Regression I

COMP9417, 22T2

What do you prefer?

What do you prefer?

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

Thinking Machine Learning

Thinking Machine Learning

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

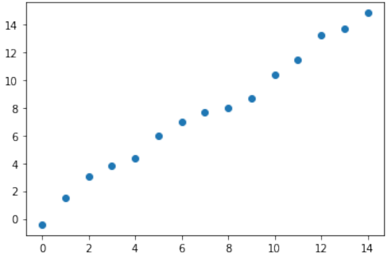
Linear Regression

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 $\rightarrow$ c)

1a

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

i.e Solve:

$$\arg\min_{w_0, w_1} L(w_0, w_1)$$

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

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

$$\begin{aligned}\frac{\partial L(w_0, w_1)}{\partial w_0} &= -\frac{2}{n}\sum_{i=1}^{n}(y_i - w_0 - w_1 x_i) \\ &= -\frac{2}{n}\left(\sum_{i=1}^{n} y_i - n w_0 - w_1 \sum_{i=1}^{n} x_i\right)\end{aligned}$$

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,

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

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

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

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

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

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

Sub (1) into (2):

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

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 $\rightarrow$ h)

2a

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

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

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

$$\frac{\partial \mathcal{L}(w)}{\partial w} = -\frac{1}{n}(-2X^T y + 2X^T X w)$$

To solve for $\hat{w}$,

$$\begin{aligned} -2X^T y + 2X^T X\hat{w} &= 0 \\ \hat{w} &= (X^T X)^{-1} X^T y \end{aligned}$$

2b

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

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

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

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

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

2c

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

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

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

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

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

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

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

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

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

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

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

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

2d

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

2e - Lab

Onto Jupyter.

2f

Say we have the classic regression problem with data $X \in \mathbb{R}^{n \times p}$ and target variable $y \in \mathbb{R}^n$. We can define a feature mapping $\phi : \mathbb{R}^p \to \mathbb{R}^K$. For example, say we have $p = 1$ and we choose $K = 4$, our mapping can be as follows

$$\phi(x) = \begin{bmatrix} x, & x^2, & x^3, & x^4 \end{bmatrix}^T$$

So our original model for a data point $i \in [1, n]$ becomes

$$\hat{y}_i = w^t \phi(x_i).$$

We can generalise our transformation to the matrix:

$$\Phi(x) = \begin{bmatrix} \phi(x_1)^T \\ \phi(x_2)^T \\ \vdots \\ \phi(x_n)^T \end{bmatrix} \in \mathbb{R}^{n \times K}$$

As we use the transpose of our transformation, our model now takes the form $\hat{y} = \Phi w$.

This allows us to solve

$$\hat{w} = \arg\min_{w} \frac{1}{n} \|y - \Phi w\|_2^2$$

Which gives us the classic form of the LS solution:

$$\hat{w} = (\Phi^T \Phi)^{-1} \Phi^T y$$

2h

$$\text{MSE}(w) = \arg\min_{w} \frac{1}{n}\|y - Xw\|_2^2 \text{ and } \text{SSE}(w) = \arg\min_{w} \|y - Xw\|_2^2$$

i) Is the minimiser of MSE and SSE the same?

ii) Is the minimum value of MSE and SSE the same?

3 (a $\rightarrow$ b)

3a

What is the difference between a population and a sample?

3b

What is population parameter? How can we estimate it?