therefore called the sufficient statistic of the distribution

Question Verify the above MLE for multivariate Gaussian distribution

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The ML estimates are:

$$\mu_{ML} = rac{1}{N}\sum_{n=1}^{N} \mathbf{x}_n$$
, and $\mathbf{\Sigma}_{ML} = rac{1}{N}\sum_{n=1}^{N} (\mathbf{x}_n - \mu_{ML}) (\mathbf{x}_n - \mu_{ML})^T$

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Observation Note that the partition function $g(\eta)$ for the exponential family

$$p(\mathbf{x}; \boldsymbol{\eta}) = g(\boldsymbol{\eta}) \exp\{\boldsymbol{\eta}^{\mathsf{T}} \mathbf{u}(\mathbf{x})\} h(\mathbf{x}),$$

normalizes the distribution.

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Then the unnormalized distribution

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Then

$$\ln \widetilde{p}(\mathbf{x}, \boldsymbol{\eta}) = \boldsymbol{\eta}^{\mathsf{T}} \mathbf{u}(\mathbf{x}) + \ln h(\mathbf{x})$$

is known as energy function, which is linear in η .

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Observation Note that the partition function $g(\eta)$ for the exponential family

$$p(\mathbf{x}; \boldsymbol{\eta}) = g(\boldsymbol{\eta}) \exp\{\boldsymbol{\eta}^{\mathsf{T}} \mathbf{u}(\mathbf{x})\} h(\mathbf{x}),$$

normalizes the distribution.

Then the unnormalized distribution

$$\widetilde{
ho}(\mathbf{x}, oldsymbol{\eta}) = \exp\left(oldsymbol{\eta}^{ op} \mathbf{u}(\mathbf{x})
ight) h(\mathbf{x})$$

Then

$$\ln \widetilde{p}(\mathbf{x}, \boldsymbol{\eta}) = \boldsymbol{\eta}^{\mathsf{T}} \mathbf{u}(\mathbf{x}) + \ln h(\mathbf{x})$$

is known as energy function, which is linear in η . Thus the $p(\mathbf{x}; \eta)$ is referred as log-linear