Regression I

COMP9417, 22T2

What do you prefer?

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More theory, more practice (i.e Python and using packages), going through questions, consultation etc.

Thinking Machine Learning

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We try to make sense of data using mathematics to help us quantify what we *know*.

A standard way to break the problem down is as follows:

- We have 'input' data X and targets/outputs y
- Our data can be modelled as $y = f(X)$
- Goal is to find the best approximation for f as $\hat{f}$

We define the quality of our approximation $(\hat{f})$ by using a error/loss function.

Linear Regression

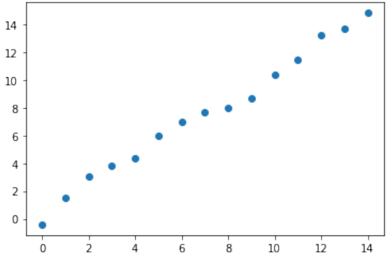
Linear Regression

We deduct and assume a linear relationship between X and y.

In this simple case, our model will take the form:

$$\hat{y} = w_0 + w_1 X$$

How do we find the optimal w_0 and w_1?



What will our loss function need? Boils down to the properties of the target function.

- Target function has ≈ 0 distance to all points
- We can define a basic loss function with one glaring issue:

$$L(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)$$

To make life easy, we define our loss function as:

$$
\begin{aligned}
L(w_0, w_1) &= \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 && \text{a.k.a MSE} \\
&= \frac{1}{n}\sum_{i=1}^{n}(y_i - w_0 - w_1 x_i)^2 && \text{by definition}
\end{aligned}
$$

The minimum of our loss function w.r.t w_0 and w_1 will be their optimal values respectively.

Question 1 (a, b, c)

1a

Derive the least-squares estimates for the univariate linear regression model.

i.e Solve:

$$\underset{w_0, w_1}{\arg\min} L(w_0, w_1)$$

$$\underset{w_0, w_1}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2$$

First we differentiate $L(w_0, w_1)$ with respect to w_0,

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = -\frac{2}{n}\sum_{i=1}^{n}(y_i - w_0 - w_1 x_i)$$

$$= -\frac{2}{n}\left(\sum_{i=1}^{n} y_i - n w_0 - w_1 \sum_{i=1}^{n} x_i\right)$$

For the minimum, $\frac{\partial L(w_0, w_1)}{\partial w_0} = 0$,

$$-\frac{2}{n}\left(\sum_{i=1}^{n} y_i - n w_0 - w_1 \sum_{i=1}^{n} x_i\right) = 0$$

$$\begin{aligned} \frac{1}{n}\sum_{i=1}^{n} y_i - w_0 - w_1 \frac{1}{n}\sum_{i=1}^{n} x_i &= 0 \\ \bar{y} - w_0 - w_1\bar{x} &= 0 \\ w_0 = \bar{y} - w_1\bar{x} \end{aligned} \tag{1}$$

To find w_1, we follow a similar process and use simple simultaneous equations to solve for the final solution.

So,

$$\frac{\partial L(w_0, w_1)}{\partial w_1} = -\frac{2}{n}\sum_{i=1}^{n} x_i(y_i - w_0 - w_1 x_i)$$

$$= -\frac{2}{n}\left(\sum_{i=1}^{n} x_i y_i - w_0 \sum_{i=1}^{n} x_i - w_1 \sum_{i=1}^{n} x_i^2\right)$$

$\frac{\partial L(w_0,w_1)}{\partial w_1} = 0,$

$$\frac{1}{n}\left(\sum_{i=1}^{n} x_i y_i - w_0 \sum_{i=1}^{n} x_i - w_1 \sum_{i=1}^{n} x_i^2\right) = 0$$

$$\overline{xy} - w_0\bar{x} - w_1\overline{x^2} = 0$$

$$
\begin{aligned}
\overline{xy} - w_0\bar{x} - w_1\overline{x^2} &= 0 \\
w_1 &= \frac{\overline{xy} - w_0\bar{x}}{\overline{x^2}}
\end{aligned}
\tag{2}
$$

Sub (1) into (2):

$$
\begin{aligned}
w_1 &= \frac{\overline{xy} - (\bar{y} - w_1\bar{x})\bar{x}}{\overline{x^2}} \\
w_1 &= \frac{\overline{xy} - \bar{x}\bar{y} + w_1\bar{x}^2}{\overline{x^2}} \\
w_1\left(\frac{\overline{x^2} - \bar{x}^2}{\bar{x}^2}\right) &= \frac{\overline{xy} - \bar{x}\bar{y} + w_1\bar{x}^2}{\overline{x^2}} \\
w_1 &= \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2}
\end{aligned}
$$

Finally, we have

$$w_1 = \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2} \text{ and } w_0 = \bar{y} - w_1\bar{x}$$

1b

Problem: Prove $(\bar{x}, \bar{y})$ is on the line.

From 1(a), the equation of our line ($\hat{y} = w_0 + w_1 x$) becomes:

$$\hat{y} = \bar{y} - \bar{x}\frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2} + \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2}x$$

Sub $x = \bar{x}$,

$$\hat{y} = \bar{y} - \bar{x}\frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2} + \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2}\bar{x}$$

$$\hat{y} = \bar{y}$$

$\therefore (\bar{x}, \bar{y})$ is on the line

1c

Similar to 1a, though take care with the partial derivatives:

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = -\frac{2}{n}\sum_{i=1}^{n}(y_i - w_0 - w_1 x_i)$$

$$\frac{\partial L(w_0, w_1)}{\partial w_1} = -\frac{2}{n}\sum_{i=1}^{n}x_i(y_i - w_0 - w_1 x_i) + 2\lambda w_1$$

Final result is:

$$w_0 = \bar{y} - w_1 \bar{x}$$
$$w_1 = \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2 + \lambda}$$

Notice how the coefficients have an inverse relationship with λ.

Question 2 (a, b, c, d)

2a

Problem: Show that $\mathcal{L}(w) = \frac{1}{n}\|y - Xw\|_2^2$ has critical point $\hat{w} = (X^T X)^{-1} X^T y$.

To find optimal w, solve $\dfrac{\partial \mathcal{L}(w)}{\partial w} = 0$

$$\begin{aligned}
\mathcal{L}(w) &= \frac{1}{n}(y - Xw)^T(y - Xw) \\
&= \frac{1}{n}\left(y^T y - y^T X w - w^T X^T y + w^T X^T X w\right) \\
&= \frac{1}{n}\left(y^T y - 2y^T X w + w^T X^T X w\right)
\end{aligned}$$

To solve for $\hat{w}$,

$$-2X^t y + 2X^T X\hat{w} = 0$$
$$\hat{w} = (X^T X)^{-1} X^T y$$

2b

Problem: Prove $\hat{w} = (X^T X)^{-1} X^T y$ is a global minimum.

$$\begin{aligned}
\nabla_w^2 \mathcal{L}(w) &= \nabla_w(\nabla_w \mathcal{L}(w)) \\
&= \nabla_w(-2X^T y + 2X^T X w) \\
&= 2X^T X
\end{aligned}$$

So, for a vector $u \in \mathbb{R}^p$,

$$\begin{aligned}
u^T(2X^T X)u &= 2(u^T X^T)(Xu) \\
&= 2(u^T X^T)(Xu) \\
&= 2(Xu)^T(Xu) \\
&= 2\|Xu\|_2^2 \geq 0
\end{aligned}$$

Therefore, $\mathcal{L}$ is convex and $\hat{w}$ is the unique global minimum.

2c

$$x_i = \begin{bmatrix} 1 \\ x_{i1} \end{bmatrix} \text{ to represent our input \& the bias } (w_0)$$

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \text{ to represent the target variable}$$

$$w = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \text{ to represent the parameters}$$

$$X = \begin{bmatrix} 1 & x_{11} \\ 1 & x_{21} \\ \vdots & \vdots \\ 1 & x_{n1} \end{bmatrix}$$

$$X^T X = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_{11} & x_{21} & \cdots & x_{n1} \end{bmatrix} \begin{bmatrix} 1 & x_{11} \\ 1 & x_{11} \\ \vdots & \vdots \\ 1 & x_{n1} \end{bmatrix}$$

$$= \begin{bmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{bmatrix}$$

$$= \begin{bmatrix} n & n\bar{x} \\ n\bar{x} & n\overline{x^2} \end{bmatrix}$$

$$X^T y = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_{11} & x_{21} & \cdots & x_{n1} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$X^T y = \begin{bmatrix} n\bar{y} \\ n\overline{xy} \end{bmatrix}$$

$$X^TX = \begin{bmatrix} n & n\bar{x} \\ n\bar{x} & n\overline{x^2} \end{bmatrix}$$

$$(X^TX)^{-1} = \frac{1}{n^2\overline{x^2} - n^2\bar{x}^2} \begin{bmatrix} n\overline{x^2} & -n\bar{x} \\ -n\bar{x} & n \end{bmatrix}$$

$$= \frac{1}{n(\overline{x^2} - \bar{x}^2)} \begin{bmatrix} \overline{x^2} & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix}$$

2d

$$
\begin{aligned}
(X^T X)^{-1} X^T y &= \frac{1}{n(\overline{x^2} - \bar{x}^2)} \begin{bmatrix} \overline{x^2} & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix} \begin{bmatrix} n\bar{y} \\ n\overline{xy} \end{bmatrix} \\
&= \frac{1}{(\overline{x^2} - \bar{x}^2)} \begin{bmatrix} \overline{x^2}\bar{y} - \bar{x}\overline{xy} \\ \overline{xy} - \bar{x}\bar{y} \end{bmatrix} \\
&= \begin{bmatrix} \bar{y} - \hat{w}_1 \bar{x} \\ \frac{\overline{xy} - \bar{x}\bar{y}}{(\overline{x^2} - \bar{x}^2)} \end{bmatrix}
\end{aligned}
$$

2e - Lab