Statistical Machine Learning

4주차
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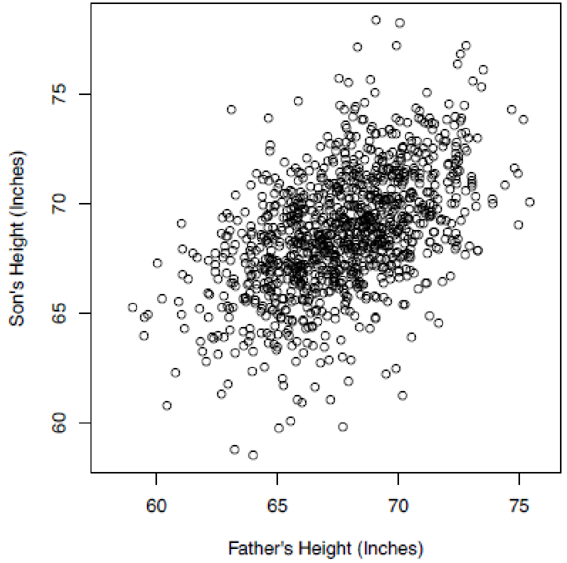
Regression

1. Linear Model
2. Linear Regression
3. MSE
4. Regularization

What is Regression?



Linearity

- Linearity?

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_p X_{pi} + \epsilon_i$$

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \beta_3 X_{1i} X_{2i} + \epsilon_i$$

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \cdots + \beta_p X_i^p + \epsilon_i$$

Linear Model

- Linearity? $\longrightarrow$ Linear Model

$$Y_i \overset{ind}{\sim} (\mu_i(\mathbf{X}_i),\ \sigma^2) \qquad \text{where} \quad E[Y_i] = \mu_i(\mathbf{X}_i)$$

$$\mu_i(\mathbf{X}_i) = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_p X_{pi} = \boldsymbol{\beta}^T \mathbf{X}_i$$

$$\boldsymbol{\mu}(\mathbf{X}) = \mathbf{X}\ \boldsymbol{\beta}$$

Linear Regression

- Least Square Estimator

$$\sum \epsilon_i^2 = \sum (Y_i - \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_p X_{pi})^2$$

$$\frac{\partial}{\partial \beta_0} \sum (Y_i - \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_p X_{pi})^2 \overset{set}{=} 0$$

$$\frac{\partial}{\partial \beta_1} \sum (Y_i - \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_p X_{pi})^2 \overset{set}{=} 0$$

$$\vdots$$

$$\frac{\partial}{\partial \beta_p} \sum (Y_i - \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_p X_{pi})^2 \overset{set}{=} 0$$

Linear Regression

- Error term?
  - Mean 0
  - Identical, Independent
  - Normal?

Linear Regression and likelihood function

- Normal distribution

$$\log L(\mu) \approx -\frac{\sum_{i=1}^{n}(y_i - \mu)}{\sigma^2}$$

Likelihood function and Loss function

- Binary Cross Entropy
- Categorical Cross Entropy
- MSE

Generalized Linear Model

	Normal	Poisson	Binomial	Gamma	Inv Gaussian
Notation	$N(\mu, \sigma^2)$	$P(\mu)$	$B(n, \pi)/n$	$G(\mu, v)$	$IG(\mu, \sigma^2)$
Support	$(-\infty, \infty)$	$\{0, 1, \cdots\}$	$\{0, \cdots, n\}/n$	$(0, \infty)$	$(0, \infty)$
$a(\phi)$	$\phi = \sigma^2$	1	$1/m$	v^{-1}	σ^2
$b(\theta)$	$\theta^2/2$	e^θ	$\log(1 + e^\theta)$	$-\log(-\theta)$	$-(-2\theta)^{1/2}$
$b'(\theta) = E(Y)$	θ	e^θ	$\frac{e^\theta}{1+e^\theta}$	$-1/\theta$	$(-2\theta)^{-1/2}$
$(b')^{-1}(\mu) = g(\mu)$	μ	$\log(\mu)$	$\log \frac{\mu}{1-\mu}$	μ^{-1}	μ^{-2}
$b''(\theta)$	1	μ	$\mu(1-\mu)$	μ^2	μ^3

Table: Summary of some popular GLM models.

Stein's Paradox

- Let $\mathbf{X} = [X_1, \cdots, X_p]^T \sim N_p(\boldsymbol{\theta}, I)$

- The UMVUE and MLE of $\boldsymbol{\theta}$ is

$$\widehat{\boldsymbol{\theta}}_{MLE,UMVUE} = \mathbf{X}$$

- Using squared error loss, the risk of $\widehat{\boldsymbol{\theta}}_{MLE,UMVUE}$ is

$$R(\boldsymbol{\theta}, \widehat{\boldsymbol{\theta}}_{UMVUE}) = E[||\mathbf{X} - \boldsymbol{\theta}||^2] = p$$

Stein's Paradox

- James and Stein (1961) Estimator

$$\widehat{\boldsymbol{\theta}}_{JS} = \left(1 - \frac{p-2}{||\mathbf{X}||^2}\right)\mathbf{X}$$

- When $p \geq 3$,

$$R(\boldsymbol{\theta}, \widehat{\boldsymbol{\theta}}_{JS}) = p - (p-2)E\left(\frac{1}{||\mathbf{X}||^2}\right) < p$$

Stein's Paradox

- Proof

$$R(\boldsymbol{\theta}, \widehat{\boldsymbol{\theta}}_{JS}) = E\left[||\mathbf{X} - \boldsymbol{\theta} - \frac{(p-2)\mathbf{X}}{||\mathbf{X}||^2}||^2 \right]$$

$$= p - 2(p-2)\sum_{j}^{p} E\left(\frac{X_j(X_j - \theta_j)}{||\mathbf{X}||^2}\right) + (p-2)^2 E\left(\frac{1}{||\mathbf{X}||^2}\right)$$

$$= p - (p-2)E\left(\frac{1}{||\mathbf{X}||^2}\right)$$

Since $\sum_j^p E\left(\frac{X_j(X_j-\theta_j)}{||\mathbf{X}||^2}\right) = (p-2)E\left(\frac{1}{||\mathbf{X}||^2}\right)$

Stein's Paradox

- JS estimator shrinks each component of $\mathbf{X}$ towards the origin, and thus the biggest improvement comes when $\| \boldsymbol{\theta} \|$ is close to zero.
- Normality assumption is not critical, and similar results can be shown for a wide class of distributions.

Ridge Regression

- We can consider

$$\widehat{\boldsymbol{\beta}}_{Ridge} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{Y}$$

- Ridge estimator is

$$\widehat{\boldsymbol{\beta}}_{Ridge} = \underset{\boldsymbol{\beta}}{argmin}\,(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda\boldsymbol{\beta}^T\boldsymbol{\beta}$$

Lagrange Multiplier Theorem

- Primal Problem

$$\min_{\boldsymbol{\beta}} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$$

subject to $||\boldsymbol{\beta}||_2^2 \leq C,$ where $||\boldsymbol{\beta}||_2^2 = \boldsymbol{\beta}^T \boldsymbol{\beta} = \sum_j^p \beta_j^2$

- Dual Problem

$$\min_{\boldsymbol{\beta}} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda(\, ||\boldsymbol{\beta}||_2^2 - C\,)$$

Lagrange Multiplier Theorem

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KKT

1. $\nabla f(\mathbf{x}) + \sum_i^m \alpha_i \nabla g_i(\mathbf{x}) + \sum_j^{\mathrm{k}} \gamma_j \nabla h_i(\mathbf{x}) = 0$ (Stationary)

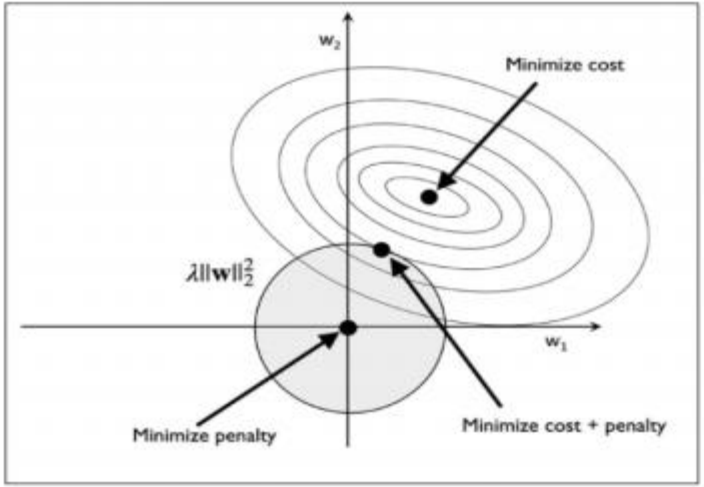
2. $\alpha_i g_i(\mathbf{x}) = 0, \quad$ for $\quad i = 1, \cdots, m$ (Complementary Slackness)

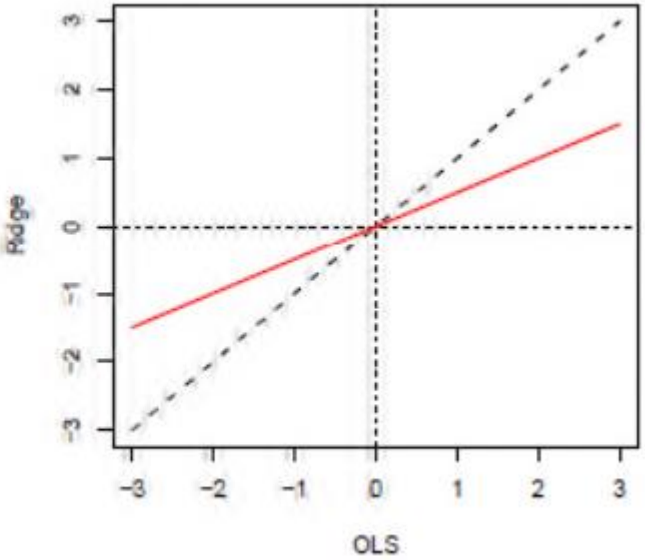
3. $g_i(\mathbf{x}) \leq 0, \quad$ for $\quad i = 1, \cdots, m \quad$ *and* (Primal Feasibility)

   $h_j(\mathbf{x}) = 0, \quad$ for $\quad j = 1, \cdots, \mathrm{k}$

4. $\alpha_i \geq 0, \quad$ for $\quad i = 1, \cdots, m$ (Dual Feasibility)

Ridge Regression





Lasso Regression

- Ridge Regression solves

$$\min_{\boldsymbol{\beta}} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda ||\boldsymbol{\beta}||_2^2 \qquad (L2\ penalty)$$

- LASSO Regression solves

$$\min_{\boldsymbol{\beta}} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda ||\boldsymbol{\beta}||_1 \qquad (L1\ penalty)$$

Lasso Regression

- LASSO (Least Absolute Shrinkage and Selection Operator)

$$(\widehat{\boldsymbol{\beta}}^{\lambda,1} =)\ \widehat{\boldsymbol{\beta}}_{LASSO} = \underset{\boldsymbol{\beta}}{argmin}\ (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda\ ||\boldsymbol{\beta}||_1$$

where $||\boldsymbol{\beta}||_1 = \sum_j^p |\beta_j|$

Lasso Regression