#### **PS5841**

#### Data Science in Finance & Insurance

# Linear Regression

Yubo Wang

Autumn 2021



### **Linear Regression Model**

$$y = X\beta + \epsilon$$

where

$$\mathbf{y} = [Y_1, \dots, Y_n]^T$$

 $Y_1, \dots Y_n$  are independent RVs with

$$Y_{i} = \mu_{i}(\boldsymbol{\beta}) + \epsilon_{i} = \boldsymbol{x}_{i}^{T} \boldsymbol{\beta} + \epsilon_{i}$$

$$\boldsymbol{X} = [\boldsymbol{x}_{1}^{T}, ..., \boldsymbol{x}_{n}^{T}]^{T}, \boldsymbol{\beta} = [\beta_{1}, ..., \beta_{p}]^{T}, \boldsymbol{\epsilon} = [\epsilon_{1}, ..., \epsilon_{n}]^{T}$$

$$E(\boldsymbol{y}) = \boldsymbol{\mu}(\boldsymbol{\beta}) = \boldsymbol{X}\boldsymbol{\beta}$$

$$Var(\boldsymbol{y}) = E[(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^{T}] = \boldsymbol{\Sigma}$$



### Least Squares Estimation

Minimize

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

Set

de-emphasize high variance RV's

$$\frac{\partial S_w}{\partial \boldsymbol{\beta}} = -2\boldsymbol{X}^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) = 0$$

Get

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



### **Least Squares Estimator**

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

• If  $Y_i's$  are homoscedastic  $\mathbf{\Sigma} = \mathbf{I}\sigma^2$ , LSE is  $\widehat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ 

with

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

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

$$\widehat{\sigma}^{2} = \frac{1}{n-p}(\mathbf{y} - X\widehat{\boldsymbol{\beta}})^{T}(\mathbf{y} - X\widehat{\boldsymbol{\beta}})$$



#### Coefficient of Determination

RSS of the model

$$\hat{S} = (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^T (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) = \mathbf{y}^T \mathbf{y} - \hat{\boldsymbol{\beta}} \mathbf{X}^T \mathbf{y}$$

•  $\hat{S}_0$ , the worst value of RSS, is associated with the naïve model  $E(Y_i) = \mu, \forall i$  $\hat{S}_0 = \mathbf{y}^T \mathbf{y} - N \bar{y}^2 = \Sigma (y_i - \bar{y})^2 \propto Var(y)$ 

Relative improvement

$$R^{2} = \frac{\hat{S}_{0} - \hat{S}}{\hat{S}_{0}} = \frac{\widehat{\boldsymbol{\beta}} \boldsymbol{X}^{T} \boldsymbol{y} - N \bar{y}^{2}}{\boldsymbol{y}^{T} \boldsymbol{y} - N \bar{y}^{2}}$$



Proportion of the total variation in the data which is explained by the model

#### The Naïve Model

$$E(Y_i) = \mu, \forall i$$

$$\widehat{\boldsymbol{\beta}} = \hat{\mu} = \overline{y}$$

$$X = \boldsymbol{j}$$

$$\hat{S}_{0} = \mathbf{y}^{T} \mathbf{y} - \widehat{\boldsymbol{\beta}} \mathbf{X}^{T} \mathbf{y} 
= \mathbf{y}^{T} \mathbf{y} - \overline{\mathbf{y}} \Sigma \mathbf{y}_{i} 
= \mathbf{y}^{T} \mathbf{y} - N \overline{\mathbf{y}}^{2} 
= \Sigma (y_{i} - \overline{y})^{2} \propto Var(y)$$



#### **Gauss-Markov Theorem**

• When  $\Sigma = I\sigma^2$ , the least squares estimator  $\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$  is BLUE



### Categorical Features

- Categorical features are often modeled by binary (dummy) variables in a regression
- For a feature (factor) with J levels
  - Need J binary variables if there is no intercept
  - Need (J-1) binary variables if intercept
  - Baseline is the level with no dummy variable
- Example: 1 factor with 3 levels (A,B,C)
  - with baseline A (A as the reference level)

$$y = \beta_0 + \beta_1 x_B + \beta_2 x_C + \beta_3 x_3 + \beta_4 x_4 + \epsilon$$

– How are  $\hat{\beta}_i$ 's interpreted?



### Example (1)

- 1 factor with 3 levels (A,B,C)
  - with baseline A (A as the reference level)

$$y = \beta_0 + \beta_1 x_B + \beta_2 x_C + \beta_3 x_3 + \beta_4 x_4 + \epsilon$$

– How are  $\hat{\beta}_i$ 's interpreted?



### Example (2)

- 1 factor with 3 levels (A,B,C)
  - with baseline A (A as the reference level)

$$y = \beta_0 + \beta_1 x_B + \beta_2 x_C + \beta_3 x_3 + \beta_4 x_4 + \epsilon$$

If level A is present, all else being equal

$$\hat{y}_A = \hat{\beta}_0 + \hat{\beta}_3 x_3 + \hat{\beta}_4 x_4$$

If level B is present, all else being equal

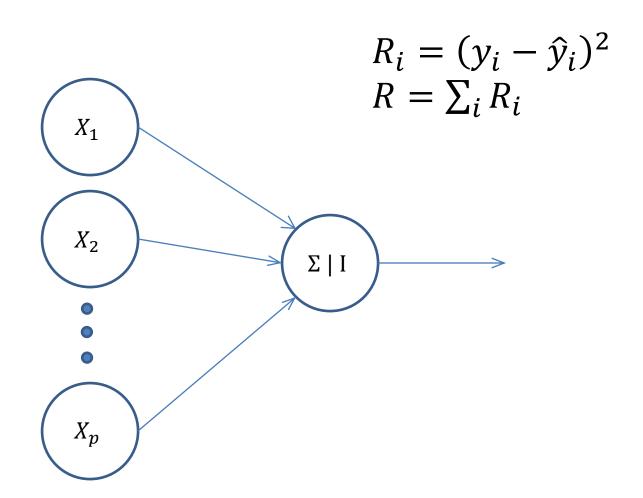
$$\hat{y}_B = \hat{\beta}_0 + \hat{\beta}_1 + \hat{\beta}_3 x_3 + \hat{\beta}_4 x_4$$

• Interpretation of  $\hat{\beta}_1$ 

$$\hat{y}_B - \hat{y}_A = \hat{\beta}_1$$



### Linear Regression with a Neuron





#### **Gradient Descent**

Gradient operator (del operator)

$$\nabla = \left(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_n}\right)^T$$

– when operating on a real valued function  $f: \mathbb{R}^n - \mathbb{R}$ 

$$\nabla(f) = \nabla f = \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n}\right)^T$$



#### Gradient

• For  $f: \mathbb{R}^n - \mathbb{R}$ , differentiable at x, the gradient of f at x is

$$\nabla f(\mathbf{x}) = \left(\frac{\partial f}{\partial x_1}(\mathbf{x}), \dots, \frac{\partial f}{\partial x_n}(\mathbf{x})\right)^T$$

- 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 (1)

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

• Moving d units from  $x_0=\binom{1}{1}$  in the direction of  $\nabla f(1,1)=\binom{1}{2}, |\nabla f(1,1)|=\sqrt{5}$ 

lands at

$$\boldsymbol{x}_1 = \begin{pmatrix} 1 + \frac{d}{\sqrt{5}} \\ 1 + \frac{2d}{\sqrt{5}} \end{pmatrix}$$



## Example (2)

						pre	edic
gradient ascent						rat	e
	f[1+(1/sqrt(5))d,						
d	1+(2/sqrt(5))d]	f(1,1)		chg (f)	sqrt(5)*d	error	
1	5.036067977		2	3.036068	2.23606798	0.8	
0.1	2.231606798		2	0.231607	0.2236068	0.008	
0.01	2.02244068		2	0.022441	0.02236068	8E-05	<b>↓</b>
non-optin	nal direction						
	f[1+(1/sqrt(2))d,						
d	1+(1/sqrt(2))d]	f(1,1)		chg (f)	See! It's true!		
1	4.621320344		2	2.62132	<	3.036068	
0.1	2.217132034		2	0.217132	<	0.231607	
0.01	2.021263203		2	0.021263	<	0.022441	

COLUMBIA

Same as

#### **Gradient Descent**

To minimize the objective function

$$R(\boldsymbol{\beta}) = \sum_{i=1}^{n} R_i(\boldsymbol{\beta})$$

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

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



#### Stochastic Gradient Descent

- SGD is a stochastic approximation of GD.
   SGD uses randomly selected samples to evaluate the gradients
- At extreme, updating would involve only a single observation

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



#### Normal Linear Model

•  $Y_i \sim N(\mu_i, \sigma^2)$ 

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

$$\widehat{\sigma}^{2} = \frac{1}{n-p} (\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}})^{T} (\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}) \sim \frac{\sigma^{2}}{n-p} \chi_{n-p}^{2}$$



### NLM: Inference (3)

Variance of fit at x

$$\mathbf{x}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x} \sigma^2$$

• Variance of prediction at x

$$[1 + \boldsymbol{x}^T (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{x}] \sigma^2$$



#### General Linear Model

• 
$$Y_i \sim N(\mu_i, \sigma^2)$$

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

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

- Features (Explanatory Variables, Independent Variables) can come from different sources
  - Quantitative or their transformations
  - Basis expansions (e.g. polynomial regression)
  - Numeric or dummy coding of categorical levels
  - Interactions between variables (e.g.  $X_1X_2$ )
- Linear regression, ANOVA, ANCOVA



#### **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  $(y > -\alpha)$ 

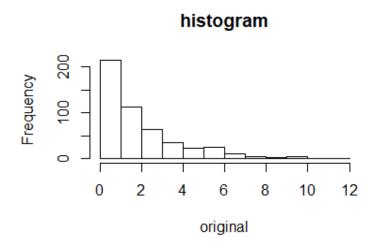
$$y^{(\lambda)} = \begin{cases} \frac{(y+\alpha)^{\lambda} - 1}{\lambda}, & \lambda \neq 0\\ \ln(y+\alpha), & \lambda = 0 \end{cases}$$

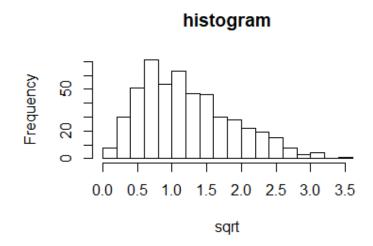
Yeo-Johnson family of transforms

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



### Box-Cox Transform Example



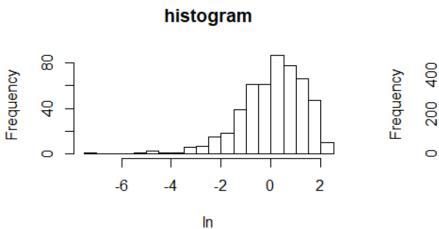


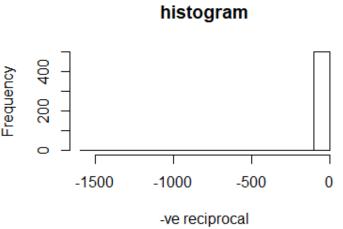
**Heavily Skewed** 

Approximately Symmetric



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



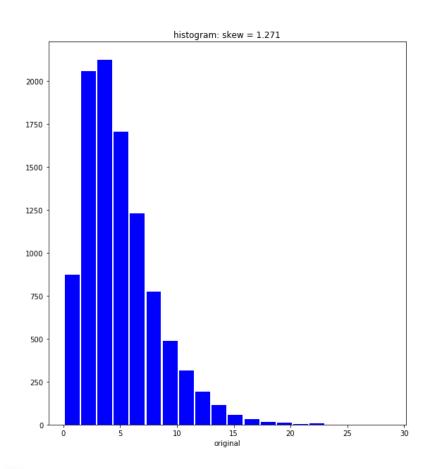


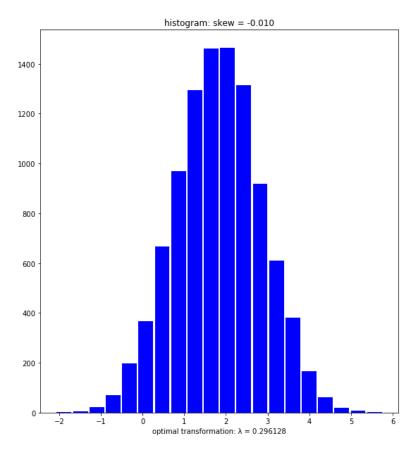
Approximately Symmetric

**Heavily Skewed** 



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







#### Generalized Linear Models

$$Y_i \sim D($$

$$g[E(Y_i)] = \boldsymbol{x}_i^T \boldsymbol{\beta}$$



### Example: Normal Linear Model

$$Y_i \sim N(\mu_i, \sigma^2), \qquad Y \sim MVN(X\beta, \sigma^2 I)$$

$$g[E(Y_i)] = \mu_i = \boldsymbol{x}_i^T \boldsymbol{\beta}$$

**MLE** 

$$l \propto \sum_{i} (y_i - \boldsymbol{x}_i^T \boldsymbol{\beta})^2$$
,  $l \propto (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^T (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})$ 

$$\frac{\partial l}{\partial \boldsymbol{\beta}} = -2\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) = 0$$

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



### That was



