Simple Linear Regression

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Simple linear regression in Weisberg's notation

Mean Function:

$$\mathrm{E}[Y|X=x] = \beta_0 + \beta_1 x,$$

Variance Function:

$$\mathrm{Var}[Y|X=x] = \sigma^2,$$

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Other common notation:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \text{ where } i = 1, \ldots, n, \epsilon_i \text{ iid, with}$$
$$\mathrm{E}[\epsilon_i|X = x] = 0 \text{ and } \mathrm{Var}[\epsilon_i|X = x] = \sigma^2.$$

Simple linear regression: Assumptions

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- Errors ϵ are independent (the error for one case gives no information about the error for another case).
- Errors are assumed to be normally distributed.
  Note: The normality assumption is much stronger than we need in many cases (e.g., see Weisberg p.22). It is used primarily for inference (tests and confidence intervals) with small sample sizes.

OLS Estimation

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One way to estimate β_0 and β_1 is to find values $\hat{\beta}_0$ and $\hat{\beta}_1$ that minimize the residual sum of squares:

$$
\begin{aligned}
RSS(\beta_0, \beta_1) &= \sum_{i=1}^{n} [y_i - (\beta_0 + \beta_1 x_i)]^2 \\
&= \sum_{i=1}^{n} \epsilon_i^2
\end{aligned}
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- setting the partial derivatives of RSS (residual sum of squares) with respect to β_0 and β_1 equal to zero

$$\frac{\partial RSS}{\partial \beta_0} = \sum_{i=1}^{n}(2\beta_0 - 2y_i + 2\beta_1 x_i) = 0$$

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The values of $\hat{\beta}_0$ and $\hat{\beta}_1$ obtained in such a way are called **ordinary least squares estimates** (OLS estimates) of β_0 and β_1.

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For example:

- Errors: $\epsilon_i = y_i - \beta_0 - \beta_1 x_i$, $i = 1, \dots, n$,
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And also:

- Observed value: y_i, $i = 1, \ldots, n$,
- Fitted value: $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$, $i = 1, \ldots, n$.

The OLS estimates for slope and intercept

$$\hat{\beta}_1 = \frac{SXY}{SXX}$$
$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x},$$

where SXY is the sum of cross-products of the deviations of x_i and y_i from their means:

$$SXY = \sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y}),$$

and SXX is the sum of squared deviations of x_i from the sample mean of x:

$$SXX = \sum_{i=1}^{n} (x_i - \overline{x})^2$$

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Then

$$\hat{\beta}_1 = \frac{s_{xy}}{SD_x^2} = \frac{SXY(n-1)}{(n-1)SXX} = \frac{SXY}{SXX}.$$

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Verify by plugging in $\overline{x}$, $\overline{y}$ and the OLS estimates into the mean function for the simple regression:

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Interpretation of $\hat{\beta}_0$ and $\hat{\beta}_1$: Fitting the regression

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \text{ with } \epsilon_i \sim \mathcal{N}(0, \sigma^2), \epsilon_i \text{ iid},$$

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we obtain estimates for $\hat{\beta}_0$ and $\hat{\beta}_1$.

- $\hat{\beta}_0$ - The estimated average value of y for $x = 0$,
- $\hat{\beta}_1$ - For every unit increase of x, we estimate that y increases by $\hat{\beta}_1$ on average.

Example: Forbes data

Find the OLS estimates for the regression of pressure on temperature, given:

$$\bar{x} = 202.9529$$

$$\bar{y} = 25.05882$$

$$SXX = 530.7824$$

$$SXY = 277.5421$$

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$$SXX = 530.7824$$
$$SXY = 277.5421$$

Using the formulae for OLS estimates of $\hat{\beta}_0$ and $\hat{\beta}_1$, we obtain

$$\hat{\beta}_1 = \frac{277.5421}{530.7824} \approx 0.523$$
$$\hat{\beta}_0 = 25.05882 - 0.523 * 202.9529 \approx -81.064$$

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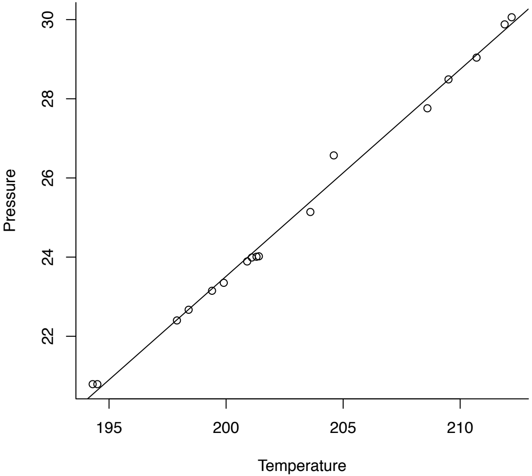

OLS properties

Property 1.

$\hat{\beta}_0$ and $\hat{\beta}_1$ can be written as linear functions of $y_1, \ldots, y_n$, e.g.,

$$\hat{\beta}_1 = \sum_{i=1}^{n} c_i y_i, \text{ where } c_i = \frac{x_i - \bar{x}}{SXX}.$$

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Proof:

$$\begin{aligned}
\hat{\beta}_1 &= \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{SXX} \\
&= \frac{\sum_{i=1}^{n}(x_i - \overline{x})y_i}{SXX} - \overline{y}\frac{\sum_{i=1}^{n}(x_i - \overline{x})}{SXX} \\
&= \sum_{i=1}^{n} c_i y_i - \frac{\overline{y}}{SXX}\left(\frac{n\sum_{i=1}^{n} x_i}{n} - n\overline{x}\right) = \sum_{i=1}^{n} c_i y_i
\end{aligned}$$

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Exercise: Find d_i, $i = 1, \ldots, n$ such that $\hat{\beta}_0 = \sum_{i=1}^{n} d_i y_i$.

OLS properties

Property 2. If $\mathrm{E}[\epsilon_i | X = x] = 0$, for all $i = 1, \ldots, n$, $\hat{\beta}_0$ and $\hat{\beta}_1$ are unbiased estimators of β_0 and β_1, that is, $\mathrm{E}[\hat{\beta}_0 | X = x] = \beta_0$ and $\mathrm{E}[\hat{\beta}_1 | X = x] = \beta_1$.

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Proof:

$$\begin{aligned}
\mathrm{E}[\hat{\beta}_1|X=x] &= \mathrm{E}[\sum_{i=1}^{n} c_i y_i|X=x] = \sum_{i=1}^{n} c_i \mathrm{E}[y_i|X=x] \\
&= \sum_{i=1}^{n} c_i(\beta_0+\beta_1 x_i) = \beta_0 \sum_{i=1}^{n} c_i + \beta_1 \sum_{i=1}^{n} c_i x_i \\
&= \frac{\beta_0}{SXX}\sum_{i=1}^{n}(x_i-\overline{x}) + \beta_1 \sum_{i=1}^{n} \frac{x_i(x_i-\overline{x})}{SXX}
\end{aligned}$$

OLS properties

Proof continued: (For $\hat{\beta}_1$, given $X = x$)

$$
\begin{aligned}
\mathrm{E}[\hat{\beta}_1 | X = x] &= \frac{\beta_0}{SXX} \sum_{i=1}^{n} (x_i - \overline{x}) + \beta_1 \sum_{i=1}^{n} \frac{x_i (x_i - \overline{x})}{SXX} \\
&= \beta_1 \frac{\sum_{i=1}^{n} x_i (x_i - \overline{x})}{\sum_{i=1}^{n} (x_i - \overline{x})(x_i - \overline{x})} \\
&= \beta_1 \frac{[\sum_{i=1}^{n} x_i (x_i - \overline{x}) - \overline{x}(x_i - \overline{x}) + \overline{x}(x_i - \overline{x})]}{\sum_{i=1}^{n} (x_i - \overline{x})(x_i - \overline{x})} \\
&= \beta_1 \frac{[\sum_{i=1}^{n} (x_i - \overline{x})(x_i - \overline{x})]}{\sum_{i=1}^{n} (x_i - \overline{x})(x_i - \overline{x})} + \beta_1 \frac{\sum_{i=1}^{n} \overline{x}(x_i - \overline{x})}{SXX} \\
&= \beta_1
\end{aligned}
$$

For the last step, we use the same trick as before to show that the second term is 0.

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Exercise: Show that $\hat{\beta}_0$ is an unbiased estimator of β_0.

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Property 3. If $\mathrm{E}[\epsilon_i|X=x]=0$, $\mathrm{Var}[\epsilon_i|X=x]=\sigma^2$ and the errors ϵ_i are uncorrelated for all $i=1,\ldots,n$,
then the variances of the OLS estimators are:

$$\mathrm{Var}[\hat{\beta}_1|X=x]=\frac{\sigma^2}{SXX},$$

$$\mathrm{Var}[\hat{\beta}_0|X=x]=\sigma^2\left(\frac{1}{n}+\frac{\overline{x}^2}{SXX}\right),$$

$$\mathrm{Cov}[\hat{\beta}_0,\hat{\beta}_1|X=x]=-\sigma^2\frac{\overline{x}}{SXX}.$$

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Proof: Exercise.

OLS properties

Property 4.

The sum of residuals form an OLS fit is zero (as long as $\beta_0 \neq 0$):

$$\sum_{i=1}^{n} \hat{\epsilon}_i = 0.$$

Proof: Exercise.

OLS properties

Gauss-Markov Theorem. Assume $\mathrm{E}[\epsilon_i|X = x] = 0$, $\mathrm{Var}[\epsilon_i|X = x] = \sigma^2$ and the errors ϵ_i are uncorrelated for all $i = 1, \ldots, n$.
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- Note 1: The Gauss-Markov Theorem as stated does not require the assumption of normality of the error terms. Adding the assumption of normality of the errors, one can show that OLS estimators are BLUE estimators among all unbiased estimators (not only linear functions of y's).
- Note 2: The Gauss-Markov Theorem does not tell one to use least squares all the time, but it strongly suggests it.

Residuals

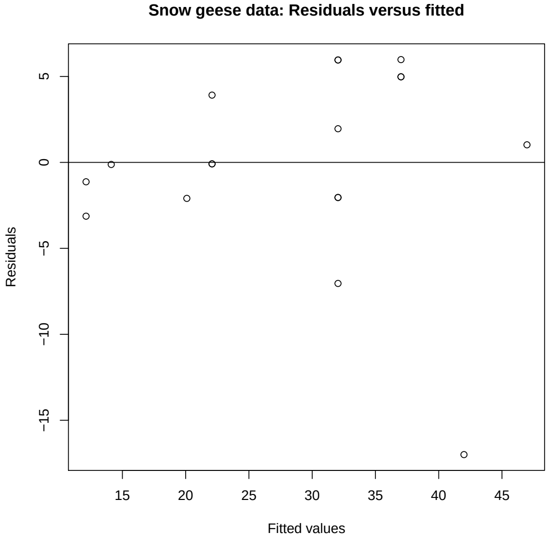
$$\hat{\epsilon}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i$$

Let's examine plot of residuals versus fitted values for the Snow Geese data for violations of the regression assumptions.

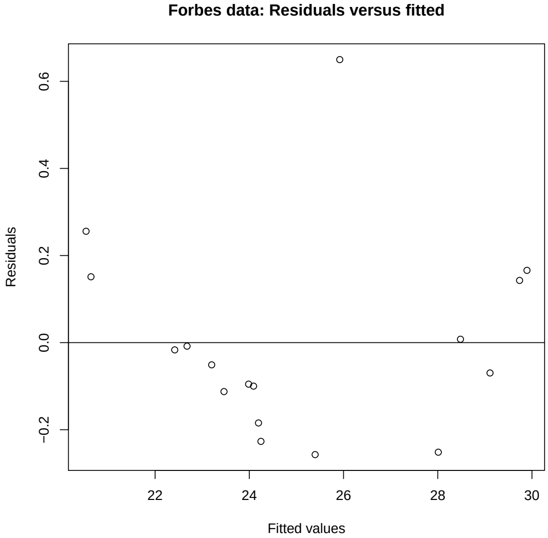
Things we are looking for:

- Curvature of the mean trend (indicates that the mean function is inappropriate);
- Increase or decrease in magnitude when fitted values are increasing (indicates non-constant variance);
- Residuals that are large in magnitude compared to the rest (indicates outliers).

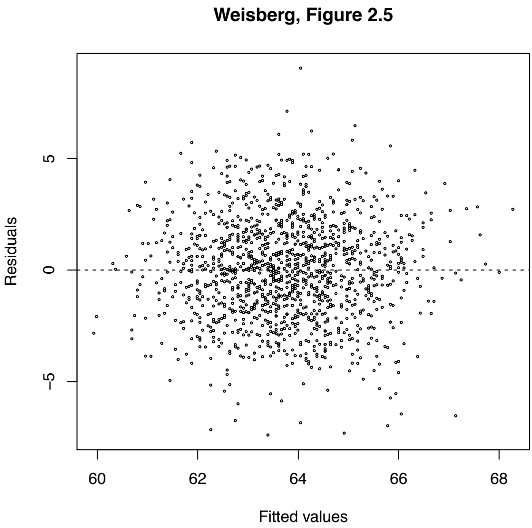
Snow geese data: Residual plot



Forbes data: Residual plot



Heights data: Residual plot



Residual assumption violations

Outliers: What to do with outliers?

In some cases we may know about specific reasons why an outlier was observed. You should not simply remove an outlier from your data without careful consideration.

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Mean trend and non-constant variance:
We will address some remedies for dealing with curvature in the mean trend and with non-constant variance later in the class.

Normality:
To check for the normality of the errors you can use histograms or normal qq-plots, these will be discussed later in the course.

Independence:
Plot residuals versus index and look for trends. Alternatives: turning point test, runs test, portmanteau test, Durbin-Watson test etc.

Estimating the Residual Variance

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Why? Because estimating parameters imposes constraints, e.g.,

$$\frac{\partial RSS}{\partial \beta_0} = \sum_{i=1}^{n} (2\beta_0 - 2y_i + 2\beta_1 x_i) = 0$$

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$$\hat{\sigma}^2 = \frac{RSS}{n-2},$$

If $\mathrm{E}[\epsilon_i | X = x] = 0$, $\mathrm{Var}[\epsilon_i | X = x] = \sigma^2$ and the errors ϵ_i are uncorrelated for all $i = 1, \ldots, n$, then

$$\mathrm{E}[\hat{\sigma}^2 | X = x] = \sigma^2,$$

the estimate is unbiased.

Estimating the Residual Variance

Note also that

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$$\hat{\sigma}^2 = \frac{0.813143}{17 - 2} \approx 0.054.$$

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Distribution of estimates

Let us come back to simple linear regression:

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Since $\hat{\beta}_0$ and $\hat{\beta}_1$ are linear combinations of $y_1, \ldots, y_n$ (Property 1), then $(\hat{\beta}_0, \hat{\beta}_1)$ follows a **bivariate normal** distribution.

Confidence Intervals

Because $(\hat{\beta}_0, \hat{\beta}_1)$ follow a bivariate normal distribution, when σ^2 is known, the marginal distributions for $\hat{\beta}_0$ and $\hat{\beta}_1$ are univariate normal.

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given that $\epsilon_i | X = x$ iid $\mathcal{N}(0, \sigma^2)$, $i = 1, \ldots, n$. Then

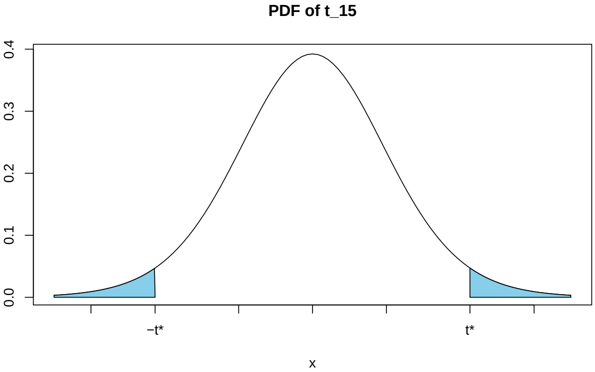
$$\frac{\hat{\beta}_0 - \beta_0}{\sigma^2(\frac{1}{n} + \frac{\overline{x}^2}{SXX})} | X = x \sim \mathcal{N}(0, 1).$$

Since σ^2 is usually not known and is instead estimated as $\hat{\sigma}^2$,

$$\frac{\hat{\beta}_0 - \beta_0}{\hat{\sigma}^2(\frac{1}{n} + \frac{\overline{x}^2}{SXX})} | X = x \sim t_{n-2}.$$

The t-distribution with $n - 2$ degrees of freedom is the appropriate reference distribution for constructing the confidence intervals for $\hat{\beta}_0$ and $\hat{\beta}_1$.

$n = 17$ and we are interested in a 90% CI for β_0



$P\left(\frac{\hat{\beta}_0-\beta_0}{\sqrt{\hat{\sigma}^2/SXX}} \leq |t^*| \middle| X=x\right) = 0.9$, so $t^* = t_{0.95,15}$. Then

$$P\left(-t^* \leq \frac{\hat{\beta}_0-\beta_0}{SE(\hat{\beta}_0|X=x)} \leq t^*\right) = 0.9.$$

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Estimate ± $(1-\alpha/2)$-quantile of the prob. dist. × SE of estimate.

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The interpretation of confidence intervals is based on repeated sampling. If samples of size n are drawn repeatedly and, say, 95% confidence intervals are estimated for the intercept, then 95% of those intervals (on average) would contain the true parameter β_0.

Example: Confidence Interval for $\hat{\beta}_0$

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Given that

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Interpret.