Linear Regression

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Model Diagnostics:

Overview

Assumptions of Normal Error Model

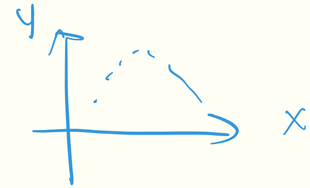
- **Linearity** of the regression relation $y = \beta_0 + \beta_1 x_i + \varepsilon_i$
- **Normality** of the error terms
- **Constant variance** of the error terms
- **Independence** of the error terms

$\varepsilon_i \overset{iid}{\sim} N(0, \sigma^2)$

equal variance

Consequences of Model Departures

violation of assumption



- With regard to regression relation: serious
  - **Nonlinearity** of the regression relation
  - **Omission of important predictor variable(s)**
- With regard to error distribution: less serious
  - **Nonconstant variance (a.k.a. heteroscedasticity)** or **Nonindependence** $\Longrightarrow$ invalid variance estimation $\Longrightarrow$ invalid inference

    b/c: central limit theorem (CLT) { ① large sample size ② small departure
  - **Nonnormality**: small departures – not serious; major departures – could be serious especially for small sample sizes
- **Outliers**: could be serious for small data sets

Residual Plots

$e_i = y_i - \hat{y}_i$, $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$

- Examine regression relation and error variance:
  - today ✲ residual vs. fitted value
  - ✲ residual vs. X variable(s)
  - residual vs. omitted X variable(s)
- Examine error distribution:
  - ✲ Normality: normal probability plot (Q-Q plot) of residuals
  - Independence: sequence plot of residuals
- Examine outliers or influential cases: studentized residuals, cook's distance

Remedial Measures

Mild departures often do not need to be fixed. For more serious departures:

- Fix regression relation: transformation of the response variable and/or transformation(s) of the X variable(s)
- Fix error distribution: transformation of the response variable
- Fix outliers: exclusion or robust regression

Model Diagnostics:

Nonlinearity Detection

Detection of Nonlinearity

e_i vs $\hat{y}_i$ or e_i vs x_i

↳ same ∵ $\hat{y}_i$ linearly with x_i

residual vs. fitted value plot or residual vs. X variable plot:

- If these show a clear nonlinear pattern, then it is an indication of possible nonlinearity in the regression relation.
- This is because the nonlinearity unaccounted for by the model would be left in the residuals.

Simulation Experiment

if mean ≠ 0, should be absorbed into y_i

- Data: 30 cases with $X \sim N(100, 16^2)$, $\varepsilon \sim N(0, 10^2)$,

$$Y_i = 5 - X_i + \underbrace{0.1X_i^2}_{\text{non-linear}} + \varepsilon_i, \quad i = 1, \cdots, 30$$

- Fitted model: simple linear regression

Coefficients	Estimate	Std. Error	t value	$Pr(>\|t\|)$
Intercept	-811.8518	35.2767	-23.01	<2e-16 ***
X	17.2787	0.3695	46.76	<2e-16 ***

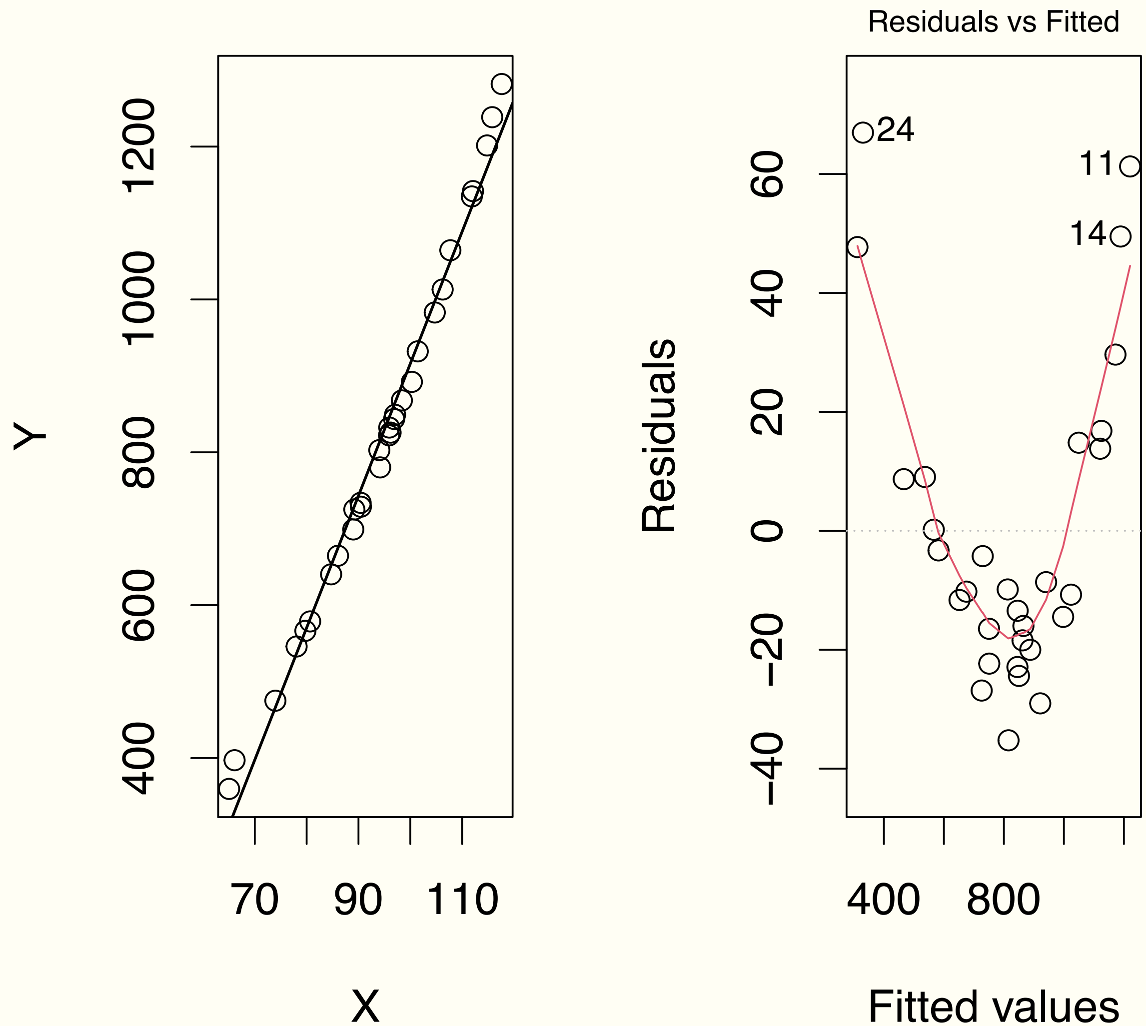
$\sqrt{MSE} = 27.6$, $R^2 = 0.9874$ → good fit

Figure: Left: scatter plot; Right: residual vs. fitted value

variance in tens

scale of hundreds

non-linearity mask by



non-linear trend

Model Diagnostics:

Unequal Variance

Detection

Unequal Variance

- Sometimes variance increases (or decreases) with the value of the X variable. E.g., in financial data, the volume of transactions often has a role in the volatility of market.
- Data may come from different strata with different variability. E.g., measuring instruments with different precision may have been used to obtain the observations.

eg. average (county of diff. sizes)
↳ reduce variance. ↓ with ↑n

Detection of Nonconstancy in Variance

residual vs. fitted value plot:

- If it shows an unequal spread of the residuals along the horizontal axis, then this is an indication of unequal variance.

Simulation Experiment

- Data: 100 cases with $X_i = \frac{i}{10}$, $\varepsilon_i \sim N(0, 1)$,

error term

$$Y_i = 2 + 3X_i + \underbrace{\sigma(X_i)\varepsilon_i}, \quad i = 1, \cdots, 100,$$

scalar ≈ a function of x

where $\log \sigma^2(x) = 1 + 0.1x$.

$\varepsilon \uparrow$ with $x_i \uparrow$

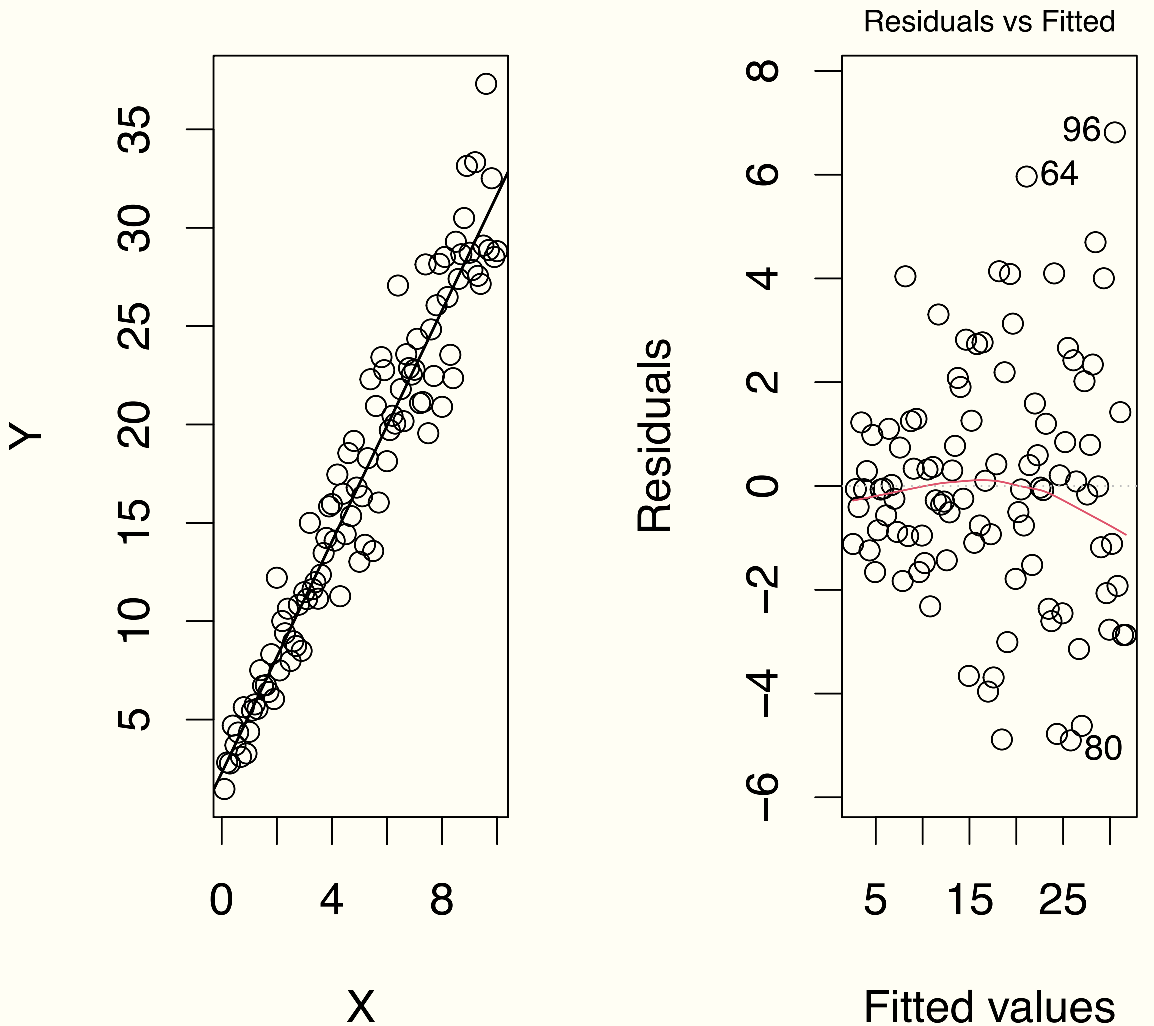
- Fitted model: simple linear regression

Coefficients	Estimate	$\boxed{\text{Std. Error}}$	t value	$Pr(> \|t\|)$
Intercept	2.29130	0.46689	4.908	3.67e-06 ***
X	2.93869	0.08027	36.612	< 2e-16 ***

$\sqrt{MSE} = 2.317$, $R^2 = 0.9319$. wrong?

Figure: Left: scatter plot; Right: residual vs. fitted value

fluctuation ↑



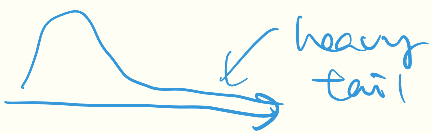
Model Diagnostics:

Non-normality Detection

Detection of Non-normality

Normal probability plot (a.k.a. Normal Q-Q plot) of residuals:

- If the residuals are normally distributed, then the points on the Q-Q plot should be (nearly) on a straight line.
- Departures from that could indicate **skewed** (non-symmetry) or **heavy-tailed** (more probability mass on tails than a Normal distribution) distributions.



- Other types of departures (e.g., nonlinearity) may affect the distribution of the residuals, thus it is better to examine these before checking normality.

Q-Q Plot

Q-Q stands for quantile-quantile. Q-Q plot is a graphical tool to compare the empirical distribution (of a sample) with a reference distribution.

- $e_{(k)}$'s – the *sample quantiles or empirical quantiles*: the kth smallest data in the sample (roughly) the $\left(\frac{k}{n}\right)$th quantile of data
- $z_{(k)}$'s – the *theoretical quantiles* under the reference distribution $z\left(\frac{k}{n}\right)$
- Q-Q plot is simply the scatter plot of $e_{(k)}$'s vs. $z_{(k)}$'s
- A (nearly) straight line pattern indicates that the sample is likely from the reference distribution.

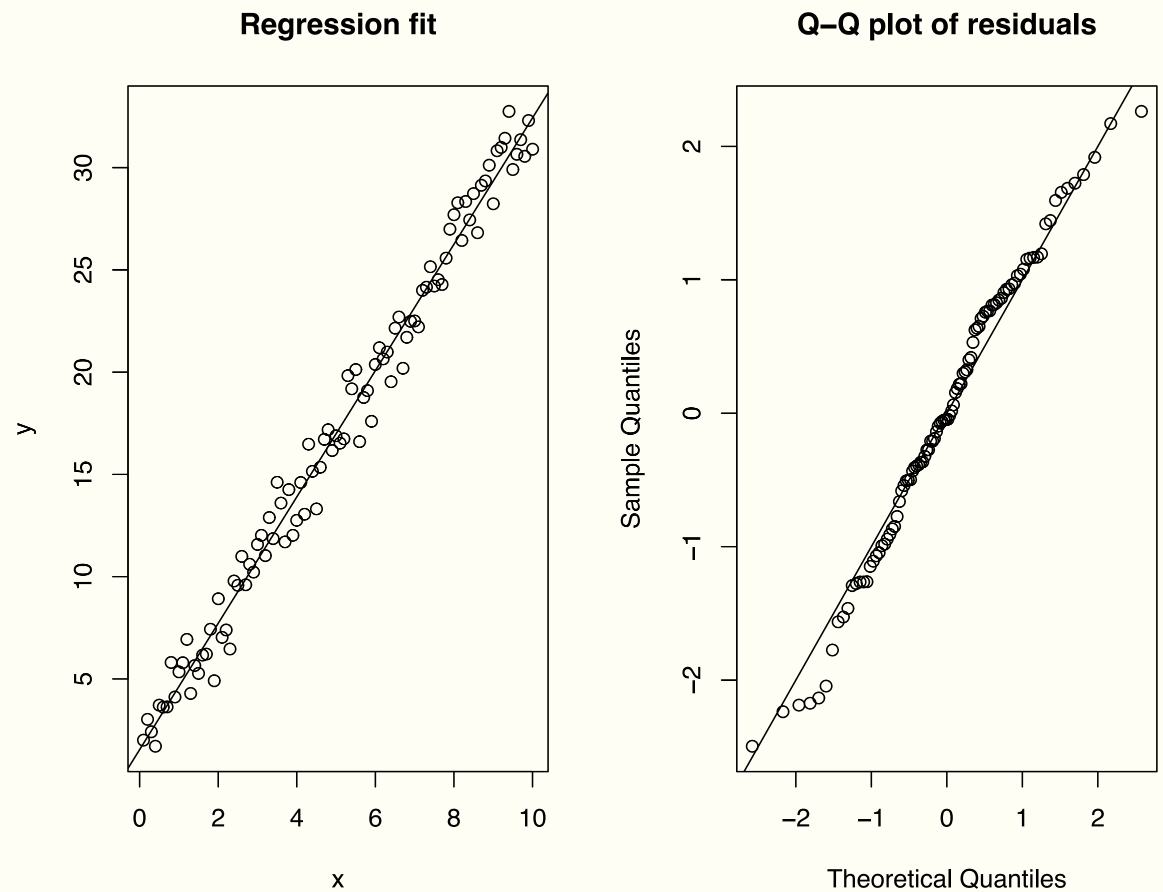
Case i	X_i	Y_i	$\widehat{Y}_i$	e_i
1	0.22	1.79	2.33	-0.54
2	3.55	5.66	5.90	-0.23
3	1.86	3.34	4.09	-0.75
4	3.29	5.83	5.62	0.22
5	1.25	4.74	3.43	1.31

$e_{(2)}$, the second smallest residual, is -0.54 and its corresponding theoretical quantile under Normality is:

$$z_{(2)} = \sqrt{MSE} \times Z\left((2 - 0.375)/(5 + 0.25)\right)$$

$$= \sqrt{0.8905} \times Z(0.31) = 0.944 \times (-0.497) = -0.469.$$

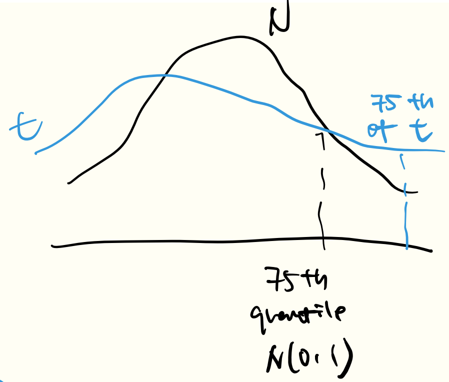
Error distribution: Normal$(0, 1)$

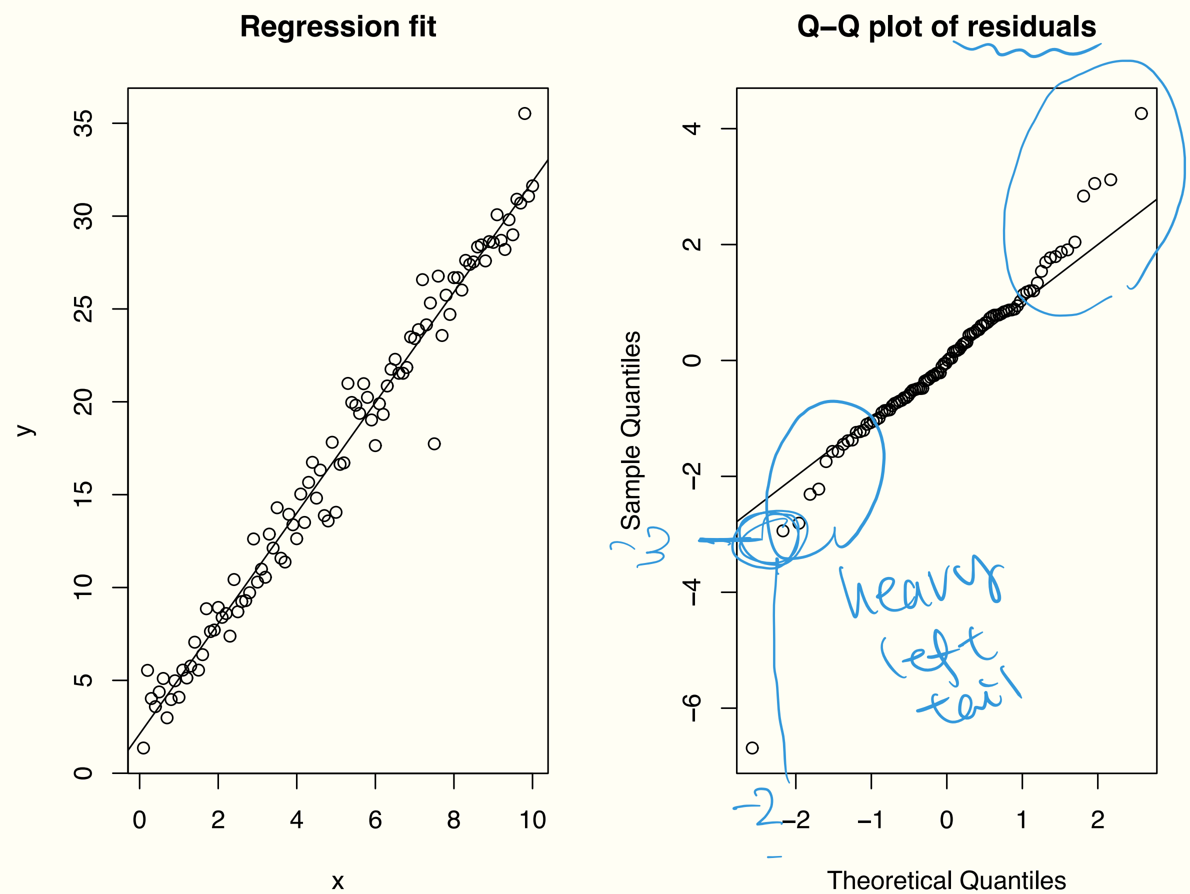


Normal Q-Q plot shows a straight line pattern.

↳ normality assumption ✓

Error distribution: $t_{(5)}$ – symmetrical but heavy-tailed

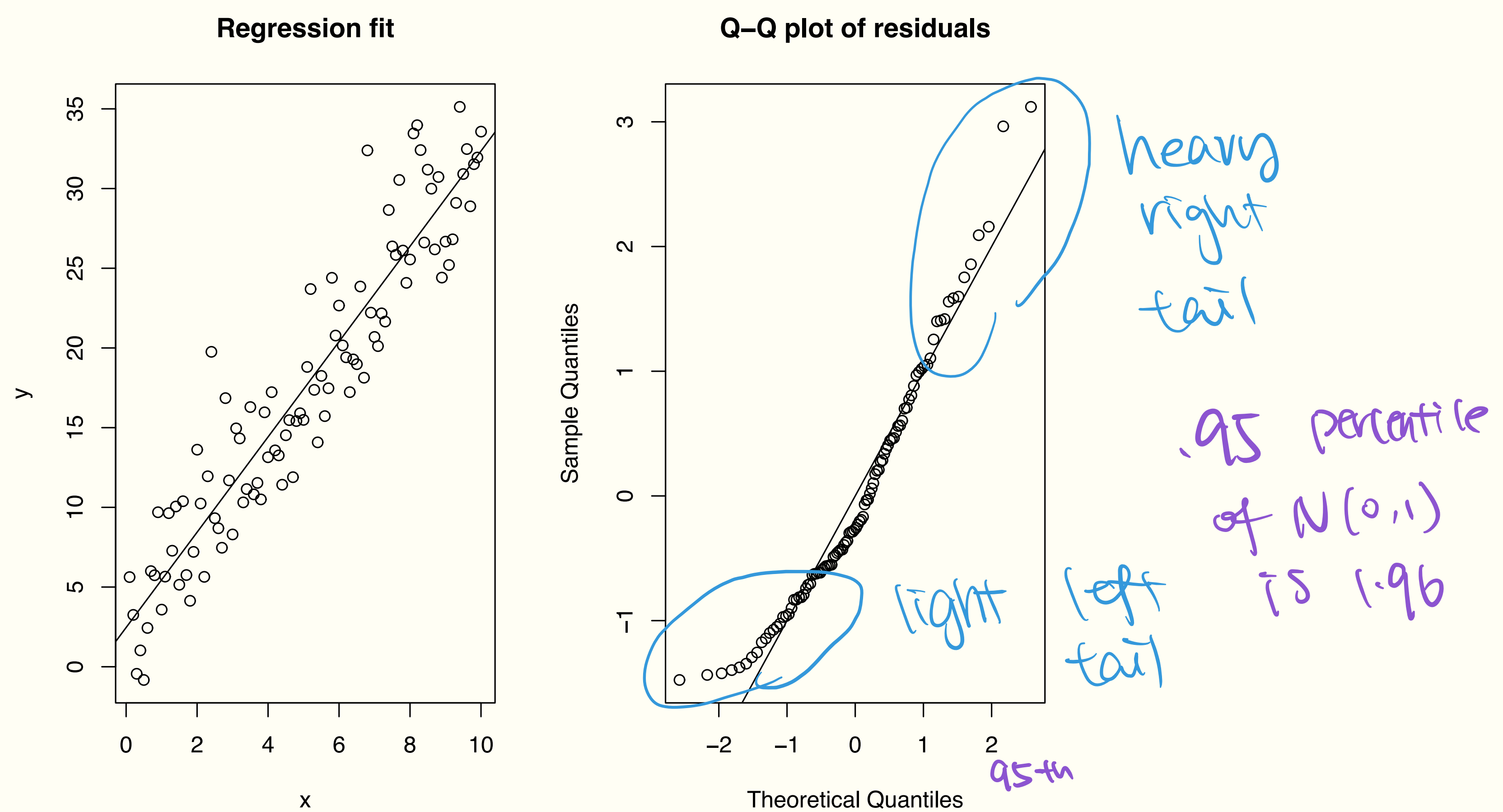




Normal Q-Q plot shows more probability mass on both tails compared to a Normal distribution.

heavy-tailed error distrib.

Error distribution: centered $\chi^2_{(5)}$ – right-skewed



Normal Q-Q plot shows more probability mass on the right tail and less probability mass on the left tail compared to a Normal distribution.

Remedial Measures: Transformations

Transformation of X

Linearize a nonlinear relationship:

- Increasing and concave downward: $X' = \log X$ or $X' = \sqrt{X}$
- Increasing and concave upward: $X' = X^2$ or $X' = \exp(X)$
- Decreasing and concave upward: $X' = 1/X$ or $X' = \exp(-X)$.
- Sometimes, add a constant to the transformation, e.g.

  $X' = 1/(c + X)$, to avoid negative or nearly zero values.

Transformation of Y

Fix error distribution such as unequal variance or non-normality.

- Unequal variance and non-normality often appear together.
- Commonly used transformations:
  - $Y' = \sqrt{Y}$
  - $Y' = \log Y$
  - $Y' = 1/Y$
  - Sometimes, add a constant to the transformation, e.g., $Y' = \log(c + Y)$, to avoid negative or nearly zero values.
- A simultaneous transformation of X might be needed to maintain a linear relationship.

Box-Cox Procedure

Choose a power transformation:

- For each $\lambda \in R$, define the transformed observations as

$$Y_i^* = \begin{cases} K_1 \frac{Y_i^\lambda - 1}{\lambda}, & if, \quad \lambda \neq 0 \\ K_2 \log(Y_i), & if, \quad \lambda = 0 \end{cases}, \quad K_2 = (\prod_{j=1}^{n} Y_j)^{1/n}, \quad K_1 = 1/K_2^{\lambda-1}$$

↳ log transform

- For each λ, fit a regression model on the transformed data Y^* and derive $SSE(\lambda)$ (or maximum loglikelihood).
- Find the λ that minimizes SSE (or maximizes maximum loglikelihood) and apply the corresponding power transformation ($\lambda = 0$: logarithm transformation).

Simple Regression: Matrix Form

Simple Linear Regression in Matrix Form

The regression equations:

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i, \quad i = 1, \cdots n$$

a set of n equations

$\varepsilon_i \sim N(0, \sigma^2)$
uncorrelated

can be expressed in a compact matrix form:

$$\underset{n\times1}{\mathbf{Y}} = \underset{n\times2}{\mathbf{X}} \ \underset{2\times1}{\boldsymbol{\beta}} + \underset{n\times1}{\boldsymbol{\epsilon}}$$

$$\vec{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} = X = \begin{array}{c} \begin{array}{cc} \beta_0 & \beta_1 \end{array} \\ \begin{pmatrix} 1 & X_1 \\ 1 & X_2 \\ 1 & X_3 \\ \vdots & \vdots \\ 1 & X_n \end{pmatrix} \end{array} \times \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} + \varepsilon = \begin{pmatrix} \varepsilon_0 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

- **Response vector Y** and **error vector** : $n \times 1$ column vectors

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_i \\ \vdots \\ Y_n \end{bmatrix}, \qquad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_i \\ \vdots \\ \epsilon_n \end{bmatrix}$$

response vector

error vector

both random vector

- **Design matrix**: $n \times 2$ matrix:

$$\mathbf{X} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_i \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix}$$

- **Coefficient vector**: 2×1 column vector:

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

The model assumptions:

$$E(\epsilon_i) = 0, \quad Var(\epsilon_i) = \sigma^2, \quad \text{for all } i = 1, \cdots, n$$

$$Cov(\epsilon_i, \epsilon_j) = 0, \quad \text{for all } i \neq j$$

can be expressed in matrix form:

$$\mathbf{E}\{\boldsymbol{\epsilon}\} = \mathbf{0}_n, \quad \boldsymbol{\sigma}^{\mathbf{2}}\{\boldsymbol{\epsilon}\} = \sigma^2 \mathbf{I}_n.$$

Mean of the error vector:

$$\mathbf{E}\{\boldsymbol{\epsilon}\} := \begin{bmatrix} E(\epsilon_1) \\ E(\epsilon_2) \\ \vdots \\ E(\epsilon_n) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \mathbf{0}_n,$$

where $\mathbf{0}_n$ is the $n \times 1$ zero vector.

Variance-covariance matrix of the error vector:

symmetric ∵ cov(a,b) = cov(b,a)

$$\boldsymbol{\sigma}^2\{\vec{\boldsymbol{\epsilon}}\} : \overset{def}{=} \begin{bmatrix} Var(\epsilon_1) & Cov(\epsilon_1, \epsilon_2) & \cdots & Cov(\epsilon_1, \epsilon_n) \\ Cov(\epsilon_2, \epsilon_1) & Var(\epsilon_2) & \cdots & Cov(\epsilon_2, \epsilon_n) \\ \vdots & \vdots & \vdots & \vdots \\ Cov(\epsilon_n, \epsilon_1) & Cov(\epsilon_n, \epsilon_2) & \cdots & \underset{\sim}{Var(\epsilon_n)} \end{bmatrix} = \left(\left(cov(\varepsilon_i, \varepsilon_j)\right)\right)$$

$(i,j^{th}$ element$)$

$n \times n$

$cov(\vec{\varepsilon}, \vec{\varepsilon}) = var(\vec{\varepsilon})$

var on diag.

$$= \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} = \sigma^2 \mathbf{I}_n,$$

scalar matrix

$$I_n = \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix}$$

where $\mathbf{I}_n$ is the $n \times n$ identity matrix.

EZ: 1st moment
EZ^2: 2nd
$E(Z-E(Z))^2$: centered 2nd

$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$

$E(y_i) = \beta_0 + \beta_1 x_i$

Mean response vector: $n \times 1$ column vector:

$$
\underset{n\times 1}{\mathbf{E}\{\mathbf{Y}\}} = \begin{bmatrix} E(Y_1) \\ E(Y_2) \\ \vdots \\ E(Y_i) \\ \vdots \\ E(Y_n) \end{bmatrix} = \begin{bmatrix} \beta_0 + \beta_1 X_1 \\ \beta_0 + \beta_1 X_2 \\ \vdots \\ \beta_0 + \beta_1 X_i \\ \vdots \\ \beta_0 + \beta_1 X_n \end{bmatrix} = \underset{n\times 2}{\begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_i \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix}} \underset{2\times 1}{\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}} = \underset{n\times 1}{\mathbf{X}\boldsymbol{\beta}}.
$$

$y = x\beta + \varepsilon$, $E(y) = E(x\beta + \varepsilon) = x\beta + E(\varepsilon) = x\beta + \vec{0} = x\beta$

E(nonrandom) = itself

Summary

simple regression in matrix form:

unknown parameter

$$\underset{n\times 1}{\mathbf{Y}} = \underbrace{\underset{n\times 2}{\mathbf{X}} \; \underset{2\times 1}{\boldsymbol{\beta}}}_{\text{non-random}} + \underset{n\times 1}{\boldsymbol{\epsilon}}$$

- $\boldsymbol{\epsilon}$ is a random vector with $\mathbf{E}\{\boldsymbol{\epsilon}\} = \mathbf{0}_n$, $\boldsymbol{\sigma}^2\{\boldsymbol{\epsilon}\} = \sigma^2 \mathbf{I}_n$. ← assumption
- Normal error model: $\boldsymbol{\epsilon} \sim \text{Normal}_n(\underset{\text{mean}}{\mathbf{0}_n}, \sigma^2 \mathbf{I}_n)$.
  ↳ multivariant normal distribution
- In terms of the response vector:

together says

$$\mathbf{E}\{\mathbf{Y}\} = \mathbf{X}\boldsymbol{\beta}, \quad \boldsymbol{\sigma}^2\{\mathbf{Y}\} = \sigma^2 \mathbf{I}_n.$$

= variance-cov matrix of Y

$= \sigma^2\{\varepsilon\}$ ∵ Xβ nonrandom does not affect var, cov

Least Squares Estimation:

Matrix Form

Least Squares Estimation in Matrix Form

vector $\underset{n\times 1}{\vec{V}} = \begin{pmatrix} V_1 \\ V_2 \\ \vdots \\ V_n \end{pmatrix}$

$\vec{V}^T = (V_1, V_2 \ldots V_n)$

$\sum_{i=1}^{n} V_i^2 = V^T \cdot V$

$= \|V\|^2$

square of length

Least squares criterion:

$$Q(b_0, b_1) = \sum_{i=1}^{n} (Y_i - (b_0 + b_1 X_i))^2$$

$$\begin{pmatrix} y_1 - (b_0 + b_1 x_1) \\ \vdots \\ y_n - (b_0 + b_1 x_n) \end{pmatrix}$$

can be expressed in matrix form : $\mathbf{b} = (b_0, b_1)^T$

$$= \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} - \begin{pmatrix} b_0 + b_1 x_1 \\ \vdots \\ b_0 + b_1 x_n \end{pmatrix}$$

$$Q(\mathbf{b}) = (\mathbf{Y} - \mathbf{X}\mathbf{b})' (\mathbf{Y} - \mathbf{X}\mathbf{b}) = \mathbf{Y}'\mathbf{Y} - \mathbf{b}'\mathbf{X}'\mathbf{Y} - \mathbf{Y}'\mathbf{X}\mathbf{b} + \mathbf{b}'\mathbf{X}'\mathbf{X}\mathbf{b}.$$

2×1

$= (y' - b'X')(y - Xb) =$

$= \underset{(n\times 1)}{\vec{y}} - \underset{n\times 2}{X} \underset{2\times 1}{\vec{b}}$

$\frac{\partial Q(\vec{b})}{\partial \vec{b}} = \ldots = 0$

$\Rightarrow (X^T X) b = X^T y$ [Normal Equation]

$(Xb)^T = b^T \cdot X^T$

Solve $\underbrace{(X^TX)}_{2\times 2}\underset{2\times 1}{b} = \underbrace{X^T y}_{2\times 1}$ $\quad b = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}$

$\Rightarrow \hat{\beta}$ is solution $= (X^TX)^{-1} X^T y =$

LS estimators:

$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \begin{bmatrix} \overline{Y} - \hat{\beta}_1 \overline{X} \\ \frac{\sum_{i=1}^{n}(X_i - \overline{X})(Y_i - \overline{Y})}{\sum_{i=1}^{n}(X_i - \overline{X})^2} \end{bmatrix},$$

provided that X_is are not all equal.
↳ X_i invertible

- $\hat{\boldsymbol{\beta}}$ is linear in the observations $\mathbf{Y}$.

$x = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}$ $y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} n & \sum_{i=1}^n X_i \\ \sum_{i=1}^n X_i & \sum_{i=1}^n X_i^2 \end{bmatrix}, \quad \mathbf{X}'\mathbf{Y} = \begin{bmatrix} \sum_{i=1}^n Y_i \\ \sum_{i=1}^n X_i Y_i \end{bmatrix}.$$

inverse of 2x2 matrix
$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad-bc} \cdot \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$
provided $ad-bc \neq 0$

When

$$D := n\sum_{i=1}^n X_i^2 - \left(\sum_{i=1}^n X_i\right)^2 = n\sum_{i=1}^n (X_i - \overline{X})^2 \neq 0$$

determinant of $x^T x$

if only if x_i not all zero

$$(\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix} \frac{\sum_{i=1}^n X_i^2}{n\sum_{i=1}^n (X_i - \overline{X})^2} & -\frac{\sum_{i=1}^n X_i}{n\sum_{i=1}^n (X_i - \overline{X})^2} \\ -\frac{\sum_{i=1}^n X_i}{n\sum_{i=1}^n (X_i - \overline{X})^2} & \frac{n}{n\sum_{i=1}^n (X_i - \overline{X})^2} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{n} + \frac{\overline{X}^2}{\sum_{i=1}^n (X_i - \overline{X})^2} & -\frac{\overline{X}}{\sum_{i=1}^n (X_i - \overline{X})^2} \\ -\frac{\overline{X}}{\sum_{i=1}^n (X_i - \overline{X})^2} & \frac{1}{\sum_{i=1}^n (X_i - \overline{X})^2} \end{bmatrix}.$$

$\Rightarrow$ get $\hat{\beta}$

Deriving LS Estimator

- Differentiate $Q(\cdot)$ with respect to $\mathbf{b}$: $\frac{\partial}{\partial \mathbf{b}} Q = -2\mathbf{X}'\mathbf{Y} + 2\mathbf{X}'\mathbf{X}\mathbf{b}$.
- Set the gradient to zero $\Longrightarrow$ *normal equation*:

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y}.$$

- Multiply both sides by $(\mathbf{X}'\mathbf{X})^{-1}$:

$$(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}.$$

- The left hand side becomes $\mathbf{I}_2\mathbf{b} = \mathbf{b}$, and the right hand side is the solution.

Fitted Value and Residual:

Matrix Form

Fitted Values and Residuals

$$\hat{y} = \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{pmatrix} = \begin{pmatrix} \hat{\beta}_0 + \hat{\beta}_1 x_1 \\ \vdots \\ \hat{\beta}_0 + \hat{\beta}_1 x_n \end{pmatrix} = X\hat{\beta}$$

- Fitted values vector: $n \times 1$ column vector:

$$X = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \quad \hat{\beta} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{pmatrix} = (X^T X)^{-1} X^T y$$

$$\underset{n\times 1}{\widehat{\mathbf{Y}}} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \underset{n\times n}{\mathbf{H}}\underset{n\times 1}{\mathbf{Y}},$$

where $\mathbf{H} := \underset{n\times 2}{\mathbf{X}}\underset{2\times 2}{(\mathbf{X}'\mathbf{X})^{-1}}\underset{2\times n}{\mathbf{X}'}$ is called the **hat matrix**.

- Residuals vector: $n \times 1$ column vector:

$$\vec{e} = \begin{pmatrix} e_1 \\ \vdots \\ e_n \end{pmatrix} = \begin{pmatrix} y_1 - \hat{y}_1 \\ \vdots \\ y_n - \hat{y}_n \end{pmatrix} = \vec{y} - \hat{y} = \vec{y} - H\vec{y} = (I_n - H)\cdot\vec{y}$$

$$\mathbf{e} = \mathbf{Y} - \widehat{\mathbf{Y}} = (\mathbf{I}_n - \mathbf{H})\mathbf{Y}.$$

- Fitted values $\widehat{\mathbf{Y}}$ and residuals $\mathbf{e}$ are linear in the observations $\mathbf{Y}$.

Hat Matrix

matrix transpose: $(ABCD)^T = D^T C^T B^T A^T$, $(X^T X)^T = X^T X$

b/c $X^T X$ is symmetric

$(A^T)^T = A$

$(A-B)^T = A^T - B^T$

H plays an important role in model diagnostics.

$$\underset{n\times n}{\mathbf{H}} := \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}', \quad \mathbf{I}_n - \mathbf{H} = \mathbf{I}_n - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$$

$H^T = X \cdot (X^T X)^{-1} \times X^T = H$

are $n \times n$ **projection matrices**:

- **Symmetric**: $\mathbf{H}' = \mathbf{H}, \quad (\mathbf{I}_n - \mathbf{H})' = \mathbf{I}_n - \mathbf{H}$

  Transpose = Matrix itself

- **Idempotent**: $\mathbf{H}^2 := \mathbf{H}\mathbf{H} = \mathbf{H}, \quad (\mathbf{I}_n - \mathbf{H})^2 = \mathbf{I}_n - \mathbf{H}.$

  raise power = itself

assume x_i not all equal $\Rightarrow$ rank$(X)=2$

max # of linearly independent column / row ; cannot exceed 2

- $rank(\mathbf{H}) = 2$, $rank(\mathbf{I}_n - \mathbf{H}) = n - 2$.

$H^2 = H \cdot H = \underbrace{X \cdot (X^T X)^{-1} \cdot X^T}_{H} \cdot \underbrace{X \cdot (X^T X)^{-1} \cdot X^T}_{H} = X \cdot \cancel{I_n} \cdot (X^T X)^{-1} \cdot X^T$

$= X \cdot (X^T X^{-1}) X^T = H$

$ABC = A(BC)$

$= (AB)C$

Error Sum of Squares

$\vec{e} = (I_n - H)\, Y$

$e^T = Y^T (I_n - H)^T$

$= Y^T \cdot (I_n - H)$

$$SSE = \sum_{i=1}^{n} e_i^2$$

$\because I_n - H$ symmetric

can be expressed in matrix form:

$(I_n - H)^2 = I_n - H$ idempotent

$$SSE = \mathbf{e}'\mathbf{e} = \underbrace{\mathbf{Y}'(\mathbf{I}_n - \mathbf{H})'}_{e'}\underbrace{(\mathbf{I}_n - \mathbf{H})\mathbf{Y}}_{e} = \mathbf{Y}'\underbrace{(\mathbf{I}_n - \mathbf{H})}_{\text{projection matrix}}\mathbf{Y}$$

- $\mathbf{I}_n - \mathbf{H}$ is a projection matrix.
- $df(SSE) = rank(\mathbf{I}_n - \mathbf{H}) = n - 2.$

LS Estimation: Mean and Variance

Linear Transformations of Random Vector

If $\mathbf{Z}$ is an $r \times 1$ random vector, and $\mathbf{A}$ is an $s \times r$ non-random matrix,

then

random vector — random

$$\underset{s \times 1}{\mathbf{W}} = \underset{s \times r}{\mathbf{A}} \; \underset{r \times 1}{\mathbf{Z}}$$

is an $s \times 1$ random vector with

if $E(z) = \vec{0}_{(r)}$

then $E(w) = \vec{0}_{(s)}$

$$\mathbf{E}\{\mathbf{W}\} = \mathbf{E}\{\mathbf{AZ}\} = \mathbf{A}\mathbf{E}\{\mathbf{Z}\}$$

$$\sigma^2\{\mathbf{W}\} = \sigma^2\{\mathbf{AZ}\} = \underset{s \times r}{\mathbf{A}} \underbrace{\sigma^2\{\mathbf{Z}\}}_{r \times r} \underset{r \times s}{\mathbf{A}'}$$

var-cov. matrix of W

if $\sigma^2\{z\} = \sigma^2 \cancel{I_r}$

then $\sigma^2\{W\} = \sigma^2 \cdot \underbrace{A A^T}_{s \times s}$

$\mathrm{cov}(AZ, BZ) = A \cdot \sigma^2\{Z\} \cdot B^T$

If 2 linear combination, can exchange order

LS Estimation: Expectations

$\hat{\beta} = \underbrace{(X^T X)^{-1} X^T}_{A} y$

$E(y) = X\beta$

$\sigma^2\{y\} = \sigma^2 I_n$

- LS estimator is unbiased:

$\hat{\beta} = Ay$, $E(\hat{\beta}) = A \cdot E(y) = A \cdot X\beta$

$= (X^T X)^{-1} \cdot X^T \cdot X\beta$

$= I_2 \cdot \beta = \beta$

$$\mathbf{E}\{\hat{\boldsymbol{\beta}}\} = \underbrace{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'}_{A}\mathbf{E}\{\mathbf{Y}\} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \boldsymbol{\beta}$$

- Expectation of the fitted values:

$$\mathbf{E}\{\widehat{\mathbf{Y}}\} = \mathbf{E}\{\mathbf{X}\hat{\boldsymbol{\beta}}\} = \mathbf{X}\mathbf{E}\{\hat{\boldsymbol{\beta}}\} = \mathbf{X}\boldsymbol{\beta} = \mathbf{E}\{\mathbf{Y}\}$$

- Expectation of the residuals:

$$\mathbf{E}\{\mathbf{e}\} = \mathbf{E}\{\mathbf{Y} - \widehat{\mathbf{Y}}\} = \mathbf{E}\{\mathbf{Y}\} - \mathbf{E}\{\widehat{\mathbf{Y}}\} = \mathbf{0}_n$$

$= X\beta - X\beta$

LS Estimation: Variance-Covariance Matrices

$$\begin{cases} \hat{\beta} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{pmatrix} = (X^T X)^{-1} X^T y \\ \sigma^2\{y\} = \sigma^2 \cdot I_n \end{cases}$$

Variance-covariance of the LS estimator:

$$= \begin{pmatrix} var(\hat{\beta}_0) & cov(\hat{\beta}_0, \hat{\beta}_1) \\ cov(\hat{\beta}_0, \hat{\beta}_1) & var(\hat{\beta}_1) \end{pmatrix}$$

$A = (X^T X)^{-1} X^T y$

$\sigma^2\{\hat{\beta}\} = \sigma^2\{Ay\} = A\,\sigma^2\{y\}\,A^T = A \cdot \sigma^2 \cdot I_n \cdot A^T$

$$\begin{aligned} \sigma^2\{\hat{\beta}\} &= \sigma^2\{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}\} = \left((\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\right)\sigma^2\{\mathbf{Y}\}\left((\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\right)' \\ &= \sigma^2(\mathbf{X}'\mathbf{X})^{-1} = \sigma^2 \underbrace{\begin{bmatrix} \frac{1}{n} + \frac{\overline{X}^2}{\sum_{i=1}^n (X_i - \overline{X})^2} & -\frac{\overline{X}}{\sum_{i=1}^n (X_i - \overline{X})^2} \\ -\frac{\overline{X}}{\sum_{i=1}^n (X_i - \overline{X})^2} & \frac{1}{\sum_{i=1}^n (X_i - \overline{X})^2} \end{bmatrix}}_{(X^T X)^{-1}} \end{aligned}$$

$= \sigma^2 \cdot A \cdot A^T$

$= \sigma^2 \cdot \underbrace{(X^T X)^{-1} X^T}_{A} \cdot \underbrace{X (X^T X)^{-1}}_{A^T}$

$= \sigma^2 \cdot (X^T X)^{-1}$

$\Rightarrow var(\hat{\beta}_0) = \sigma^2 \left\{ \frac{1}{n} + \frac{\bar{x}^2}{\sum (x_i - \bar{x})^2} \right\}$

$var(\hat{\beta}_1) = \sigma^2 / \sum (x_i - \bar{x})^2$

$cov(\hat{\beta}_0, \hat{\beta}_1) = -\sigma^2 \cdot \frac{\bar{x}}{\sum (x_i - \bar{x})^2}$

$\hat{y} = Hy$ $\quad H = X(X^TX)^{-1}X^T$ $\quad H^T = H$ $\quad H^2 = H$

non-random $\quad \sigma^2\{y\} = \sigma^2 \cdot I_n$

- Variance-covariance of the fitted values: $= H \cdot \sigma^2 I_n \cdot H^T = \sigma^2 \cdot H \cdot H^T$

$= \sigma^2 \cdot H^2$

$= \sigma^2 \cdot H$

$$\sigma^2\{\widehat{\mathbf{Y}}\} = \mathbf{H}\sigma^2\{\mathbf{Y}\}\mathbf{H}' = \sigma^2\mathbf{H}$$

error variance

$\Rightarrow \text{cov}(\hat{y}_i, \hat{y}_j) = \sigma^2 \cdot h_{ij}$ (i,jth element of H)

↳ fitted values correlated among themselves

- Variance-covariance of the residuals:

$$\sigma^2\{\mathbf{e}\} = (\mathbf{I}_n - \mathbf{H})\underbrace{\sigma^2\{\mathbf{Y}\}}_{\sigma^2 I_n}(\mathbf{I}_n - \mathbf{H})' = \sigma^2(\mathbf{I}_n - \mathbf{H})$$

$e = (I_n - H)y$ $\quad = \sigma^2(I_n - H^2)$

$\Rightarrow \text{cov}(e_i, e_j) = \sigma^2(0 - h_{ij})$

$= -\sigma^2 \cdot h_{ij}$

residuals correlated among themselves

$\text{cov}(e, \hat{\beta}) = \text{cov}\left((I_n - H)y, (X^TX)^{-1}X^Ty \right)$

$= (I_n - H) \cdot \text{cov}(y, y) \cdot X(X^TX)^{-1}$

$= (I_n - H) \cdot \sigma^2 \cdot I_n \cdot X(X^TX)^{-1} = \sigma^2 \cdot \underbrace{(I_n - H)X}_{0} \cdot (X^TX)^{-1} = 0$

$\text{var}(e_i) = \sigma^2(1 - h_{ii})$

Expectation of SSE

$$
\begin{aligned}
E(SSE) &= E\left(\mathbf{Y}'(\mathbf{I}_n - \mathbf{H})\mathbf{Y}\right) = E\left(Tr((\mathbf{I}_n - \mathbf{H})\mathbf{Y}\mathbf{Y}')\right) \\
&= Tr\left((\mathbf{I}_n - \mathbf{H})E(\mathbf{Y}\mathbf{Y}')\right) \\
&= Tr\Big((\mathbf{I}_n - \mathbf{H})(\sigma^2\mathbf{I}_n + \mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}')\Big) \\
&= \sigma^2 Tr\left(\mathbf{I}_n - \mathbf{H}\right) + Tr\left((\mathbf{I}_n - \mathbf{H})\mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}'\right) \\
&= (n-2)\sigma^2.
\end{aligned}
$$

The last equality is because $Tr\left(\mathbf{I}_n - \mathbf{H}\right) = n - 2$ and $(\mathbf{I}_n - \mathbf{H})\mathbf{X} = \mathbf{0}$.