LEAST-SQUARES PROOF (MATRIX FORM)

Deriving b = $(X'X)^{-1}X'Y$ — Simple Step-by-Step

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The Goal

The multiple regression model in matrix form is:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

Y is the vector of responses, X the matrix of predictors, β the unknown coefficients, and ε the errors. We want the vector b that makes the total squared error as small as possible.

Step 1 — Write the total squared error

The errors are ε = Y − Xβ (actual minus predicted). Squaring and adding them up is, in matrix form, the vector times its own transpose:

$$S = \boldsymbol{\varepsilon}'\boldsymbol{\varepsilon} = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$$

Reading it simply: ε is a column of the n errors, and ε′ is the same numbers written as a row. Multiplying row × column gives $\varepsilon_1^2 + \varepsilon_2^2 + \ldots + \varepsilon_n^2$ — the sum of squared errors as a single number. So ε′ε is just shorthand for “square every error and add them,” and replacing ε with Y − Xβ shows this total depends on β — the quantity we now minimise. (Squaring is used so positive and negative errors do not cancel, and larger errors are penalised more.)

Step 2 — Expand the brackets

Multiply out, exactly like $(a - b)^2 = a^2 - 2ab + b^2$. The two middle terms are equal (each is a single number), so they combine:

$$S = \mathbf{Y}'\mathbf{Y} - 2\boldsymbol{\beta}'\mathbf{X}'\mathbf{Y} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta}$$

Step 3 — Differentiate and set to zero

To find the minimum, take the derivative with respect to β and set it to zero (using the rules d(β′X′Y)/dβ = X′Y and d(β′X′Xβ)/dβ = 2X′Xβ):

$$\frac{\partial S}{\partial \boldsymbol{\beta}} = -2\mathbf{X}'\mathbf{Y} + 2\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \mathbf{0}$$

Step 4 — Get the normal equations

Cancel the 2 and rearrange. Writing b for the solution:

$$\mathbf{X}'\mathbf{X}\,\mathbf{b} = \mathbf{X}'\mathbf{Y}$$

Step 5 — Solve for b

Multiply both sides on the left by $(X'X)^{-1}$, which exists because X′X is nonsingular:

$$\boxed{\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}}$$

This is a genuine minimum: the second derivative is 2X′X, which is positive-definite.

In plain words: square the errors, add them up, slide β until the slope of that total becomes zero, and the point where the slope vanishes is $b = (X'X)^{-1}X'Y$.