

DATA 558: Homework 2

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Exercise 1

In this section, I will that the coefficient of determination:

$$R^2 = \frac{\text{TSS-RSS}}{\text{TSS}} = 1 - \frac{\text{RSS}}{\text{TSS}}$$

With:

$$\text{RSS} = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \text{ and } \text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2$$

Has a domain given by:

$$0 \leq R^2 \leq 1$$

I will do this by showing that the TSS is equal to the sum of the RSS and the ESS, that is:

$$\sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 + \sum_{i=1}^n (\hat{y}_i - \bar{y})^2$$

Proof. Let us begin with the LHS:

$$\begin{aligned} \sum_{i=1}^n (y_i - \bar{y})^2 &= \sum_{i=1}^n (y_i - \bar{y} + \hat{y}_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^n ((\hat{y}_i - \bar{y}) + (y_i - \hat{y}_i))^2 \\ &= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n (y_i - \hat{y}_i)^2 + 2 \sum_{i=1}^n (y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) \end{aligned}$$

Now recall that $\hat{\beta}$ is chosen to minimize the RSS, that is to say:

$$\frac{\partial}{\partial \beta^{(j)}} \text{RSS} = -2 \sum_{i=1}^n (y_i - \beta^T x_i) x_i^{(j)}$$

And with $\hat{\beta}$ we have:

$$-2 \sum_{i=1}^n (y_i - \beta^T x_i) x_i^{(j)} = 0$$

Now, breaking down the final addend from our initial derivation we have:

$$2 \sum_{i=1}^n (y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) = 2 \left(\sum_{i=1}^n \hat{y}_i (y_i - \hat{y}_i) - \bar{y} \sum_{i=1}^n (y_i - \hat{y}_i) \right)$$

However, because we know:

$$\sum_{i=1}^n (y_i - \hat{y}_i) = 0$$

We just need to show:

$$\sum_{i=1}^n \hat{y}_i (y_i - \hat{y}_i) = 0$$

Consider the partial derivative of the RSS with respect to $\beta^{(j)}$, then we have:

$$\begin{aligned} \sum_{i=1}^n x_i (y_i - \hat{y}_i) &= 0 \\ \sum_{i=1}^n \beta^T x_i (y_i - \hat{y}_i) &= 0 \\ \sum_{i=1}^n \hat{\beta}^T x_i (y_i - \hat{y}_i) + \sum_{i=1}^n \hat{\beta}_0 (y_i - \hat{y}_i) &= 0 \\ \sum_{i=1}^n (\hat{\beta}_0 + \hat{\beta}^T x_i) (y_i - \hat{y}_i) &= 0 \\ \sum_{i=1}^n \hat{y}_i (y_i - \hat{y}_i) &= 0 \end{aligned}$$

Therefore:

$$2 \sum_{i=1}^n (y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) = 0$$

Giving us:

$$\sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

And we are done. □

Exercise 2

Now, I will prove the following identity:

$$E_y[(y - \bar{\beta}^T x)^2] = E_y[(y - f(x))^2] + (f(x) - \bar{\beta}^T x)^2$$

With $f(x)$ learned from the data, that is:

$$f(x) \approx \hat{\beta}^T x$$

Proof. Beginning with the LHS:

$$\begin{aligned} E_y[(y - \bar{\beta}^T x)^2] &= E_y[((y - f(x)) + (f(x) - \bar{\beta}^T x))^2] \\ &= E_y[(y - f(x))^2] + 2E_y[(y - f(x))(f(x) - \bar{\beta}^T x)] + E_y[(f(x) - \bar{\beta}^T x)^2] \\ &= E_y[(y - f(x))^2] + (f(x) - \bar{\beta}^T x)^2 + 2E_y[(y - f(x))]E_y[(f(x) - \bar{\beta}^T x)] \end{aligned}$$

Note that we were able to distribute the expectation across the product because $(f(x) - \bar{\beta}^T x)$ is independent of y . Moreover, because the expected value of the residual is equal to zero:

$$E_y[(y - f(x))] = 0$$

The final term in the addition is eliminated, leaving us with:

$$E_y[(y - \bar{\beta}^T x)^2] = E_y[(y - f(x))^2] + (f(x) - \bar{\beta}^T x)^2$$

And we are done. □