

## 0.1 reviewer comment for reference

The statistical evaluation of the fitted model describes a situation to avoid, as I have repeatedly stressed in my graduate level statistics classes. I find that the R2 statistics is overly simplified and overly emphasized. When using the R2 value, students will naturally equate a model with a higher value as a better model, a simplistic, and often misleading, view. Once this idea is introduced, we cannot easily correct the misconception. So, please do not plant the misconception in the first place. The R2 value is a measure of linear association. For a simple linear regression model (with one predictor), the R2 value is the square of the correlation coefficient between x and y when the relationship between x and y is actually linear.

## 0.2 Walk through the regression portion [my potalk](#)

### What is our model?

For linear regression, the model is:

$$y \sim \theta_1 x + \theta_0 + \epsilon \quad (1)$$

Where the slope  $\theta_1$  and the intercept  $\theta_0$  are (in the frequentist interpretation) numbers we have estimated somehow, and  $\epsilon$  is a random variable that represents variability that isn't captured by the linear relationship. Note that this means that y is also a random variable, and we strictly need to write ( $\sim$ : "has the probability distribution of") rather than ( $=$ : "is equal to"). This nuance makes a big difference in everything that follows.

### 0.3 Modeling $\epsilon$

For standard ordinary least squares regression, there are some strong constraints on  $\epsilon$ . It is assumed to be normally distributed with mean 0 and constant variance  $\sigma^2$ . That is," it takes the form:

$$\epsilon(y; \sigma) \approx \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(y - (\theta_1 x + \theta_0))^2}{2\sigma^2}} \quad (2)$$

and this means that the full model also has a probability distribution that is given by:

$$p(y|x; \theta_0, \theta_1, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(y - (\theta_1 x + \theta_0))^2}{2\sigma^2}} \quad (3)$$

How do we use the model to make a prediction? If the underlying process is accurately captured by (3) then if you give me  $(x, \theta_0, \theta_1, \sigma)$  I can say that, if we sampled the process repeatedly, 95% of the time we would get a measurement of y that lay in the range  $\theta_0 + \theta_1 x \pm 2\sigma$  (See [slide 8](#) )

## But I want a number not a confidence interval!

Because we have  $p(y)$ , we can find  $\bar{y}$ , the mean value, or first moment, of  $y$ :

$$\bar{y} = \int_{-\infty}^{\infty} y p(y|x; \theta_0, \theta_1, \sigma^2) dy = \int_{-\infty}^{\infty} (\theta_1 x + \theta_0 + \epsilon) dy = \theta_1 x + \theta_0 \quad (4)$$

This follows since the only thing that is a function of  $y$  is  $\epsilon$ , and  $\bar{\epsilon} = 0$ .

Note that we can also find the probability, for example, that if  $x = 5$ ,  $y > 10$  by doing this integral:

$$\int_{10}^{\infty} p(y|10; \theta_0, \theta_1, \sigma^2) dy \quad (5)$$

## Estimating $\theta_0$ and $\theta_1$

How does a frequentist find estimates of the slope and the intercept? They start with this model, and assume that we have [universes as plenty as blackberries](#) each generating  $(x,y)$  values from the process described by (1).

We can imagine independently drawing a large number of measurements of  $(y,x)$  pairs from the different universes. Since we have the probability distribution of our model, we can calculate the probability that any particular sample  $(x_i, y_i)$  will be observed:

$$p(y_i|x_i; \theta_0, \theta_1, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - (\theta_1 x_i + \theta_0))^2}{2\sigma^2}} \quad (6)$$

Since we are making independent draws, the probability that will see a particular set of  $X \in (x_i, y_i)$  pairs is just the product of each of their individual probabilities:

$$L_X(\theta_0, \theta_1, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \prod_{(x,y) \in X} e^{-\frac{(y - (\theta_1 x + \theta_0))^2}{2\sigma^2}} \quad (7)$$

This is called the “likelihood”.

## Maximum likelihood

Solve this for the set of parameters that give the **maximum likelihood** by taking the log and finding the maximum by setting the derivative = 0 and solving for  $(\theta_0, \theta_1)$ . This gives you the usual relationship for the slope and intercept in terms of the sample statistics  $(\bar{x}, \bar{y})$ . Note that we don't need to know  $\sigma$ , because we're assuming it's constant.

$$l_X(\theta_0, \theta_1, \sigma^2) = \log \left[ \frac{1}{\sqrt{2\pi\sigma^2}} \prod_{(x,y) \in X} e^{-\frac{(y - (\theta_1 x + \theta_0))^2}{2\sigma^2}} \right]$$

$$= -\log(\sqrt{2\pi\sigma^2}) - \frac{1}{2\sigma^2} \sum_{(x,y) \in X} [y - (\theta_1 x + \theta_0)]^2$$

Which yields

$$\bar{y} = \theta_1 \bar{x} + \theta_0 \quad (8)$$

$$\theta_0 = \bar{y} - \theta_1 \bar{x} \quad (9)$$

$$\theta_1 = \frac{\sum_i^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_i^n (x_i - \bar{x})^2} \quad (10)$$

To repeat, we've assumed  $\sigma = \text{constant}$  so the value of particular value of  $\sigma$  doesn't change the location of the maximum. That doesn't mean that it is not still part of the model though.

### Link to ordinary least squares

Miraculously, in the specific case of this model, maximising the likelihood is the same as minimizing  $\chi^2$  so we can just turn that crank, but hopefully not forget all of the above.

### Uncertainty in $\theta_0$ and $\theta_1$

We've found a single estimate of  $(\theta_0, \theta_1)$  for a single sample. What if we draw other samples from different universes? Then you get something like [slide 18](#) and [slide 19](#)

## 0.4 Estimating $\sigma^2$ (Bayesian)

How do we estimate the variance? In my talk, I show how a Bayesian would do this – see [slide 25](#)

## 0.5 Frequentist results

(for completeness, here's a typical set of textbook equations)

### Estimating $\sigma^2$ (frequentist)

Define:

$$\bar{y}_i = \theta_1 x_i + \theta_0 \quad (11)$$

and

$$\widehat{\sigma^2} = \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y}_i)^2 \quad (12)$$

Then an unbiased estimator of  $\sigma^2$  is:

$$\frac{n}{n-2} \widehat{\sigma^2} \quad (13)$$

### Frequentist confidence interval for $\overline{y_i}$

The 95% confidence interval for a prediction  $\overline{y_i}$  at a particular  $x_i$  is

$$\overline{y_i} \pm t_{n-2} s_y \sqrt{\frac{1}{n} + \frac{(x_i - \bar{x})^2}{(n-1)s_x^2}} \quad (14)$$

where

$$s_y = \sqrt{\frac{\sum (y_i - \overline{y_i})^2}{n-2}} \quad (15)$$

## 0.6 Summary

In light of the above, a sentence like:

“The linear regression model can still only weakly predict the October CO2 values based on time.” isn’t quite right, because it’s ignoring the  $\epsilon$  specification that is part of the model. A good model that properly captures an intrinsically large  $\sigma^2$  is going to have low covariance, but that’s the right answer, not a failure of the model.