A College Algebra Approach to Least Squares

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Abstract

In this article we present a way of deriving the formulas for the regression coefficients which is understandable to students with no mathematics preparation beyond that of a good college algebra course. The solution is quite elementary and could be used as a project for interested students in a mathematics modeling or introductory statistics class.

Linear Regression and the Least Squares Criterion

In an introductory mathematics modeling or statistics class is very common for a student to face the situation where he or she needs to find a function *f* that, in a sense to be specified, will best approximate a given set of data points $\{(x_k, y_k),\ k = 1,2,\ldots,n\}$. The least squares criterion is most common approach to solving this problem and consists in finding the function *f* that minimizes the value of

$$E(f) := \sum_{k=1}^{n} (f(x_k) - y_k)^2$$

for all *f* within a given class $\mathcal{F}$ of functions.

When $\mathcal{F}$ is the class of all linear functions, $\hat{y} = f(x) = mx + b$, the problem reduces to that of finding the values of the slope *m*, $-\infty < m < \infty$, and the intercept *b*, $-\infty < b < \infty$, that will minimize the sum of the squares of the errors

$$E(m,b) = \sum_{k=1}^{n} e_k^{\,2} = \sum_{k=1}^{n} (mx_k + b - y_k)^2$$

where the errors are defined as $e_k = \hat{y}_k - y_k = mx_k + b - y_k$, which is the difference between the predicted value $\hat{y}_k = mx_k + b$ and the observed value y_k. This specific version of the problem is called linear regression and the corresponding optimal values of *m* and *b* are called the regression coefficients.

Here are some of the approaches to solving linear regression problem commonly found in textbooks.

1. Just present the students the formulas for finding the regression coefficients or ask the students to use a graphing calculator to find them.

2. Use partial derivatives to find the minimum of $E(m,b)$ as a function of the two variables m and b. See, for instance, the statistics book by Wackerly, Mendenhall, and Schaeffer [6] or the article by Dunn III in [3].
3. Use lots of linear algebra and vector projection to find the correct value of m and b. See, for instance, the statistics book by Bickel and Doksum [1] or the linear algebra book by Lay [5].
4. Present a derivation of the formulas which already makes use of knowing in advance what the answer is. See for instance the statistics book by Casella and Berger [2] (their derivation uses Theorem 5.2.4 on page 212) or the article by Key in [4] which makes use of knowing one point on the regression line.

In an introductory class, the students lack the mathematical expertise to follow any of the derivations of the formulas that provide the values of m and b that minimize the value of $E(m,b)$ and therefore the only available option is the method mentioned above in bullet 1. We thought this was unacceptable and tried to find a way out of this situation.

In our case, one of the authors of this article was a highly motivated undergraduate student with little mathematics background carrying out several undergraduate projects and confronted with the situation of trying to understand where the regression coefficients come from. Thus, we were forced to look for a solution to the problem based of tools learnt in a college algebra course. We even avoid the explicit use of rotation of axes by exploiting the usual symmetries taught in basic algebra. The solution presented below is truly elementary and can be followed by any motivated student and could be used as a project in a mathematics modeling or statistics class.

How do we find *m* and *b*?

We begin by expanding $E(m,b)=\sum_{k=1}^{n}(mx_k+b-y_k)^2$ to obtain

$$E(m,b)=\sum_{k=1}^{n}\left[x_k{}^2m^2+2x_kmb+b^2-2x_ky_km-2y_kb+y_k{}^2\right]$$

$$=\left[\sum_{k=1}^{n}x_k{}^2\right]m^2+2\left[\sum_{k=1}^{n}x_k\right]mb+\left[n\right]b^2+\left[-2\sum_{k=1}^{n}x_ky_k\right]m+\left[-2\sum_{k=1}^{n}y_k\right]b+\left[\sum_{k=1}^{n}y_k{}^2\right]$$

If we rename all of the coefficients, the expressions in the square brackets, to be a,b,c,d,e,f , respectively, and if we let $m=u$ and $b=v$, then the expression has the generic form

$$E(u,v) = au^2 + buv + cv^2 + du + ev + f$$

where it is important to observe that $a > 0$ and $c > 0$. In order to find the smallest value $E(u,v)$ can have for $-\infty < u, v < \infty$, we will complete the square in the variables u and v to make the expression look like

$$E(u,v) = c_1\left(u-h\right)^2 + c_2\left(v-k\right)^2 + c_3$$

If this is possible, then the minimum of $E(u,v)$ is attained at $(u,v) = (h,k)$. Notice that if this is the case, then the fact that $E(u,v) \geq 0$ for all $-\infty < u, v < \infty$ implies that c_1 and c_2 are nonnegative and that the minimum value of E exists.

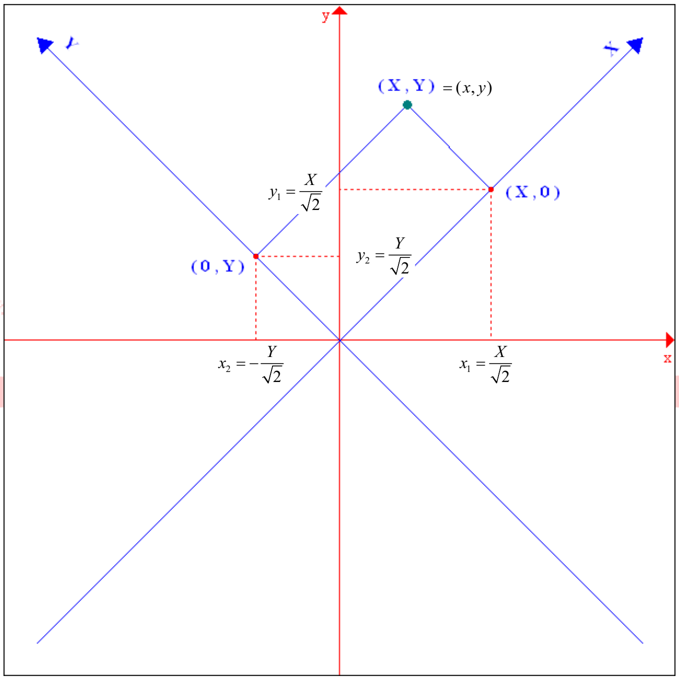
The presence of the cross term buv in $E(u,v)$ makes it very difficult to directly complete the squares in the variables u and v. We will eliminate the presence of the cross term by using some simple transformations to change $E(u,v)$ in a way that we can exploit the symmetry of E in the right coordinate system. The first step consists in rescaling the variables u and v to make the coefficients of u^2 and v^2 the same. That is, we let $u = x$ and $v = \frac{\sqrt{a}}{\sqrt{c}}y$. We can think of this rescaling as changing units in the y axis. Now, a direct substitution into $E(u,v)$ leads to the expression

$$E(x,y) = ax^2 + b\frac{\sqrt{a}}{\sqrt{c}}xy + ay^2 + dx + \frac{e\sqrt{a}}{\sqrt{c}}y + f$$

which, by renaming the coefficients, has the more compact and symmetric form

$$E(x,y) = Ax^2 + Bxy + Ay^2 + Dx + Ey + F$$

By symmetric, we mean that the principal part of $E(x,y)$ defined by the second order terms, is symmetric about the straight lines $y = x$ and $y = -x$. That is, $Ax^2 + Bxy + Ay^2$ remains unchanged if we replace (x,y) with either, (y,x) or $(-y,-x)$. The lines, $y = x$ and $y = -x$, are perpendicular to each other and therefore, make up a new XY-coordinate system which could be interpreted as a counterclockwise rotation of 45 degrees of the original xy-coordinate system. The following figure, depicting both coordinate systems, shows how a simple application of Pythagoras theorem relates the (x,y) coordinates with the (X,Y) coordinates of a given point in the plane.



Following the picture we see that

$$
\begin{aligned}
(X,Y) = (X,0) + (0,Y) &= \left(\frac{X}{\sqrt{2}}, \frac{X}{\sqrt{2}}\right) + \left(-\frac{Y}{\sqrt{2}}, \frac{Y}{\sqrt{2}}\right) \\
&= \left(\frac{X}{\sqrt{2}} - \frac{Y}{\sqrt{2}}, \frac{X}{\sqrt{2}} + \frac{Y}{\sqrt{2}}\right) = (x, y)
\end{aligned}
$$

If in the expression for $E(x,y)$ we let $x = \dfrac{X-Y}{\sqrt{2}}$ and $y = \dfrac{X+Y}{\sqrt{2}}$, then we get

$$
\begin{aligned}
E(X,Y) = {} & A\left(\frac{X-Y}{\sqrt{2}}\right)^2 + B\left(\frac{X-Y}{\sqrt{2}}\right)\left(\frac{X+Y}{\sqrt{2}}\right) + A\left(\frac{X+Y}{\sqrt{2}}\right)^2 + D\left(\frac{X-Y}{\sqrt{2}}\right) \\
& + E\left(\frac{X+Y}{\sqrt{2}}\right) + F
\end{aligned}
$$

And after expanding, simplifying, and collecting like terms we obtain

$$E(X,Y) = X^2\left(A+\frac{B}{2}\right)+Y^2\left(A-\frac{B}{2}\right)+X\left(\frac{E+D}{\sqrt{2}}\right)+Y\left(\frac{E-D}{\sqrt{2}}\right)+F$$

which, after renaming the coefficients, has the form,

$$E(X,Y) = A'X^2 + D'X + C'Y^2 + E'Y + F'$$

The full symmetry, with respect to the *XY*-coordinate system, of the principal part of $E(x,y)$ is what causes the coefficient of the cross term *XY* to vanish.

An additional algebraic effort completing the squares in *X* and *Y* in the previous expression, leads to the form

$$E(X,Y) = A'\left(X+\frac{D'}{2A'}\right)^2 + C'\left(Y+\frac{E'}{2C'}\right)^2 + F' - \frac{(D')^2C'+(E')^2A'}{4A'C'}$$

It is now evident that the minimum value of $E(X,Y)$ is attained when $X = -\frac{D'}{2A'}$ and $Y = -\frac{E'}{2C'}$. Now rewriting A', B', D', E' in terms of A, B, D, E we have that the *XY*-point where the minimum is attained is

$$(X,Y) = \left(\frac{-(E+D)}{\sqrt{2}(2A+B)}, \frac{-(E-D)}{\sqrt{2}(2A-B)}\right)$$

Using the fact that $x = \frac{X-Y}{\sqrt{2}}$ and $y = \frac{X+Y}{\sqrt{2}}$, we can transform back to the *xy*-coordinate system to obtain

$$(x,y) = \left(\frac{BE-2AD}{4A^2-B^2}, \frac{BD-2AE}{4A^2-B^2}\right)$$

Thus $E(x,y)$ has a minimum when $x = \frac{BE-2AD}{4A^2-B^2}$ and $y = \frac{BD-2AE}{4A^2-B^2}$.

Now recalling that $u = x$, $v = \frac{\sqrt{a}}{\sqrt{c}}y$, and the expressions of A, B, D, E in terms of *a, b, c, d,* and *e* we can say that the minimum of $E(u,v)$ occurs when

$$u = \frac{be-2cd}{4ac-b^2} \text{ and } v = \frac{bd-2ae}{4ac-b^2}$$

And finally, recalling that $m = u$ and $b = v$, and the definition of *a, b, c, d,* and *e* from the expression

$$E(u,v) = \underbrace{\left[\sum_{k=1}^{n} x_k^{\,2}\right]}_{a} u^2 + 2\underbrace{\left[\sum_{k=1}^{n} x_k\right]}_{b} uv + \underbrace{[n]}_{c} v^2 + \underbrace{\left[-2\sum_{k=1}^{n} x_k y_k\right]}_{d} u + \underbrace{\left[-2\sum_{k=1}^{n} y_k\right]}_{e} v + f$$

we obtain that the minimum value of $E(m,b)$ occurs at

$$m = \frac{n\sum_{k=1}^{n} x_k y_k - \sum_{k=1}^{n} x_k \sum_{k=1}^{n} y_k}{n\sum_{k=1}^{n} x_k^{\,2} - \left(\sum_{k=1}^{n} x_k\right)^2} \text{ and } b = \frac{\sum_{k=1}^{n} x_k^{\,2} \sum_{k=1}^{n} y_k - \sum_{k=1}^{n} x_k \sum_{k=1}^{n} x_k y_k}{n\sum_{k=1}^{n} x_k^{\,2} - \left(\sum_{k=1}^{n} x_k\right)^2}$$

which are one version of the usual formulas for *m* and *b*.

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