Example: Cats Data

- Let's look at the cats data, where the goal is to describe the relationship between Hwt (heart weight) and Bwt (body weight). As a starting point, we assume the relationship is linear.
- Data $(y_i, x_i)_{i=1}^n$, where $y_i, x_i \in \mathbb{R}$.
- Apparently the data won't be able to fit on a straight line. Assume

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

$$\begin{aligned} (\beta_0, \beta_1) &: \quad \text{unknown regression coefficients,} \\ e_i's &: \quad \text{often assume to have mean } 0 \text{ and variance } \sigma^2 \end{aligned}$$

Overview for SLR (I)

- How to use LS to estimate (β_0, β_1)? We can obtain an explicit expression for $(\hat{\beta}_0, \hat{\beta}_1)$. There is a nice connection between the LS estimate of the slope, $\hat{\beta}_1$, and sample correlation/variance of X and Y, which will help you to remember the expression.

- Throughout we'll pick up some jargons: fitted value, residual, RSS, R-square (used to access the overall model fit).

- How would the LS fitting/inference be affected if the data, X and/or Y, are shifted and/or scaled (i.e., linear transformed)?

- SLR without the intercept: fit a regression line passing the origin.

- How to use `R` to carry out all the analysis and produce relevant graphs.

Parameter Estimation by Least Squares

We would like to choose a line which is close to the data points. We measure the closeness by squared errors[a].

Least Squares Estimation: find $(\hat{\beta}_0, \hat{\beta}_1)$ that minimize the residual sum of squares (RSS)

$$\mathsf{RSS} = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2.$$

To find the solution, we have

$$\begin{aligned} \frac{\partial \mathsf{RSS}}{\partial \beta_0} &= -2 \sum_i (y_i - \beta_0 - \beta_1 x_i) = 0, \\ \frac{\partial \mathsf{RSS}}{\partial \beta_1} &= -2 \sum_i x_i (y_i - \beta_0 - \beta_1 x_i) = 0. \end{aligned}$$

[a] Why squared error? Why not absolute error?

Re-arrange the equations,

$$
\begin{aligned}
\beta_0 n + \beta_1 \sum x_i &= \sum y_i, && (1)\\
\beta_0 \sum x_i + \beta_1 \sum x_i^2 &= \sum x_i y_i. && (2)
\end{aligned}
$$

From (1), we have

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

Plug it back to (2),

$$\left(\bar{y} - \hat{\beta}_1 \bar{x}\right) \sum x_i + \beta_1 \sum x_i^2 = \sum x_i y_i$$

$$\beta_1 \left(\sum x_i^2 - \sum x_i \bar{x} \right) = \sum x_i y_i - \sum x_i \bar{y}$$

$$\hat{\beta}_1 = \frac{\sum x_i y_i - \sum x_i \bar{y}}{\sum x_i^2 - \sum x_i \bar{x}} = \frac{\sum x_i (y_i - \bar{y})}{\sum x_i (x_i - \bar{x})}.$$

Some equalities (basically centering one side is the same as centering both sides for cross-products):

$$\sum_i (x_i - \bar{x})(y_i - \bar{y}) = \sum_i x_i (y_i - \bar{y}) = \sum_i (x_i - \bar{x}) y_i.$$

So the LS estimates of (β_0, β_1) can be expressed as

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x}, \\ \hat{\beta}_1 &= \frac{\mathsf{Sxy}}{\mathsf{Sxx}} = r_{\mathsf{XY}} \left(\frac{\mathsf{Syy}}{\mathsf{Sxx}} \right)^{1/2}, \end{aligned}$$

where

$$\begin{aligned} \mathsf{Sxy} &= \sum (x_i - \bar{x})(y_i - \bar{y}), \\ \mathsf{Sxx} &= \sum (x_i - \bar{x})^2, \quad \mathsf{Syy} = \sum (y_i - \bar{y})^2, \\ r_{\mathsf{XY}} &= \frac{\mathsf{Sxy}}{\sqrt{(\mathsf{Sxx})(\mathsf{Syy})}} \quad \text{(the sample correlation).} \end{aligned}$$

It is not surprising that the LS estimates are related to the sample correlation between X and Y. Recall that SLR assumes the dependence between X and Y is linear. Correlation is exactly the measure used to quantify the linear dependence between two variables[a].

[a] It is easy to construct an example, where Y depends on X via a nonlinear function and their correlation is zero.

Suppose we know the mean, variance of X and Y, and their correlation r. What is your guess of y given x? It seems reasonable to guess the "unit-free, location/scale invariant" version of Y by r times the "unit-free, location/scale invariant" version of X, i.e.,

$$\frac{y-\mu_y}{\sigma_y} \approx r_{\mathsf{xy}} \frac{x-\mu_x}{\sigma_x}.$$ [a]

Replace the mean, variance and correlation by the corresponding sample version:

$$\begin{aligned} \frac{y-\bar{y}}{\sqrt{\mathsf{Syy}}} \approx r_{\mathsf{xy}} \frac{x-\bar{x}}{\sqrt{\mathsf{Sxx}}} \quad &\Longrightarrow \quad y-\bar{y} \approx r_{\mathsf{xy}} \sqrt{\frac{\mathsf{Syy}}{\mathsf{Sxx}}}(x-\bar{x}) \\ &\Longrightarrow \quad y \approx \left(\bar{y} - r_{\mathsf{xy}}\sqrt{\frac{\mathsf{Syy}}{\mathsf{Sxx}}}\bar{x}\right) + \left(r_{\mathsf{xy}}\sqrt{\frac{\mathsf{Syy}}{\mathsf{Sxx}}}\right)x \end{aligned}$$

[a] Of course, if you are given y and want to predict x, then you need to place r_{xy} on the y-side.

Some jargons.

- Fitted value at x_i or the prediction of y_i: $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$.

- Residual at x_i: $r_i = y_i - \hat{y}_i$. Note that the two equations on p6 imply that

$$\sum_i r_i = 0, \quad \sum_i r_i x_i = 0.$$ [a]

- RSS $= \sum_{i=1}^n r_i^2$.

- The error variance is estimated by

$$\hat{\sigma}^2 = \frac{1}{n-2}\text{RSS} = \frac{1}{n-2}\sum_{i=1}^n r_i^2.$$

  The degree of freedom (df) of the residuals is $n-2$. In general

$$df\,(\text{residuals}) = \text{sample-size} - \text{number-of-parameters}.$$

[a] $\sum_i r_i = 0$ implies that the sample mean of $\hat{y}_i$ is just $\bar{y}$.

Goodness of Fit: R-square

Note the total variation (TSS) in y can be decomposed into the summation of RSS and the total variation in the fitted value $\hat{y}$ (FSS):

$$
\begin{aligned}
\sum_i (y_i - \bar{y})^2 &= \sum_i (y_i - \hat{y}_i + \hat{y}_i - \bar{y})^2 = \sum_i (r_i + \hat{y}_i - \bar{y})^2 \\
&= \sum_i r_i^2 + \sum_i (\hat{y}_i - \bar{y})^2 \qquad (3) \\
&= \mathsf{RSS} + \mathsf{FSS},
\end{aligned}
$$

where the cross-product

$$
\sum_i r_i(\hat{y}_i - \bar{y}) = \hat{\beta}_0 \sum_i r_i + \hat{\beta}_1 \sum_i r_i x_i - \bar{y} \sum_i r_i = 0.
$$

Also note that the average of $\hat{y}_i$'s, $\bar{\hat{y}}$, is the same as the average of y_i; this is true because the intercept is included in the model.

A common measure on how well the model fits the data is the so-called coefficient of determination or simply R-square:

$$R^2 = \frac{\sum(\hat{y}_i - \bar{y})^2}{\sum(y_i - \bar{y})^2} = \frac{\mathsf{FSS}}{\mathsf{TSS}} = \frac{\mathsf{TSS} - \mathsf{RSS}}{\mathsf{TSS}} = 1 - \frac{\mathsf{RSS}}{\mathsf{TSS}}.$$

For a given data set where TSS is fixed, so smaller the RSS, larger the R^2.

We can also show that $R^2 = r^2_{\mathsf{XY}}$ (see PP1).

$R^2 = \frac{\mathsf{Var}(\hat{y})}{\mathsf{Var}(y)}$ measures how much variation in the original data y_i's is explained or reduced by the LS fitting. If Y and X are strongly linear dependent, a linear function of X can help to reduce the uncertainty (i.e., variation) of Y.

How Affine Transformations on the Data Affect Regression?

Suppose we have run a SLR model of Y on X.

- If we rescale the data y_i by $\tilde{y}_i = ay_i + b$, and then regress $\tilde{y}_i$ on x_i. How would the LS estimates and R^2 be affected?

- If we rescale the covariates x_i by $\tilde{x}_i = ax_i + b$, and then regress y_i on $\tilde{x}_i$. How would the LS estimates and R^2 be affected?

- If we regression X on Y instead, will the LS line be the same? How about R^2?

Regression Through the Origin

Sometimes we want to fit a line with no intercept (regression through the origin): $y_i \approx \beta_1 x_i$. For example, x_i denotes the intensity level of various exercises and y_i denotes the additional calories you burn with those exercises.

We can estimate β_1 using the LS principle

$$\min_{\beta_1} \sum_{i=1}^{n} (y_i - \beta_1 x_i)^2 \Longrightarrow \hat{\beta}_1 = \frac{\sum_i x_i y_i}{\sum_i x_i^2}.$$

The ordinary definition of R-square is no longer meaningful; you could have RSS bigger than TSS, and therefore have a negative R-square, if you use formula $R^2 = 1 - \text{RSS}/\text{TSS}$.

The ordinary R-square measures the effect of X after removing the effect of the intercept by centering both y_i's and $\hat{y}_i$'s. For regression models with no intercept, we shouldn't do the centering when computing R-square.

Let's look at the following decomposition (slightly different from (3))

$$\sum_i y_i^2 = \sum_i (y_i - \hat{y}_i + \hat{y}_i)^2 = \sum_i (y_i - \hat{y}_i)^2 + \sum_i \hat{y}_i^2.$$

Then define R-square for regression with no intercept as

$$\tilde{R}^2 = \frac{\sum_i \hat{y}_i^2}{\sum_i y_i^2} = 1 - \frac{\mathsf{RSS}}{\sum_i y_i^2}.$$

Remarks

- I want to emphasize here that $(\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2)$ are not the values of the true parameters $(\beta_0, \beta_1, \sigma^2)$, but estimates/estimators. This is why we put a hat on those symbols. If we happen to collect another data set, their values would be different; they are functions of the data, and therefore they are random variables.

- Next we'll *1)* check the statistical properties (such as unbiasedness or MSE) of those estimates, and *2)* do some statistical inference under the normal assumption.

Overview for SLR (II)

- Regarding the statistical properties of the LS estimates, we first check the properties of $(\hat{\beta}_0, \hat{\beta}_1)$ as an estimate of the true coefficient vector (β_0, β_1).
- We'll compute their mean, variance and covariance, and then show that they are unbiased.
- We can also show that they achieve the smallest MSE among all unbiased estimators, but we'll show this result as a general result when discussing MLR.
- Till this point, we only need to assume the 1st and 2nd moments of e_i's, i.e., $\mathbb{E}e_i = 0$, Var$(e_i) = \sigma^2$, Cov$(e_i, e_j) = 0, \; i \neq j$.

- For hypothesis testing and construct confidence/prediction intervals, we need to derive the distribution of $(\hat{\beta}_0, \hat{\beta}_1)$.

- We'll make iid normal assumptions on e_i's, and will use t-dist in testing and interval estimation.

  Of course we could stick to the original weaker assumption on just the 1st and 2nd moments, and then call CLT to approximate the distribution of $(\hat{\beta}_0, \hat{\beta}_1)$, as well as some test statistics, by normals, when the sample size n is large enough.

- In most other stat courses, we use uppercase letters for random variables and lowercase for their observed values. However, in stat425, sometimes the uppercase letters are reserved for matrices, so I'll use lowercase letters for random variables as well. Whether a lowercase letter is a rv or a constant is usually clear from the context, but feel free to ask whenever you are confused.

Properties of LS Estimates

Assume: $y_i = \beta_0 + \beta_1 x_i + e_i$, and

$$\mathbb{E}[e_i] = 0, \quad \mathsf{Cov}(e_i, e_j) = \sigma^2 \delta_{ij}, \tag{4}$$

where $\delta_{ij} = 1$, if $i = j$ and 0, otherwise. The assumption (4) on the 1st and 2nd moments of the error term leads to the following assumption on the 1st and 2nd moments of Y conditioning on X:

$$\mathbb{E}[y_i \mid x_i] = \beta_0 + \beta_1 x_i, \quad \mathsf{Cov}[y_i, y_j \mid x_i, x_j] = \sigma^2 \delta_{ij},$$

where $\delta_{ij} = 1$ if $i = j$ and 0 if $i \neq j$.

In stat425, the statistical assumption is on the conditional distribution of Y given X. So when we evaluate expectations, only y_i's are random and x_i's are treated as given, non-random constants.

LS estimates are unbiased.

$$
\begin{aligned}
\hat{\beta}_1 &= \sum_i \frac{(x_i - \bar{x})}{\mathsf{Sxx}} y_i = \sum_i c_i y_i, \quad \sum_i c_i = 0 \\
\mathbb{E}\hat{\beta}_1 &= \sum_i c_i \mathbb{E} y_i = \sum_i c_i(\beta_0 + \beta_1 x_i) = \beta_1 \Big(\sum_i c_i x_i \Big) = \beta_1 \\
\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\
\mathbb{E}\hat{\beta}_0 &= \Big(\frac{1}{n} \sum_i \mathbb{E} y_i \Big) - \bar{x} \cdot \mathbb{E}\hat{\beta}_1 = \beta_0 + \beta_1 \bar{x} - \beta_1 \bar{x} = \beta_0
\end{aligned}
$$

MSE of the LS estimates (since they are unbiased, MSE $=$ Var).

$$\mathsf{Var}(\hat{\beta}_1) = \mathsf{Var}\big(\sum_i c_i y_i\big) = \sigma^2 \sum c_i^2 = \sigma^2 \frac{1}{\mathsf{Sxx}}.$$

$$\mathsf{Var}(\hat{\beta}_0) = \sigma^2 \Big(\frac{1}{n} + \frac{\bar{x}^2}{\mathsf{Sxx}}\Big).^{\mathrm{a}}$$

Both MSEs reciprocally depend on Sxx. So to reduce the error, we should only include kittens and overweight cats?

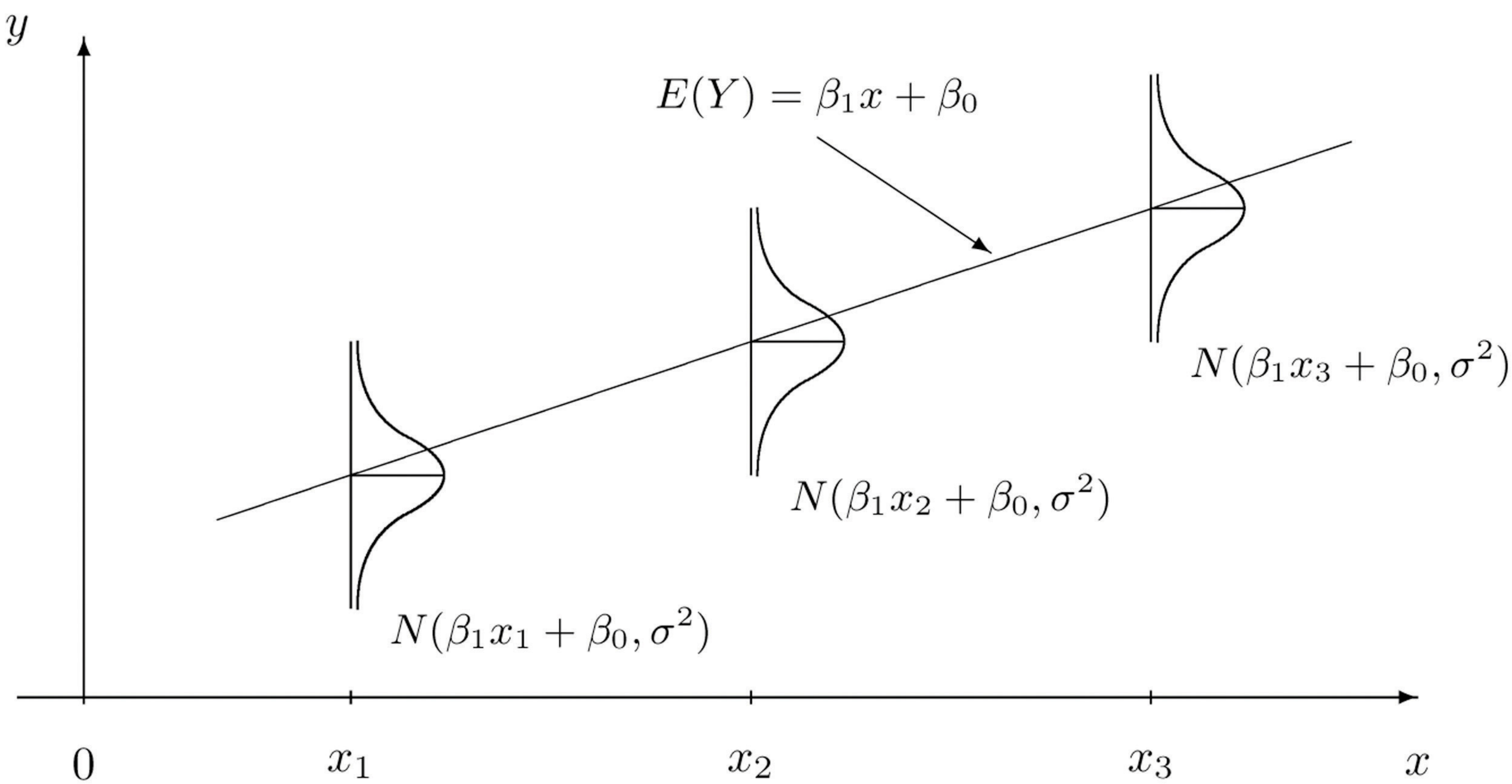
[a] We can write $\hat{\beta}_0 = \bar{y} - \sum_i c_i y_i \bar{x} = \sum_i \Big(\frac{1}{n} - c_i \bar{x}\Big) y_i$.

Normal Assumptions

Assume: $y_i = \beta_0 + \beta_1 x_i + e_i$, and

$$e_i \text{ iid } \sim \mathsf{N}(0, \sigma^2), \text{ or equivalently, } y_i \text{ indep.} \sim \mathsf{N}(\beta_0 + \beta_1 x_i, \sigma^2).$$

- The mean function is linear: $\mathbb{E}(y_i) = \beta_0 + \beta_1 x_i$.
- Errors e_i's are independent; data y_i's are independent.
- Errors e_i's have homogeneous variance: $\mathrm{Var}(e_i) = \sigma^2$, and so are data y_i's.
- Each e_i is normally distributed and each y_i is normally distributed.
- Note that each e_i is normal + independence, so they are jointly normal. Consequently y_i's are jointly normal, and so are any linear combinations of y_i's, which is an important result that will be used later in our inference.


y
$E(Y) = \beta_1 x + \beta_0$
$N(\beta_1 x_3 + \beta_0, \sigma^2)$
$N(\beta_1 x_2 + \beta_0, \sigma^2)$
$N(\beta_1 x_1 + \beta_0, \sigma^2)$
0
x_1
x_2
x_3
x

Distributions of the LS estimates

- $\hat{\beta}_0$ and $\hat{\beta}_1$ are jointly normally distributed with

$$
\begin{aligned}
\mathbb{E}\hat{\beta}_1 &= \beta_1, & \mathsf{Var}(\hat{\beta}_1) &= \sigma^2 \frac{1}{\mathsf{Sxx}} \\
\mathbb{E}\hat{\beta}_0 &= \beta_0, & \mathsf{Var}(\hat{\beta}_0) &= \sigma^2 \Big(\frac{1}{n} + \frac{\bar{x}^2}{\mathsf{Sxx}} \Big) \\
& & \mathsf{Cov}(\hat{\beta}_0, \hat{\beta}_1) &= -\sigma^2 \frac{\bar{x}}{\mathsf{Sxx}}.
\end{aligned}
$$

- $\mathsf{RSS} \sim \sigma^2 \chi^2_{n-2}$ and therefore

$$\mathbb{E}\hat{\sigma}^2 = \frac{\mathbb{E}\ \mathsf{RSS}}{n-2} = \sigma^2.$$

- $(\hat{\beta}_0, \hat{\beta}_1)$ and RSS are independent (which will be proved for MLR later).

Hypothesis Testing

- Test $H_0 : \beta_1 = c$ versus $H_a : \beta_1 \neq c$
- The test statistic

$$t = \frac{\hat{\beta}_1 - c}{\mathsf{se}(\hat{\beta}_1)} = \frac{\hat{\beta}_1 - c}{\hat{\sigma}/\sqrt{\mathsf{Sxx}}} \sim T_{n-2} \text{ under } H_0.$$

- p-value $= 2 \times$ the area under the T_{n-2} dist more extreme than the observed statistic t.
- The p-value returned by the R command lm is for the test with $H_0 : \beta_1 = 0$.

F-test and ANOVA

An alternative way to test $\beta_1 = 0$ is based on the F-test. Recall the following decomposition of the variance: TSS $=$ FSS $+$ RSS.

Sum of Squares	Expression	df
TSS	$\sum_i (y_i - \bar{y})^2$	$n-1$
FSS	$\sum_i (\hat{y}_i - \bar{y})^2$	1
RSS	$\sum_i (y_i - \hat{y}_i)^2$	$n-2$

If $\beta_1 \neq 0$, we would expect a large amount of variation in Y is explained by the regression model, i.e., FSS is large. But how *large* is large? For the `cats` data, if we measure `Hwt` by kg, FSS will be much smaller, but whether `Bwt` is a good predictor for `Hwt` shouldn't be affected by the scale of `Hwt`.

Source	df	SS	MS	F
Regression	1	FSS	FSS/1	MS(reg)/MS(err)
Error	$n-2$	RSS	RSS/$(n-2)$	
Total	$n-1$	TSS		

Under $H_0 : \beta_1 = 0$, the F-test statistic (scale-invariant)

$$F = \frac{\text{MS(reg)}}{\text{MS(err)}} = \frac{\text{FSS}}{\text{RSS}/(n-2)} \sim F_{1,n-2}.$$

It can be shown that the F-test statistic is equal to the square of the t-test statistic (for testing $\beta_1 = 0$) and their p-values (for testing $\beta_1 = 0$) are the same. So they are essentially the same test; in other words, you can ignore the F-test in the `R` output for SLR.

Estimation/Prediction at A New Case

The LS line can be used to obtain values of the response (Y_*) for given values of the predictor ($X = x_*$). There are two variants of this problem. [a]

1. Estimation of the mean response at x_*, i.e., we aim to estimate

$$\beta_0 + \beta_1 x_*$$

2. Prediction of an outcome Y^* that we might observe at x_*, where

$$Y_* \sim \mathsf{N}(\beta_0 + \beta_1 x_*, \sigma^2)$$

Point estimation and prediction are the same, i.e., the fitted value at x_*

$$\hat{\beta}_0 + \hat{\beta}_1 x_*.$$

[a] "estimation" is associate with a parameter which takes a fixed but unknown value (i.e., not random); "prediction" is associated with a random variable.

However accuracy for estimation and the one for prediction are different. Here we measure accuracy by the averaged squared discrepancy between the point estimation/prediction and their target.

- estimation, the target is $\beta_0 - \beta_1 x_*$, and

$$
\begin{aligned}
& \mathbb{E}(\hat{\beta}_0 + \hat{\beta}_1 x_* - \beta_0 - \beta_1 x_*)^2 \\
= \quad & \mathsf{Var}(\hat{\beta}_0 + \hat{\beta}_1 x_*) \\
= \quad & \mathsf{Var}(\hat{\beta}_0) + (x_*)^2 \mathsf{Var}(\hat{\beta}_1) + 2x_* \mathsf{Cov}(\hat{\beta}_0, \hat{\beta}_1) \\
= \quad & \sigma^2 \Big(\frac{1}{n} + \frac{(x_* - \bar{x})^2}{\mathsf{Sxx}} \Big)
\end{aligned}
$$

- For prediction, the target is $Y_* = \beta_0 + \beta_1 x_* + e_*$ where $e_* \sim \mathsf{N}(0, \sigma^2)$ and e_*, as the error incurred with a new sample Y_*, is independent of the previous n data points, i.e., independent of $(\hat{\beta}_0, \hat{\beta}_1)$.

$$
\begin{aligned}
& \mathbb{E}(\hat{\beta}_0 + \hat{\beta}_1 x_* - Y_*)^2 \\
= \quad & \mathbb{E}(\hat{\beta}_0 + \hat{\beta}_1 x_* - \beta_0 - \beta_1 x_* - e_*)^2 \\
= \quad & \mathbb{E}(\hat{\beta}_0 + \hat{\beta}_1 x_* - \beta_0 - \beta_1 x_*)^2 + \mathbb{E}(e_*)^2 \\
= \quad & \sigma^2 \Big(1 + \frac{1}{n} + \frac{(x_* - \bar{x})^2}{\mathsf{Sxx}} \Big)
\end{aligned}
$$

$$\text{Error for Estimation} = \sigma^2\Big(\frac{1}{n} + \frac{(x_* - \bar{x})^2}{\text{Sxx}}\Big)$$

$$\text{Error for Prediction} = \sigma^2\Big(1 + \frac{1}{n} + \frac{(x_* - \bar{x})^2}{\text{Sxx}}\Big)$$

- Errors are not the same at all x_*: smaller when x_* is near $\bar{x}$.
- Error for prediction is larger.

There are two sources of uncertainty when doing prediction at x_*: 1) one is from the n sample points $(x_i, y_i)_{i=1}^n$, which is used to estimate the LS line, and 2) one is from the random error $e_* \sim \text{N}(0, \sigma^2)$, which is the error we couldn't avoid if we knew (β_0, β_1). There is why even when the sample size n goes to infinity, we can have the estimation error go to 0 but not the prediction error.

- The $(1-\alpha)$ confidence interval (CI) for $\beta_0 + \beta_1 x_*$

$$\hat{\beta}_0 + \hat{\beta}_1 x_* \ \pm \ t_{n-2}^{(\alpha/2)} \hat{\sigma} \sqrt{\frac{1}{n} + \frac{(x_* - \bar{x})^2}{\mathsf{Sxx}}}$$

- The $(1-\alpha)$ prediction interval (PI) for y^*

$$\hat{\beta}_0 + \hat{\beta}_1 x_* \ \pm \ t_{n-2}^{(\alpha/2)} \hat{\sigma} \sqrt{1 + \frac{1}{n} + \frac{(x_* - \bar{x})^2}{\mathsf{Sxx}}}$$

Here we replace σ, which is usually unknown, by its estimate $\hat{\sigma} = \sqrt{\mathsf{RSS}/(n-2)}$.

Association/Correlation vs Causation

- The statement "X causes Y" means that changing the value of X will change the distribution of Y. When X causes Y , X and Y will be associated but the reverse is not, in general, true. Association does not necessarily imply causation.
- If the data are from a randomized study, then the causal interpretation is correct.
- If the data are from a observational study, then the association interpretation is correct.