Big Data Analysis (MA60306)

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Spring 2022-23, IIT Kharagpur

Lecture 5 January 12, 2023

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Theorem If  $Loss(y, \hat{y}) = (y - \hat{y})^2$  then the optimal prediction function  $g^*$  is equal to the conditional expectation of Y given  $\mathbf{X} = \mathbf{x}$ :

$$g^*(\mathbf{x}) = \mathbb{E}[Y|\mathbf{X} = \mathbf{x}]$$

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#### Consequence

 $\triangleright$  The conditional **X** = **x**, the random response Y can be written as

$$Y = g^*(\mathbf{x}) + \epsilon(\mathbf{x})$$

where  $\epsilon(\mathbf{x})$  can be thought of as a random deviation of the response from its conditional mean at  $\mathbf{x}$ .

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$$\label{eq:expansion} \begin{split} & \triangleright \ \mathbb{E}[\epsilon(\mathbf{x})] = \mathbf{0} \\ & \triangleright \ \mathbb{V}\mathrm{ar}[\epsilon(\mathbf{x})] = \nu^2(\mathbf{x}) \text{ for some function } \nu(\mathbf{x}) \end{split}$$

Geometry Relate it to a data set: Where x measures height and y measures age of a person. Suppose we want to write y as a function of x through the predictor function:

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$$\begin{aligned} f(x,y) &= \\ \frac{1}{2\pi\sqrt{(1-\rho^2)}\sigma_x\sigma_y} \times \\ &\exp\left\{-\frac{1}{2(1-\rho^2)}\left[\frac{(x-\mu_x)^2}{\sigma_x^2} - 2\rho\frac{(x-\mu_x)(y-\mu_y)}{\sigma_x\sigma_y} + \frac{(y-\mu_y)^2}{\sigma_y^2}\right]\right\} \\ &\text{where } \sigma_x > 0, \, \sigma_y > 0, \, \text{and } |\rho| < 1. \end{aligned}$$

Note that if x denotes the total marks that one student has obtained and y denotes the grade then it becomes a classification problem.

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- → Let  $X_1, \ldots, X_n$  be independent  $\mathcal{N}(0, 1)$  random variables. Then  $\mathbf{X} = (X_1, \ldots, X_n)$  has the density function  $\mathcal{N}_n(\mathbf{0}, \mathbf{I}_n)$
- $\rightarrow$  Let  $\mathbf{X} \sim \mathcal{N}_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , *C* be an  $m \times n$  matrix of rank *m*, and *d* be an *m* dimensional vector. Then  $C\mathbf{X} + d \sim \mathcal{N}_m(C\boldsymbol{\mu} + d, C\boldsymbol{\Sigma}C^T)$

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Note that if x denotes the total marks that one student has obtained and y denotes the grade then it becomes a classification problem.

Multivariate normal distribution Let  $\Sigma$  be a positive definite  $n \times n$  matrix and  $\mu$  an n dimensional vector. Then the pdf of a multivariate normal rv  $\mathbf{X} = (X_1, \ldots, X_n)$  i.e.  $\mathbf{X} \sim \mathcal{N}_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  is

$$f(x_1,\ldots,x_n) = \frac{1}{\sqrt{(2\pi)^n \det(\boldsymbol{\Sigma})}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

- $\rightarrow \mathbb{E}[\mathbf{X}] = \boldsymbol{\mu}, \mathbb{V}ar[\mathbf{X}] = \mathbf{\Sigma} = [\Sigma_{ij}] \text{ where } \Sigma_{ij} = \mathbb{E}[(X_i \mu_i)(X_j \mu_j)]$
- → Let  $X_1, \ldots, X_n$  be independent  $\mathcal{N}(0, 1)$  random variables. Then  $\mathbf{X} = (X_1, \ldots, X_n)$  has the density function  $\mathcal{N}_n(\mathbf{0}, \mathbf{I}_n)$
- $\rightarrow$  Let  $\mathbf{X} \sim \mathcal{N}_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , C be an  $m \times n$  matrix of rank m, and d be an m dimensional vector. Then  $C\mathbf{X} + d \sim \mathcal{N}_m(C\boldsymbol{\mu} + d, C\boldsymbol{\Sigma}C^T)$
- $\rightarrow \text{ If } \mathbf{X} = A\mathbf{Z} + \mu \text{ where } A \text{ is an } n \times n \text{ nonsingular matrix and } \\ \mathbf{Z} \sim \mathcal{N}_n(\mathbf{0}, \mathbf{I}_n) \text{ then } \mathbf{X} \sim \mathcal{N}_n(\mu, AA^T)$

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Method of least square Recall  $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}(\mathbf{x})$ 

$$\min_{\beta} \sum_{i} \epsilon_i^2$$

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*i.e.* 
$$\min_{\boldsymbol{\theta} \in \mathcal{C}(\mathbf{X}) = \Omega} \boldsymbol{\epsilon}^{\mathsf{T}} \boldsymbol{\epsilon} = \|\mathbf{Y} - \boldsymbol{\theta}\|^2$$

where  $\theta = \mathbf{X}\boldsymbol{\beta}$  and  $\Omega$  is the column space of  $\mathbf{X}$  i.e.  $\Omega = \{\mathbf{y} : \mathbf{y} = \mathbf{X}\mathbf{x} \text{ for any } \mathbf{x}\}$ 

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From the geometry, what is your guess for  $\theta$  which can minimize the function?

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From the geometry, what is your guess for  $\theta$  which can minimize the function?

Obviously, 
$$\hat{\theta} = \theta$$
 will minimize  $\|\mathbf{Y} - \theta\|^2$  if  $(\mathbf{Y} - \hat{\theta}) \perp \Omega$ 

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Obviously.  $\hat{\theta}$  can be obtained via a projection matrix P, namely  $\hat{\theta} = P\mathbf{Y}$ , where P is the orthogonal projection onto  $\Omega$  i.e.  $P\theta = \theta$ .  $P^T = P$  and  $P^2 = P$ 

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Then

$$\mathbf{Y} - oldsymbol{ heta} = (\mathbf{Y} - \widehat{oldsymbol{ heta}}) + (\widehat{oldsymbol{ heta}} - oldsymbol{ heta})$$

and

$$(\mathbf{Y} - \widehat{\theta})^T (\widehat{\theta} - \theta) = (\mathbf{Y} - P\mathbf{Y})^T P(\mathbf{Y} - \theta)$$
  
=  $\mathbf{Y}^T (I_n - P) P(\mathbf{Y} - \theta)$   
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Thus

$$\|\mathbf{Y} - \mathbf{ heta}\|^2 = \|Y - \widehat{\mathbf{ heta}}\|^2 + \|\widehat{\mathbf{ heta}} - \mathbf{ heta}\|^2 \ge \|\mathbf{Y} - \widehat{\mathbf{ heta}}\|^2,$$

with equality iff  $\theta = \widehat{\theta}$ .

Now since  $\mathbf{Y} - \hat{\boldsymbol{\theta}}$  is perpendicular to  $\Omega$ ,

$$\mathbf{X}^{T}(\mathbf{Y} - \widehat{\mathbf{\theta}}) = 0$$
 i.e.  $\mathbf{X}^{T}\widehat{\mathbf{\theta}} = \mathbf{X}^{T}\mathbf{Y}$ 

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$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}^{\mathsf{T}} \mathbf{Y}$$

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$$\widehat{\boldsymbol{\mathbf{eta}}} = (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}^{\mathsf{T}} \mathbf{Y}$$

 $\hat{\beta}$  is called the least squares estimate of  $\beta$ . However, finding inverse is computationally not stable!!

Bibhas Adhikari (Spring 2022-23, IIT Kharag

Question What is a stable algorithm?

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Floating point number system A floating point number system  $F \subset \mathbb{R}$  is a set whose elements have the form

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The range of floating point numbers in F is :

$$|\beta^{e_{\min}-1} \leq |y| \leq \beta^{e_{\max}}(1-\beta^{-t})$$

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Image: A matrix

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Note An alternative way of expressing y is

$$y = \pm \beta^{e} \left( \frac{d_{1}}{\beta} + \frac{d_{2}}{\beta^{2}} + \ldots + \frac{d_{t}}{\beta^{t}} \right) = \pm \underbrace{.d_{1}d_{2}\ldots d_{t}}_{t-\text{digit fraction}} \times \beta^{e}$$

where  $0 \le d_i \le \beta - 1$  and  $d_1 \ne 0$  (for normalized numbers)

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Observation Floating points are not equally spaced. Set  $\beta = 2, t = 3, e_{\min} = -1, e_{\max} = 3$ 

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