#### **PS5841**

#### Data Science in Finance & Insurance

Linear Regression

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#### Model

$$E(Y_i) = \mu_i(\boldsymbol{\beta}) = \boldsymbol{x}_i^T \boldsymbol{\beta}$$
$$\boldsymbol{y} = X \boldsymbol{\beta} + \boldsymbol{\epsilon}$$

- $Y_1, ... Y_n$  are independent random variables
- Homoscedasticity

$$Var(Y_i) = \sigma^2, \quad Var(\mathbf{y}) = \sigma^2 I$$

$$\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \sum_{i} (Y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2$$

Heteroscedasticity

$$Var(Y_i) = \sigma_i^2, \quad Var(\mathbf{y}) = V$$

$$\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \sum_{i} \frac{1}{\sigma_i^2} (Y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2$$

#### Least Squares Estimator

$$\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} S_{w}(\boldsymbol{\beta})$$

$$= \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \sum_{i} (\boldsymbol{y} - \boldsymbol{\mu})^{T} V^{-1} (\boldsymbol{y} - \boldsymbol{\mu})$$

Set 
$$\frac{\partial S_W(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = -2X^T V^{-1} (\boldsymbol{y} - X\boldsymbol{\beta}) = 0$$
  
 $\widehat{\boldsymbol{\beta}} = (X^T V^{-1} X)^{-1} X^T V^{-1} \boldsymbol{y}$ 

If homoscedasticity

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

## If homoscedasticity

• 
$$\widehat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T y$$

• 
$$E(\widehat{\boldsymbol{\beta}}) = \boldsymbol{\beta}$$

• 
$$Var(\widehat{\beta}) = \sigma^2 (X^T X)^{-1}$$

LSE is BLUE (Gauss-Markov)

$$\bullet \hat{\sigma}^2 = \frac{\hat{e}^T \hat{e}}{n-p}$$

#### Coefficient of Determination

• 
$$TSS = ESS + RSS$$
  

$$\sum_{i}^{n} (y_{i} - \overline{y})^{2} = \sum_{i}^{n} (y_{i} - \hat{y}_{i})^{2} + \sum_{i}^{n} (\hat{y}_{i} - \overline{y})^{2}$$

$$TSS = \mathbf{y}^{T} \mathbf{y} - n(\overline{y})^{2}$$

$$ESS = \mathbf{y}^{T} \mathbf{y} - \mathbf{y}^{T} \hat{\mathbf{y}}$$

$$RSS = \hat{\mathbf{y}}^{T} \hat{\mathbf{y}} - n(\overline{y})^{2}$$

$$\mathbf{y}^{T} \hat{\mathbf{y}} = \hat{\mathbf{y}}^{T} \hat{\mathbf{y}}$$

• 
$$\hat{R}^2 = \frac{RSS}{TSS} = \left(r_{y,\hat{y}}\right)^2$$

## **Categorical Features**



#### Categorical Features

- *J* levels
- Use a coding scheme to encode it
  - Treatment (Dummy) coding
    - Dummy variables indicate the presence of levels
    - Effect beyond that of the reference level
  - Sum (Deviation) coding
    - Coefficients on coded variables sum to zero
    - Effect beyond the grand mean

#### **Treatment Coding**

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_A I_A + \hat{\beta}_B I_B + \hat{\beta}_C I_C + \hat{\beta}_x x$$

Contrast matrix

strong multicollinearity singular design matrix

If level A is present,

$$I_A = 1$$
,  $I_B = I_C = 0$   
 $\hat{y}_A = \hat{\beta}_0 + \hat{\beta}_A + \hat{\beta}_x x$ 

•  $\hat{\beta}_A$  is the effect, the increase in  $\hat{y}$ , if level A is present, ceteris paribus.

### Treatment Coding w/ a Reference Level

$$\hat{y} = (\hat{\beta}_0 + \hat{\beta}_B) + \hat{\beta}_A I_A + \hat{\beta}_C I_C + \hat{\beta}_x x$$

Contrast matrix

If level A is present,

$$I_A = 1, I_C = 0$$

$$\hat{y}_A = (\hat{\beta}_0 + \hat{\beta}_B) + \hat{\beta}_A + \hat{\beta}_x x$$

$$\hat{\beta}_A = \hat{y}_A - \hat{y}_B$$

•  $\hat{\beta}_A$  is the effect beyond that of level B, if level A is present, ceteris paribus.

### Sum-to-Zero Coding (1)

$$\hat{y} = GM + \hat{\beta}_A I_A + \hat{\beta}_B I_B + \hat{\beta}_{\chi} \chi$$

- GM is the mean of the group/category/level means
- Contrast matrix

$$egin{array}{cccc} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{array}$$

The level C coding forces coefficients to sum to zero

### Sum-to-Zero Coding (2)

$$\hat{y} = GM + \hat{\beta}_A I_A + \hat{\beta}_B I_B + \hat{\beta}_{\chi} \chi$$

If level A is present,

$$I_A = 1, I_B = 0$$

$$\hat{y}_A = GM + \hat{\beta}_A + \hat{\beta}_X x$$

•  $\hat{\beta}_A$  is the effect beyond GM, if level A is present, ceteris paribus.

### Sum-to-Zero Coding (3)

$$\hat{y} = GM + \hat{\beta}_A I_A + \hat{\beta}_B I_B + \hat{\beta}_{\mathcal{X}} X$$

If level C is present,

$$I_A = -1, I_B = -1$$

$$\hat{y}_A = GM - \hat{\beta}_A - \hat{\beta}_B + \hat{\beta}_{\chi} \chi$$

$$"\hat{\beta}_C" = -(\hat{\beta}_A + \hat{\beta}_B)$$

•  $-(\hat{\beta}_A + \hat{\beta}_B)$  is the effect beyond GM, if level C is present

### **Detecting & Modeling Interaction Effects**



#### Between Quantitative & Categorical

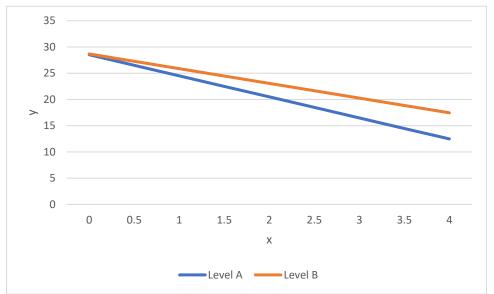
Model

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_x x + \hat{\beta}_B I_B + \hat{\beta}_{xB} x I_B$$

Margin is dependent on x

$$\hat{y}_B - \hat{y}_A = \hat{\beta}_B + \hat{\beta}_{xB} x$$

example



### Between Categorical & Categorical

Model

$$y \sim ... + FactorA + FactorB + FactorA: FactorB$$

example

SEX FEMALE 44.188130 MALE 44.186982

Name: PRESTG10, dtype: float64

SEX MARITAL

FEMALE MARRIED 45.994792

NEVER MARRIED 40.905363

MALE MARRIED 47.692449

NEVER MARRIED 37.884106

Name: PRESTG10, dtype: float64



#### Between Quantitative & Quantitative

Model

$$y \sim ... + x_1 + x_2 + x_1 : x_2$$

example

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_{12} x_1 x_2$$

$$= \hat{\beta}_0 + (\hat{\beta}_1 + \hat{\beta}_{12} x_2) x_1 + \hat{\beta}_2 x_2$$

$$= \hat{\beta}_0 + \hat{\beta}_1 x_1 + (\hat{\beta}_2 + \hat{\beta}_{12} x_1) x_2$$

- For  $\hat{\beta}_{12} > 0$ ,
  - the greater the  $x_2$ , the more positive the effect of  $x_1$  on the response is
  - the greater the  $x_1$ , the more positive the effect of  $x_2$  on the response is

#### Normal Linear Model

Assume

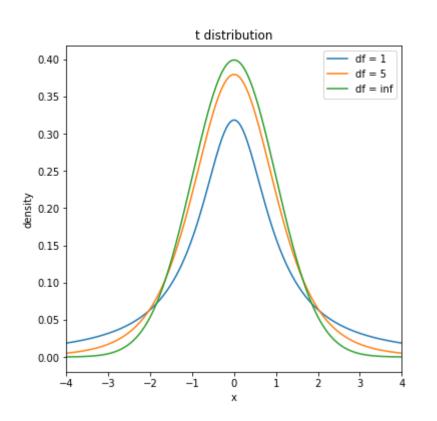
$$\mathbf{y} = (Y_1, \dots, Y_n)^T \sim \mathcal{N}(X\boldsymbol{\beta}, \sigma^2 I)$$

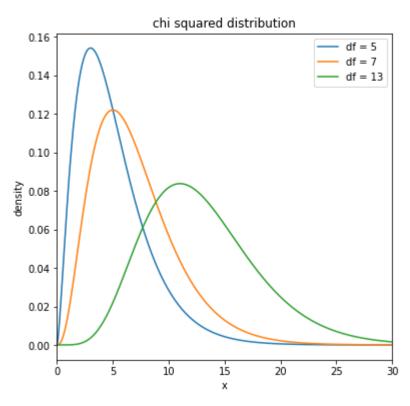
•  $\widehat{\boldsymbol{\beta}} \sim \mathcal{N}(\boldsymbol{\beta}, (X^T X)^{-1} \sigma^2)$ 

• 
$$\frac{\hat{\epsilon}^T \hat{\epsilon}}{\sigma^2} = \frac{(n-p)\hat{\sigma}^2}{\sigma^2} \sim \chi_{n-p}^2$$

• 
$$t = \frac{\widehat{\beta}_j - \beta_j}{\widehat{\sigma}\sqrt{(X^T X)_{jj}^{-1}}} \sim t_{n-p}$$

## T and $\chi^2$ Distributions





#### NLM: inference on a coefficient

- $H_0$ :  $\beta_j = d$  vs
- $H_1: \beta_j \neq d \rightarrow |t| > t_{n-p,1-0.5\alpha}$
- $H_1: \beta_j > d \rightarrow t > t_{n-p,1-\alpha}$
- $H_1: \beta_j < d \to t < -t_{n-p,1-\alpha}$

- where 
$$t = \frac{\widehat{\beta}_j - d}{\widehat{\sigma} \sqrt{(X^T X)_{jj}^{-1}}} \sim t_{n-p}$$

•  $100(1-\alpha)\%$  confidence interval for  $\hat{\beta}_i$ 

$$\hat{\beta}_j \pm t_{n-p,1-\alpha/2} \hat{\sigma}_{\sqrt{(X^T X)_{jj}^{-1}}}$$

#### NLM: inference for prediction

•  $100(1-\alpha)\%$  confidence interval for the predicted mean function at  $x_0$ 

$$\mathbf{x}_{0}^{T}\widehat{\boldsymbol{\beta}} \pm t_{n-p,1-\alpha/2} \, \widehat{\sigma}(\mathbf{x}_{0}^{T}(X^{T}X)^{-1}\mathbf{x}_{0})^{1/2}$$

•  $100(1-\alpha)\%$  prediction interval for the prediction at  ${\it x}$ 

$$\mathbf{x}_0^T \widehat{\boldsymbol{\beta}} \pm t_{n-p,1-\alpha/2} \widehat{\sigma} (1 + \mathbf{x}_0^T (X^T X)^{-1} \mathbf{x}_0)^{1/2}$$

#### **Power Transforms**

 To make the assumption of normality (if desired) more plausible

### Strictly Positive Data

• Box-Cox family of transforms (y > 0)

$$y^{(\lambda)} = \begin{cases} \frac{y^{\lambda} - 1}{\lambda}, & \lambda \neq 0 \\ \ln y, & \lambda = 0 \end{cases}$$

- Estimate  $\lambda$  via maximum likelihood
- In practice,
  - Typically,  $\lambda = 1, 0.5, 0, -1$
  - No need to -1 and  $\div \lambda$  for operations unaffected by location and scale shifts (e.g. some regressions)

#### **General Data**

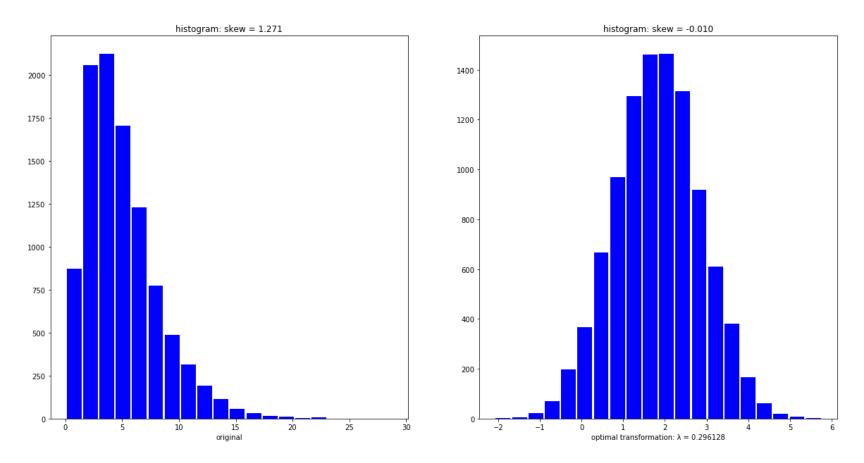
• Box-Cox family of transforms  $(y > -\alpha)$ 

$$y^{(\lambda)} = \begin{cases} \frac{(y+\alpha)^{\lambda} - 1}{\lambda}, & \lambda \neq 0\\ \ln(y+\alpha), & \lambda = 0 \end{cases}$$

Yeo-Johnson family of transforms

$$y^{(\lambda)} = \begin{cases} \frac{(y+1)^{\lambda} - 1}{\lambda}, & \lambda \neq 0, y \ge 0\\ \ln(y+1), & \lambda = 0, y \ge 0\\ -\frac{(-y+1)^{2-\lambda} - 1}{2-\lambda}, & \lambda \neq 2, y < 0\\ -\ln(-y+1), & \lambda = 0, y < 0 \end{cases}$$

### **Box-Cox Transform Example**



sklearn.preprocessing.PowerTransformer()



#### The Bootstrap

- Emulate the process of obtaining new samples without generating additional samples
- Obtain distinct data sets by repeatedly sampling, with replacement, observations from the original data set
- Works well if the original data set is a good representation of the population
  - Risk of "garbage in, garbage out"

#### The Bootstrap

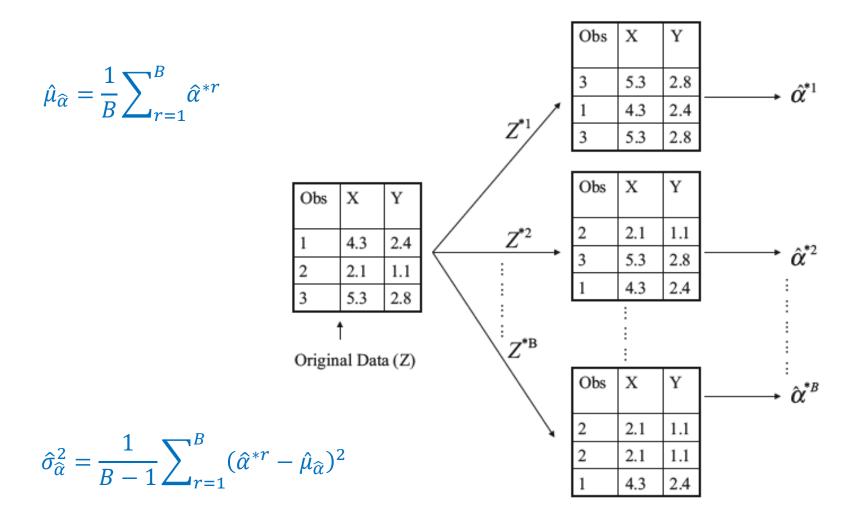
quantity of interest

bootstrap data sets

 $S(\mathbf{Z}^{*1})$  $S(\mathbf{Z}^{*2})$  $S(\mathbf{Z}^{*B})$  $\mathbf{Z}^{*2}$  $\mathbf{Z}^{*1}$  $\mathbf{Z}^{*B}$  $Z = (z_1, z_2, \dots, z_N)$ 

original data set

#### **Bootstrap Data Sets**



#### Gradient

Directional Derivative

$$D_{\boldsymbol{u}}f(\boldsymbol{x}) \equiv \lim_{h \to 0} \frac{1}{h} [f(\boldsymbol{x} + h\boldsymbol{u}) - f(\boldsymbol{x})]$$
$$= \nabla f(\boldsymbol{x}) \cdot \boldsymbol{u} = |\nabla f(\boldsymbol{x})| |\boldsymbol{u}| \cos \theta = |\nabla f(\boldsymbol{x})| \cos \theta$$

where

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_p}\right)^T$$
 $\mathbf{u} = (u_1, \dots, u_p)^T, \quad ||\mathbf{u}|| = 1$ 

•  $D_{\boldsymbol{u}}f(\boldsymbol{x})$  is maximized at  $|\nabla f(\boldsymbol{x})|$  when  $\boldsymbol{u}$  has the same direction as  $\nabla f(\boldsymbol{x})$ .

# $D_{\boldsymbol{u}}f(\boldsymbol{x}) = \boldsymbol{\nabla}f(\boldsymbol{x}) \cdot \boldsymbol{u}$

$$g(h) = f(\mathbf{x} + h\mathbf{u}) = \begin{cases} f(x_1 + hu_1, ..., x_p + hu_p), & [A] \\ f(x_1^*, ..., x_p^*), & [B] \end{cases}$$

• From [A]

$$g'(0) = \lim_{s \to 0} \frac{1}{s} [g(0+s) - g(0)]$$
$$= \lim_{s \to 0} \frac{1}{s} [f(x+(0+s)u) - f(x+0u)] = D_u f(x)$$

• From [B]

$$g'(h) = \frac{dg(h)}{dh} = \frac{\partial f(\mathbf{x}^*)}{\partial x_1^*} \frac{\partial x_1^*}{\partial h} + \dots + \frac{\partial f(\mathbf{x}^*)}{\partial x_p^*} \frac{\partial x_p^*}{\partial h}$$

$$= \frac{\partial f(\mathbf{x}^*)}{\partial x_1^*} u_1 + \dots + \frac{\partial f(\mathbf{x}^*)}{\partial x_p^*} u_p$$

$$\to g'(0) = \frac{\partial f(\mathbf{x})}{\partial x_1} u_1 + \dots + \frac{\partial f(\mathbf{x})}{\partial x_p} u_p = \nabla f(\mathbf{x}) \cdot \mathbf{u}$$

### Maximum Rate of Change

- When  $\nabla f(x) \neq 0$ 
  - the maximum rate of increase of f is  $|\nabla f(x)|$  and is in the direction of  $\nabla f(x)$
  - the maximum rate of decrease of f is  $|\nabla f(x)|$  and is in the direction of  $-\nabla f(x)$

#### Example

• 
$$f(\mathbf{x}) = x_1 + x_2^2$$
,  $\nabla f(\mathbf{x}) = \begin{pmatrix} 1 \\ 2x_2 \end{pmatrix}$ 

• The unit vector in the direction of the gradient at

$$\mathbf{x}_0 = (1,1)^T \text{ is } \mathbf{u} = \left(\frac{1}{\sqrt{5}}, \frac{2}{\sqrt{5}}\right)^T \text{ since}$$

$$\nabla f(\mathbf{x}_0) = (1,2)^T, \quad |\nabla f(\mathbf{x}_0)| = \sqrt{5}$$

• Moving d units from  $x_0 = (1,1)^T$  in the direction of

the gradient vector will land at 
$$x_1 = x_0 + ud = \left(1 + \frac{d}{\sqrt{5}}, 1 + \frac{2d}{\sqrt{5}}\right)^T$$
, with rate of increase 
$$f(x_1) = f(x_0) + \sqrt{5}d + \frac{4d^2}{5}$$
 predicted "error" on large increase on large yields

#### **Gradient Descent**

To minimize the loss function

$$R(\widehat{\boldsymbol{\beta}}) = \sum_{i=1}^{n} R_i(\widehat{\boldsymbol{\beta}}) = \sum_{i=1}^{n} (y_i - \widehat{y}_i(\widehat{\boldsymbol{\beta}}))^2$$

with learning rate  $\eta > 0$ , updating involves all observations

$$\widehat{\boldsymbol{\beta}}^{(r+1)} = \widehat{\boldsymbol{\beta}}^{(r)} - \eta \nabla R(\widehat{\boldsymbol{\beta}}^{(r)})$$

$$= \widehat{\boldsymbol{\beta}}^{(r)} - \eta \sum_{i=1}^{n} \nabla R_i(\widehat{\boldsymbol{\beta}}^{(r)})$$

#### Stochastic Gradient Descent

- SGD is a stochastic approximation of GD.
- SGD uses randomly selected samples/subset from the training set for each iteration
- At extreme, updating would involve only a single (randomly selected) observation

$$\widehat{\boldsymbol{\beta}}^{(r+1)} = \widehat{\boldsymbol{\beta}}^{(r)} - \eta \nabla R_i (\widehat{\boldsymbol{\beta}}^{(r)})$$

### **Gradient Descent for Linear Regression**

Loss function

$$R(\widehat{\boldsymbol{\beta}}) = \sum_{i=1}^{n} R_i(\widehat{\boldsymbol{\beta}}) = \sum_{i=1}^{n} (y_i - \boldsymbol{x}_i^T \widehat{\boldsymbol{\beta}})^2$$

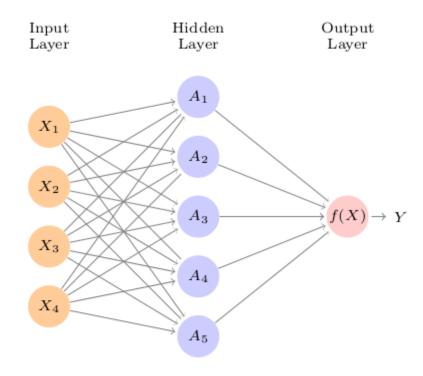
Gradient

$$\nabla R_i(\widehat{\boldsymbol{\beta}}) = -2(y_i - \boldsymbol{x}_i^T \widehat{\boldsymbol{\beta}}) \boldsymbol{x}_i = -2\hat{e}_i(\widehat{\boldsymbol{\beta}}^{(r)}) \boldsymbol{x}_i$$

Updating

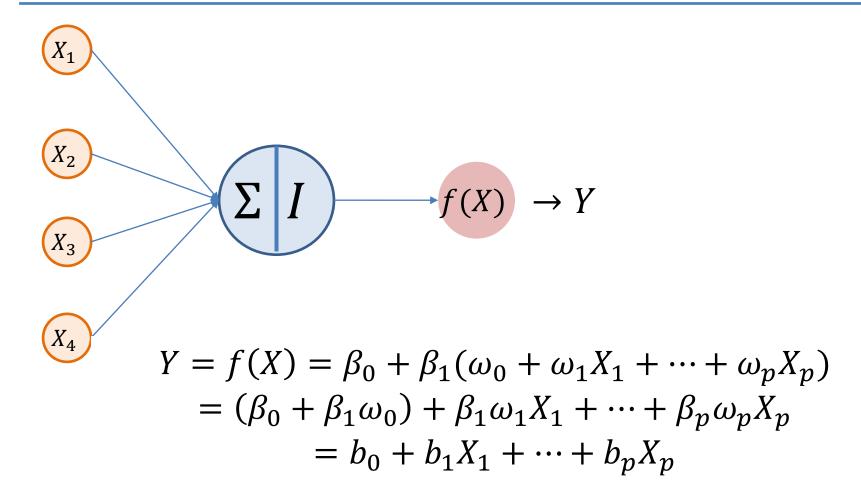
$$\widehat{\boldsymbol{\beta}}^{(r+1)} = \widehat{\boldsymbol{\beta}}^{(r)} - \eta \nabla R(\widehat{\boldsymbol{\beta}}^{(r)})$$
$$= \widehat{\boldsymbol{\beta}}^{(r)} + 2\eta \sum_{i=1}^{n} \hat{e}_i(\widehat{\boldsymbol{\beta}}^{(r)}) x_i$$

#### Single Layer Neural Network



$$\hat{y} = f(X) = \beta_0 + \sum_{k=1}^K \beta_k A_k, \qquad A_k = g(\mathbf{x}_i^T \boldsymbol{\omega}_k)$$

#### NN: Linear Regression



#### Bayesian Approach

$$f_{\mathrm{D}|\Theta}(\boldsymbol{d}) = \frac{f_{\Theta,D}(\boldsymbol{\theta},\boldsymbol{d})}{f_{\Theta}(\boldsymbol{\theta})}$$

$$f_{\Theta|D}(\boldsymbol{\theta}) = \frac{f_{\Theta,D}(\boldsymbol{\theta},\boldsymbol{d})}{f_{\mathrm{D}}(\boldsymbol{d})} = \frac{f_{\mathrm{D}|\Theta}(\boldsymbol{d})f_{\Theta}(\boldsymbol{\theta})}{f_{\mathrm{D}}(\boldsymbol{d})}$$

$$f_{\mathrm{D}}(\boldsymbol{d}) = \int f_{\mathrm{D}|\Theta}(\boldsymbol{d}) d\boldsymbol{\Theta}$$

- Prior
- Likelihood
- Posterior

### Example

• 
$$\Theta = \{\mu, \sigma\}$$

– Assumption:  $\mu$  and  $\sigma$  are independent

$$Y_i \sim^{iid} \mathcal{N}(\mu, \sigma)$$
  
 $\mu \sim \mathcal{N}(\mu_{\mu}, \sigma_{\mu})$   
 $\sigma \sim \mathcal{U}(\sigma_L, \sigma_H)$ 

#### Example: Likelihood

Prior

$$f_{\Theta}(\boldsymbol{\theta}) = \prod_{j=1}^{p} f_{\Theta_{j}}(\theta_{j}) = \frac{\exp\left[-\left(\frac{\mu - \mu_{\mu}}{\sigma_{\mu}}\right)^{2}\right]}{\sqrt{2\pi}\sigma_{\mu}} \cdot \frac{1}{(\sigma_{H} - \sigma_{L})}$$

Likelihood

$$f_{\mathrm{D}|\Theta}(\boldsymbol{d}) = \prod_{i=1}^{n} \frac{\exp[-\left(\frac{y_i - \mu}{\sigma}\right)^2]}{\sqrt{2\pi}\sigma}$$

$$f_{\Theta|D}(\boldsymbol{\theta}) = \frac{f_{\mathrm{D}|\Theta}(\boldsymbol{d})f_{\Theta}(\boldsymbol{\theta})}{f_{\mathrm{D}}(\boldsymbol{d})} \propto f_{\mathrm{D}|\Theta}(\boldsymbol{d})f_{\Theta}(\boldsymbol{\theta})$$

#### Example: Log Likelihood

Posterior

$$f_{\Theta|D}(\boldsymbol{\theta}) = \frac{f_{\mathrm{D}|\Theta}(\boldsymbol{d})f_{\Theta}(\boldsymbol{\theta})}{f_{\mathrm{D}}(\boldsymbol{d})}$$

Log Posterior

$$\ln f_{\mathrm{D}|\Theta}(\boldsymbol{d}) + \ln f_{\Theta}(\boldsymbol{\theta}) + \mathrm{const}$$

$$l(\boldsymbol{\theta} \mid \boldsymbol{d}) = -\sum_{i=1}^{n} \left(\frac{y_i - \mu}{\sigma}\right)^2 - \left(\frac{\mu - \mu_{\mu}}{\sigma_{\mu}}\right)^2 + \mathrm{const}$$

•  $\widehat{\boldsymbol{\theta}}$  maximizes  $l(\boldsymbol{\theta} \mid \boldsymbol{d})$ 

#### **Bayesian Regression**

$$Y_i \sim^{iid} \mathcal{N}(\mu_i, \sigma)$$

$$\mu_i = \boldsymbol{x}_i^T \boldsymbol{\beta}$$

$$\beta_j \sim$$

$$\sigma \sim$$

#### Fitting a Bayesian Regression

- Numerically minimize  $-l(\beta \mid data)$ 
  - GD-like?
- Numerically represent the posterior
  - Grid approximation
- Posterior Sampling
  - Markov Chain Monte Carlo

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### Linear Regression: Gibbs Sampling

example

$$\beta_j \sim N\left(\mu_{\beta_j}, \sigma_{\beta_j}^2\right)$$

$$\sigma^2 \sim IG(a, b)$$

Conditional posterior

$$\beta | y, \sigma^2 \sim N((X'X)^{-1}X'y, \sigma^2(X'X)^{-1})$$
  
 $\sigma^2 | y, \beta \sim IG(a + 0.5n, b + 0.5e'e)$ 

### Linear Regression: Gibbs Sampling

Gibbs Sampling

Initialize 
$$\widehat{\pmb{\beta}}^{(1)}$$

Draw 
$$\hat{\sigma}^{2^{(1)}}$$
 from  $\sigma^2 | y$ ,  $\hat{\beta}^{(1)}$ 

Draw 
$$\hat{\beta}^{(2)}$$
 from  $\boldsymbol{\beta}|y$ ,  $\hat{\sigma}^{2^{(1)}}$ 

Draw 
$$\hat{\sigma}^{2}$$
 from  $\sigma^2 | y$ ,  $\hat{\beta}^{(2)}$ 

Draw 
$$\hat{\beta}^{(3)}$$
 from  $\boldsymbol{\beta}|y$ ,  $\hat{\sigma}^{2^{(2)}}$ 

. . .