Lecture 3: Linear Regression

If $\underset{\sim}{x} = (x^{(1)}, \ldots, x^{(P)})$

and $\beta = (\beta^{(0)}, \ldots, \beta^{(P+1)})$

and $\underline{x} = (1, x^{(1)}, \ldots, x^{(P)})$

LR proposes the model

$$Y = f_\beta(\underset{\sim}{x}) = \underbrace{\underline{x}^T \beta = \beta^{(0)} + \sum_{j=1}^{P} x^{(j)} \beta^{(j)}}$$

Looking at least-squares linear regression (OLS)

$$L(y_n, f_\beta(\underset{\sim}{x}_n)) = (y_n - f_\beta(x_n))^2$$

So if we use ERM to get $\hat{f}$

$$\hat{f} = \underset{f \in F}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} L(y_n, f_\beta(\underset{\sim}{x}_n))$$

$$= \underset{f \in F}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} (y_n - \underline{x}^T \beta)^2$$

Notice: to determine f — I simply need to determine β

So equivalently $\hat{f} = f_{\hat{\beta}}$ i.e. $\hat{f}(\underset{\sim}{x}) = \underline{x}^T \hat{\beta}$

where $\hat{\beta}$ minimizes ER:

$$\hat{f} = f_{\hat{\beta}} \quad \text{where} \quad \hat{\beta} = \underset{\beta}{\operatorname{argmin}} \underbrace{\frac{1}{N} \sum_{n=1}^{N} (y_n - \underline{x}^T \beta)^2}$$

$$= \underset{\beta}{\operatorname{argmin}} \underbrace{\sum_n \left(y_n - \overset{\alpha}{x_n^T} \beta\right)^2}_{RSS(\beta)}$$

So equiv.

$$\hat{f}(\underline{x}) = \underline{x}^T \hat{\beta} \quad \text{whe} \quad \hat{\beta}^{(OLS)} = \underset{\beta}{\operatorname{argmin}}\, RSS(\beta)$$

So ERM = Ordinary Least Squares Regression

Practically, How do we find $\hat{\beta}^{(OLS)}$?

Let X be our <u>design matrix</u> so that

$$X = \begin{bmatrix} \vdots \\ - \underline{x}_n^T - \\ \vdots \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & x_1^{(2)} & \cdots & x_1^{(p)} \\ \vdots & x_2^{(1)} & \vdots & & \vdots \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_N^{(1)} & x_N^{(2)} & \cdots & x_N^{(p)} \end{bmatrix}_{N \times (p+1)}$$

and $y = (y_1, \dots, y_n)^T \in \mathbb{R}^{N \times 1}$

then I want to minimize $RSS(\beta)$

$$RSS(\beta) = \sum_{n=1}^{N} \left(y_n - \underline{x}^T \beta\right)^2$$

$$= \| \underset{N\times 1}{y} - \underbrace{\underset{N\times(p+1)}{X}\ \underset{(p+1)\times 1}{\beta}}_{N \times 1} \|^2$$

X

$\|y - X\beta\|^2$

$\hookrightarrow y - X\beta = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} - \underline{x}_1^T - \\ \vdots \\ - \underline{x}_N^T - \end{bmatrix} \beta$

$= \underset{N\times 1}{\begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}} - \underset{N\times 1}{\begin{bmatrix} - \underline{x}_1^T\beta - \\ \vdots \\ - \underline{x}_N^T\beta - \end{bmatrix}}$

$\|a\| = \sqrt{\sum_i a_i^2}$

$\|a\|^2 = \sum_i a_i^2$

$= \begin{bmatrix} y_1 - \underline{x}_1^T\beta \\ y_2 - \underline{x}_2^T\beta \\ \vdots \\ y_N - \underline{x}_N^T\beta \end{bmatrix}$

So $\|y - X\beta\|^2 = \sum_n (y_n - \underline{x}_n^T\beta)^2 = RSS(\beta)$.

So $\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \underbrace{\|y - X\beta\|^2}_{RSS:\ \mathbb{R}^{P+1} \to \mathbb{R}}$

How do I find the minimizer of RSS?

MV Calc Problem: get $\underbrace{\text{derivative}}_{\text{gradient}}$ and set equal to zero

Turns Out:

gradient of $RSS(\beta)$ w.r.t. $\beta = \frac{\partial RSS}{\partial \beta} = \underbrace{-2\overbrace{(y - X\beta)^T}^{1\times N}\overbrace{X}^{N\times(P+1)}}_{1\times(P+1) \text{ row vector}}$

So if $\frac{\partial RSS}{\partial \beta} = -2(y - X\beta)^T X$

then Calc 3 says set equal to zero

$$\frac{\partial RSS}{\partial \beta} = -2(y - X\beta)^T X = 0$$

$$\Rightarrow -\cancel{2}(y^T - \beta^T X^T) X = 0$$

$$\Rightarrow \quad y^T X - \beta^T X^T X = 0$$

$$\Rightarrow \boxed{X^T y = X^T X \beta}$$

Normal equations

If $\underbrace{X^T X}_{\substack{p+1 \times N \times p+1 \\ (p+1)\times(p+1)}}$ is invertible then

$$(X^T X)^{-1} X^T y = \cancel{(X^T X)^{-1} X^T X}^{\,I} \beta$$

So $\boxed{\hat{\beta}^{(LS)} = (X^T X)^{-1} X^T y}$

So $\hat{f}(\underset{\sim}{x}) = \underset{\sim}{x}^T \hat{\beta}$ when $\hat{\beta} = (X^T X)^{-1} X^T y$

$$= \underset{\sim}{x}^T (X^T X)^{-1} X^T y$$

Consider predictions on training data

$$\hat{y}_n = \hat{f}(\underset{\sim}{x}_n) = \underline{x_n}^T \underbrace{(X^T X)^{-1} X^T y}_{\hat{\beta}}$$

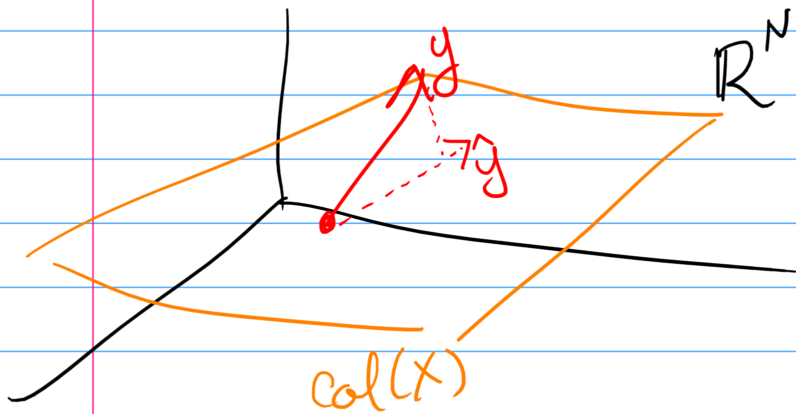
$$\hat{y} = \begin{bmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_N \end{bmatrix} = \begin{bmatrix} \text{—} & \underline{x_n}^T \hat{\beta} & \text{—} \end{bmatrix} = X\hat{\beta}$$

For training data

$$\hat{y} = X\hat{\beta}$$

notice then that

$$\hat{y} = X\hat{\beta} = \underbrace{X(X^TX)^{-1}X^T}_{\text{projection mtx onto } Col(X)} y = \text{proj. of } y \text{ onto } Col(X)$$



How flexible is OLS?

Is this regression?

$$Y = \beta^{(0)} + \sum_{j=1}^{p} \beta^{(j)} X^{(j)2} \quad ?$$

Yes. This is still linear in βs.

lets just change the design

$$\underline{X} = (1, \underbrace{X^{(1)2}, X^{(2)2}, \ldots, X^{(p)2}})$$

then $Y = \underline{X}^T \beta$

this is still a linear operation wrt β

So as before

$\hat{\beta} = (X^TX)^{-1}X^Ty$ but now I'm using a slightly different X

Ex. What about this:

$$Y = f(\underset{\sim}{x}) = \underline{\beta^{(0)}} + \underline{\beta^{(1)}} X^{(1)2} + \underline{\beta^{(2)}} \log(X^{(2)}) + \underline{\beta^{(3)}} \sin(X^{(1)} X^{(2)}) \ ?$$

Is this linear regression?

Yes. All we need to do is change the design

$$\underline{x} = (1, X^{(1)2}, \log(X^{(2)}), \sin(X^{(1)} X^{(2)}))$$

So if

$$X = \begin{bmatrix} 1 & | & | & | \\ \vdots & X^{(1)2} & \log(X^{(2)}) & \sin(X^{(1)} X^{(2)}) \\ 1 & | & | & | \end{bmatrix}$$

then $\hat{\beta} = (X^T X)^{-1} X^T y$

and $\hat{f}(\underline{x}) = \underline{x}^T \hat{\beta}$.

Generically we still have an OLS method in any basis expansion so long as the bases don't depend on βs:

$\underline{x}^{(j)} = \varphi_j(\underset{\sim}{x})$ for arb. φ_j doesn't depend on βs

then

$$X = \begin{bmatrix} | & | & \\ \varphi_1(\underset{\sim}{x}) & \varphi_2(\underset{\sim}{x}) & \cdots \\ | & | & \end{bmatrix}$$ and $\hat{\beta} = (X^T X)^{-1} X^T y$

What about categorical vars? (factors in R)

e.g. race, color, gender etc.

How do I do something like

$$Y = \beta^{(0)} + \beta^{(1)} \underbrace{\text{Gender}}^{x^{(1)}} ?$$

Can do this using dummy variable encoding.

$\underline{x} = (1, 0)$ if female

$x^{(1)} = \begin{cases} 0 & \text{fem} \\ 1 & \text{male} \end{cases}$

$\underline{x} = (1, 1)$ if male

then my design mtx X will look somethg like

$$X = \begin{bmatrix} 1 & 0 \\ \vdots & 1 \\ \vdots & 1 \\ \vdots & 0 \\ 1 & 1 \end{bmatrix}$$

females

males

then $\hat{\beta} = (X^T X)^{-1} X^T y$

How do I interpret $\hat{\beta}$?

Ex. $(\hat{\beta}^{(0)}, \hat{\beta}^{(1)})$ interpret?

If gender = F then $Y \approx \hat{\beta}^{(0)} + \hat{\beta}^{(1)} \cdot 0 = \hat{\beta}^{(0)}$

gender = M then $Y \approx \hat{\beta}^{(0)} + \hat{\beta}^{(1)} \cdot 1$

So $\hat{\beta}^{(0)}$ as the typ. val. for Y (w/ other vars fixed) for a female

$$\hat{\beta}^{(1)} = \underbrace{\hat{\beta}^{(0)} + \hat{\beta}^{(1)}}_{\text{typ val for M}} - \underbrace{\hat{\beta}^{(0)}}_{\text{typ val for F}} = \text{contrast} = \text{diff. btwn typ. vals for M and F}$$

Generically I can encode a K level factor using K-1 dummy vars.

Hogwarts House

4-level

$$\text{data} = \begin{bmatrix} \cdots & \begin{array}{c} \text{Hogwarts} \\ H \\ R \\ G \\ H \\ S \\ \vdots \end{array} & \cdots \end{bmatrix} \Rightarrow X = \begin{array}{c} \begin{array}{ccc} H & R & G \end{array} \\ \begin{bmatrix} & 1 & 0 & 0 & \\ & 0 & 1 & 0 & \\ & 0 & 0 & 1 & \\ \cdots & 1 & 0 & 0 & \cdots \\ & 0 & 0 & 0 & \\ & & \vdots & & \end{bmatrix} \end{array}$$

How do I interpret $\hat{\beta}$?

difference in typical values for Y

Holding other vars. constant what is the diff btwn (in typ. val for Y) H/R/G and S

Fitting Issues

Recall that $\frac{\partial RSS}{\partial \beta} = 0$ yielded "normal equations"

$$X^T X \beta = X^T y.$$

IF $X^T X$ is invertible then $\hat{\beta} = (X^T X)^{-1} X^T y$.

When can this fail? when X^TX isn't invertible.

$$\rightarrow \boxed{X^TX \text{ isn't invertible} \iff \operatorname{rank}(X) < \# \text{cols } X}$$

$\Leftarrow$ $\operatorname{rank}(X) < \#$ cols X then $\exists v \neq 0$ s.t. $Xv = 0$.

Recall that Xv is a linear combination of columns of X

Consequently $X^TXv = X^T0 = 0$

So $\exists v \neq 0$ s.t. $(X^TX)v = 0$ i.e. X^TX is rank defficient so its not invertible.

$\Rightarrow$ If X^TX isn't invertible then $\exists v \neq 0$ s.t.

$X^TXv = 0$ $\qquad \|u\| = \sqrt{u^Tu}$

hence $0 = v^T0 = v^TX^TXv = (Xv)^T(Xv) = \|Xv\|^2$

So $\exists v \neq 0$ when $\|Xv\| = 0$ hence $Xv = 0$

$(\|a\| = 0 \iff a = 0)$

So X is rank difficient i.e. $\operatorname{rank}(X) < \#$ cols.

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when does this happen in reality?

(1) If I accidentically incl. a var. twice in design

$$X = \begin{bmatrix} 1 & 1 & 1 \\ & 2 & 2 \\ \vdots & \cdots\ 3 & \cdots\ 3 \\ 1 & 4 & 4 \end{bmatrix}$$

lin. dep. $\Rightarrow$ X rank def.

this is like saying

$$\hat{Y} = \hat{\beta}^{(0)} + \hat{\beta}^{(1)} X^{(1)} + \hat{\beta}^{(2)} X^{(1)}$$

e.g. $= 1 + 5x^{(1)} + 7x^{(1)}$

this has exactly same preds as

$$= 1 + \underbrace{3x^{(1)} + 9x^{(1)}}_{12x^{(1)}}$$

or any model where sum of $\hat{\beta}^{(1)} + \hat{\beta}^{(2)} = 12$

2) If # cols of X > N having variables more than observations

if X is $N \times P+1$

and $P+1 > N$

then $\text{rank}(X) \leq \min\{\#\text{rows}, \#\text{cols}\} = N < P+1$