The Mathematical Derivation of Least Squares

The Bivariate Case

For the case in which there is only one independent variable, the classical OLS (ordinary least squares) regression model can be expressed as follows:

$$y_i = \beta_0 + \beta_1 x_i + e_i \qquad (1)$$

where y_i is dependent response variable, x_i is the independent explanatory variable, β_0 is the regression constant, β_1 is the regression coefficient for the effect of x, and e_i is the error we make in predicting y from x.

Now, in running the regression model, what are trying to do is to minimize the sum of the squared errors (SSE) of prediction – i.e., of the e_i values – across all cases. Mathematically, this quantity can be expressed as:

$$SSE \ \sum_1^n e_i^2 \qquad (2)$$

Specifically, what we want to do is find the values of b_0 *(The estimate of β_0)* and b_1 *(The estimate of β_1)* that minimize the quantity in Equation 2 above.

So, how do we do this? The key is to think back to differential calculus and remember how one goes about *finding the minimum value* of a mathematical function. This involves taking the *derivative* of that function.

If we want to find the values of b_0 and b_1 that minimize SSE, we need to express SSE in terms of b_0 and b_1, take the derivatives of SSE with respect to b_0 and b_1, set these derivatives to zero, and solve for b_0 and b_1.

However, since SSE is a function of two critical variables, b_0 and b_1, we will need to take the *partial derivatives* of SSE with respect to b_0 and b_1. In practice, this means we will need to take the derivative of SSE with regard to each of these critical variables one at a time, while treating the other critical variable as a constant (keeping in mind that the derivative of a constant always equals zero). In effect, what this does is take the derivative of SSE with respect to one variable while holding the other constant.

We begin by rearranging the basic OLS equation for the bivariate case so that we can express e_i in terms of y_i, x_i, b_0, and b_1. This gives us:

$$e_i = y_i - b_0 - b_1 x_i \tag{3}$$

Substituting this expression back into Equation (2), we get

$$SSE = \sum_1^n (y_i - b_0 - b_1 x_i)^2 \tag{4}$$

where n = the sample size for the data. It is this expression that we actually need to differentiate with respect to b_0 and b_1. Let's start by taking the partial derivative of SSE with respect to the regression constant, b_0, i.e.,

$$\frac{\partial SSE}{\partial b_0} = \frac{\partial}{\partial b_0}\left[\sum_1^n (y_i - b_0 - b_1 x_1)^2\right]$$

In doing this, we can move the summation operator (Σ) out front, since the derivative of a sum is equal to the sum of the derivatives:

$$\frac{\partial SSE}{\partial b_0} = \sum_1^n \left[\frac{\partial}{\partial b_0}(y_i - b_0 - b_1 x_1)^2\right]$$

We then focus on differentiating the squared quantity in parentheses. Since this quantity is a composite – we do the math in parentheses and then square the result – we need to use the chain rule in order to obtain the partial derivative of SSE with respect to the regression constant. In order to do this, we treat y_i, b_1, and x_i as constants. This gives us:

$$\frac{\partial SSE}{\partial b_0} = \sum_1^n \left[-2(y_i - b_0 - b_1 x_1)\right]$$

Further rearrangement gives us a final result of:

$$\frac{\partial SSE}{\partial b_0} = -2\sum_1^n (y_i - b_0 - b_1 x_1) \tag{5}$$

For the time being, let's put this result aside and take the partial derivative of SSE with respect to the regression coefficient, b_1, i.e.,

$$\frac{\partial SSE}{\partial b_1} = \frac{\partial}{\partial b_1}\left[\sum_{1}^{n}(y_i - b_0 - b_1 x_1)^2\right]$$

Again, we can move the summation operator (Σ) out front:

$$\frac{\partial SSE}{\partial b_1} = \sum_{1}^{n}\left[\frac{\partial}{\partial b_{10}}(y_i - b_0 - b_1 x_1)^2\right]$$

We then differentiate the squared quantity in parentheses, again using the chain rule. This time, however, we treat y_i, b_0, and x_i as constants. With some subsequent rearrangement, this gives us:

$$\frac{\partial SSE}{\partial b_1} = -2\sum_{1}^{n} x_i (y_i - b_0 - b_1 x_1) \qquad (6)$$

With that, we have our two partial derivatives of SSE – in Equations (5) and (6) The next step is to set each one of them to zero:

$$0 = -2\sum_{1}^{n}(y_i - b_0 - b_1 x_1) \qquad (7)$$

$$0 = -2\sum_{1}^{n} x_i (y_i - b_0 - b_1 x_1) \qquad (8)$$

Equations (7) and (8) form a system of equations with two unknowns – our OLS estimates, b_0 and b_1. The next step is to solve for these two unknowns. We start by solving Equation (7) for b_0. First, we get rid of the -2 by multiplying each side of the equation by -1/2:

$$0 = \sum_{1}^{n}(y_i - b_0 - b_1 x_1)$$

Next, we distribute the summation operator though all of the terms in the expression in parentheses:

$$0 = \sum_{1}^{n} y_i - \sum_{1}^{n} b_0 - \sum_{1}^{n} b_1 x_1$$

Then, we add the middle summation term on the right to both sides of the equation, giving us:

$$\sum_{1}^{n} b_0 = \sum_{1}^{n} y_i - \sum_{1}^{n} b_1 x_1$$

Since b_0 and b_1 the same for all cases in the original OLS equation, this further simplifies to:

$$nb_0 = \sum_{1}^{n} y_i - \sum_{1}^{n} b_1 x_1$$

To isolate b_0 on the left side of the equation, we then divide both sides by n:

$$\boldsymbol{b_0} = \frac{\sum_{1}^{n} \boldsymbol{y_i}}{\boldsymbol{n}} - \boldsymbol{b_1} \frac{\sum_{1}^{n} \boldsymbol{x_i}}{\boldsymbol{n}} \tag{9}$$

Equation (9) will come in handy later on, so keep it in mind. Right now, though, it is important to note that the first term on the right of Equation (9) is simply the mean of y_i, while everything following b_1 in the second term on the right is the mean of x_i.

$$b_0 = \bar{y} - b_1 \bar{x} \tag{10}$$

Now, we need to solve Equation (8) for b_1. Again, we get rid of the -2 by multiplying each side of the equation by -1/2:

$$0 = \sum_{1}^{n} x_i (y_i - b_0 - b_1 x_1)$$

Next, we distribute x_i through all of the terms in parentheses:

$$0 = \sum_{1}^{n}(x_i y_i - x_i b_0 - b_1 x_i^2)$$

We then distribute the summation operator through all of the terms in the expression in parentheses:

$$0 = \sum_{1}^{n} x_i y_i - \sum_{1}^{n} x_i b_0 - \sum_{1}^{n} b_1 x_i^2$$

Next, we bring all of the constants in these terms (i.e., b_0 and b_1) out in front of the summation operators, as follows:

$$0 = \sum_{1}^{n} x_i y_i - b_0 \sum_{1}^{n} x_i - b_1 \sum_{1}^{n} x_i^2$$

We then add the last term on the right side of the equation to both sides:

$$b_1 \sum_{1}^{n} x_i^2 = \sum_{1}^{n} x_i y_i - b_0 \sum_{1}^{n} x_i$$

Next, we go back to the value for b_0 from Equation (9) and substitute it into the result we just obtained. This gives us:

$$b_1 \sum_{1}^{n} x_i^2 = \sum_{1}^{n} x_i y_i - \left[\frac{\sum_{1}^{n} y_i}{n} - b_1 \frac{\sum_{1}^{n} x_i}{n} \right] \sum_{1}^{n} x_i$$

Multiplying out the last term on the right, we get:

$$b_1 \sum_{1}^{n} x_i^2 = \sum_{1}^{n} x_i y_i - \frac{\sum_{1}^{n} y_i \sum_{1}^{n} x_i}{n} + b_1 \left[\frac{\left(\sum_{1}^{n} x_i \right)^2}{n} \right]$$

If we then add the last term on the right to both sides of the equation, we get:

$$b_1 \sum_1^n x_i^2 - b_1 \left[\frac{\left(\sum_1^n x_i \right)^2}{n} \right] = \sum_1^n x_i y_i - \frac{\sum_1^n y_i \sum_1^n x_i}{n}$$

On the left side of the equation, we can then factor out b_1:

$$b_1 \left[\sum_1^n x_i^2 - \frac{\left(\sum_1^n x_i \right)^2}{n} \right] = \sum_1^n x_i y_i - \frac{\sum_1^n y_i \sum_1^n x_i}{n}$$

If we divide both sides of the equation by the quantity in the large brackets on the left side, we can isolate *b*.

$$b_1 = \frac{\sum_1^n x_i y_i - \frac{\sum_1^n y_i \sum_1^n x_i}{n}}{\sum_1^n x_i^2 - \frac{\left(\sum_1^n x_i \right)^2}{n}}$$

Finally, if we multiply top and bottom by n we obtain the least-square estimator for the regression coefficient in the bivariate case. This is the form from lecture:

$$b_1 = \frac{n \sum_1^n x_i y_i - \sum_1^n y_i \sum_1^n x_i}{n \sum_1^n x_i^2 - \left(\sum_1^n x_i \right)^2} \qquad (11)$$