Statistical Machine Learning

4주차

담당:11기 명재성



Logistic Regression Optimization

$$Loss[Y, \hat{Y}] = -\sum_{i=1}^{n} [y_i(\boldsymbol{\beta}^T \mathbf{X}_i) - \log(1 + \exp(\boldsymbol{\beta}^T \mathbf{X}_i))]$$

$$\widehat{\beta} = \underset{\beta}{\operatorname{argmin}} L[Y, \ \widehat{Y}]$$

⇒ Do not have an explicit solution!

Quadratic approximation (2nd order Taylor Expansion)

$$L(\mathbf{\theta}) \approx L(\mathbf{\theta}_0) + \nabla L(\mathbf{\theta}_0)^T (\mathbf{\theta} - \mathbf{\theta}_0) + \frac{1}{2} (\mathbf{\theta} - \mathbf{\theta}_0)^T \mathbf{H}(\mathbf{\theta}_0) (\mathbf{\theta} - \mathbf{\theta}_0)$$
where
$$\nabla L(\mathbf{\theta}_0) = \frac{\partial}{\partial \mathbf{\theta}} L(\mathbf{\theta}) \bigg|_{\mathbf{\theta} = \mathbf{\theta}_0}$$

$$\mathbf{H}(\mathbf{\theta}_0) = \frac{\partial^2}{\partial \mathbf{\theta} \partial \mathbf{\theta}^T} L(\mathbf{\theta}) \bigg|_{\mathbf{\theta} = \mathbf{\theta}_0}$$

Newton-Raphson Method

$$\mathbf{\theta}^{(t+1)} = \mathbf{\theta}^{(t)} - \mathbf{H}^{-1}(\mathbf{\theta}^{(t)}) \nabla L(\mathbf{\theta}^{(t)})$$
$$= \mathbf{\theta}^{(t)} - \mathbf{H}^{-1}(\mathbf{\theta}^{(t)}) \frac{\partial}{\partial \mathbf{\theta}^{(t)}} L(\mathbf{\theta}^{(t)})$$

$$cf. \ \theta^{(t+1)} = \theta^{(t)} - \frac{f'(\theta^{(t)})}{f''(\theta^{(t)})}$$

$$L[\boldsymbol{\beta}] = -\sum_{i=1}^{n} [y_i(\boldsymbol{\beta}^T \mathbf{X}_i) - \log(1 + \exp(\boldsymbol{\beta}^T \mathbf{X}_i))]$$

$$\nabla L(\mathbf{\beta}) = \frac{\partial}{\partial \mathbf{\beta}} L(\mathbf{\beta}) = -\sum_{i=1}^{n} \left[y_i \mathbf{X}_i - \frac{\exp(\mathbf{\beta}^T \mathbf{X}_i)}{1 + \exp(\mathbf{\beta}^T \mathbf{X}_i)} \mathbf{X}_i \right]$$

$$\mathbf{H}(\boldsymbol{\beta}) = \frac{\partial^2}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^T} L(\boldsymbol{\beta}) = \sum_{i=1}^n \left[\left(\frac{\exp(\boldsymbol{\beta}^T \mathbf{X}_i)}{1 + \exp(\boldsymbol{\beta}^T \mathbf{X}_i)} \right) \left(\frac{1}{1 + \exp(\boldsymbol{\beta}^T \mathbf{X}_i)} \right) \mathbf{X}_i \mathbf{X}_i^T \right]$$



$$L[\boldsymbol{\beta}] = -\sum_{i=1}^{n} [y_i(\boldsymbol{\beta}^T \mathbf{X}_i) - \log(1 + \exp(\boldsymbol{\beta}^T \mathbf{X}_i))]$$

Update

$$\boldsymbol{\beta}^{(t+1)} = \boldsymbol{\beta}^{(t)} - \mathbf{H}^{-1} (\boldsymbol{\beta}^{(t)}) \nabla L(\boldsymbol{\beta}^{(t)})$$

until

$$||\mathbf{\beta}^{t+1} - \mathbf{\beta}^t|| < \epsilon$$
 for small $\epsilon > 0$

					Solvers
Penalties	'lib <mark>l</mark> inear'	'lbfgs'	'newton-cg'	'sag'	'saga'
Multinomial + L2 penalty	no	yes	yes	yes	yes
OVR + L2 penalty	yes	yes	yes	yes	yes
Multinomial + L1 penalty	no	no	no	no	yes
OVR + L1 penalty	yes	no	no	no	yes
Behaviors					
Penalize the intercept (bad)	yes	no	no	no	no
Faster for large datasets	no	no	no	yes	yes
Robust to unscaled datasets	yes	yes	yes	no	no

Gradient Descent

$$\mathbf{\theta}^{(t+1)} = \mathbf{\theta}^{(t)} - \mathbf{H}^{-1}(\mathbf{\theta}^{(t)}) \nabla L(\mathbf{\theta}^{(t)})$$

$$\Rightarrow \quad \mathbf{\theta}^{(t+1)} = \mathbf{\theta}^{(t)} - \mathbf{\eta}^{(t)} \, \nabla L(\mathbf{\theta}^{(t)})$$

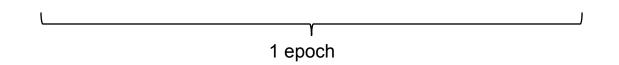
Gradient Descent

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \mathbf{H}^{-1}(\boldsymbol{\theta}^{(t)}) \nabla L(\boldsymbol{\theta}^{(t)})$$

$$\Rightarrow \quad \boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta^{(t)} \nabla L(\boldsymbol{\theta}^{(t)}) \quad \rightarrow \quad \text{in Deep Learning}$$

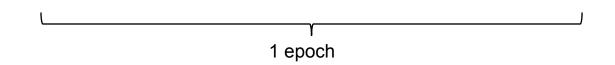
$$\Rightarrow \quad \boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta \nabla L(\boldsymbol{\theta}^{(t)})$$

• (Batch) Gradient Descent



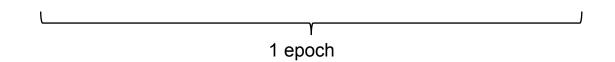
Batch size = n

Stochastic Gradient Descent

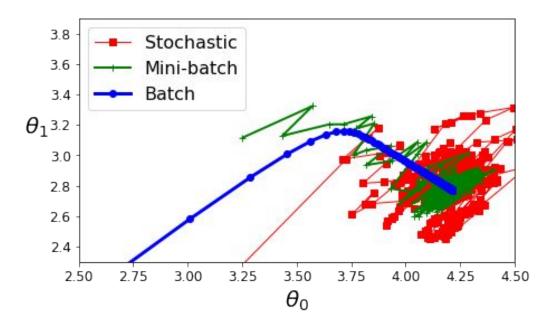


■ Batch size = 1

Mini-Batch Gradient Descent



• Batch size = p, where $p \times k = n$



Stein's Paradox

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

The UMVUE and MLE of θ is

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

• Using squared error loss, the risk of $\widehat{m{ heta}}_{MLE,UMVUE}$ is

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

Stein's Paradox

James and Stein (1961) Estimator

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

• When $p \ge 3$,

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

Steins Paradox

Proof

$$\begin{split} R(\pmb{\theta}, \widehat{\pmb{\theta}}_{JS}) &= E\left[||\mathbf{X} - \pmb{\theta} - \frac{(p-2)\mathbf{X}}{||\mathbf{X}||^2}||^2\right] \\ &= p - 2(p-2)\sum_{j}^{p} E\left(\frac{X_j(X_j - \theta_j)}{||\mathbf{X}||^2}\right) + (p-2)^2 E\left(\frac{1}{||\mathbf{X}||^2}\right) \\ &= p - (p-2)E\left(\frac{1}{||\mathbf{X}||^2}\right) \\ &= \sum_{j}^{p} E\left(\frac{X_j(X_j - \theta_j)}{||\mathbf{X}||^2}\right) = (p-2)E\left(\frac{1}{||\mathbf{X}||^2}\right) \end{split}$$
 Since $\sum_{j}^{p} E\left(\frac{X_j(X_j - \theta_j)}{||\mathbf{X}||^2}\right) = (p-2)E\left(\frac{1}{||\mathbf{X}||^2}\right)$

Steins Paradox

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

Normal Equation

$$(\mathbf{X}^T\mathbf{X})\mathbf{\beta} = \mathbf{X}^T\mathbf{Y}$$

The OLS estimator

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

Normal Equation

$$(\mathbf{X}^T\mathbf{X})\mathbf{\beta} = \mathbf{X}^T\mathbf{Y}$$

The OLS estimator

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

• What if $\mathbf{X}^T\mathbf{X}$ is not invertible?

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

$$\begin{aligned} \min_{\boldsymbol{\beta}} \ (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) \\ \text{subject to} \quad ||\boldsymbol{\beta}||_2^2 &\leq \mathcal{C}, \quad \text{where} \quad ||\boldsymbol{\beta}||_2^2 = \boldsymbol{\beta}^T \boldsymbol{\beta} = \sum_i^p \beta_i^2 \end{aligned}$$

Dual Problem

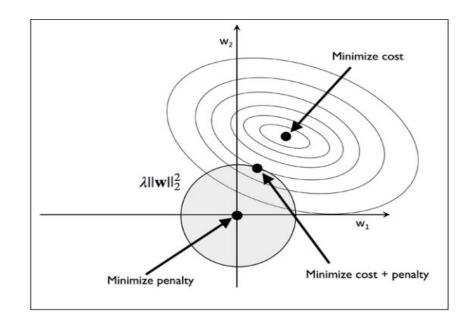
$$\min_{\boldsymbol{\beta}} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda(||\boldsymbol{\beta}||_2^2 - C)$$

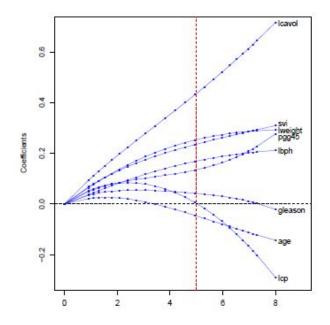
Lagrange Multiplier Theorem

$$(\widehat{\boldsymbol{\beta}}^{\lambda,2} =) \widehat{\boldsymbol{\beta}}_{Ridge} = \underset{\boldsymbol{\beta}}{argmin} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^{T} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda ||\boldsymbol{\beta}||_{2}^{2}$$

$$\Leftrightarrow \underset{\boldsymbol{\beta}}{argmin} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^{T} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda (||\boldsymbol{\beta}||_{2}^{2} - C)$$

```
# Logistic regression from sklearn.linear_model import LogisticRegression Logit = LogisticRegression(C=1e2, random_state=1023) # C = 1/\lambda. 口譽트: L2, One-versus-Rest. Logit.fit(X_train_std, y_train)
```





Bias-Variance Trade off

Expected Prediction Error

$$E[(Y_0 - \hat{Y}_0)^2] = \sigma^2 + E[(\mu_0 - \hat{Y}_0)^2]$$

Irreducible error

model error

where
$$Y_0 = \mu_0 + \epsilon_0 = \mathbf{X}_0^T \mathbf{\beta} + \epsilon_0$$

and
$$\widehat{Y}_0 = \mathbf{X}_0^T \widehat{\boldsymbol{\beta}}$$

Bias-Variance Trade off

Model Error

$$E[(\mu_0 - \hat{Y}_0)^2] = E[(\mu_0 - E[\hat{Y}_0] + E[\hat{Y}_0] - \hat{Y}_0)^2]$$

$$= (\mu_0 - E[\hat{Y}_0])^2 + Var[\hat{Y}_0]$$
Bias² variance

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



Ridge Regression solves

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

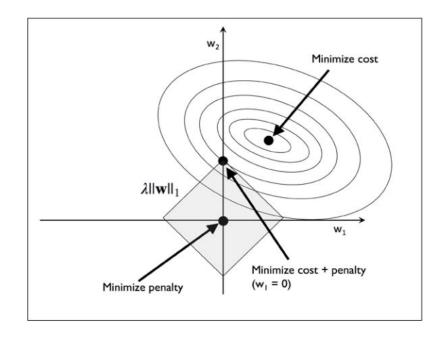
LASSO Regression solves

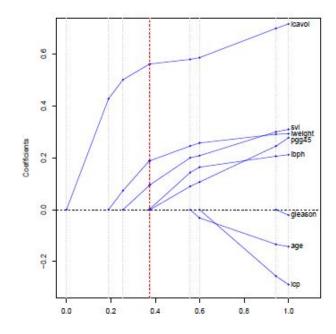
$$\min_{\mathbf{\beta}} (\mathbf{Y} - \mathbf{X}\mathbf{\beta})^{T} (\mathbf{Y} - \mathbf{X}\mathbf{\beta}) + \lambda ||\mathbf{\beta}||_{1} \qquad (L1 \ penalty)$$

LASSO (Least Absolute Shrinkage and Selection Operator)

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

where
$$||\boldsymbol{\beta}||_1 = \sum_{j=1}^p |\beta_j|$$





- For simplicity, let $y_i = \beta x_i + \epsilon_i$, where $\sum_i^n x_i = 0$ and $\sum_i^n x_i^2 = n$
- Least Square estimator is

$$\hat{\beta}_{OLS} = \frac{1}{n} \sum x_i y_i$$

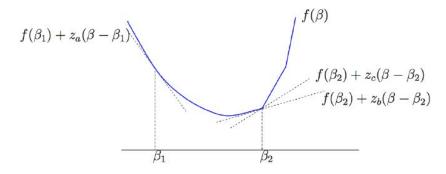
Ridge estimator is

$$\hat{\beta}_{Ridge} = \frac{\hat{\beta}_{OLS}}{1+\lambda}$$

Definition (Subgradient)

For a convex function $f: \mathbb{R}^p \to \mathbb{R}$, a vector $\mathbf{z} \in \mathbb{R}^p$ is to be a *subgradient* of f at $\boldsymbol{\beta}$ if

$$f(\boldsymbol{\beta}') \ge f(\boldsymbol{\beta}) + \mathbf{z}^T(\boldsymbol{\beta}' - \boldsymbol{\beta})$$
 for all $\boldsymbol{\beta}' \in \mathbb{R}^p$.



For LASSO, the objective function is

$$f(\beta) = \frac{1}{n} \sum (y_i - \beta x_i)^2 + \lambda |\beta|$$

and its subdifferential is

$$\partial f(\beta) = \begin{cases} \beta - \hat{\beta}_{OLS} + \lambda & \text{if } \beta > 0 \\ \beta - \hat{\beta}_{OLS} + \lambda[-1,1] & \text{if } \beta = 0 \\ \beta - \hat{\beta}_{OLS} - \lambda & \text{if } \beta < 0 \end{cases}$$

LASSO estimator is

$$\hat{\beta}_{LASSO} = \begin{cases} \hat{\beta}_{OLS} - \lambda & \text{if } \hat{\beta}_{OLS} > \lambda \\ 0 & \text{if } |\hat{\beta}_{OLS}| \le \lambda \\ \hat{\beta}_{OLS} + \lambda & \text{if } \hat{\beta}_{OLS} < -\lambda \end{cases}$$

LASSO estimator is

$$\hat{\beta}_{LASSO} = \begin{cases} \hat{\beta}_{OLS} - \lambda & \text{if } \hat{\beta}_{OLS} > \lambda \\ 0 & \text{if } |\hat{\beta}_{OLS}| \le \lambda \\ \hat{\beta}_{OLS} + \lambda & \text{if } \hat{\beta}_{OLS} < -\lambda \end{cases}$$

Soft-thresholding operator

$$S_{\lambda}(x) = sign(x) (|x| - \lambda)_{+}$$

One-dimensional Case

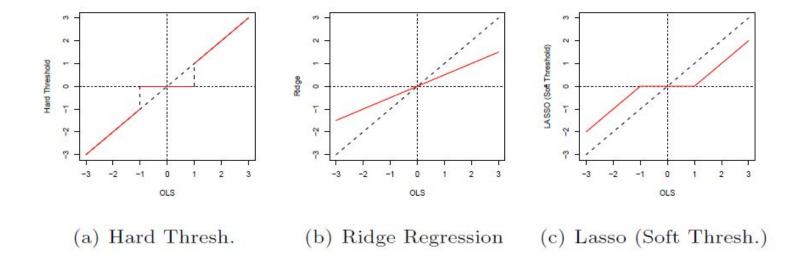
LASSO estimator is

$$\hat{\beta}_{LASSO} = S_{\lambda}(\hat{\beta}_{OLS})$$

Soft-thresholding operator

$$S_{\lambda}(x) = sign(x) (|x| - \lambda)_{+}$$

One-dimensional Case



LASSO (Least Absolute Shrinkage and Selection Operator)

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

where
$$||\boldsymbol{\beta}||_1 = \sum_{j=1}^p |\beta_j|$$

LASSO (Least Absolute Shrinkage and Selection Operator)

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

where
$$||\boldsymbol{\beta}||_1 = \sum_{j=1}^p |\beta_j|$$

LASSO (Least Absolute Shrinkage and Selection Operator)

LASSO estimator gives a sparse solution

⇒ Thus, features are selected automatically!

- Feature Selection
 - Subset selection, Stepwise method, LASSO, Least Angle Regression etc...
- Feature Extraction (Dimension Reduction)
 - Principal Component Analysis, Partial Least Square, Discriminant Analysis, Factor Analysis, Latent Class Analysis, etc..

Elastic Net solves

$$\min_{\boldsymbol{\beta}} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda \left[\alpha ||\boldsymbol{\beta}||_1 + \frac{1}{2} (1 - \alpha) ||\boldsymbol{\beta}||_2^2 \right]$$

⇒ middle ground of LASSO and Ridge penalty

L_p penalty

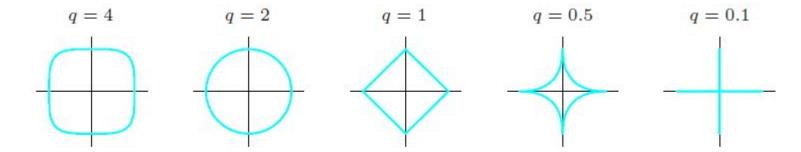


FIGURE 3.12. Contours of constant value of $\sum_{j} |\beta_{j}|^{q}$ for given values of q.

Elastic Net

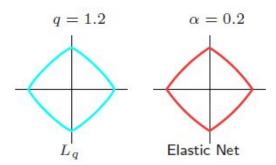


FIGURE 3.13. Contours of constant value of $\sum_{j} |\beta_{j}|^{q}$ for q = 1.2 (left plot), and the elastic-net penalty $\sum_{j} (\alpha \beta_{j}^{2} + (1-\alpha)|\beta_{j}|)$ for $\alpha = 0.2$ (right plot). Although visually very similar, the elastic-net has sharp (non-differentiable) corners, while the q = 1.2 penalty does not.

Elastic Net

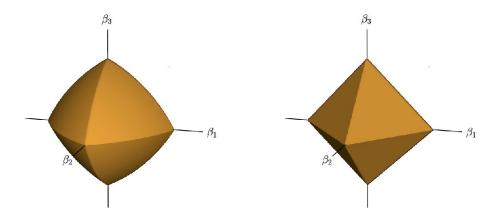


Figure 4.2 The elastic-net ball with $\alpha = 0.7$ (left panel) in \mathbb{R}^3 , compared to the ℓ_1 ball (right panel). The curved contours encourage strongly correlated variables to share coefficients (see Exercise 4.2 for details).

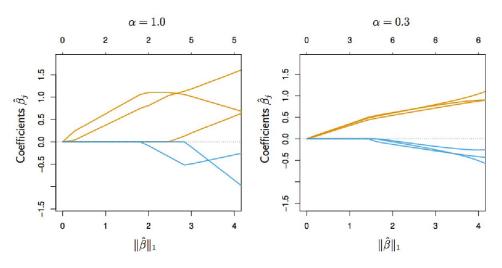
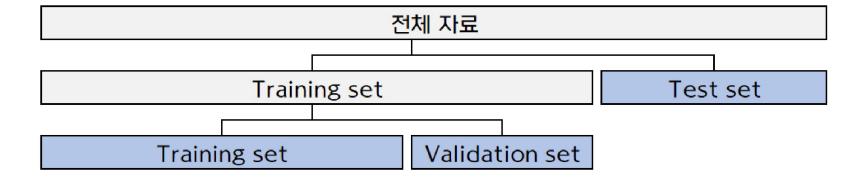


Figure 4.1 Six variables, highly correlated in groups of three. The lasso estimates $(\alpha=1)$, as shown in the left panel, exhibit somewhat erratic behavior as the regularization parameter λ is varied. In the right panel, the elastic net with $(\alpha=0.3)$ includes all the variables, and the correlated groups are pulled together.

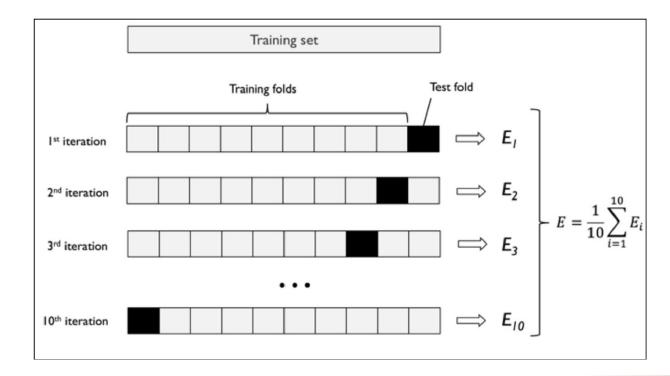
library(glmnet)

```
fit = glmnet(x, y, alpha = 0.2, weights = c(rep(1,50), rep(2,50)), nlambda = 20)
```

Cross Validation



K-fold Cross Validation



K-fold Cross Validation



K-fold Cross Validation

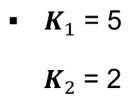
CV accuracy: 0.965 +/- 0.022

```
[ ] ### K-fold cross-validation using pipeline ###
    from sklearn.model_selection import cross_val_score
    scores = cross_val_score(estimator=pipe_Ir, X=X_train, y=y_train, cv=10) # Accuracy scores
    print('CV accuracy scores: %s' % scores)

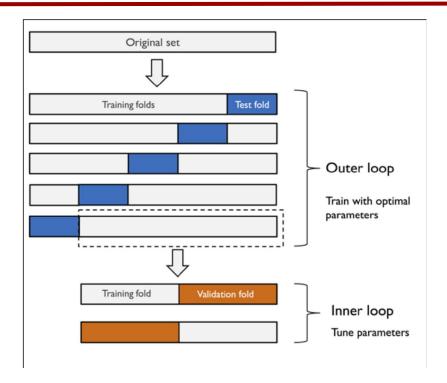
import numpy as np
    print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores), np.std(scores)))

CY accuracy scores: [0.97826087 0.95652174 0.95652174 0.95652174 0.91304348 0.95555556
    0.97777778 0.97777778 1. 0.97777778]
```

Nested Cross Validation



$$K_2 = 2$$



Grid Search CV

```
# Decision tree
from sklearn.tree import DecisionTreeClassifier
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import KFold
inner_cv=KFold(n splits=3, shuffle=True, random state=0)
outer cv=KFold(n splits=5, shuffle=True, random state=0)
gs = GridSearchCV(estimator=DecisionTreeClassifier(random state=0),
                  param_grid=[{'max_depth': [1, 2, 3, 4, 5, 6, 7, None]}],
                  scoring='accuracy', cv=inner_cv)
scores = cross_val_score(gs, X, y, scoring='accuracy', cv=outer_cv)
print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores), np.std(scores)))
```

CY accuracy: 0.942 +/- 0.012



Grid Search CV

cv.glmnet {glmnet} R Documentation

Cross-validation for glmnet

Description

Does k-fold cross-validation for glmnet, produces a plot, and returns a value for lambda (and gamma if relax=TRUE)

Usage

```
cv.glmnet(x, y, weights = NULL, offset = NULL, lambda = NULL,
  type.measure = c("default", "mse", "deviance", "class", "auc", "mae",
  "C"), nfolds = 10, foldid = NULL, alignment = c("lambda",
  "fraction"), grouped = TRUE, keep = FALSE, parallel = FALSE,
  gamma = c(0, 0.25, 0.5, 0.75, 1), relax = FALSE, trace.it = 0, ...)
```



reference

자료

19-2 STAT424 통계적 머신러닝 - 박유성 교수님

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- R. Tibshirani, , T. Hastie, M. Wainwright