Regression I

COMP9417, 23T1

Section 1

Intro

Intro

Who am I?

Intro

Who am I? Who are you?

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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 math or 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.

Linear Regression

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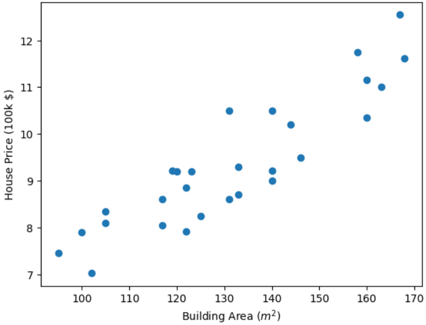
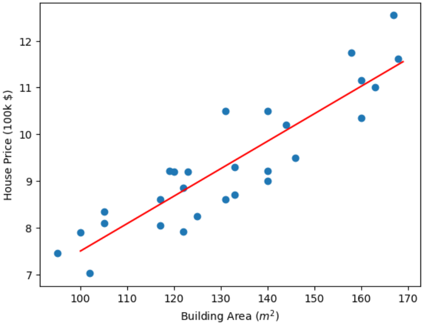


Let's try fitting a line of best fit:



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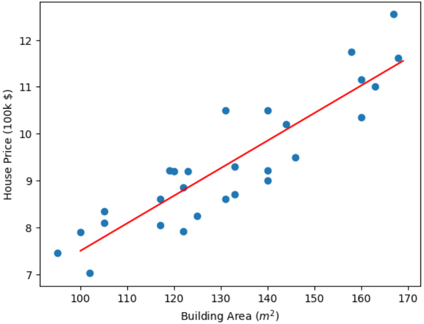

How do we know that this is the line of *best* fit?

Let's define our error as

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We can generalise this to a function in nicer form:

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

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:

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

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

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

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

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

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

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

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Sub (1) into (2):

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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

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Simple, just add another parameter:

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Multiple Linear Regression

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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:

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

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So,

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

$$\hat{y} = Xw$$

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Squared 2-Norm Identity

For a vector v,

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

Vector Calculus

Say we have our weight vector w and a constant vector c,

$$\frac{\partial(cw)}{\partial w} = c^T$$
$$\frac{\partial(w^T cw)}{\partial w} = 2cw$$
$$\frac{\partial(cw^2)}{\partial w} = 2cw$$

Section 5

Question 2 (a $\rightarrow$ h)

2a

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

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

2a

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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 Xw - w^T X^T y + w^T X^T Xw\right) \\
&= \frac{1}{n}\left(y^T y - 2y^T Xw + w^T X^T Xw\right)
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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.

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$$\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
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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

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

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

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

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

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

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

2d

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

2d

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

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?