Stat 206: Linear Models

Lecture 6

October 14, 2019

Adjusted Coefficient of Determination R_a^2

- A modified measure for degree of linear association between X and Y:

$$R_a^2 = 1 - \frac{MSE}{MSTO} = 1 - \frac{n-1}{n-2}\frac{SSE}{SSTO}.$$

- $R_a^2 \leq R^2 = 1 - \frac{SSE}{SSTO}$.
- Heights.

$$R_a^2 = 1 - \frac{927}{926} \times \frac{4659}{5893} = 0.2085.$$

Model Diagnostics

- Assumptions of the simple linear model with Normal errors:
  -
  -
  -
  -
- Diagnostic plots can be used to examine the appropriateness of these assumptions.
  - **Residual plots**.
- Remedial measures: transformations.

Model Diagnostics

- Assumptions of the simple linear model with Normal errors:
  - **linearity** of the regression relation
  - **normality** of the error terms
  - **constant variance** of the error terms
  - **independence** of the error terms
- Diagnostic plots can be used to examine the appropriateness of these assumptions.
  - **Residual plots**.
- Remedial measures: transformations.

Residual Plots

- Examine regression relation and error variance.
  - Residual vs. predictor variable or residual vs. fitted value.
  - Residual vs. omitted predictor variable(s). (Later)
- Examine error distributions.
  - Normality: normal probability plot (Q-Q plot) of residuals.

Detection of Nonlinearity

- **If the residual vs. predictor variable plot (or residual vs. fitted value plot) shows a**
  , then it is an indication of possible nonlinearity in regression relation.
- True model : $Y = 5 - X + 0.1X^2 + \varepsilon$.
  - 30 cases with $X \sim N(100, 16^2)$ and $\varepsilon \sim N(0, 10^2)$.
  - Summary statistics:

$$\overline{X} = 104.13, \overline{Y} = 1004.79, \sum_i X_i^2 = 330962.9, \sum_i Y_i^2 = 32466188, \sum_i X_i Y_i = 3249512.$$

  - Simple linear regression model was fitted to this data.

Coefficients	Estimate	Std. Error	t-statistic	P-value
Intercept	-1021.3803	40.0648	-25.49	$< 2 \times 10^{-16}$
Slope	19.4587	0.3814	51.01	$< 2 \times 10^{-16}$

$\sqrt{MSE} = 28.78$, $R^2 = 0.9894$, $R_a^2 = 0.989$.

Detection of Nonlinearity

- If the residual vs. predictor variable plot (or residual vs. fitted value plot) shows a clear nonlinear pattern, then it is an indication of possible nonlinearity in regression relation as the nonlinearity would be left to the residuals.
- True model : $Y = 5 - X + 0.1X^2 + \varepsilon$.
  - 30 cases with $X \sim N(100, 16^2)$ and $\varepsilon \sim N(0, 10^2)$.
  - Summary statistics:

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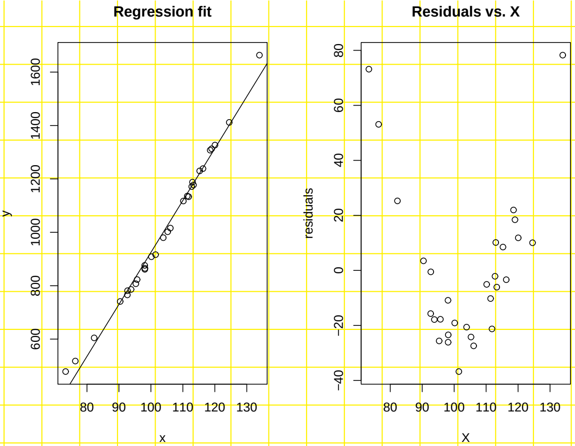
$\sqrt{MSE} = 28.78$, $R^2 = 0.9894$, $R_a^2 = 0.989$.

Note that R^2 is very large.



Here, the scatter plot (left) is not very effective in showing the nonlinearity: the observations Y_i are close to the fitted values $\widehat{Y}_i$ due to the steep slope of the fitted regression line.

Detection of Nonconstancy in Variance

- **If the residual vs. predictor variable plot (or residual vs. fitted value plot) shows**

  , then this is an indication of unequal variance.

Detection of Nonconstancy in Variance

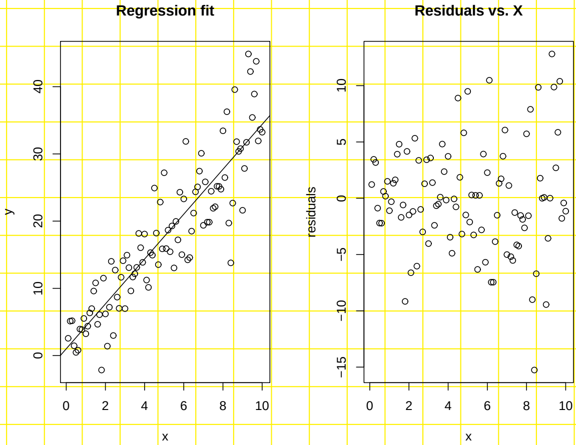
- **If the residual vs. predictor variable plot (or residual vs. fitted value plot) shows an unequal spread of the residuals along the x-axis, then this is an indication of unequal variance.**
- Sometimes, the variance of the error may depend on the value of the predictor variable.
    - Variance increases (or decreases) with the value of X: e.g., in financial data, the volume of transactions usually has a role in the uncertainty of the market.
    - Data may come from different strata with different variabilities: e.g., different measuring instruments with different precisions may have been used to obtain the observations.

True model : $Y = 2 + 3X + \sigma(X)\varepsilon$, where $\log\sigma^2(X) = 1 + 0.1X$.

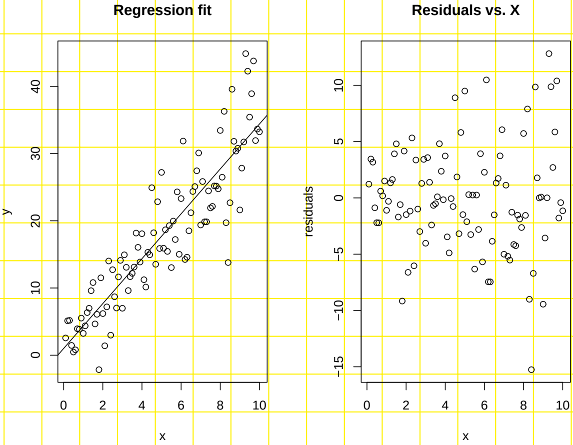
- 100 cases with $X_i = \frac{i}{10}$ and $\varepsilon_i \sim N(0,1)$, $i = 1, \ldots, 100$.
- Simple linear regression model was fitted to this data.

Coefficients	Estimate	Std. Error	t-statistic	P-value
Intercept	1.0074	0.9729	1.035	0.303
Slope	3.3382	0.1673	19.958	$< 2 \times 10^{-16}$

$\sqrt{MSE} = 4.828$, $R^2 = 0.8026$.



Note the spread of the residuals with the value of X.



Note the spread of the residuals increases with the value of X.

Detection of Nonnormality

- **Normality of the errors can be examined by a normal probability plot, a.k.a. Q-Q plot.**
    - $z_{(k)}$'s: the *theoretical quantiles* under Normality
    - $e_{(k)}$'s: the *sample quantiles or empirical quantiles*.
    - Q-Q plot is simply a scatter plot of $e_{(k)}$'s vs. $z_{(k)}$'s.

Notes: Q-Q stands for quantile-quantile.

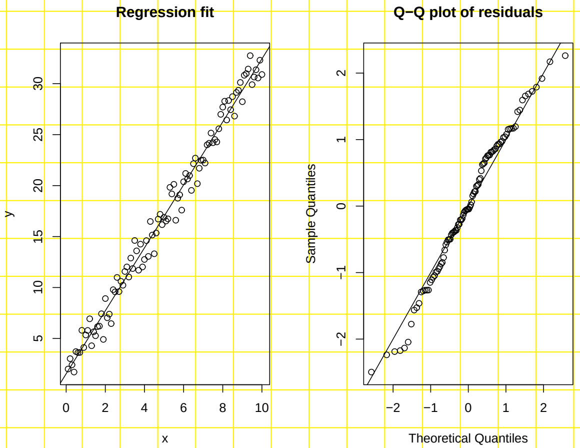
How to Read a Q-Q Plot?

- If the errors are indeed normally distributed, then the points on the Q-Q plot should be .
- Departures from that could indicate **skewed** (non-symmetry) or **heavy-tailed** (probability mass in tails than a Normal distribution) distributions.
- Other types of departures (e.g., nonlinearity) may affect the distribution of the residuals and render them non-normal. **Thus it is better to examine other types of departures before checking normality.**

How to Read a Q-Q Plot?

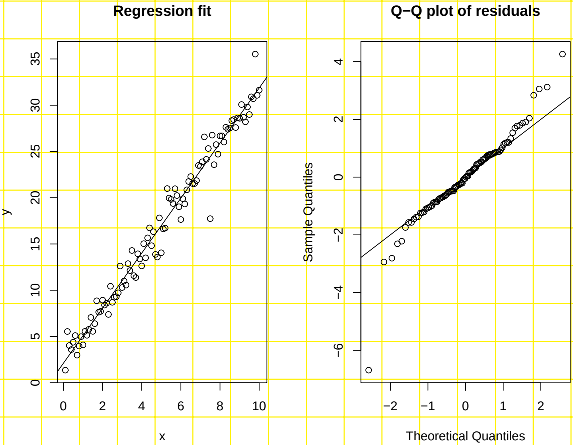
- If the errors are indeed normally distributed, then the points on the Q-Q plot should be nearly on a straight line.
- Departures from that could indicate **skewed** (non-symmetry) or **heavy-tailed** (more probability mass in tails than a Normal distribution) distributions.
- Other types of departures (e.g., nonlinearity) may affect the distribution of the residuals and render them non-normal. **Thus it is better to examine other types of departures before checking normality.**

True model : $Y = 2 + 3X + \varepsilon$. $\varepsilon \sim N(0, 1)$.



Q-Q plot shows a pattern.

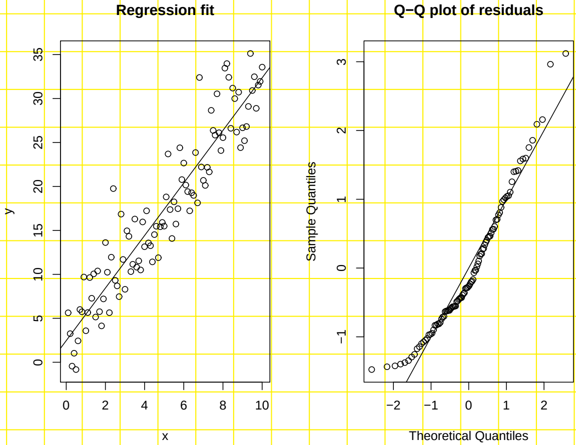
True model : $Y = 2 + 3X + \varepsilon$. $\varepsilon \sim t_{(5)}$ – symmetrical but heavy-tailed errors.



Q-Q plot shows

than a Normal distribution.

True model : $Y = 2 + 3X + \varepsilon$. $\varepsilon \sim \chi^2_{(5)}$ – right-skewed errors.



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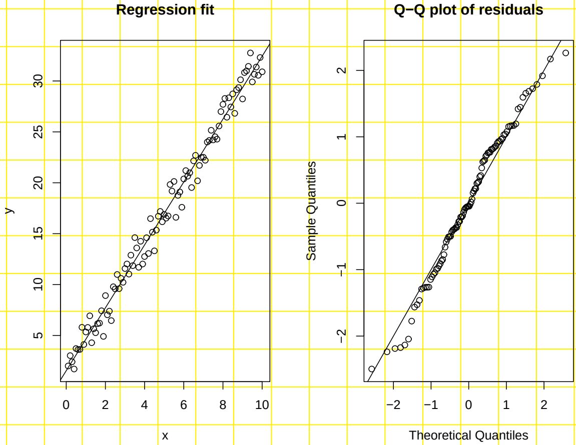
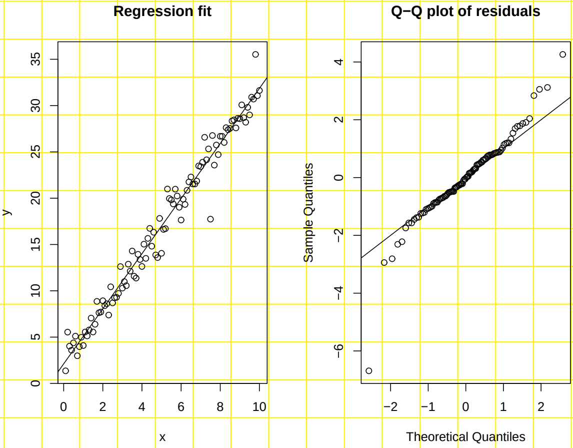


Q-Q plot shows a straight line pattern.

True model : $Y = 2 + 3X + \varepsilon$. $\varepsilon \sim t_{(5)}$ – symmetrical but heavy-tailed errors.



Q-Q plot shows more probabilities in both tails compared with Normal distribution.

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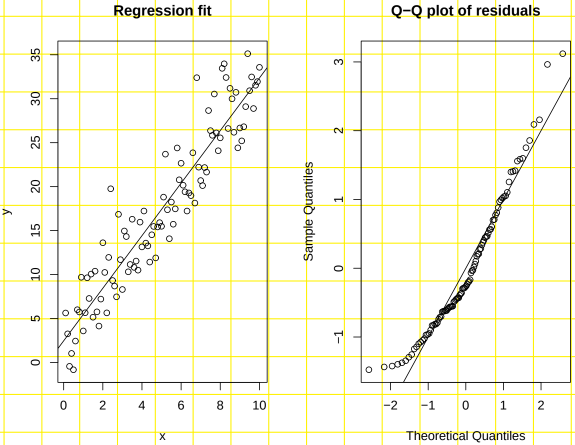

Q-Q plots shows more probabilities in the right tail and less probabilities in the left tail compared with Normal distribution.

Transformations to Treat Unequal Variance and Nornormality

- Unequal variance and nornormality often appear together.
- Transformations on Y may fix the error distributions.
  - $Y' = \sqrt{Y}$
  - $Y' = \log Y$
  - $Y' = 1/Y$
  - Sometimes, add a constant to the transformation, e.g., $Y' = \log(c + Y)$, to avoid negative or nearly zero values.
- A member from the family of power transformations may be chosen automatically by the **Box-Cox** procedure.
- Sometimes, a simultaneous transformation on X may be needed to maintain a linear relationship.

Box-Cox Procedure

- For each $\lambda \in R$, standardize Y_i^λ such that the magnitude of SSE does not depend on λ:

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

with

$$K_2 = (\prod_{i=1}^{n} Y_i)^{1/n}, \;\; K_1 = 1/K_2^{\lambda-1}.$$

- Notes: $\lambda = 0$ corresponds to the logarithm transformation.
- For each λ, fit a regression model on the transformed data Y_i^* and derive $SSE(\lambda)$ (or maximum loglikelihood).
- Find the λ that maximizes loglikelihood.

(*Notes:* Read the lab 2 handout on Box-Cox procedure.)

Simple Linear Regression in Matrix Form

The regression equations:

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

can be written in a compact matrix form:

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

Simple Linear Regression in Matrix Form

The regression equations:

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

can be written in a compact matrix form:

$$\underset{n\times 1}{\mathbf{Y}} = \underset{n\times 2}{\mathbf{X}} \underset{2\times 1}{\boldsymbol{\beta}} + \underset{n\times 1}{\boldsymbol{\epsilon}}.$$

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

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

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

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

- **Design matrix**: an $n \times 2$ 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**: a 2×1 column vector:

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

- Model assumptions:

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

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

- Matrix form:

- In terms of the response vector **Y**:

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- Matrix form:

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

- In terms of the response vector:

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

- $\mathbf{0}_n$ is the $n \times 1$ zero vector, $\mathbf{I}_n$ is the $n \times n$ identity matrix.
- Mean of the error vector:

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

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Variance-covariance matrix of the error vector:

$$\boldsymbol{\sigma}^{2}\{\boldsymbol{\epsilon}\} : \quad = \begin{bmatrix} Var(\epsilon_1) & Cov(\epsilon_1, \epsilon_2) & \cdots & Cov(\epsilon_1, \epsilon_n) \\ Cov(\epsilon_2, \epsilon_1) & Var(\epsilon_2) & \cdots & Cov(\epsilon_2, \epsilon_n) \\ \vdots & \vdots & \vdots & \vdots \\ Cov(\epsilon_n, \epsilon_1) & Cov(\epsilon_n, \epsilon_2) & \cdots & Var(\epsilon_n) \end{bmatrix}$$

$$=$$

Variance-covariance matrix of the error vector:

$$
\begin{aligned}
\boldsymbol{\sigma}^{\mathbf{2}}\{\boldsymbol{\epsilon}\} : \quad &= \begin{bmatrix} Var(\epsilon_1) & Cov(\epsilon_1, \epsilon_2) & \cdots & Cov(\epsilon_1, \epsilon_n) \\ Cov(\epsilon_2, \epsilon_1) & Var(\epsilon_2) & \cdots & Cov(\epsilon_2, \epsilon_n) \\ \vdots & \vdots & \vdots & \vdots \\ Cov(\epsilon_n, \epsilon_1) & Cov(\epsilon_n, \epsilon_2) & \cdots & Var(\epsilon_n) \end{bmatrix} \\
&= \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} = \sigma^2 \mathbf{I}_n.
\end{aligned}
$$

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

$$\mathbf{E}\{\mathbf{Y}\} = \begin{bmatrix} E(Y_1) \\ E(Y_2) \\ \vdots \\ E(Y_i) \\ \vdots \\ E(Y_n) \end{bmatrix} =$$

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

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

Summary: Simple Linear Regression in Matrix Form

$$\underset{n\times 1}{\mathbf{Y}} = \underset{n\times 2}{\mathbf{X}}\ \underset{2\times 1}{\boldsymbol{\beta}} + \underset{n\times 1}{\boldsymbol{\epsilon}}.$$

- $\boldsymbol{\epsilon}$ is a random vector with $\mathbf{E}\{\boldsymbol{\epsilon}\} = \mathbf{0}_n,\ \boldsymbol{\sigma}^2\{\boldsymbol{\epsilon}\} = \sigma^2\mathbf{I}_n$.
- Normal error model: $\boldsymbol{\epsilon} \sim \mathrm{Normal}_n(\mathbf{0}_n, \sigma^2\mathbf{I}_n)$.

Least Squares Estimation in Matrix Form

- Least squares criterion:

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

- Matrix form :

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

- Differentiate Q 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:

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y}. \tag{1}$$

Least-square estimators are the solutions of equation (1).

- Multiply both sides of equation (1) 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

- **LS estimators**:

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

- The left hand side becomes

$$\mathbf{I}_2\mathbf{b} = \mathbf{b}$$

- **LS estimators**:

$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}. \tag{2}$$

$$\mathbf{X}'\mathbf{X} =$$

Note that $\mathbf{X}'\mathbf{X}$ *and* $(\mathbf{X}'\mathbf{X})^{-1}$ *are* *matrices.*

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

When

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

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

Note that $\mathbf{X}'\mathbf{X}$ *and* $(\mathbf{X}'\mathbf{X})^{-1}$ *are symmetric positive definite matrices.*

- LS estimators:

$$\begin{bmatrix}\hat{\beta}_0 \\ \hat{\beta}_1\end{bmatrix} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \qquad\qquad ,$$

  provided that X_is are .
- $n \times 1$ vector of fitted values:

$$\widehat{\mathbf{Y}} = \qquad\qquad ,$$

  where $\mathbf{H} := \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ is called the .
- $n \times 1$ vector of residuals:

$$\mathbf{e} = \qquad\qquad .$$

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

- LS estimators:

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

provided that X_is are not all equal.

- $n \times 1$ vector of fitted values:

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

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

- $n \times 1$ vector of residuals:

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

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

Hat Matrix

$$\underset{n\times n}{\mathbf{H}} := \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'.$$

$\mathbf{H}$ and $\mathbf{I}_n - \mathbf{H}$ are **projection matrices.**

- Symmetric:
- **Idempotent**:
- Moreover, $rank(\mathbf{H}) =$, $rank(\mathbf{I}_n - \mathbf{H}) =$.

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$\mathbf{H}$ and $\mathbf{I}_n - \mathbf{H}$ are **projection matrices**.

- Symmetric:

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

- **Idempotent**:

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

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

Column Space of the Design Matrix X

- Let $\mathbf{1}_n$ denote the $n \times 1$ vector of ones and $\mathbf{x} = (X_1, \cdots, X_n)^T$ denote the $n \times 1$ vector of design points.
- The design matrix
$$\mathbf{X} = (\mathbf{1}_n, \mathbf{x}).$$
- $\langle X \rangle$ is the
- $\langle X \rangle =$

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- Let $\mathbf{1}_n$ denote the $n \times 1$ vector of ones and $\mathbf{x} = (X_1, \cdots, X_n)^T$ denote the $n \times 1$ vector of design points. item The design matrix
$$\mathbf{X} = (\mathbf{1}_n, \mathbf{x}).$$
- $\langle X \rangle$ is the linear subspace of $\mathbf{R}^n$ generated by the columns of $\mathbf{X}$.
- $\langle X \rangle = \{c_0 \mathbf{1}_n + c_1 \mathbf{x} = \mathbf{X}\mathbf{c} : c_0, c_1 \in R, \mathbf{c} = (c_0, c_1)^T\}$.