Assessing accuracy of the LSR line

Chris Cornwell

Feb 13, 2025

Outline

Assuming the data does have a linear relationship

Measuring how well LSR line fits

Outline

Assuming the data does have a linear relationship

Measuring how well LSR line fits

Underlying assumption

- Modeled points in a plane as being from a line, but with noise in the y-coordinate direction. In other words, we assumed an underlying relationship
$$y = mx + b + \varepsilon$$
for some m and b, and a random variable ε[1] that has expected value 0. Alternatively, among the "entire population" there is an LSR line $mx + b$.

[1] ε is called the error term.

Underlying assumption

- Modeled points in a plane as being from a line, but with noise in the y-coordinate direction. In other words, we assumed an underlying relationship
$$y = mx + b + \varepsilon$$
for some m and b, and a random variable ε[1] that has expected value 0. Alternatively, among the "entire population" there is an LSR line $mx + b$.
- Assumption: ε is independent of x.

When we have a data set $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, from the population, our procedure determines an LSR line $\hat{m}x + \hat{b}$. However, $\hat{m}$ and $\hat{b}$ are not the slope and intercept for the population curve m and b.

[1] ε is called the error term.

Example

Simulate noisy linear data: make 30 points, using a standard deviation $\sigma = 0.5$. We'll use slope -1.6 and intercept 0.8.

Example

Simulate noisy linear data: make 30 points, using a standard deviation $\sigma = 0.5$. We'll use slope -1.6 and intercept 0.8.

```
x = np.random.uniform(0, 2, size=30)

def simulate_data(x, std):
    return -1.6*x + 0.8 + np.random.normal(0, std, size=len(x))
y = simulate_data(x, 0.5)
```

Example

Simulate noisy linear data: make 30 points, using a standard deviation $\sigma = 0.5$. We'll use slope -1.6 and intercept 0.8.

```
x = np.random.uniform(0, 2, size=30)

def simulate_data(x, std):
    return -1.6*x + 0.8 + np.random.normal(0, std, size=len(x))
y = simulate_data(x, 0.5)
```

In groups, compute slope and intercept of the LSR line for a size 30 simulated data set; store $\hat{m}$ and $\hat{b}$ (in two lists). Iterate this 1000 times $\longrightarrow$ a list of 1000 slopes and intercepts.

Example

Simulate noisy linear data: make 30 points, using a standard deviation $\sigma = 0.5$. We'll use slope -1.6 and intercept 0.8.

```
x = np.random.uniform(0, 2, size=30)

def simulate_data(x, std):
    return -1.6*x + 0.8 + np.random.normal(0, std, size=len(x))
y = simulate_data(x, 0.5)
```

In groups, compute slope and intercept of the LSR line for a size 30 simulated data set; store $\hat{m}$ and $\hat{b}$ (in two lists). Iterate this 1000 times $\longrightarrow$ a list of 1000 slopes and intercepts.

What is the mean of the slopes and of the intercepts?

Sample statistic, relation to population statistic

This is fundamental to statistics.

- Say that a sample of 2000 people are selected from around the country and their height is measured. Mean of these 2000 heights: sample mean.

Sample statistic, relation to population statistic

This is fundamental to statistics.

- Say that a sample of 2000 people are selected from around the country and their height is measured. Mean of these 2000 heights: sample mean.
- Sample mean differs from the true mean height of the entire population of the country. (Not by much, perhaps.)
  - Weak Law of Large Numbers: if s random samples of 2000 people taken, and each sample mean calculated, as $s \longrightarrow \infty$, mean of the sample means limits (in probability) to population mean.

Sample statistic, relation to population statistic

This is fundamental to statistics.

- Say that a sample of 2000 people are selected from around the country and their height is measured. Mean of these 2000 heights: sample mean.
- Sample mean differs from the true mean height of the entire population of the country. (Not by much, perhaps.)
  - Weak Law of Large Numbers: if s random samples of 2000 people taken, and each sample mean calculated, as $s \longrightarrow \infty$, mean of the sample means limits (in probability) to population mean.
- Analogous thing happens with data from linear relationship with noise – think of parameters $\hat{m}$ and $\hat{b}$ as sample statistics (like sample mean).

Confidence intervals

How close do we suspect $\hat{m}$ and $\hat{b}$ to be to the “true” (population) slope and intercept?

Confidence intervals

How close do we suspect $\hat{m}$ and $\hat{b}$ to be to the "true" (population) slope and intercept?

Standard error (SE): Suppose that for our error term ε, we have $\mathrm{Var}(\varepsilon) = \sigma^2$. Sample size: n.

Confidence intervals

How close do we suspect $\hat{m}$ and $\hat{b}$ to be to the "true" (population) slope and intercept?

Standard error (SE): Suppose that for our error term ε, we have $\mathrm{Var}(\varepsilon) = \sigma^2$. Sample size: n.

Using $\bar{x}$ for the average of $x_1, \ldots, x_n$,

$$SE(\hat{m})^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2};$$

$$SE(\hat{b})^2 = \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \right).$$

Confidence intervals

How close do we suspect $\hat{m}$ and $\hat{b}$ to be to the "true" (population) slope and intercept?

Standard error (SE): Suppose that for our error term ε, we have $\mathrm{Var}(\varepsilon) = \sigma^2$. Sample size: n.

Using $\bar{x}$ for the average of $x_1, \ldots, x_n$,

$$SE(\hat{m})^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2};$$

$$SE(\hat{b})^2 = \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \right).$$

Roughly, these are the amount, on average, that $\hat{m}$ (resp. $\hat{b}$) differs from true slope m (resp. true intercept b).

Confidence intervals

How close do we suspect $\hat{m}$ and $\hat{b}$ to be to the "true" (population) slope and intercept?

Standard error (SE): Suppose that for our error term ε, we have $\mathrm{Var}(\varepsilon) = \sigma^2$. Sample size: n.

Using $\bar{x}$ for the average of $x_1, \ldots, x_n$,

$$SE(\hat{m})^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2};$$

$$SE(\hat{b})^2 = \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \right).$$

Roughly, these are the amount, on average, that $\hat{m}$ (resp. $\hat{b}$) differs from true slope m (resp. true intercept b).

σ is unknown, but can estimate it with **residual standard error**:

$$\hat{\sigma}^2 = RSE^2 = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n-2}.$$

Confidence intervals

How close do we suspect $\hat{m}$ and $\hat{b}$ to be to the "true" (population) slope and intercept?

Formulae:

$$SE(\hat{m})^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2};$$

$$SE(\hat{b})^2 = \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \right).$$

Estimate:

$$\sigma^2 \approx RSE^2 = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n-2}.$$

[2] 95% of the time, these intervals contain m, b.

Confidence intervals

How close do we suspect $\hat{m}$ and $\hat{b}$ to be to the "true" (population) slope and intercept?

Formulae:

$$SE(\hat{m})^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2};$$

$$SE(\hat{b})^2 = \sigma^2\left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right).$$

Estimate:

$$\sigma^2 \approx RSE^2 = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n-2}.$$

Can get (roughly) 95% confidence interval[2] with $\pm 2SE$:

$$(\hat{m} - 2SE(\hat{m}), \hat{m} + 2SE(\hat{m}))$$

and

$$(\hat{b} - 2SE(\hat{b}), \hat{b} + 2SE(\hat{b})).$$

[2] 95% of the time, these intervals contain m, b.

Outline

Assuming the data does have a linear relationship

Measuring how well LSR line fits

Mean Squared Error

How to measure how well the data fits to regression line?

Mean Squared Error

How to measure how well the data fits to regression line?

In linear regression, we found $\hat{y}_i, 1 \le i \le n$ so that the points $(x_1, \hat{y}_1), \ldots, (x_n, \hat{y}_n)$ fit exactly to a line. Could use average of $(y_i - \hat{y}_i)^2$ as our measure.

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2.$$

Mean Squared Error

How to measure how well the data fits to regression line?
In linear regression, we found $\hat{y}_i, 1 \leq i \leq n$ so that the points $(x_1, \hat{y}_1), \ldots, (x_n, \hat{y}_n)$ fit exactly to a line. Could use average of $(y_i - \hat{y}_i)^2$ as our measure.

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2.$$

- Called the mean squared error, MSE, of the LSR line.
- Larger MSE (for same sample size), the farther y_i is from $\hat{y}_i$, on average.

Mean Squared Error

How to measure how well the data fits to regression line?
In linear regression, we found $\hat{y}_i, 1 \leq i \leq n$ so that the points $(x_1, \hat{y}_1), \ldots, (x_n, \hat{y}_n)$ fit exactly to a line. Could use average of $(y_i - \hat{y}_i)^2$ as our measure.

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2.$$

- Called the mean squared error, MSE, of the LSR line.
- Larger MSE (for same sample size), the farther y_i is from $\hat{y}_i$, on average.

Closely related to RSE (residual standard error). Recall,

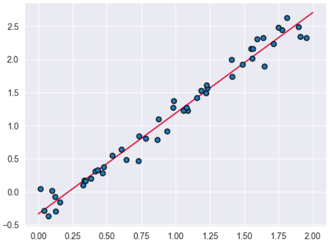
$$\text{RSE} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}.$$

So $\text{MSE} = \frac{n-2}{n}\text{RSE}^2$.

Mean Squared Error, example

Recall, `'Example1.csv'` data. Its LSR line is

$$y = 1.520275x - 0.33458.$$

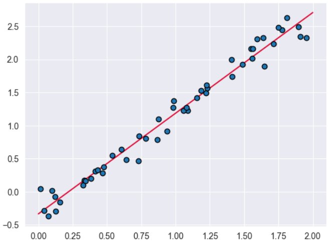


Mean Squared Error, example

Recall, `'Example1.csv'` data. Its LSR line is

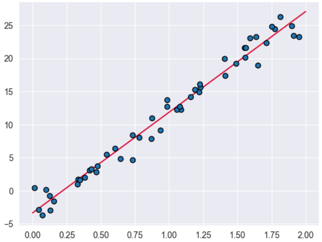
$$y = 1.520275x - 0.33458.$$

The MSE for this data and its LSR line is ≈ 0.0197.
Does that mean that the linear model is a "good fit"?



Mean Squared Error, scaling

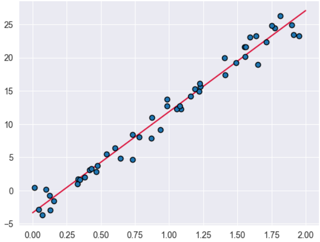
What about the following data and its LSR line? Here, the MSE is 1.9746.



Is it still a good fit?

Mean Squared Error, scaling

What about the following data and its LSR line? Here, the MSE is 1.9746.



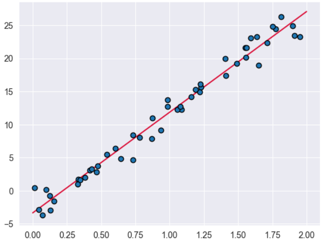
Is it still a good fit?

The data here is from `'Example1.csv'` again, except that the y-coordinates have been multiplied by 10. Its LSR line is

$$y = 15.20275x - 3.3458.$$

Mean Squared Error, scaling

What about the following data and its LSR line? Here, the MSE is 1.9746.



Is it still a good fit?

The data here is from `'Example1.csv'` again, except that the y-coordinates have been multiplied by 10. Its LSR line is

$$y = 15.20275x - 3.3458.$$

MSE is still a good measure to think about, but its size depends on scale of y-coordinates (equivalently, depends on units y is measured in).

R^2: Proportion of "variance explained"

Get a measure that is unchanged by scaling: first, set **total sum of squares** (TSS) to

$$\mathrm{TSS} = \sum_{i=1}^{n} (y_i - \bar{y})^2,$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$.

R^2: Proportion of "variance explained"

Get a measure that is unchanged by scaling: first, set **total sum of squares** (TSS) to

$$\mathrm{TSS} = \sum_{i=1}^{n} (y_i - \bar{y})^2,$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$.
Then,

$$R^2 = \frac{\mathrm{TSS} - n\mathrm{MSE}}{\mathrm{TSS}} = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y}_i)^2}.$$

R^2: Proportion of "variance explained"

Get a measure that is unchanged by scaling: first, set **total sum of squares** (TSS) to

$$\mathrm{TSS} = \sum_{i=1}^{n} (y_i - \bar{y})^2,$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$.
Then,

$$R^2 = \frac{\mathrm{TSS} - n\mathrm{MSE}}{\mathrm{TSS}} = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y}_i)^2}.$$

- R^2 does *not* depend on the scale of the y-coordinates.

R^2: Proportion of "variance explained"

Get a measure that is unchanged by scaling: first, set **total sum of squares** (TSS) to

$$\mathsf{TSS} = \sum_{i=1}^{n} (y_i - \bar{y})^2,$$

where $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$.
Then,

$$R^2 = \frac{\mathsf{TSS} - n\mathsf{MSE}}{\mathsf{TSS}} = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}.$$

- R^2 does *not* depend on the scale of the y-coordinates.
- Any data set, have $0 \leq R^2 \leq 1$ (provided R^2 is defined; i.e., we do not have $y_1, y_2, \ldots, y_n$ all the same).
  - Can you prove this?