Assessing accuracy of the LSR line

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Outline

Assuming the data does have a linear relationship

Measuring how well LSR line fits

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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.

 $^{^{1}\}varepsilon$ 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.

```
1  x = np.random.uniform(0, 2, size=30)
2
3  def simulate_data(x, std):
4    return -1.6*x + 0.8 + np.random.normal(0, std, size=len(x))
5  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 \rightarrow 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 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 $s \to \infty$, 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?

Standard error (SE): Suppose that for our error term ε , we have

$$\mathrm{Var}(\boldsymbol{\varepsilon}) = \sigma^2$$
. Sample size: n .

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

$$\begin{split} \text{SE}(\hat{m})^2 &= \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}; \\ \text{SE}(\hat{b})^2 &= \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right). \end{split}$$

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:

$$\begin{split} \mathrm{SE}(\hat{\mathbf{m}})^2 &= \frac{\sigma^2}{\sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})^2}; \\ \mathrm{SE}(\hat{\mathbf{b}})^2 &= \sigma^2 \left(\frac{1}{n} + \frac{\bar{\mathbf{x}}^2}{\sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})^2} \right). \end{split}$$

Estimate:

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

Can get (roughly) 95% confidence interval² 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.

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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.

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

- 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,

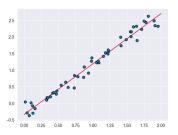
RSE =
$$\sqrt{\frac{1}{n-2} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$
.

So MSE =
$$\frac{n-2}{n}$$
RSE².

Mean Squared Error, example

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

$$y = 1.520275x - 0.33458.$$

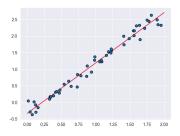


Mean Squared Error, example

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

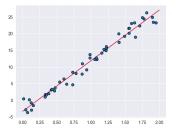
$$y = 1.520275x - 0.33458.$$

The MSE for this data and its LSR line is $\approx 0.0197.$ 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?
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

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

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

$$R^{2} = \frac{\text{TSS} - n\text{MSE}}{\text{TSS}} = 1 - \frac{\sum_{i=1}^{n} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i=1}^{n} (y_{i} - \bar{y}_{i})^{2}}.$$

- $ightharpoonup R^2$ does not depend on the scale of the y-coordinates.
- Any data set, have $0 \le R^2 \le 1$ (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?