Introduction to Machine Learning CS182

Lu Sun

School of Information Science and Technology

ShanghaiTech University

October 15, 2023

Today:

- Linear Methods for Regression I
    - Linear regression models
    - The Gauss-Markov theorem
    - Subsets selection

Readings:

- The Elements of Statistical Learning (ESL), Chapters 3
- Pattern Recognition and Machine Learning (PRML), Chapter 3

Introduction

- A linear regression model assumes that,

$$f(x) = \mathrm{E}(Y|X = x)$$

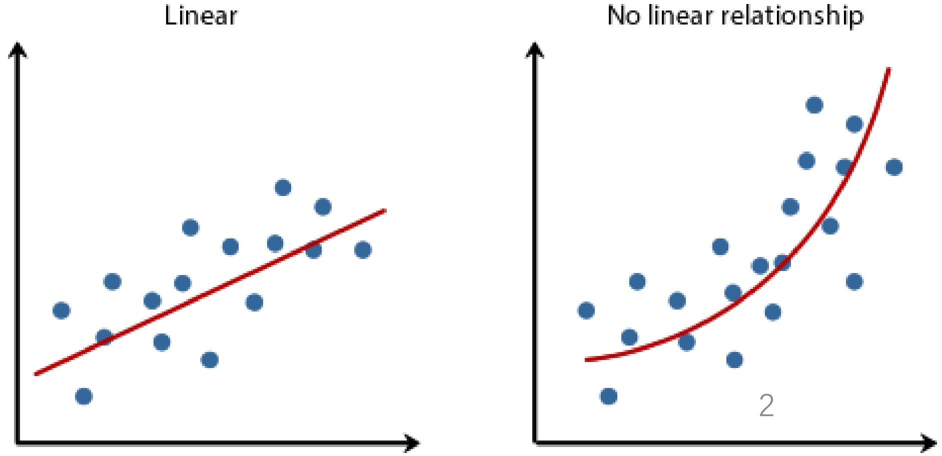
Regression function

$\min_f \mathrm{EPE}(f)$

  - linear in the inputs $X_1, X_2, \dots, X_p$.

- $p = 1$ → simple linear regression
- $p > 1$ → multiple linear regression

- Suitable for the situations:
  - small number of training samples
  - low signal-to-noise ratio
  - sparse data
- Generalize to many nonlinear techniques.



Linear Methods for Regression

--- Linear Regression Models

Simple Linear Regression

- Training set: $(x_1, y_1), \dots, (x_N, y_N)$
  - x_i: value of predictor X (covariate, independent variable, feature,…)
  - y_i: value of response Y (dependent variable, label,…)
- We denote the regression function by

$$f(x) = \mathrm{E}(Y|X = x)$$

  - conditional expectation of Y given x
- The linear regression model assumes a specific linear form

$$f(x) = \beta_0 + \beta x$$

  - usually thought of as an approximation to the truth

Simple Linear Regression

- Fitting the model by least squares

the values of β_0, β for which RSS(β_0, β) attains it's minimum.

$$\hat{\beta}_0, \hat{\beta} = \boxed{\text{argmin}_{\beta_0,\beta}} \sum_{i=1}^{N} (y_i - \beta_0 - \beta x_i)^2$$

- Solutions are

$$\hat{\beta} = \frac{\sum_{i=1}^{N} (x_i - \bar{x})(y_i - \boxed{\bar{y}})}{\sum_{i=1}^{N} (x_i - \boxed{\bar{x}})^2}$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}\bar{x}$$

sample mean:

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

$$\bar{y} = \frac{1}{N} \sum_{i=1}^{N} y_i$$

Q: How to get the solutions?

- $\hat{y}_i = \hat{\beta}_0 + \hat{\beta} x_i$ are called the *fitted* or *predicted* values
- $r_i = y_i - \hat{y}_i = y_i - \hat{\beta}_0 - \hat{\beta} x_i$ are called the *residuals*

Multiple Linear Regression

- Given $X = (X_1, X_2, \ldots, X_p)^T$
- $\mathrm{E}(Y|X)$ is (approximately) linear:

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j$$

- Sources of the variable X_j
  - quantitative inputs
  - transformation
  - basis expansions
  - dummy coding
  - interaction
- Linear in the parameters β

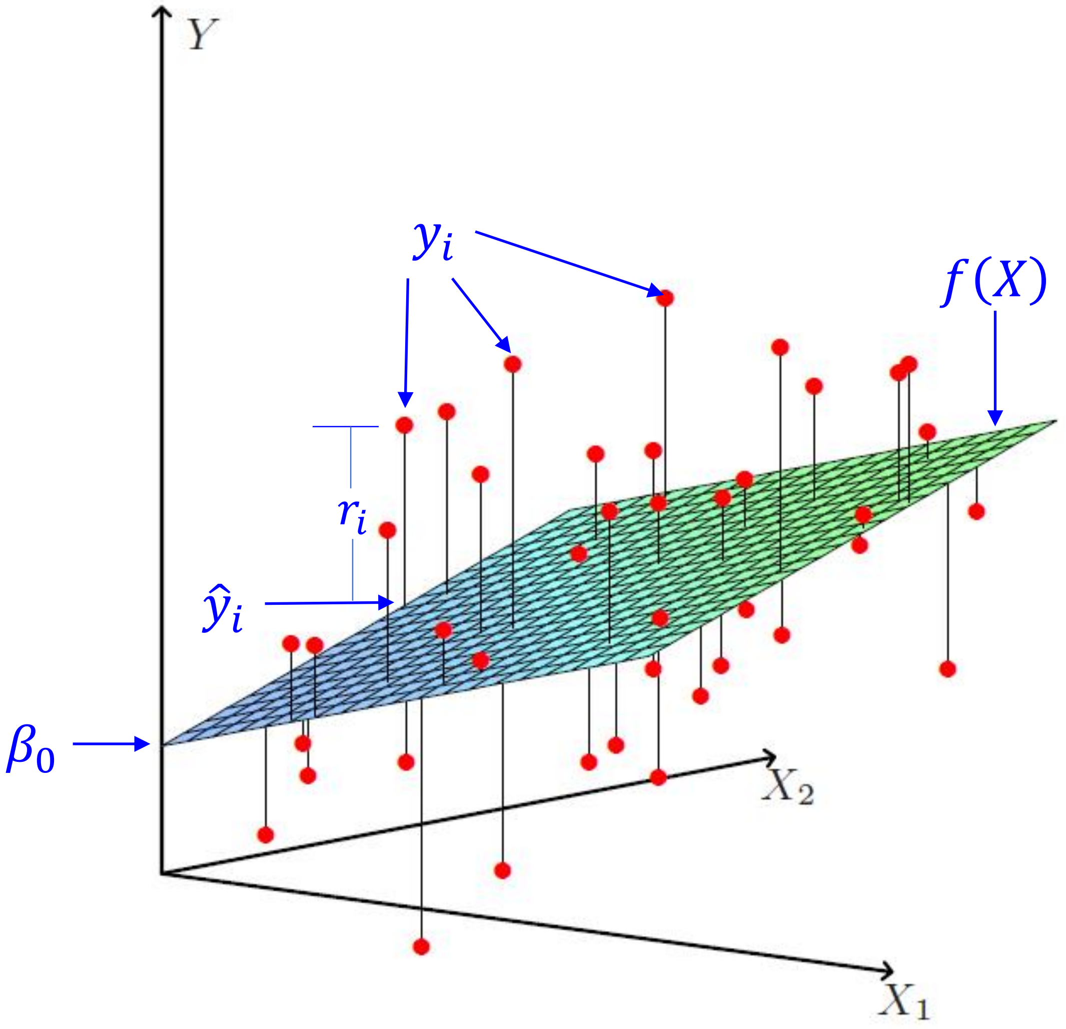
- Training data $(x_1, y_1), \ldots, (x_N, y_N)$
- *Least squares:*

$$\mathrm{RSS}(\beta) = \sum_{i=1}^{N} (y_i - f(x_i))^2$$

$$= \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j)^2$$

- It is reasonable once
  - Observations (x_i, y_i) are randomly sampled from their population
  - Output y_i is conditionally independent w.r.t. the inputs x_i
- No guarantee on the validity of model

Multiple Linear Regression



- Training data $(x_1, y_1), \ldots, (x_N, y_N)$
- *Least squares*:

$$\mathrm{RSS}(\beta) = \sum_{i=1}^{N} (y_i - f(x_i))^2$$

$$= \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\,\beta_j)^2$$

- It is reasonable once
  - Observations (x_i, y_i) are randomly sampled from their population
  - Output y_i is conditionally independent w.r.t. the inputs x_i
- No guarantee on the validity of model

Multiple Linear Regression

- Minimization of $\text{RSS}(\beta)$
- Rewrite it by the vector form:

$$\text{RSS}(\beta) = (\mathbf{y} - \mathbf{X}\beta)^T \boxed{(\mathbf{y} - \mathbf{X}\beta)}$$

- Differentiating w.r.t. β

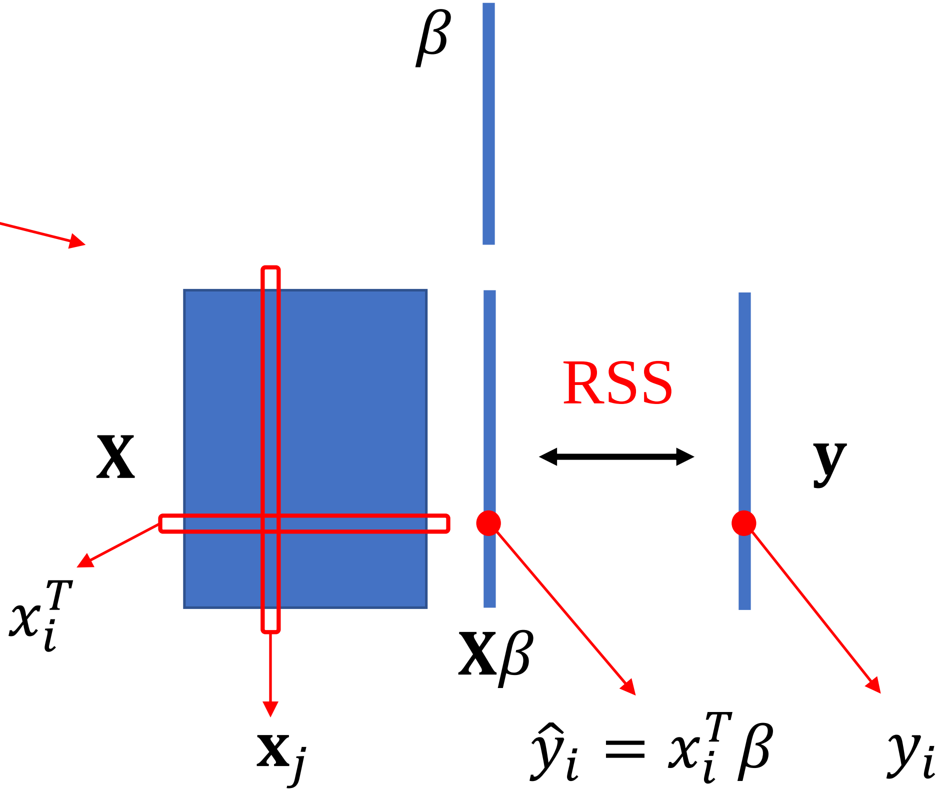
$$\frac{\partial \text{RSS}}{\partial \beta} = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta)$$

- Set the first derivative to zero

$$\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta) = 0$$

- If $\mathbf{X}$ has full column rank,

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



Multiple Linear Regression

- Minimization of RSS(β)
- Rewrite it by the vector form:

$$\mathrm{RSS}(\beta) = (\mathbf{y} - \mathbf{X}\beta)^T(\mathbf{y} - \mathbf{X}\beta)$$

- Differentiating w.r.t. β

$$\frac{\partial \mathrm{RSS}}{\partial \beta} = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta)$$

- Set the first derivative to zero

$$\boxed{\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta) = 0}$$

- If $\mathbf{X}$ has full column rank,

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

- Prediction on a test sample x_0

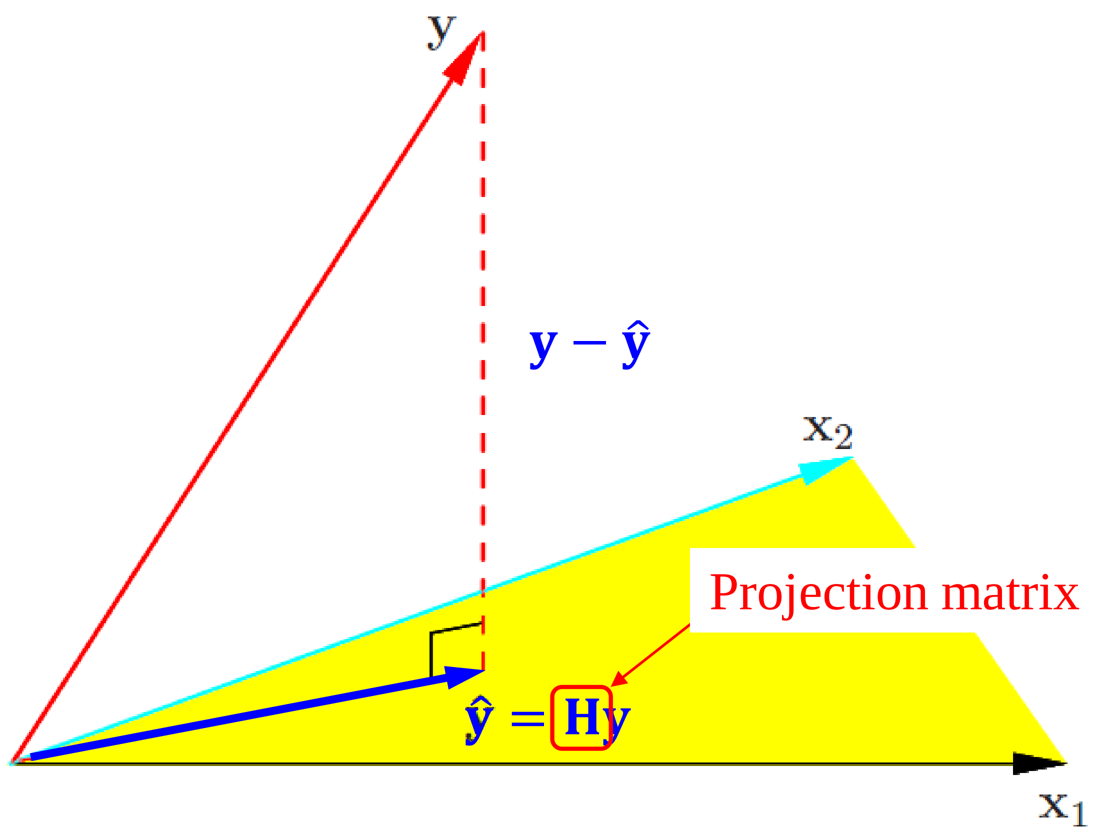
$$\hat{f}(x_0) = (1{:}\, x_0)^T\hat{\beta}$$

- The fitted values at the training inputs

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{H}\mathbf{y}$$

- The “hat” matrix **H**
  - like a hat put on **y**
- Geometrical interpretation
  - The optimal $\hat{\beta}$ makes the residual vector $\mathbf{y} - \hat{\mathbf{y}}$ orthogonal to the subspace spanned by the columns of **X**

Multiple Linear Regression



y
$\mathbf{y}-\hat{\mathbf{y}}$
x_2
Projection matrix
$\hat{\mathbf{y}}=\boxed{\mathbf{H}}\mathbf{y}$
x_1

$\mathbf{X}=(\mathbf{x_1},\dots,\mathbf{x_p})$, where $\mathbf{x}_j=\left(x_{1j},\dots,x_{Nj}\right)^T\in\mathbb{R}^N$

- Prediction on a test sample x_0

$$\hat{f}(x_0)=(1\colon x_0)^T\hat{\beta}$$

- The fitted values at the training inputs

$$\hat{\mathbf{y}}=\mathbf{X}\hat{\beta}=\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}=\mathbf{H}\mathbf{y}$$

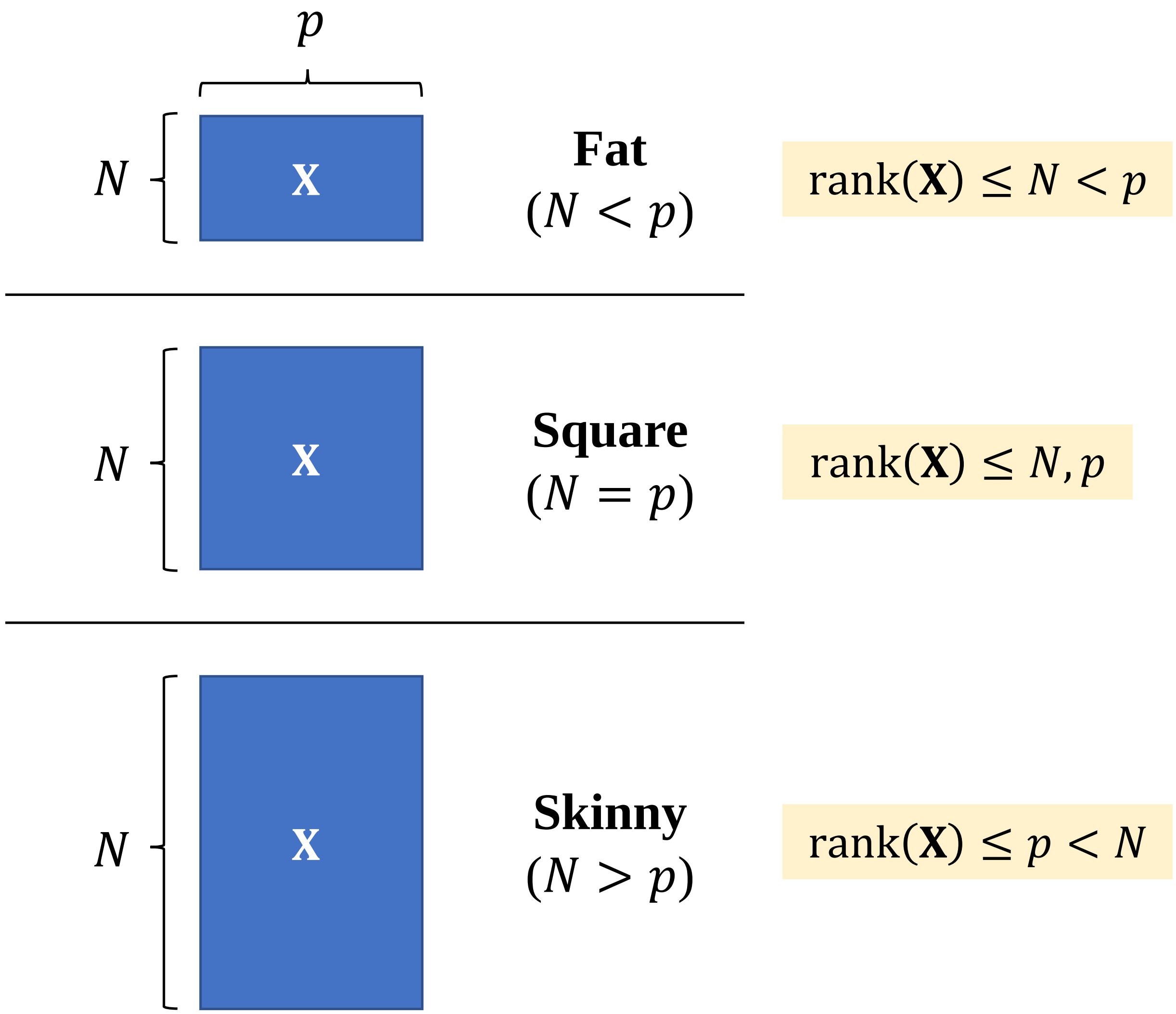
- The "hat" matrix **H**
  - like a hat put on **y**
- Geometrical interpretation
  - The optimal $\hat{\beta}$ makes the residual vector $\mathbf{y}-\hat{\mathbf{y}}$ orthogonal to the subspace spanned by the columns of **X**

Multiple Linear Regression

On the singularity of $\mathbf{X}^T\mathbf{X}$

- *Fat* data matrix $\mathbf{X}$
  - singular
- *Square* data matrix $\mathbf{X}$
  - probably singular
  - nonsingular if $\text{rank}(\mathbf{X}) = p$
- *Skinny* data matrix $\mathbf{X}$
  - probably nonsingular
  - singular if $\text{rank}(\mathbf{X}) < p$

The solution $\hat{\beta}$ is unique once $\mathbf{X}^T\mathbf{X}$ is nonsingular ($\text{rank}(\mathbf{X}) = p$)



p

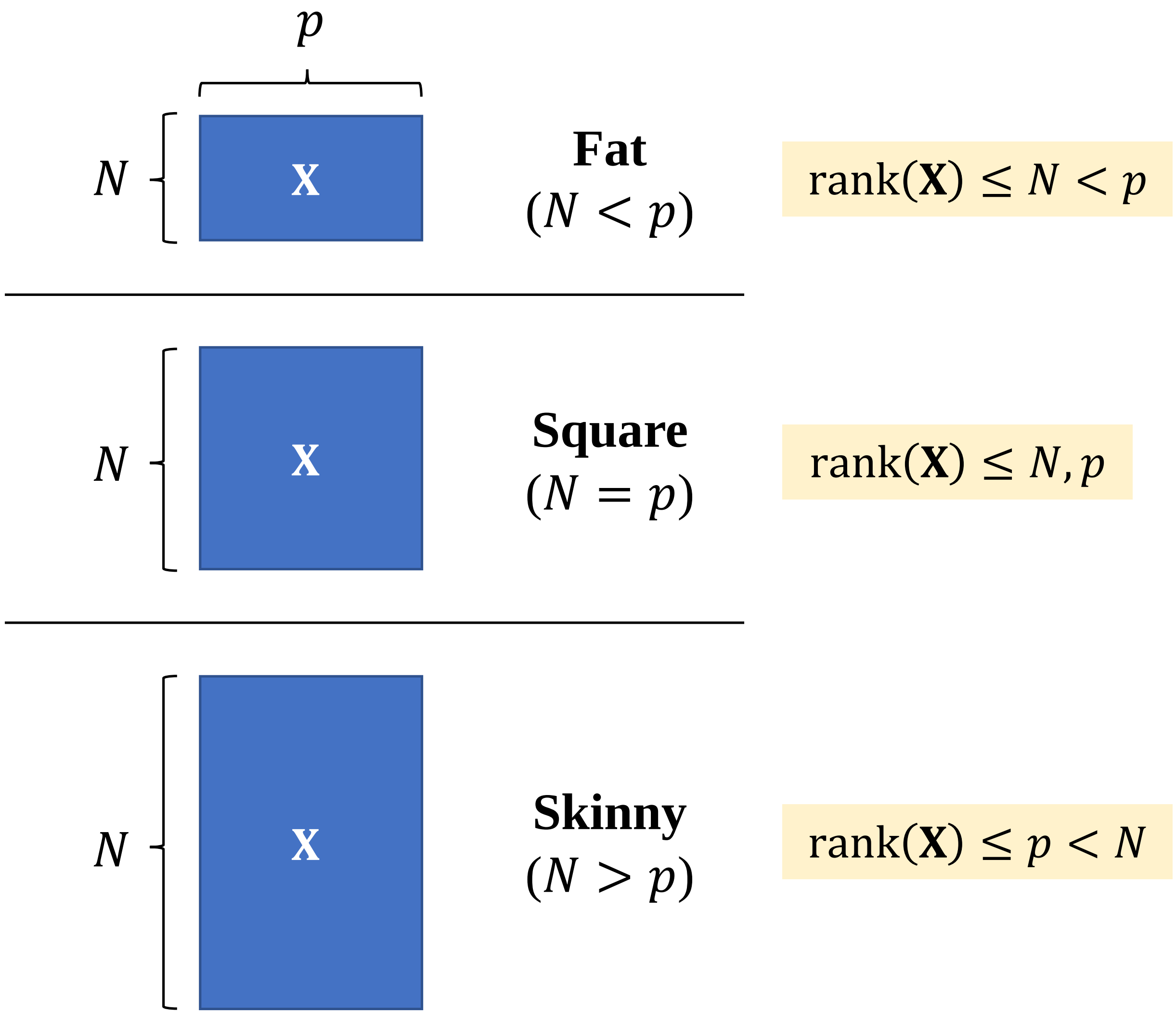
N $\mathbf{X}$ **Fat** $(N < p)$ $\text{rank}(\mathbf{X}) \leq N < p$

N $\mathbf{X}$ **Square** $(N = p)$ $\text{rank}(\mathbf{X}) \leq N, p$

N $\mathbf{X}$ **Skinny** $(N > p)$ $\text{rank}(\mathbf{X}) \leq p < N$

Multiple Linear Regression

- Rank deficient **X**
  - ❑ coding qualitative inputs
    - ➢ redundancy in columns of X
  - ❑ image and signal analysis
    - ➢ more features $(p > N)$
- Two ways to overcome it
  - ❑ feature selection (dimension reduction)
  - ❑ regularization



Fat $(N < p)$ — $\text{rank}(\mathbf{X}) \leq N < p$

Square $(N = p)$ — $\text{rank}(\mathbf{X}) \leq N, p$

Skinny $(N > p)$ — $\text{rank}(\mathbf{X}) \leq p < N$

Multiple Output Regression*

- Multiple outputs $Y_1, Y_2, \dots, Y_K$
- Assume a linear model for each output

$$Y_k = \beta_{0k} + \sum_{j=1}^{p} X_j \beta_{jk} + \varepsilon_k = f_k(X) + \varepsilon_k$$

- In matrix notation

$$\mathbf{Y} = \mathbf{X}\mathbf{B} + \mathbf{E}$$

where $\mathbf{X} \in \mathbb{R}^{N \times (p+1)}$, $\mathbf{B} \in \mathbb{R}^{(p+1) \times K}$ and $\mathbf{E} \in \mathbb{R}^{N \times K}$.

- A generalization of the univariate loss function

$$\mathrm{RSS}(\mathbf{B}) = \sum_{k=1}^{K} \sum_{i=1}^{N} \left(y_{ik} - f_k(x_i)\right)^2 = \|\mathbf{Y} - \mathbf{X}\mathbf{B}\|_F^2$$

For an arbitrary matrix $\mathbf{A}$, the Frobenius-norm is defined by $\|\mathbf{A}\|_F^2 = \mathrm{Tr}(\mathbf{A}^T\mathbf{A}) = \sum_{ij} a_{ij}^2$.

Multiple Output Regression*

- Our problem:

$$\hat{\mathbf{B}} = \mathrm{argmin}_{\mathbf{B}}\mathrm{RSS}(\mathbf{B}) = \mathrm{argmin}_{\mathbf{B}}\|\mathbf{Y}-\mathbf{X}\mathbf{B}\|_F^2$$

- A quadratic function with global minimum
- Rewrite $\mathrm{RSS}(\mathbf{B})$ as follows

Matrix trace

$\mathbb{R}^{K\times K}$

$$\begin{aligned}\mathrm{RSS}(\mathbf{B}) &= \boxed{\mathrm{Tr}}\left((\mathbf{Y}-\mathbf{X}\mathbf{B})^T(\mathbf{Y}-\mathbf{X}\mathbf{B})\right)\\ &= \mathrm{Tr}(\mathbf{Y}^T\mathbf{Y} - \boxed{\mathbf{Y}^T\mathbf{X}\mathbf{B} - \mathbf{B}^T\mathbf{X}^T\mathbf{Y}} + \mathbf{B}^T\mathbf{X}^T\mathbf{X}\mathbf{B})\\ &= \mathrm{Tr}(\mathbf{Y}^T\mathbf{Y}) - 2\mathrm{Tr}(\mathbf{B}^T\mathbf{X}^T\mathbf{Y}) + \mathrm{Tr}(\mathbf{B}^T\mathbf{X}^T\mathbf{X}\mathbf{B})\end{aligned}$$

- Differentiating w.r.t. $\mathbf{B}$

$$\frac{\partial \mathrm{RSS}(\mathbf{B})}{\partial \mathbf{B}} = -2\mathbf{X}^T\mathbf{Y} + 2\mathbf{X}^T\mathbf{X}\mathbf{B}$$

- If $\mathbf{X}^T\mathbf{X}$ is nonsingular, $\hat{\mathbf{B}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \longrightarrow \hat{\beta}_k = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}_k, \forall k$

Multiple outputs do not affect one another's least squares estimates.

Linear Methods for Regression

--- The Gauss-Markov Theorem

The Gauss-Markov Theorem

The least squares estimator has the lowest sampling variance within the class of linear unbiased estimators.

Proof: suppose $\tilde{\beta} = \mathbf{Cy}$ is a linear estimator of $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$,

where $\mathbf{C} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T + \mathbf{D}$, and $\mathbf{D} \in \mathbb{R}^{\boldsymbol{p\times N}}$ is a non-zero matrix

$$\begin{aligned}
\mathrm{E}\left[\tilde{\beta}\right] &= \mathrm{E}[Cy] \\
&= \mathrm{E}\left[\left((X'X)^{-1}X' + D\right)(X\beta + \varepsilon)\right] \\
&= \left((X'X)^{-1}X' + D\right)X\beta + \left((X'X)^{-1}X' + D\right)\boxed{\mathrm{E}[\varepsilon]} \\
&= \left((X'X)^{-1}X' + D\right)X\beta \\
&= (X'X)^{-1}X'X\beta + DX\beta \\
&= (Ip + \boxed{DX})\beta.
\end{aligned}$$

$E[\varepsilon] = 0$

If and only if $\mathbf{DX} = 0$, $\tilde{\beta}$ is unbiased.

$$\begin{aligned}
\mathrm{Var}\left(\tilde{\beta}\right) &= \mathrm{Var}(Cy) \\
&= C\,\boxed{\mathrm{Var}(y)}\,C' \\
&= \sigma^2 CC' \\
&= \sigma^2\left((X'X)^{-1}X' + D\right)\left(X(X'X)^{-1} + D'\right) \\
&= \sigma^2\left((X'X)^{-1}X'X(X'X)^{-1} + (X'X)^{-1}X'D' + DX(X'X)^{-1} + DD'\right) \\
&= \sigma^2(X'X)^{-1} + \sigma^2(X'X)^{-1}\boxed{(DX)}' + \sigma^2\boxed{DX}(X'X)^{-1} + \sigma^2DD' \\
&= \sigma^2(X'X)^{-1} + \sigma^2DD' \\
&= \boxed{\mathrm{Var}\left(\hat{\beta}\right)} + \boxed{\sigma^2DD'}
\end{aligned}$$

$\mathrm{Var}(\mathbf{y}) = E\left[\mathbf{y} - E[\mathbf{y}]\right]^2 = \mathrm{Var}(\varepsilon)$

$\mathbf{DX} = 0$

$\mathrm{Var}\left(\hat{\beta}\right) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$

Positive semidefinite

The Gauss-Markov Theorem

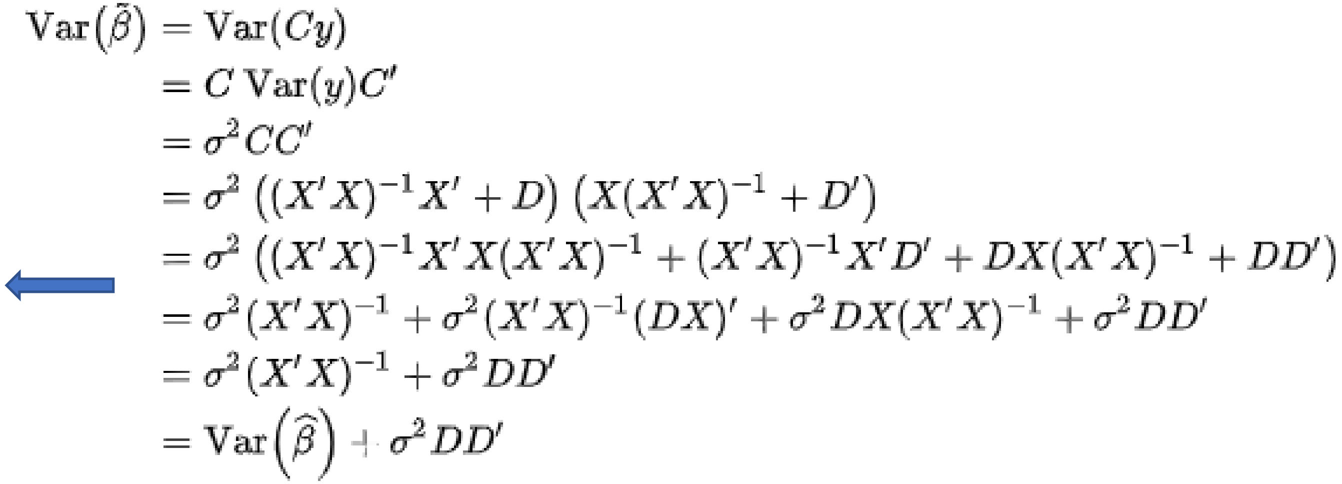
The least squares estimator has the lowest sampling variance within the class of linear unbiased estimators.

Proof: suppose $\tilde{\beta} = \mathbf{Cy}$ is a linear estimator of $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$,

where $\mathbf{C} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T + \mathbf{D}$, and $\mathbf{D} \in \mathbb{R}^{\boldsymbol{p\times N}}$ is a non-zero matrix

Given an arbitrary test point x_0, we have

$$\begin{aligned}\mathrm{Var}(\tilde{y}_0) &= \mathrm{Var}\left(x_0^T\tilde{\beta}\right)\\ &= x_0^T\mathrm{Var}\left(\tilde{\beta}\right)x_0\\ &= x_0^T\mathrm{Var}\left(\hat{\beta}\right)x_0+\sigma^2x_0^T\mathbf{DD}^{\boldsymbol{T}}x_0\\ &= \mathrm{Var}(\hat{y}_0)+\sigma^2x_0^T\mathbf{DD}^{\boldsymbol{T}}x_0\end{aligned}$$



$$\begin{aligned}\mathrm{Var}\left(\tilde{\beta}\right) &= \mathrm{Var}(Cy)\\ &= C\,\mathrm{Var}(y)C'\\ &= \sigma^2CC'\\ &= \sigma^2\left((X'X)^{-1}X'+D\right)\left(X(X'X)^{-1}+D'\right)\\ &= \sigma^2\left((X'X)^{-1}X'X(X'X)^{-1}+(X'X)^{-1}X'D'+DX(X'X)^{-1}+DD'\right)\\ &= \sigma^2(X'X)^{-1}+\sigma^2(X'X)^{-1}(DX)'+\sigma^2DX(X'X)^{-1}+\sigma^2DD'\\ &= \sigma^2(X'X)^{-1}+\sigma^2DD'\\ &= \mathrm{Var}\left(\widehat{\beta}\right)+\sigma^2DD'\end{aligned}$$

The Gauss-Markov Theorem

The least squares estimator has the lowest sampling variance within the class of linear unbiased estimators.

Remarks

- Among the unbiased linear methods, least squares has the lowest MSE
  - MSE = Var + Bias^2
- A biased methods probably has lower MSE
  - Var-Bias trade-off
  - A small increase in Bias might gives rise to a large reduction in Var ← Model selection

Linear Methods for Regression

--- Subset Selection

Introduction

Two limitations of least squares

- prediction accuracy
  - ❑ low bias and high variance

    → sacrifice a little bias to reduce the variance
- interpretation
  - ❑ hard to interpret a large number of input features

    → find a subset of features exhibiting strong effects

We use model selection to overcome the limitations

- variable subset selection, shrinkage, dimension reduction.
- not restricted to linear models

Subset Selection

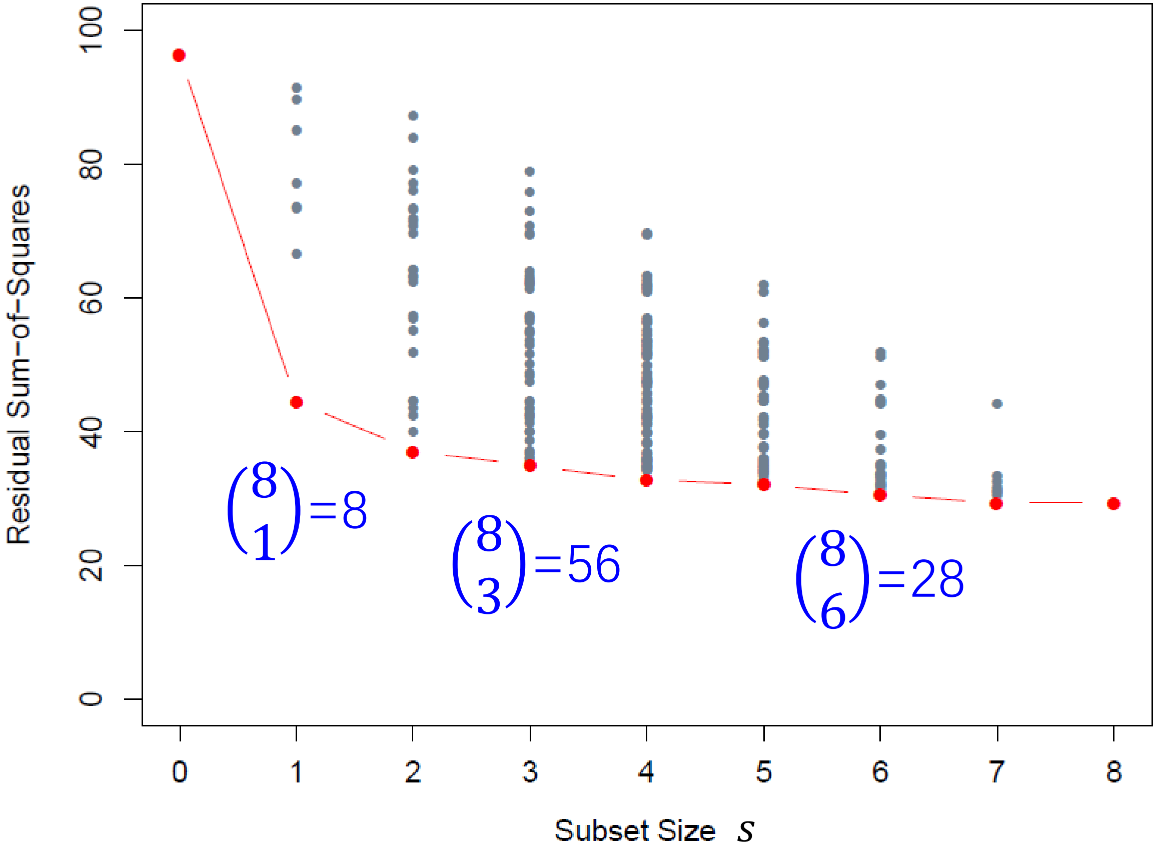
- Best-subset selection
  - For each $s \in \{0,1,\ldots,p\}$, find the subset in size of s that gives lowest $\mathrm{RSS}(\beta) = \|\mathbf{y} - \mathbf{X}^{(s)}\beta\|_2^2$

$$\binom{4}{2} = 6$$

$p = 4$ $s = 2$	X_1	X_2	X_3	X_4	$\mathbf{X}^{(s)}$
Model 1	√	√	×	×	$(\mathbf{x}_1, \mathbf{x}_2)$
Model 2	√	×	√	×	$(\mathbf{x}_1, \mathbf{x}_3)$
Model 3	√	×	×	√	$(\mathbf{x}_1, \mathbf{x}_4)$
Model 4	×	√	√	×	$(\mathbf{x}_2, \mathbf{x}_3)$
Model 5	×	√	×	√	$(\mathbf{x}_2, \mathbf{x}_4)$
Model 6	×	×	√	√	$(\mathbf{x}_3, \mathbf{x}_4)$

Subset Selection

- Best-subset selection
  - For each $s \in \{0,1,\ldots,p\}$, find the subset in size of s that gives lowest $\mathrm{RSS}(\beta) = \left\|\mathbf{y} - \mathbf{X}^{(s)}\beta\right\|_2^2$
- Example
  - prostate cancer example ($p = 8$)
  - the red lower bound denotes the models eligible for selection
  - the red lower bound keeps decreasing ($s = 8$?)
  - *cross-validation* to estimate prediction error and select s
- Typically intractable for $p > 40$



All the subset models for the prostate cancer example.

Forward- and Backward-Stepwise Selection

- Forward-stepwise
  - starts with intercept
  - sequentially adds the best predictor
- Greedy algorithm
  - sub-optimal
- Advantages
  - Computational
    - even $p \gg N$
  - Statistical
    - constrained search
    - lower variance, more bias

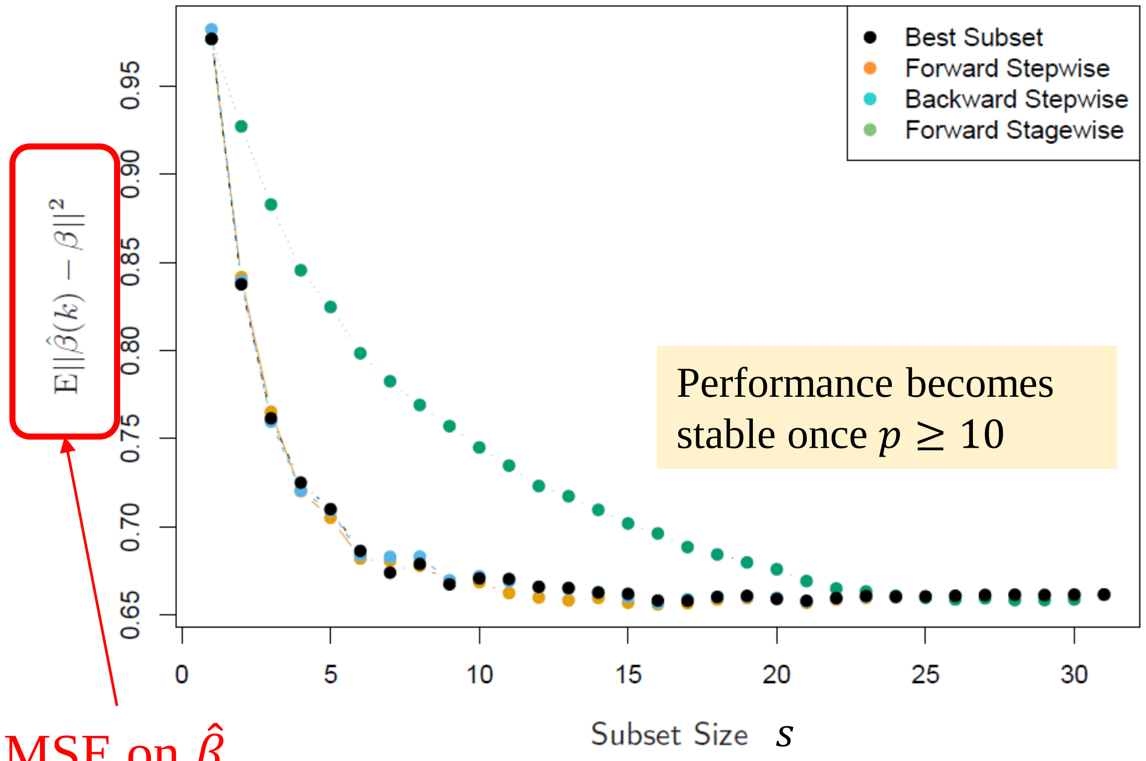
Forward- and Backward-Stepwise Selection

- Forward-stepwise
  - ❑ starts with intercept
  - ❑ sequentially adds the best predictor
- Greedy algorithm
  - ❑ sub-optimal
- Advantages
  - ❑ Computational
    - even $p \gg N$
  - ❑ Statistical
    - constrained search
    - lower variance, more bias

- Backward-stepwise
  - ❑ starts with the full model
  - ❑ sequentially deletes the worst predictor
- Greedy algorithm
- Only useful when $N > p$
  - ❑ linear regression

- Smart stepwise
  - ❑ group of variables
  - ❑ add or drop whole groups at a time

Forward- and Backward-Stepwise Selection



Performance becomes stable once $p \geq 10$

MSE on $\hat{\beta}$

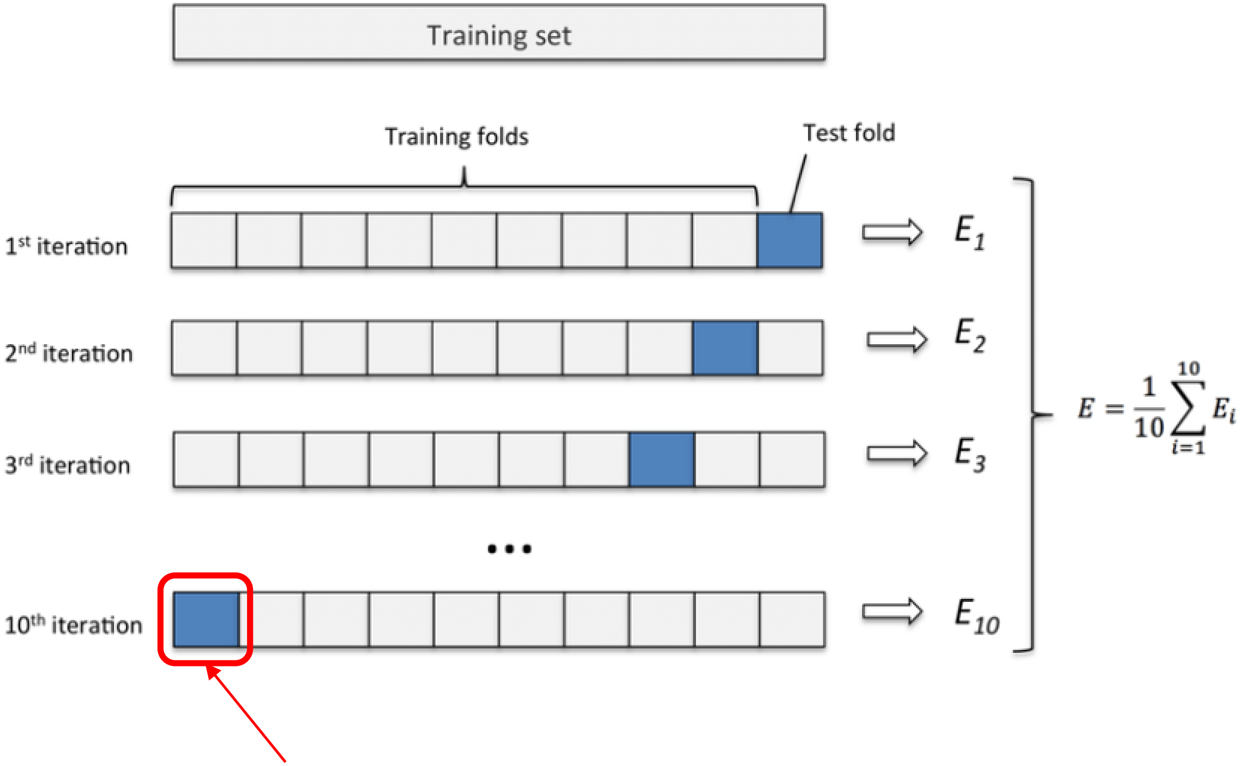
- Example
  - $Y = X^T\beta + \varepsilon$
  - $N = 300, p = 31$
  - only 10 variables are effective
  - similar performance

K-Fold Cross-Validation

- Each has a complexity parameter λ
  - the subset size in subset selection
  - the neighborhood size in k-NN
  - The coefficient of regularization
- K-fold cross validation
  - divide the training data into K roughly equal parts ($K = 5$ or 10)
  - for $k = 1, \dots, K$,
    - fit the model with $K - 1$ parts
    - compute the error E_k on the rest part
  - The K-fold cross validation error

$$E(\lambda) = \frac{1}{K}\sum_{k=1}^{K} E_k(\lambda)$$

Repeat this for many values of λ, and choose the best value that makes $E(\lambda)$ lowest.



validation set