Explore ordinary least squares

As previously mentioned, one way for finding the best fit line in regression modeling is to try different models until you find the best one. But for simple linear regression, the formulas for the best beta coefficients have been derived. In this reading, you will go through an example to gain a better understanding of how the sum of squared residuals can change as $\hat{\beta}_0$ and $\hat{\beta}_1$ change. There will be resources for further exploration if you're interested in deriving the formulas for estimating the coefficients using ordinary least squares. In this reading, we will cover:

- Formula and notation review
- Minimizing the sum of squared residuals (SSR)
- Estimating beta coefficients

Formula and notation review

Earlier, you learned about simple linear regression as a method for estimating the linear relationship between a continuous dependent variable and one independent variable. An estimate based on simple linear regression can be represented mathematically as $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 X$.

Remember that the hat symbol indicates that the beta coefficients are just estimates. As a result, the y-values derived from the regression model are also just estimates.

A common technique for calculating the coefficients of a linear regression model is called ordinary least squares, or OLS. Ordinary least squares estimates the beta coefficients in a linear regression model by minimizing a measure of error called the sum of squared residuals.

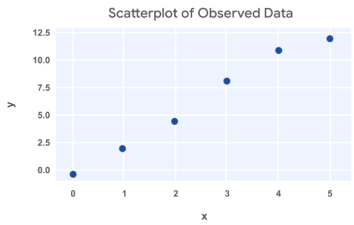
You can calculate the sum of squared residuals via this formula: $\sum_{i=1}^{N}(Observed - Predicted)^2$, which can be rewritten using mathematical notation as: $\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$.

The large E shaped symbol is the capital Greek letter, sigma, and it denotes a sum. So the sum of squared residuals is the sum of the squared differences between the observed values and the values predicted by the regression model.

Minimizing the sum of squared residuals (SSR)

For the purposes of this reading, assume that you have a dataset of 6 observations: (0, -1), (1, 2), (2, 4), (3, 8), (4, 11), and (5, 12). These can be plotted on a 2-dimensional X-Y coordinate plane.

X (observed)	Y (observed)
0	-1
1	2
2	4
3	8
4	11
5	12



Line 1: $\hat{y} = -0.5 + 3x$

Next, let's assume some values for $\hat{\beta}_0$ and $\hat{\beta}_1$ and calculate the sum of squared residuals. For the first attempt, let's assume $\hat{\beta}_0 = -0.5$ and $\hat{\beta}_1 = 3$. Then the linear equation would be $\hat{y} = -0.5 + 3x$. Since you now have the equation for y, you can calculate the predicted values by plugging in each value of x.

For example, if $x = 0$, then $\hat{y} = -0.5 + 3 * 0 = -0.5$. If $x = 1$, then $\hat{y} = -0.5 + 3 * 1 = 2.5$. So after calculating all the predicted values, then you can calculate the residual for each data point.

X (observed)	Y (actual)	Y (predicted) = -0.5 + 3x	Residual
0	-1	-0.5	-1 - (-0.5) = -1+0.5 = -0.5
1	2	2.5	2 - 2.5 = -0.5
2	4	5.5	4 - 5.5 = -1.5
3	8	8.5	8 - 8.5 = -0.5
4	11	11.5	11 - 11.5 = -0.5
5	12	14.5	12 - 14.5 = -2.5

Then you can square each of the residuals by multiplying them by themselves, and then adding them all together to calculate the sum of squared residuals.

Residual	Squared Residual
-1 - (-0.5) = -1+0.5 = -0.5	0.25
2 - 2.5 = -0.5	0.25
4 - 5.5 = -1.5	2.25
8 - 8.5 = -0.5	0.25
11 - 11.5 = -0.5	0.25
12 - 14.5 = -2.5	6.25

Sum of squared residuals =0.25+0.25+2.25+0.25+0.25+6.25=9.5

Line 2: $\hat{y} = -0.5 + 2.5x$

Next, let's adjust just the slope from the prior example. So $\hat{\beta}_0 = -0.5$ but $\hat{\beta}_1 = 2.5$. Then the linear equation would be $\hat{y} = -0.5 + 2.5x$. You can plug in values for x just like last time to calculate the predicted values and get the squared residuals.

X (observed)	Y (actual)	Y (predicted) = -0.5 + 2.5x	Residual	Squared Residuals
0	-1	-0.5	-0.5	0.25
1	2	2	0	0
2	4	4.5	-0.5	0.25
3	8	7	1	1
4	11	9.5	1.5	2.25
5	12	12	0	0

Sum of squared residuals $= 0.25 + 0 + 0.25 + 1 + 2.25 + 0 = 3.75$.

Great! This estimate is way better!

Estimating beta coefficients

You could keep adjusting the slope and intercept, and then calculating the predicted values, residuals, and squared residuals. But there's really no way to be sure you've found the best fit line. Through advanced math, some formulas have been derived to find the beta coefficients that minimize error.

There are multiple ways to write out the formulas for finding the beta coefficients. For simple linear regression, one

way to write the formulas is as follows:

- $\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(X_i - \overline{X})(Y_i - \overline{Y})}{\sum_{i=1}^{n}(X_i - \overline{X})^2}$
- $\hat{\beta}_0 = \overline{Y} - \hat{\beta}_1\overline{X}$

You won't be asked to calculate beta coefficients without help from a computer, but it can be interesting to explore if you desire. We've provided additional resources in case you're interested.

Key takeaways

Given a sample of data, you can try out different lines that could fit your data. You could calculate the sum of squared residuals for each line to determine which fits your data best. As a data professional, it's important to understand what the sum of squared residuals represents, and how to calculate it on your own. Thankfully, we have computers and programming languages that can calculate the sum of squared residuals and perform OLS for us. You can explore the deeper math behind OLS and SSR on your own if you wish!

Resources

- Parameter Estimation - Ordinary Least Squares Method: *Rudolph, A., Krois, J., Hartmann, K. (2023): Statistics and Geodata Analysis using Python (SOGA-Py). Department of Earth Sciences, Freie Universitaet Berlin.*

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