Regression I

COMP9417, 23T2

Section 1

Intro

Intro

Who am I? Who are you?

What you'll get from this course:

- Understand the basis of machine learning
- ML algorithms and the math behind them
- Ability to implement these ideas in Python

How to do well:

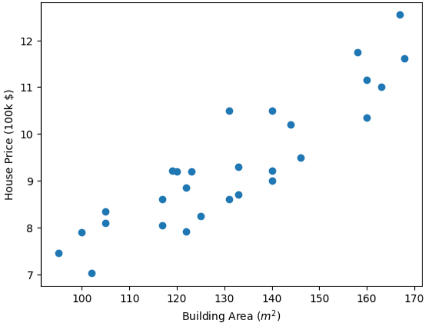
- Fully understand tut questions from week to week (they pile up)
- Don't be afraid of notation, break it all down
- Keep researching

Section 2

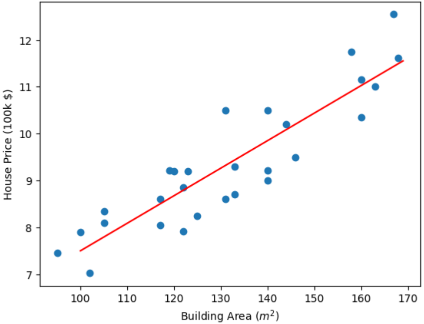
Linear Regression

Linear Regression

Say we're given a task to explain the relationship of the prices of homes based on their size in square meters.



Let's try fitting a line of best fit:



How do we know that this is the line of *best* fit?

Let's define our error as

$$
\begin{aligned}
E &= e_1 + e_2 + e_3 + \cdots + e_n \\
&= \sum_{i=1}^{n} e_i
\end{aligned}
$$

We can generalise this to a function in nicer form:

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

Something is wrong here.

Formally, we define our error/loss function as:

$$L(\hat{y}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \qquad \text{a.k.a MSE}$$

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

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

Section 3

Question 1 (a $\rightarrow$ c)

1a

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

i.e Solve:

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

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

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,

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

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

$$\begin{aligned}\frac{1}{n}\left(\sum_{i=1}^{n} x_i y_i - w_0 \sum_{i=1}^{n} x_i - w_1 \sum_{i=1}^{n} x_i^2\right) &= 0 \\ \overline{xy} - w_0 \bar{x} - w_1 \overline{x^2} &= 0\end{aligned}$$

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

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.

Section 4

Multiple Linear Regression

Multiple Linear Regression

Recall the previous problem where we were tasked with finding price patterns of homes using the size of the home. Say we're now given the number of bedrooms in the house, how do we account for this in the model?

Simple, just add another parameter:

$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2$$

What if we're given the year the house was built and the coordinates? Let's say d more features?

Let's vectorise our model, say:

$x_i = \begin{bmatrix} 1 \\ x_{i1} \end{bmatrix}$ 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

Then, let's define our entire feature set X as:

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

So,

$$Xw = \begin{bmatrix} w_0 + w_1 x_{11} \\ w_0 + w_1 x_{21} \\ \vdots \\ w_0 + w_1 x_{n1} \end{bmatrix}$$

$$\hat{y} = Xw$$

Then, what does our error become?

$$\mathcal{L}(w) = \frac{1}{n}\sum_{i=1}^{n}(y_i - [Xw]_i)^2$$

Formally,

$$\mathcal{L}(w) = \frac{1}{n}\|y - Xw\|_2^2$$

Squared 2-Norm Identity

For a vector v,

$$\|v\|_2^2 = v^T v$$

Vector Calculus

If $u \in \mathbb{R}^n$ and $v \in \mathbb{R}^n$ is a fixed vector, then

$$\frac{\partial v^T u}{\partial u} = v$$

If $A \in \mathbb{R}^{n \times n}$ is a fixed matrix,

$$\frac{\partial (u^T A u)}{\partial u} = Au + A^T u$$

Section 5

Question 2 (a → h)

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 $\dfrac{\partial \mathcal{L}(w)}{\partial w} = 0$

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

Let's find the derivative w.r.t w,

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

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 $\hat{w} = (X^T X)^{-1} X^T y$ 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 $u \in \mathbb{R}^p$,

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

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

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

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

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

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

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

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

We have:

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

Recall the inverse of a matrix $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ is $A^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$.

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

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

Given $x_1, \cdots, x_5 = 3, 6, 7, 8, 11$ and $y_1, \cdots, y_5 = 13, 8, 11, 2, 6$ compute the least squares solution by hand and using Python. Check your results with the sklearn implementation.

2g

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

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

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