

Linear regression

Machine Learning 2021-2022 - UMONS

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Consider the following optimization problem:

$$(\beta_0^*, \beta_1^*) = \underset{(\beta_0, \beta_1) \in \mathbb{R}^2}{\operatorname{argmin}} E_{\text{out}}(\beta_0, \beta_1) := \mathbb{E}_{x,y}[(y - (\beta_0 + \beta_1 x))^2]$$

where $x, y \in \mathbb{R}$.

Show that the solution is given by

$$\begin{aligned}\beta_1^* &= \frac{\operatorname{Cov}(x, y)}{\operatorname{Var}(x)}, \\ \beta_0^* &= \mathbb{E}[y] - \beta_1^* \mathbb{E}[x].\end{aligned}$$

We have

$$\begin{aligned}E_{\text{out}}(\beta_0, \beta_1) &= \mathbb{E}[(y - (\beta_0 + \beta_1 x))^2] \\ &= \mathbb{E}[y^2] - 2\beta_0 \mathbb{E}[y] - 2\beta_1 \mathbb{E}[xy] + \mathbb{E}[(\beta_0 + \beta_1 x)^2] \\ &= \mathbb{E}[y^2] - 2\beta_0 \mathbb{E}[y] - 2\beta_1 (\operatorname{Cov}(x, y) + \mathbb{E}[x]\mathbb{E}[y]) \\ &\quad + \mathbb{E}[(\beta_0 + \beta_1 x)^2] \\ &= \mathbb{E}[y^2] - 2\beta_0 \mathbb{E}[y] - 2\beta_1 (\operatorname{Cov}(x, y) + \mathbb{E}[x]\mathbb{E}[y]) \\ &\quad + \beta_0^2 + \beta_1^2 \mathbb{E}[x^2] + 2\beta_0 \beta_1 \mathbb{E}[x] \\ &= \mathbb{E}[y^2] - 2\beta_0 \mathbb{E}[y] - 2\beta_1 \operatorname{Cov}(x, y) - 2\beta_1 \mathbb{E}[x]\mathbb{E}[y] \\ &\quad + \beta_0^2 + \beta_1^2 \operatorname{Var}(x) + \beta_1^2 (\mathbb{E}[x])^2 + 2\beta_0 \beta_1 \mathbb{E}[x]\end{aligned}$$

where we used the following identities:

$$\operatorname{Cov}(x, y) = \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y], \quad \operatorname{Var}(x) = \mathbb{E}[x^2] - (\mathbb{E}[x])^2.$$

Taking the partial derivatives of $E_{\text{out}}(\beta_0, \beta_1)$ with respect to β_0 and β_1 and equaling to zero yields :

$$\begin{aligned}\frac{\partial E_{\text{out}}(\beta_0, \beta_1)}{\partial \beta_0} = 0 &\iff -2\mathbb{E}[y] + 2\beta_0 + 2\beta_1 \mathbb{E}[x] = 0 \\ &\iff \beta_0 = \mathbb{E}[y] - \beta_1 \mathbb{E}[x]\end{aligned}$$

$$\begin{aligned}\frac{\partial E_{\text{out}}(\beta_0, \beta_1)}{\partial \beta_1} = 0 &\iff -2\operatorname{Cov}(x, y) - 2\mathbb{E}[x]\mathbb{E}[y] + 2\beta_1 \operatorname{Var}(x) + 2\beta_1 (\mathbb{E}[x])^2 + 2\beta_0 \mathbb{E}[x] = 0 \\ &\iff -2\operatorname{Cov}(x, y) - 2\mathbb{E}[x]\mathbb{E}[y] + 2\beta_1 \operatorname{Var}(x) + 2\beta_1 (\mathbb{E}[x])^2 + 2\mathbb{E}[x]\mathbb{E}[y] - 2\beta_1 (\mathbb{E}[x])^2 = 0 \\ &\iff \beta_1 = \frac{\operatorname{Cov}(x, y)}{\operatorname{Var}(x)}\end{aligned}$$

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Consider a dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ with $x_i, y_i \in \mathbb{R}$, and the following optimization problem:

$$(\hat{\beta}_0, \hat{\beta}_1) = \underset{(\beta_0, \beta_1) \in \mathbb{R}^2}{\operatorname{argmin}} E_{\text{in}}(\beta_0, \beta_1),$$

where

$$E_{\text{in}}(\beta_0, \beta_1) = \frac{1}{n} \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i))^2.$$

Prove that the minimizing values $\hat{\beta}_1$ and $\hat{\beta}_0$ are given by

$$\begin{aligned} \hat{\beta}_1 &= \frac{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2} \\ \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x}, \end{aligned}$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$ and $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$.

$$\begin{aligned} \frac{\partial \text{RSS}}{\partial \beta_0} = 0 &\iff -2 \sum_i (y_i - (\beta_0 + \beta_1 x_i)) = 0, \\ &\iff \sum_i y_i = n\beta_0 + \beta_1 \sum_i x_i \\ &\iff \beta_0 = \bar{y} - \hat{\beta}_1 \bar{x} \end{aligned}$$

$$\begin{aligned} \frac{\partial \text{RSS}}{\partial \beta_1} = 0 &\iff -2 \sum_i x_i (y_i - (\beta_0 + \beta_1 x_i)) = 0 \\ &\iff \sum_i x_i y_i = \sum_i (\beta_0 x_i + \beta_1 x_i^2) \\ &\iff \sum_i x_i y_i = n\beta_0 \bar{x} + \beta_1 \sum_i x_i^2 \\ &\iff \sum_i x_i y_i = n(\bar{y} - \hat{\beta}_1 \bar{x}) \bar{x} + \beta_1 \sum_i x_i^2 \\ &\iff \sum_i x_i y_i - n\bar{x}\bar{y} = \beta_1 (\sum_i x_i^2 - n\bar{x}^2) \\ &\iff \beta_1 = \frac{\sum_i x_i y_i - n\bar{x}\bar{y}}{\sum_i x_i^2 - n\bar{x}^2} \end{aligned}$$

Using the following equalities proves the result.

$$\begin{aligned} \sum_i (x_i - \bar{x})^2 &= \sum_i x_i^2 - n\bar{x}^2 \\ \sum_i (x_i - \bar{x})(y_i - \bar{y}) &= \sum_i x_i y_i - n\bar{x}\bar{y} \end{aligned}$$

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We now assume the data has been generated by the following model

$$y_i = f(x_i) + \varepsilon_i,$$

where x_i is fixed (non-random), ε_i are i.i.d. with $E[\varepsilon_i] = 0$, $\text{Var}(\varepsilon_i) = \sigma^2$.

Show that the variance of $\hat{\beta}_1$ is given by $\text{Var}(\hat{\beta}_1) = \frac{\sigma^2}{\sum_i (x_i - \bar{x})^2}$. You can use the following equalities

$$\begin{aligned} \sum_i (x_i - \bar{x})(y_i - \bar{y}) &= \sum_i (x_i - \bar{x})y_i - \sum_i (x_i - \bar{x})\bar{y} \\ &= \sum_i (x_i - \bar{x})y_i \\ &= \sum_i (x_i - \bar{x})(\beta_0^* + \beta_1^* x_i + \varepsilon_i) \end{aligned}$$

$$\begin{aligned} \text{Var}(\hat{\beta}_1) &= \text{Var}\left(\frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2}\right) \\ &= \text{Var}\left(\frac{\sum_i (x_i - \bar{x})(\beta_0^* + \beta_1^* x_i + \varepsilon_i)}{\sum_i (x_i - \bar{x})^2}\right), \text{ using the previous equalities} \\ &= \text{Var}\left(\frac{\sum_i (x_i - \bar{x})\varepsilon_i}{\sum_i (x_i - \bar{x})^2}\right), \text{ only } \varepsilon_i \text{ is random} \\ &= \frac{\sum_i (x_i - \bar{x})^2 \text{Var}(\varepsilon_i)}{(\sum_i (x_i - \bar{x})^2)^2}, \text{ independence of } \varepsilon_i \text{ and, } \text{Var}(kX) = k^2 \text{Var}(X) \\ &= \frac{\sigma^2}{\sum_i (x_i - \bar{x})^2} \end{aligned}$$

Show that the variance of $\hat{\beta}_0$ is given by

$$\text{Var}(\hat{\beta}_0) = \frac{\sigma^2}{n} + \frac{\bar{x}^2 \sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

$$\begin{aligned} \text{Var}(\hat{\beta}_0) &= \text{Var}(\bar{y} - \hat{\beta}_1 \bar{x}) \\ &= \text{Var}(\bar{y}) + (\bar{x})^2 \text{Var}(\hat{\beta}_1) - 2\text{Cov}(\bar{y}, \hat{\beta}_1 \bar{x}) \\ &= \text{Var}(\bar{y}) + (\bar{x})^2 \text{Var}(\hat{\beta}_1) - 2\bar{x} \text{Cov}(\bar{y}, \hat{\beta}_1) \end{aligned}$$

where

$$\text{Var}(\bar{y}) = \frac{1}{n^2} \text{Var}\left(\sum_i^n y_i\right) = \frac{\sigma^2}{n},$$

$$\text{Var}(\hat{\beta}_1) = \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2},$$

$$\begin{aligned}
\text{Cov}(\bar{y}, \hat{\beta}_1) &= \text{Cov} \left(\frac{1}{n} \sum_{i=1}^n y_i, \frac{\sum_{j=1}^n (x_j - \bar{x}) y_j}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \frac{1}{n \sum_{i=1}^n (x_i - \bar{x})^2} \text{Cov} \left(\sum_{i=1}^n y_i, \sum_{j=1}^n (x_j - \bar{x}) y_j \right) \\
&= \frac{1}{n \sum_{i=1}^n (x_i - \bar{x})^2} \sum_{i=1}^n (x_i - \bar{x}) \sum_{j=1}^n \text{Cov}(y_i, y_j) \\
&= \frac{1}{n \sum_{i=1}^n (x_i - \bar{x})^2} \sum_{i=1}^n (x_i - \bar{x}) \sigma^2 \\
&= 0 \quad \left(\text{since } \sum_{i=1}^n (x_i - \bar{x}) = 0 \right).
\end{aligned}$$

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Under the same set of assumptions as the previous exercise, show that the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are unbiased, i.e. $\text{Bias}(\hat{\beta}_0) = 0$ and $\text{Bias}(\hat{\beta}_1) = 0$.

$$\text{Bias}(\hat{\beta}_1) = \mathbb{E}[\hat{\beta}_1] - \beta_1^* \quad (1)$$

$$\begin{aligned} \text{Bias}(\hat{\beta}_1) &= \mathbb{E}[\hat{\beta}_1] - \beta_1^* \\ &= \mathbb{E}\left[\frac{\frac{1}{n}\sum_i^n (x_i - \bar{x})(y_i - \bar{y})}{\frac{1}{n}\sum_i^n (x_i - \bar{x})^2}\right] - \beta_1^* \\ &= \frac{\mathbb{E}\left[\frac{1}{n}\sum_i^n (x_i y_i - x_i \bar{y} - \bar{x} y_i + \bar{x} \bar{y})\right]}{\frac{1}{n}\sum_i^n (x_i - \bar{x})^2} - \beta_1^* \quad x_i\text{'s are non-random.} \\ &= \frac{\mathbb{E}\left[\frac{1}{n}\sum_i^n x_i(\beta_0^* + \beta_1^* x_i + \varepsilon_i) - \bar{x}(\beta_0^* + \beta_1^* \bar{x} + \bar{\varepsilon})\right]}{\frac{1}{n}\sum_i^n (x_i - \bar{x})^2} - \beta_1^* \\ &= \frac{\frac{1}{n}\sum_i^n x_i(\beta_0^* + \beta_1^* x_i + \mathbb{E}[\varepsilon_i]) - \bar{x}(\beta_0^* + \beta_1^* \bar{x} + \mathbb{E}[\bar{\varepsilon}])}{\frac{1}{n}\sum_i^n (x_i - \bar{x})^2} - \beta_1^* \\ &= \frac{\beta_0^* \bar{x} + \beta_1^* \overline{x^2} - \beta_0^* \bar{x} + \beta_1^* (\bar{x})^2}{\frac{1}{n}\sum_i^n (x_i^2 - 2x_i \bar{x} + \bar{x}^2)} - \beta_1^* \quad \text{as } \mathbb{E}[\varepsilon_i] = \mathbb{E}\left[\frac{1}{n}\sum_i^n \varepsilon_i\right] = \mathbb{E}[\bar{\varepsilon}] = 0 \\ &= \frac{\beta_1^* (\overline{x^2} + (\bar{x})^2)}{\overline{x^2} + (\bar{x})^2} - \beta_1^* \\ &= 0 \end{aligned}$$

$$\begin{aligned} \text{Bias}(\hat{\beta}_0) &= \mathbb{E}[\hat{\beta}_0] - \beta_0^* \\ &= \mathbb{E}[\bar{y} - \hat{\beta}_1 \bar{x}] - \beta_0^* \\ &= \mathbb{E}[\bar{y}] - \bar{x} \mathbb{E}[\hat{\beta}_1] - \beta_0^* \\ &= \mathbb{E}[\beta_0^* + \beta_1^* \bar{x} + \bar{\varepsilon}] - \beta_1^* \bar{x} - \beta_0^* \\ &= 0 \end{aligned}$$