Machine Learning

Bhaswar Chakma

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Contents

5

1 OLS **7**

1.1 SLR 7

1.2 Review: Derivatives 9

1.3 Back to SLR 11

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Chapter 1

OLS

1.1 SLR

We define our column vector of parameters $\mathbf{w}$ (β in econometrics):

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

A single observation $\mathbf{x_n}$ is:

$$\mathbf{x_n} = \begin{bmatrix} 1 \\ x_n \end{bmatrix}$$

And thus the value predicted by the model can be written as:

$$f(x_n; w_0, w_1) = w_0 + w_1 x_n = \begin{bmatrix} w_0 & w_1 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \end{bmatrix} = \mathbf{w}^T \mathbf{x_n}$$

The matrix representing all the input data $\mathbf{X}$ and the column vector of outcomes $\mathbf{t}$ ($\mathbf{y}$ in econometrics) are:

$$\mathbf{X} = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix}$$

$$\mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_N \end{bmatrix}$$

The loss function $\mathcal{L}$ becomes

$$\mathcal{L} = \frac{1}{N}(\mathbf{t} - \mathbf{X})^T(\mathbf{t} - \mathbf{X})$$

The column vector of values predicted by the function $f(x_n; w_0, w_1)$ are:

$$\mathbf{Xw} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix} \times \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} = \begin{bmatrix} w_0 & w_1 x_1 \\ w_0 & w_1 x_2 \\ \vdots & \vdots \\ w_0 & w_1 x_N \end{bmatrix}$$

$$\underset{(N\times 2)}{\mathbf{X}} \times \underset{(2\times 1)}{\mathbf{w}} = \underset{(N\times 1)}{\mathbf{Xw}}$$

The column vector of residual is

$$\mathbf{t} - \mathbf{Xw} = \begin{bmatrix} t_1 - w_0 + w_1 x_1 \\ t_2 - w_0 + w_1 x_2 \\ \vdots \\ t_N - w_0 + w_1 x_N \end{bmatrix}$$

The sum of squared errors can be expressed as:

$$\sum_{n=1}^{N}(t_n - (w_0 + w_1 x_1))^2$$

$$= \begin{bmatrix} t_1 - (w_0 + w_1 x_1) & t_2 - (w_0 + w_1 x_2) & ... & t_N - (w_0 + w_1 x_N) \end{bmatrix} \times \begin{bmatrix} t_1 - (w_0 + w_1 x_1) \\ t_2 - (w_0 + w_1 x_2) \\ \vdots \\ t_N - (w_0 + w_1 x_N) \end{bmatrix} = (\mathbf{t} - \mathbf{Xw})^T$$

We can now write our loss function compactly with matrix notation, which produces a scalar (1×1) value:

$$\underset{(1\times 1)}{\frac{1}{N}} \underset{(1\times N)}{(\mathbf{t} - \mathbf{Xw})^T} \underset{(N\times 1)}{(\mathbf{t} - \mathbf{Xw})} = \underset{(1\times 1)}{\mathcal{L}}$$

We can expand the sum of squared errors as follows:

$$(\mathbf{t} - \mathbf{Xw})^T(\mathbf{t} - \mathbf{Xw})$$

$$= (\mathbf{t}^T - (\mathbf{Xw})^T)(\mathbf{t} - \mathbf{Xw})$$

$$= (\mathbf{t}^T - (\mathbf{w}^T\mathbf{X}^T))(\mathbf{t} - \mathbf{X}\mathbf{w})$$

$$= \underset{(1\times1)}{\mathbf{t}^T\mathbf{t}} - \underset{(1\times N)}{\mathbf{t}^T}\underset{(N\times2)}{\mathbf{X}}\underset{(2\times1)}{\mathbf{w}} - \underset{(1\times2)}{\mathbf{w}^T}\underset{(2\times N)}{\mathbf{X}^T}\underset{(N\times1)}{\mathbf{t}} + \underset{(1\times2)}{\mathbf{w}^T}\underset{(2\times N)}{\mathbf{X}^T}\underset{(N\times2)}{\mathbf{X}}\underset{(2\times1)}{\mathbf{w}} \tag{1.1}$$

Note the following:

- each of the term becomes 1×1
- the terms $\mathbf{t}^T\mathbf{X}\mathbf{w}$ and $\mathbf{w}^T\mathbf{X}^T\mathbf{t}$ are transposes of each other and are scalars. So they are the same value and can be combined.

So, sum of squared residuals can be written as

$$\mathbf{t}^T\mathbf{t} - 2\mathbf{w}^T\mathbf{X}^T\mathbf{t} + \mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w}$$

Hence, the loss function becomes:

$$\mathcal{L} = \frac{1}{N}\mathbf{t}^T\mathbf{t} - 2\mathbf{w}^T\mathbf{X}^T\mathbf{t} + \mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w}$$

Now that we have defined our loss function in matrix notation, we still want to find the value of w that will minimize the loss. Like before, this involves taking the derivative (now with respect to the vector $\mathbf{w}$), setting the derivative equal to 0, and then solving for $\mathbf{w}$. Thus, we must delve into doing vector Calculus.

1.2 Review: Derivatives

Lets say we have a function of one variable that produces a scalar output (real-valued input is mapped to real-valued output):

$$f : \mathbb{R} \to \mathbb{R}$$

The derivative of this function tells us how the function changes with respect to that variable. The derivative is:

$$f'(x) = \lim_{h\to0} \frac{f(x+h) - f(x)}{h}$$

Which can be rearranged to say that the derivative at a $f'(x)$ satisfies the following:

$$\lim_{h \to 0} \frac{f(x+h) - f(x) - f'(x)h}{h} = 0$$

Gradient

Let's say we have a function of a vector that produces a scalar output (n-dimensional real-valued input is mapped to one real-valued output):

$$f : \mathbb{R}^n \to \mathbb{R}$$

The gradient $\nabla f(x)$ is the multidimensional derivative and it tells us how the function changes with respect to each component in the vector. It satisfies the following equation:

$$\lim_{\|h\| \to 0} \frac{\|f(x+h) - f(x) - f'(x)h\|}{\|h\|} = 0$$

Again, we have a function of a vector that produces a scalar $f : \mathbb{R}^n \to \mathbb{R}$. The input to the function is a vector:

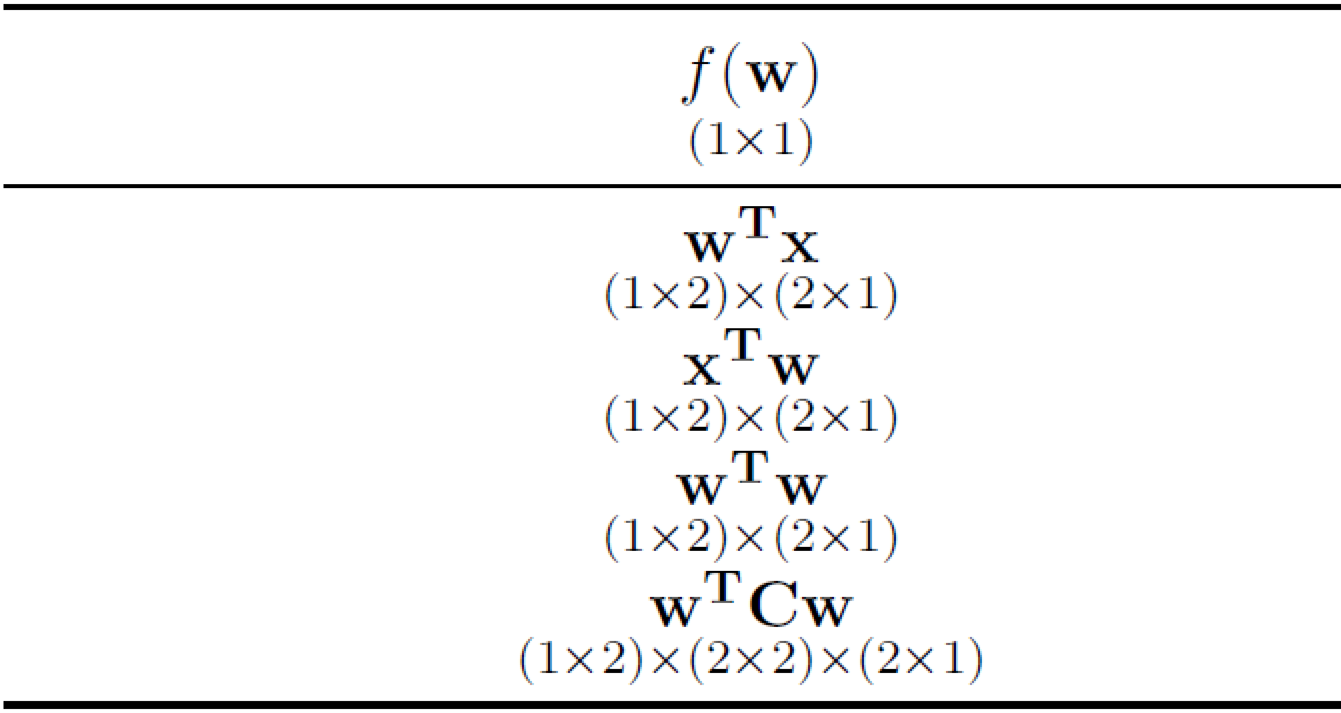
$$\mathbf{w} = (w_1, w_2, ..., w_n)^T$$

The gradient of the function with respect to $\mathbf{w}$ at $\mathbf{w}$ is itself a vector:

$$\nabla f(\mathbf{w}) = \frac{\partial f}{\partial \mathbf{w}} = (\frac{\partial f}{\partial w_1}, \frac{\partial f}{\partial w_2}, ..., \frac{\partial f}{\partial w_n})^T = \begin{bmatrix} \frac{\partial f}{\partial w_1} \\ \frac{\partial f}{\partial w_2} \\ \vdots \\ \frac{\partial f}{\partial w_n} \end{bmatrix}$$

Like the derivative, the gradient represents the slope of the tangent of the graph of the function. More precisely, the gradient points in the direction of the greatest rate of increase of the function, and its magnitude is the slope of the graph in that direction.

The gradient will always have the same dimensions as the input vector. In the following examples, $\mathbf{w}$ and $\mathbf{w}$ are 2 x 1 matrices.



$f(\mathbf{w})$ (1×1)
$\mathbf{w}^{\mathbf{T}}\mathbf{x}$ $(1\times2)\times(2\times1)$
$\mathbf{x}^{\mathbf{T}}\mathbf{w}$ $(1\times2)\times(2\times1)$
$\mathbf{w}^{\mathbf{T}}\mathbf{w}$ $(1\times2)\times(2\times1)$
$\mathbf{w}^{\mathbf{T}}\mathbf{C}\mathbf{w}$ $(1\times2)\times(2\times2)\times(2\times1)$

1.3 Back to SLR

Earlier, we found the total OLS regression loss function to be:

$$\mathcal{L} = \frac{1}{N}\mathbf{t}^T\mathbf{t} - 2\mathbf{w}^T\mathbf{X}^T\mathbf{t} + \mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w}$$

We will take the derivative of the loss with respect to the vector $\mathbf{w}$, set the derivative equal to the $\mathbf{0}$ vector, and then solve for $\mathbf{w}$.

If $\mathbf{w}$ is a 2×1 vector, then ∇f must also be 2×1.

Now note that $\underset{(1\times2)}{\mathbf{w}^T}\underset{(2\times N)}{\mathbf{X}^T}\underset{(N\times1)}{\mathbf{t}}$ could be treated as $\underset{(1\times2)}{\mathbf{w}^T}\underset{(2\times1)}{\mathbf{x}}$

$$\frac{\partial f}{\partial \mathbf{w}} = 0 - \frac{N}{2}X^T\mathbf{t} + \frac{N}{2}X^TX\mathbf{w}$$