Linear Regression

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Chapter 3

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About the Course

- Course web: https://yuany-pku.github.io/2018_math4432/
- Related courses:
  - Statistical Learning: Math 5470 by Bingyi JING
  - Unsupervised learning: CSIC5011 2017, Topological and Geometric Data Reduction (http://math.stanford.edu/~yuany/course/2017.fall/)
  - Deep learning: Math 6380o (https://deeplearning-math.github.io/)

Summary of The Bias-Variance Trade-Off

Consider $y_i = f(x_i) + \epsilon_i$, $i = 1, ..., n$ where ϵ_i are mean 0 with variance σ^2. An estimate function from data $\mathcal{D}$ is denoted as $\hat{f}(x; \mathcal{D})$ or simply $\hat{f}(x)$, then the expected predicted error is

$$\begin{aligned}
\text{EPE}(x) &= E((Y - \hat{f}(x))^2 | X = x) \\
&= E((\epsilon + f(x) - \hat{f}(x))^2 | X = x) \\
&= E\{((\epsilon + f(x) - E(\hat{f}(x)) + E(\hat{f}(x)) - \hat{f}(x))^2 | X = x\} \\
&= \sigma^2 + (f(x) - E(\hat{f}_k(x)))^2 + \text{var}(\hat{f}(x)) \\
&= \underbrace{\sigma^2}_{\textbf{Irreducible}} + \underbrace{\text{Bias}^2 + \text{Variance}}_{\textbf{Reducible}}
\end{aligned}$$

- **Bias** refers to the error that is introduced by approximating a real-life problem, which may be extremely complicated, by a much simpler model.
- **Variance** refers to the amount by which $\hat{f}$ would change if we estimated it using a different training data set. Since the training data are used to fit the statistical learning method, different training data sets will result in a different $\hat{f}$. But ideally the estimate for f should not vary too much between training sets.
- **Bias and variance trade-off**: The optimal predictive ability is the one that leads to balance between bias and variance.

Bias-variance tradeoff

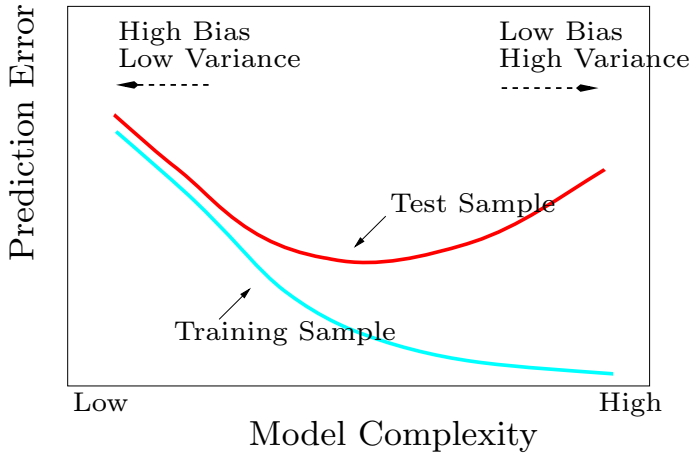

FIGURE 2.11. *Test and training error as a function of model complexity.*

General models/methods

- linear models, generalized linear models.
- K-Nearest-Neighbor (KNN)
- Kernel methods
- local polynomial regression
- regression and smoothing splines
- Tree based methods and boosting
- SVM
- projection pursuit and neural networks.

Prediction vs. Interpretability

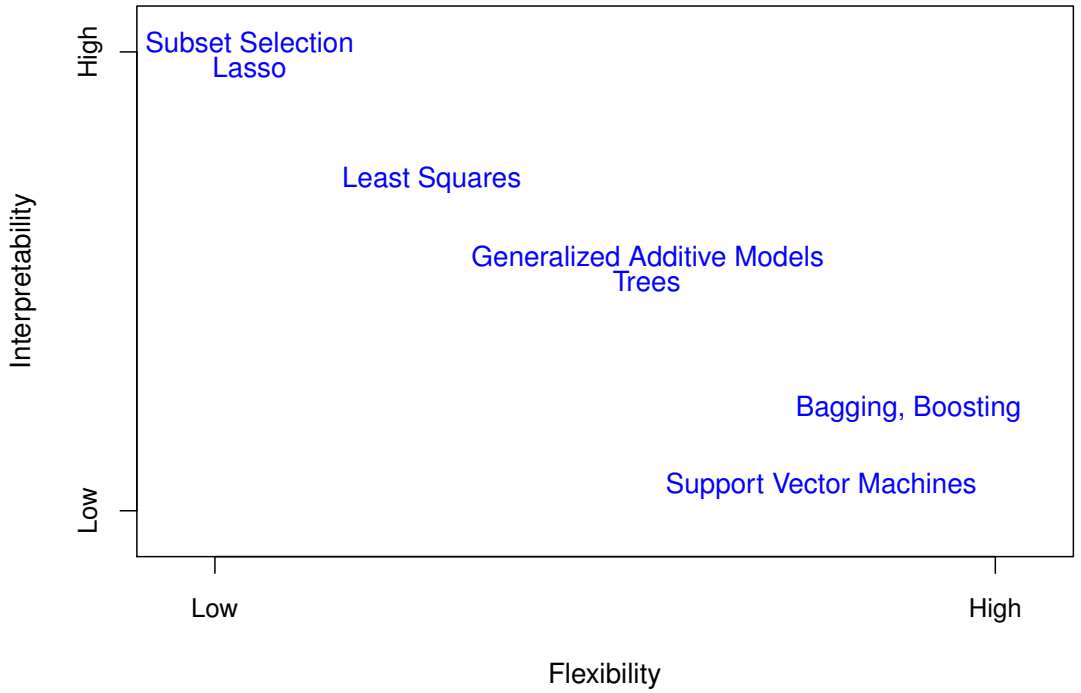

Figure: "Occam's Razor" or "Simplicity is beauty" or "Everything else the same, bring the simplest model". Vote for parsimonious models or bet on sparsity

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2. 3.2 Multiple linear regression
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About linear regression model

- Fundamental statistical models. (supervised learning)
- Covering one-sample, two-sample, multiple sample problems.
- Most illustrative on various important issues: fitting, prediciton, model checking, ...
- In-depth understanding of linear model helps learning further topics.
- This chapter is slightly more advanced than Chapter 3 of ISLR

The formulation

- Consider linear regression model:

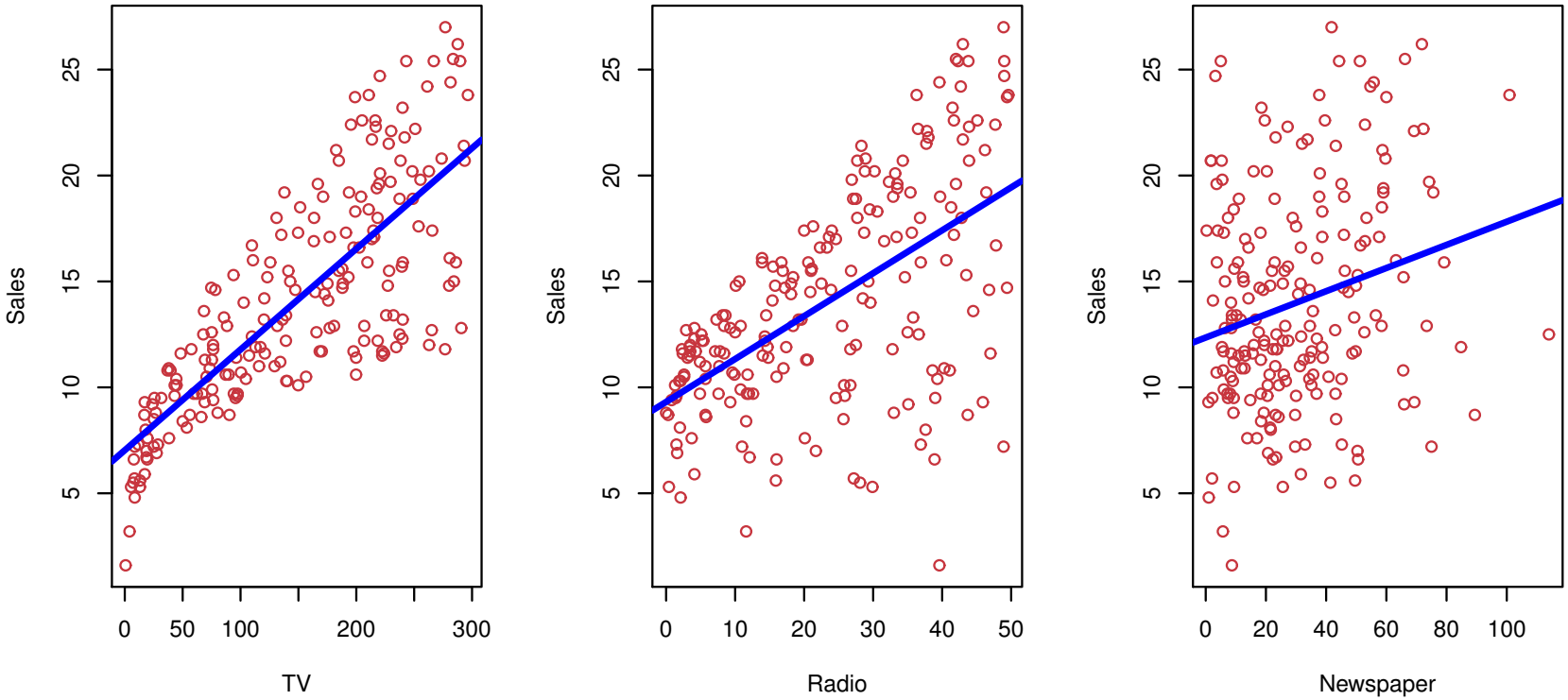
$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \qquad i = 1, ..., n$$

  where y_i, x_i are the i-th observation of the response and covariates. Here x_i is of 1-dimension.
- Responses are sometimes called dependent variables or outputs;
- covariates called independent variables or inputs or features or predictors or regressors.
- obtain the parameter estimation and making prediction of any responses on given covariates.

Example: Advertising data

The data contains 200 observations.
Sample size: $n = 200$.
Sales: y_i, $i = 1..., n$.
TV (bugdets): $x_{i1}, i = 1, ..., n$.
Radio (budgets): $x_{i2}, i = 1, ..., n$.
Newspaper (budgets): $x_{i3}, i = 1, ..., n$.

Example: Advertising data



Simple linear regression

For the time being, we only consider one covariate: TV.
The linear regression model is

$$y_i = \beta_0 + \beta_1 x_{i1} + \epsilon_i, \qquad i = 1, ..., n$$

Estimating the coefficient by the least squares

Minimizing the sum of squares of error:

$$\sum_{i=1}^{n}(y_i = \beta_0 + \beta_1 x_{i1})^2.$$

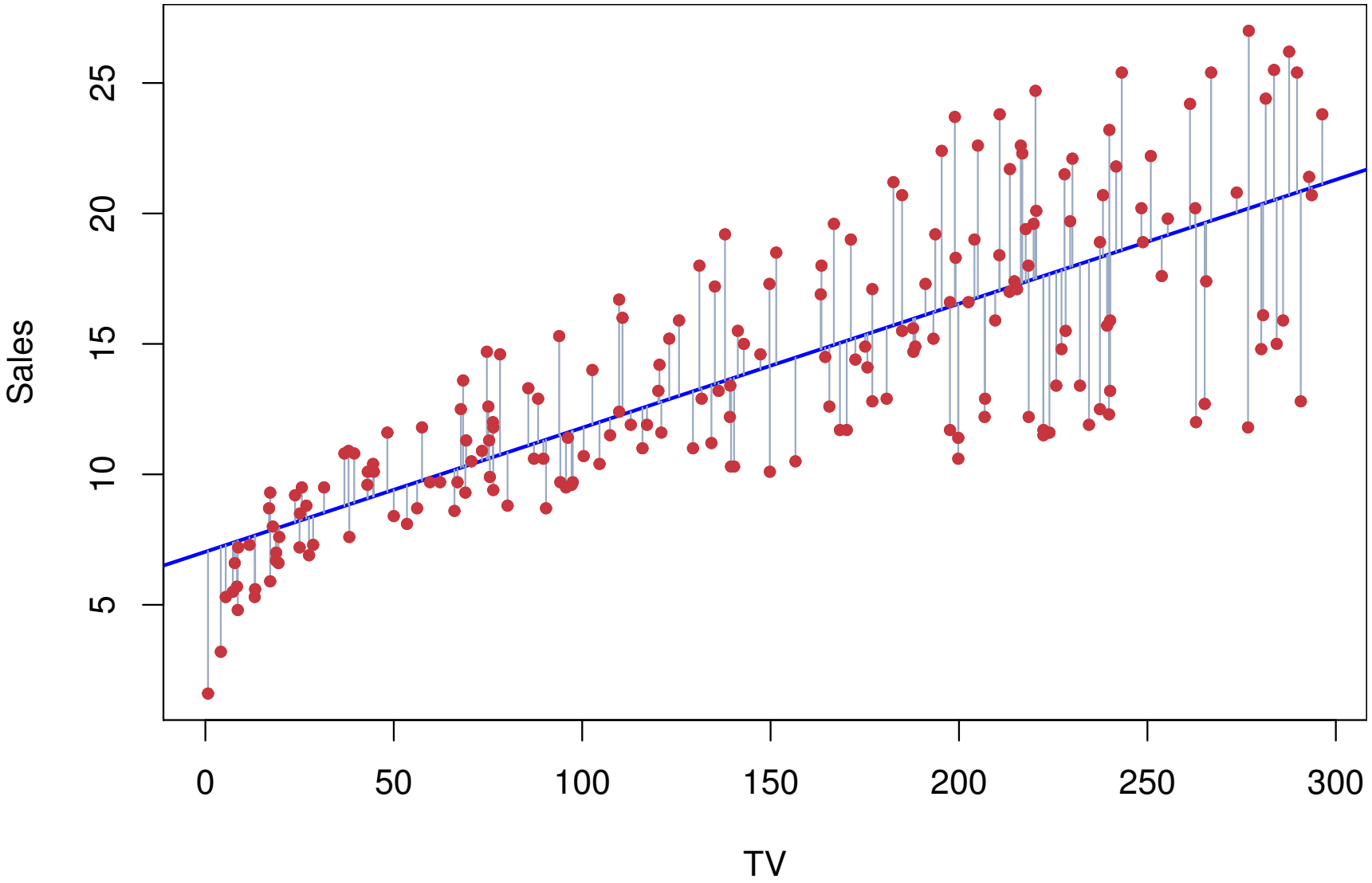
The estimator is

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

Here $x_i = x_{i1}$.

Illustrating least squares



Inference

$$\frac{\hat{\beta}_1 - \beta_1}{s\sqrt{1/\sum_{i=1}^n (x_i - \bar{x})^2}} \sim t_{n-2}$$

$$\frac{\hat{\beta}_0 - \beta_0}{s\sqrt{1/n + \bar{x}^2/\sum_{i=1}^n (x_i - \bar{x})^2}} \sim t_{n-2}$$

where

$$s^2 = \mathrm{RSS}/(n-2)$$

is an unbiased estimator of the variance of the error, and, setting $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ as the so-called fitted value,

$$\mathrm{RSS} = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

are so-called residual sum of squares.

Details would be provided in multiple linear regression.

Result of the estimation

TABLE 3.1. (from ISLR) The advertising data: coefficients of the LSE for the regression on number of units sold on TV advertising budget. An increase of $1000 in the TV advertising budget would cause an increase of sales of about 50 units.

	Coefficient	Std.error	t-statistic	p-value
Intercept	7.0325	0.4578	15.36	< 0.0001
TV	0.0475	0.0027	17.67	< 0.0001

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Linear models formulation

- Consider linear regression model:

$$y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i, \qquad i = 1, ..., n \tag{2.1}$$

  where $y_i, x_i = (x_{i1}, ..., x_{ip})$ are the i-th observation of the response and covariates.
- Responses are sometimes called dependent variables or outputs;
- covariates called independent variables or inputs or regressors.
- obtain the parameter estimation and making prediction of any responses on given covariates.

Example: Advertising data

Now, we consider three covariates: TV, radio and newspapers.
The number of covarites $p = 3$.
The linear regression model is

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \epsilon_i, \qquad i = 1, ..., n$$

Estimating the coefficient by the least squares

Minimizing the sum of squares of error:

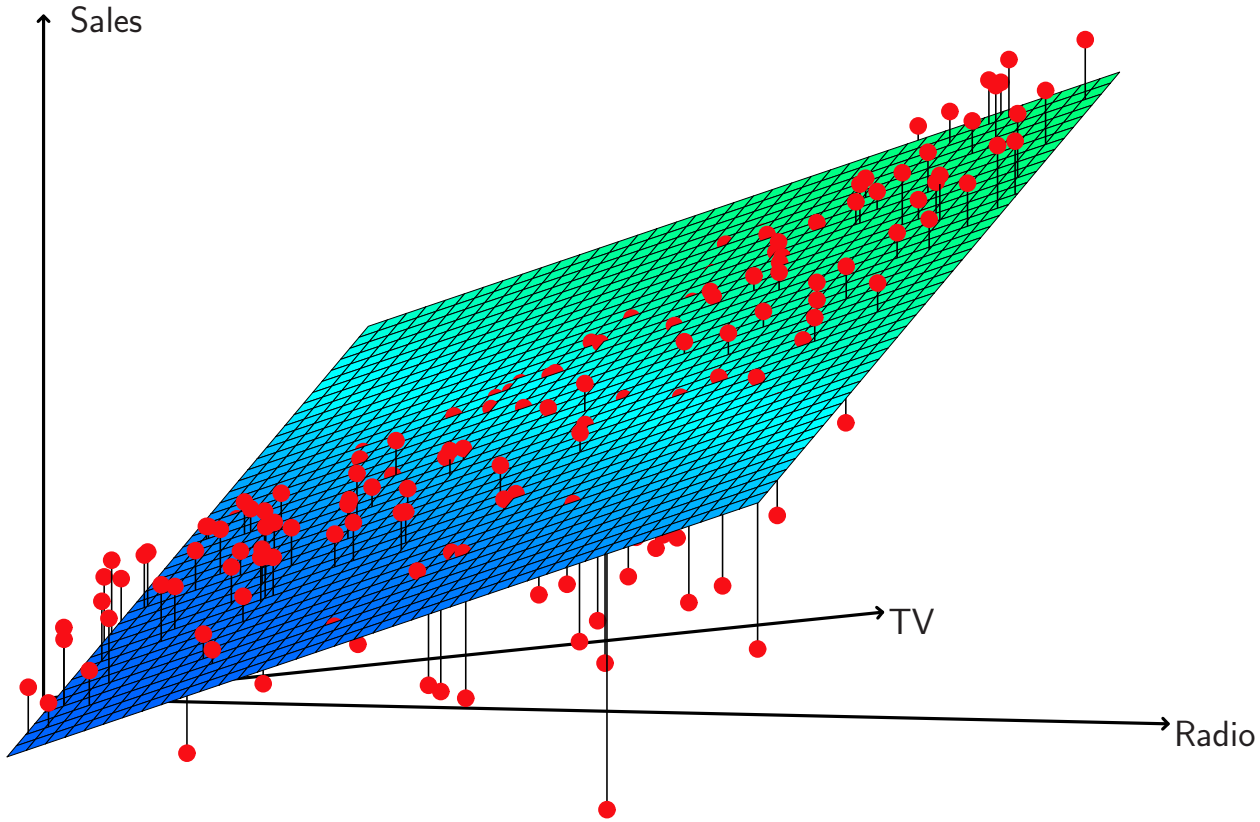
$$\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_{i1} - \beta_2 x_{i2} - \beta_3 x_{i3})^2.$$

which is

$$\sum_{i=1}^{n}(y_i - \beta^T x_i)^2$$

The expression of the LSE of β, as a vector, has a simple matrix expression, even though the estimator of the individual $\hat{\beta}_i$ is not eqaully simple.

Illustrating the least squares



Result of the estimation

TABLE 3.9. (from ISLR) The advertising data: coefficients of the LSE for the regression on number of units sold on TV, radio and newspaper advertising budgets.

	Coefficient	Std.error	t-statistic	p-value
Intercept	2.939	0.3119	9.42	< 0.0001
TV	0.046	0.0014	32.81	< 0.0001
radio	0.189	0.0086	21.89	< 0.0001
newspaper	-0.001	0.0059	-0.18	0.8599

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Notations

With slight abuse of notation, in this chapter, we use

$$\begin{aligned}\mathbf{X} &= \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{1} \vdots \mathbf{x}_1 \vdots \mathbf{x}_2 \vdots \cdots \vdots \mathbf{x}_p \end{pmatrix}.\end{aligned}$$

Here a column of ones, $\mathbf{1}$, is added, which corresponds to the intercept β_0. Then $\mathbf{X}$ is a n by $p+1$ matrix.

Recall that

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \quad \beta = \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_p \end{pmatrix}, \quad \epsilon = \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{pmatrix}, \quad \mathbf{x}_j = \begin{pmatrix} x_{1j} \\ \vdots \\ x_{nj} \end{pmatrix}$$

The least squares criterion

The least squares criterion is try to minimize the sum of squares:

$$\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_{i1} - \cdots - \beta_p x_{ip})^2.$$

Using matrix algebra, the above sum of squares is

$$\|\mathbf{y} - \mathbf{X}\beta\|^2 = (\mathbf{y} - \mathbf{X}\beta)^T(\mathbf{y} - \mathbf{X}\beta).$$

The LSE, fitted values and residuals

By some linear algebra calcuation, the least squares estimator of β is then

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

Then

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\beta}$$

is called the fitted values; viewed as the predicted values of the reponses based on the linear model.

Terminology and notation

$$\mathbf{y} - \hat{\mathbf{y}}$$

are called residuals, which is denoted as $\hat{\epsilon}$. The sum of squares of these residuals

$$\sum_{i=1}^{n} \hat{\epsilon}_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2.$$

- The zero-correlation of two variables from multivariate normal random variable implies their independence.
- Suppose $\mathbf{z} = (z_1, ..., z_n)^T$, and z_i are iid standard normal random variables.
- Let $\mathbf{z}_1 = \mathbf{A}\mathbf{z}$ and $\mathbf{z}_2 = \mathbf{B}\mathbf{z}$ with $\mathbf{A}$ and $\mathbf{B}$ are two nonrandom matrices.
- Then

$$\text{cov}(\mathbf{z}_1, \mathbf{z}_2) = \mathbf{A}\mathbf{B}^T = 0$$

  implies the independence between $\mathbf{z}_1$ and $\mathbf{z}_2$.
- We also call $\mathbf{z}_1$ and $\mathbf{z}_2$ orthogonal.

Orthogonality

- The residual $\hat{\epsilon}$ is orthogonal to all columns of $\mathbf{X}$, i.e, all $\mathbf{1}, \mathbf{x}_1, ..., \mathbf{x}_p$. This can be seen by

$$\begin{aligned} & \mathbf{X}^T \hat{\epsilon} = \mathbf{X}^T \mathbf{y} - \mathbf{X}^T \mathbf{X} \hat{\beta} \\ = \quad & \mathbf{X}^T \mathbf{y} - \mathbf{X}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = 0. \end{aligned}$$

- The residual vector $\hat{\epsilon}$ is orthogonal to the hyperplane formed by vectors $\mathbf{1}, \mathbf{x}_1, ..., \mathbf{x}_p$ in n dimensional real space.

A proof of the LSE

$$
\begin{aligned}
& \|\mathbf{y} - \mathbf{X}\mathbf{b}\|^2 \\
= \; & \|\mathbf{y} - \mathbf{X}\hat{\beta} - \mathbf{X}(\mathbf{b} - \hat{\beta})\|^2 \\
= \; & \|\mathbf{y} - \mathbf{X}\hat{\beta}\|^2 + \|\mathbf{X}(\mathbf{b} - \hat{\beta})\|^2 \qquad \text{by orthogonality} \\
\geq \; & \|\mathbf{y} - \mathbf{X}\hat{\beta}\|^2
\end{aligned}
$$

- The fitted value $\hat{\mathbf{y}} = \mathbf{X}\hat{\beta}$, which, also as a vector in n dimensional real space, is a linear combination of the vectors $\mathbf{1}, \mathbf{x}_1, ..., \mathbf{x}_p$, with the $p+1$ linear combination coefficients being the components of $\hat{\beta}$.
- The fitted values are orthogonal to the residuals, i.e., $\hat{\mathbf{y}}$ is orthogonal to $\mathbf{y} - \hat{\mathbf{y}}$ or

$$\hat{\mathbf{y}}^T(\mathbf{y} - \hat{\mathbf{y}}) = 0.$$

This implies

$$\|\mathbf{y}\|^2 = \|\hat{\mathbf{y}}\|^2 + \|\mathbf{y} - \hat{\mathbf{y}}\|^2.$$

The projection matrix

- Let $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$.
- This n by n matrix is called projection matrix or hat matrix.
- It has the property that, for any vector, $\mathbf{b}$ in n dimensional real space $\mathbf{Hb}$ projects $\mathbf{b}$ onto the linear space formed by the columns of $\mathbf{X}$.
- $\mathbf{Hb}$ is in this linear space formed by the columns of $\mathbf{X}$.
- And $\mathbf{b} - \mathbf{Hb}$ is orthogonal to this space.

The least squares projection

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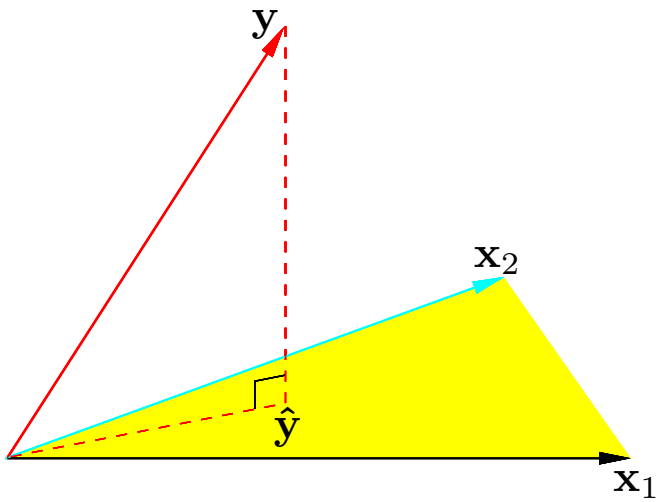

FIGURE 3.2. *The N-dimensional geometry of least squares regression with two predictors. The outcome vector $\mathbf{y}$ is orthogonally projected onto the hyperplane spanned by the input vectors $\mathbf{x}_1$ and $\mathbf{x}_2$. The projection $\hat{\mathbf{y}}$ represents the vector of the least squares predictions*

symmetric and idempotent

- projection matrix $\mathbf{H}$ is symmetric and idempotent; i.e., $\mathbf{H}^2 = \mathbf{H}$.
- eigenvalues are either 1 or 0.
- All eigenvectors associated with eigenvalue 1 form a space, say $\mathcal{L}_1$;
- Those with eigenvalue 0 form the orthogonal space, $\mathcal{L}_0$, of $\mathcal{L}_1$.
- Then $\mathbf{H}$ is the projection onto space $\mathcal{L}_1$ and $\mathbf{I} - \mathbf{H}$ is the projection onto $\mathcal{L}_0$, where $\mathbf{I}$ is the n by n identity matrix.

Matrix decomposition

- Suppose, for convenience $n \geq p$, any matrix n by p matrix A can always be decomposed into

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^T$$

where $\mathbf{U}$ is $n \times p$ orthogonal matrix, $\mathbf{D}$ is a $p \times p$ diagonal matrix and $\mathbf{V}$ is $p \times p$ orthogonal matrix. In particular

$$\mathbf{X} = \mathbf{U}\mathbf{R},$$

where $\mathbf{R} = \mathbf{D}\mathbf{V}$.

- If $\mathbf{A}$ and $\mathbf{B}^T$ are two matrices of same dimension, then

$$trace(\mathbf{A}\mathbf{B}) = trace(\mathbf{B}\mathbf{A}).$$

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Model assumptions

- The linear regression model general assumes the error ϵ_i has zero conditional mean and constant conditional variance σ^2, and the covariates x_i are non-random;
- Independence across the observations
- A more restrictive (but common) assumption: the errors follow normal distribution, i.e, $N(0, \sigma^2)$.

Statistical properties of LSE

$$\hat{\beta} \sim N(\beta, \sigma^2(\mathbf{X}^T\mathbf{X})^{-1});$$

$$\text{RSS} = \sum_{i=1}^n \hat{\epsilon}_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \sim \sigma^2 \chi^2_{n-p-1}$$

$\hat{\beta}$ and RSS are independent

$s^2 = \text{RSS}/(n-p-1)$ unbiased estimate of σ^2

$$\frac{\hat{\beta}_j - \beta_j}{s\sqrt{c_{jj}}} \sim t_{n-p-1}$$

$$\frac{(\hat{\beta}-\beta)^T(\mathbf{X}^T\mathbf{X})(\hat{\beta}-\beta)/p}{s^2} \sim F_{p+1,n-p-1}$$

where $c_{00}, c_{11}, ..., c_{pp}$ are the diagonal elements of $(\mathbf{X}^T\mathbf{X})^{-1}$.

Understanding

$$\begin{aligned} & \mathrm{cov}(\hat{\beta}, \hat{\epsilon}) \\ = \quad & \mathrm{cov}(\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon,\ (\mathbf{I}-\mathbf{H})\epsilon) \\ = \quad & \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathrm{var}(\epsilon)(\mathbf{I}-\mathbf{H}) \\ = \quad & 0 \end{aligned}$$

because $\mathbf{H}$ is idempotent.

Confidence intervals

For example,

$$\hat{\beta}_j \pm t_{n-p-1}(\alpha/2) s \sqrt{c_{jj}}$$

is a confidence interval for β_j at confidence level $1-\alpha$. Here $t_{n-p-1}(\alpha/2)$ is the $1-\alpha/2$ percentile of the t-distribution with degree of freedom $n-p-1$.

Confidence intervals

For a given value of input $\mathbf{x}$ which is a $p+1$ vector (the first component is constant 1), its mean response is $\beta^T \mathbf{x}$. The confidence interval for this mean response is

$$\hat{\beta}^T \mathbf{x} \pm t_{n-p-1}(\alpha/2) s \sqrt{\mathbf{x}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}}$$

The confidence interval for β_j is a special case of the above formula by taking $\mathbf{x}$ as a vector that all zero except the $(j+1)$ entry corresponding β_j. (Because of β_0, β_j is at the $j+1$th position of $\hat{\beta}$.)

Prediction interval

- To predict the actual response y, rather than its mean, we would use the same point estimator $\hat{\beta}^T \mathbf{x}$, but the accuracy is much decreased as more uncertainty in the randomness of the actual response from the error is involved.
- The confidence interval, often called prediction interval, for y is

$$\hat{\beta}^T \mathbf{x} \pm t_{n-p-1}(\alpha/2) s \sqrt{1 + \mathbf{x}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}}.$$

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Variance decomposition

Recall that

$$\|\mathbf{y}\|^2 = \|\hat{\mathbf{y}}\|^2 + \|\mathbf{y} - \hat{\mathbf{y}}\|^2.$$

The common variance decomposition takes a similar form, but leaving out sample mean,

$$\|\mathbf{y} - \bar{y}\|^2 = \|\hat{\mathbf{y}} - \bar{y}\|^2 + \|\mathbf{y} - \hat{\mathbf{y}}\|^2;$$

which is often written as

$$\mathrm{SS}_{total} = \mathrm{SS}_{reg} + \mathrm{SS}_{error}.$$

Understanding

- SS_{total}, the total sum of squares, measures the total variation in response.
- SS_{reg}, the sum of squares due to regression or, more precisely, due to the inputs, measures variation in response explained by that of the inputs.
- SS_{error}, the sum of squares due to error, measures the size of randomness due to error or noise.

The ANOVA table

Source of Variation	SumOfSquares	Degree of Freedom	Mean Squared	F-statistic
Regression	SS_{reg}	p	MS_{reg}	MS_{reg}/MS_{error}
Error	SS_{error}	$n-p-1$	MS_{error}	
Total	SS_{total}	$n-1$		

where $\mathrm{MS}_{reg} = \mathrm{SS}_{reg}/p$ and $\mathrm{MS}_{error} = \mathrm{SS}_{error}/(n-p-1)$.
And the F-statistic follows $F_{p,n-p-1}$ distribution under the hypothesis that $\beta_1 = \beta_2 = ...\beta_p = 0$, i.e., all inputs are unrelated with the output.
The p-value is the probability for the distribution $F_{p+1,n-p-1}$ taking value greater than the value of the F-statistic.

General variance decomposition

- The above ANOVA is a special case of a general variance decomposition.
- Let $\mathcal{L}$ be the linear space spanned by $\mathbf{1}, \mathbf{x}_1, ..., \mathbf{x}_p$, all columns of $\mathbf{X}$.
- The linear model assumption:

$$\mathbf{y} = \mathbf{X}\beta + \epsilon$$

can be written as $E(\mathbf{y}) = \mathbf{X}\beta$, or

$$E(\mathbf{y}) \in \mathcal{L}.$$

- The fitted values $\hat{\mathbf{y}}$ is projection of $\mathbf{y}$ onto $\mathcal{L}$.
- $s^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2/(n - p - 1)$ is the unbiased estimator of σ^2.