

In the name of God



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Deep Learning - 25647

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Homework 1 - Section 1

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Problem 1.

As wikipedia says: In Vapnik–Chervonenkis theory, the Vapnik–Chervonenkis (VC) dimension is a measure of the capacity (complexity, expressive power, richness, or flexibility) of a set of functions that can be learned by a statistical binary classification algorithm. It is defined as the cardinality of the largest set of points that the algorithm can shatter, which means the algorithm can always learn a perfect classifier for any labeling of that many data points.

VC dimension of a classification model: A binary classification model f with some parameter vector θ is said to shatter a set of data points (x_1, x_2, \dots, x_n) if, for all assignments of labels to those points, there exists a θ such that the model f makes no errors when evaluating that set of data points.

The VC dimension of a model f is the maximum number of points that can be arranged so that f shatters them. More formally, it is the maximum cardinal D such that some data point set of cardinality D can be shattered by f .

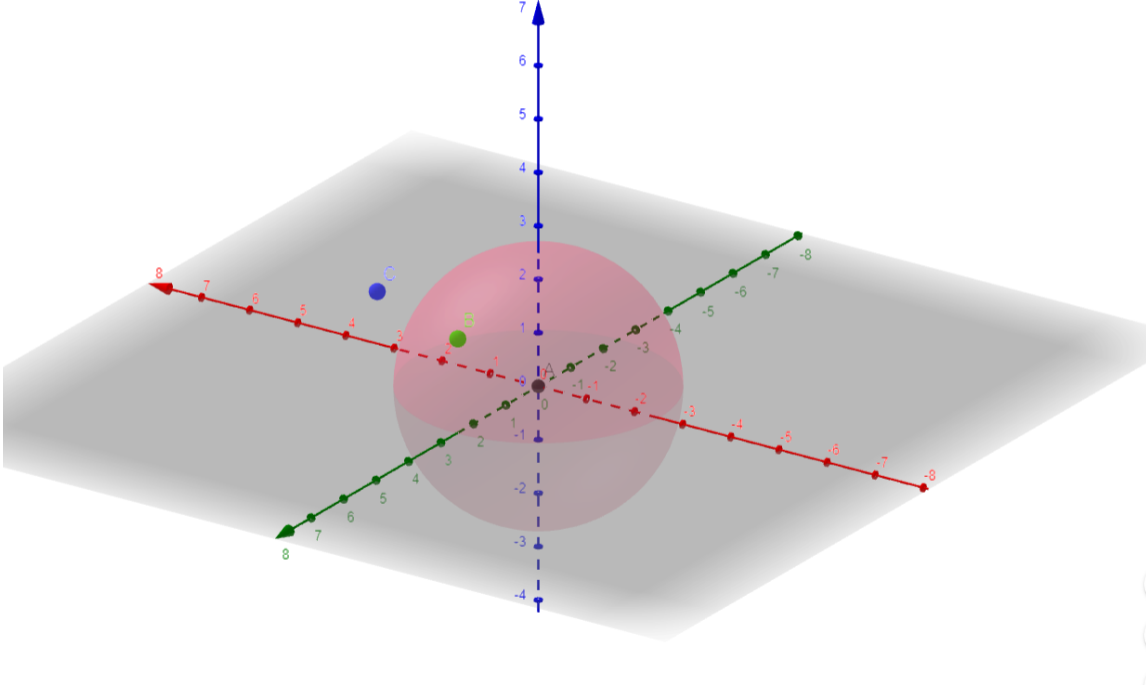


Figure 1: Green point: $\{(1, 1, 1): -1\}$, Blue point: $\{(2, 2, 2): +1\}$

(a) The VC dimension is 1.

First, we show that there exists 1 point, $x_1 \in \mathbb{R}^3$ that can be shattered. Pick $(1, 1, 1)$. Consider the following sub-cases: ($r = \sqrt{(-\theta)}$)

* The point is positive. Choose any origin-centered sphere that includes the point ($r < \sqrt{3}$)

* The point is negative. Choose any origin-centered sphere that does not include the point ($r > \sqrt{3}$).

We now need to show that an origin-centered sphere cannot shatter 2 points. Pick $(1, 1, 1)$ as +1 and $(2, 2, 2)$ as -1. An origin-centered sphere cannot shatter these two points because $r_1 < r_2$. Each origin-centered sphere of radius r , divide the space into two parts, -1 and +1. Moreover, radius of class +1 is greater than radius of class -1. Therefore, we cannot shatter two points of different classes while the point of class -1 is closer to the origin (Figure 1).

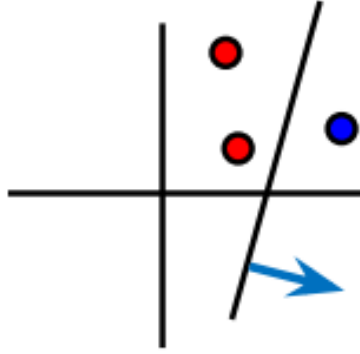


Figure 2: A two-dimensional line for splitting 3 points.

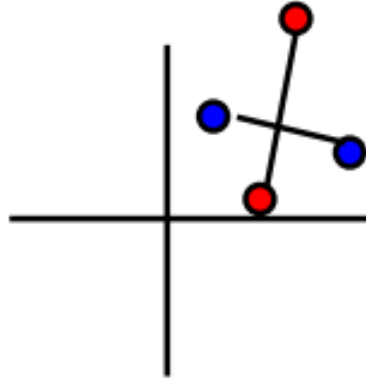


Figure 3: Two-dimensional lines for splitting 4 points.

(b) The VC dimension is 3.

First, we show that there exist 3 points, $x_1, x_2, x_3 \in \mathbb{R}^2$ that can be shattered.

* All of the points are positive or All of the points are negative: We can have a line which separates the points correctly (The points will be in one side of the line).

* Two points are positive and 1 point is negative or Two points are negative and 1 point is positive. Figure 2 shows that we can easily draw a line, which can separates the points correctly.

We now need to show that a two-dimensional line cannot shatter 4 points. Assume 4 points in 2 pairs. Any line through these points must split one pair (by crossing one of the lines) (Figure 3).

(c) We can show that the VC dimension of hyperplanes in m dimensions is $m + 1$.

Proof: Let \mathcal{H} be the set of hyperplanes in m dimensions. First, we show that there exists a set S of $m+1$ points $\in \mathbb{R}^m$ shattered by \mathcal{H} .

Suppose $S = \{x_1, \dots, x_m, x_{m+1}\}$, where x_i is a point $\in \mathbb{R}^m$, and our hyperplane is represented as $y = w^\top x + w_0$. Let y_1, \dots, y_m, y_{m+1} be any set of labels assigned to the $m+1$ points and construct the following linear system:

$$w^\top x_1 + w_0 = y_1 w^\top x_2 + w_0 = y_2 \dots w^\top x_{m+1} + w_0 = y_{m+1}$$

Notice that the above linear system has $m + 1$ variables w_0, \dots, w_m and $m + 1$ equations, hence it must have a solution as long as S satisfies the condition that $(1, x_1), \dots, (1, x_m), (1, x_{m+1})$ are linearly independent.

Hence by choosing S s.t. the matrix $\begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_{m+1} \end{pmatrix}$ is full-rank, we can always

solve for a m -dimensional hyperplane with bias term that separates the $m + 1$ points in S . Since y_1, \dots, y_m, y_{m+1} can be any set of labels, the m -dimensional hyperplane shatters the $m + 1$ points in S .

Secondly, we show that there exists no set S' of $m + 2$ points can be shattered by \mathcal{H} .

Suppose to the contrary that $S' = \{x_1, \dots, x_{m+1}, x_{m+2}\}$ can be shattered. This implies that there exist 2^{m+2} weight vectors $w^{(1)}, \dots, w^{(2^{m+2})}$ such that the matrix of inner products denoted by $z_{i,j} = x_i^\top w^{(j)}$ has columns with all possible combination of signs (note here x_i contains the constant feature and $w^{(j)}$ contains the bias term). We use A to denote this matrix and

$$A = \begin{pmatrix} z_{1,1} & \dots & z_{1,2^{m+2}} \\ \vdots & \dots & \vdots \\ z_{m+2,1} & \dots & z_{m+2,2^{m+2}} \end{pmatrix} \text{ s.t. } \text{sign}(A) = \begin{pmatrix} - & - & \dots & - & + \\ - & \cdot & \dots & \cdot & + \\ \vdots & \vdots & \dots & \vdots & \vdots \\ - & + & \dots & + & + \end{pmatrix}$$

Then the rows of A are linearly independent because there exists a column of A with the same signs which does not sum to zero hence there are no constants c_1, c_2, \dots, c_{m+2} such that $\sum_{i=1}^{m+2} c_i z_{i,:} = 0$. However, notice that row i of A can be written as $x_i^\top W$ where $W = [w^{(1)}, \dots, w^{(2^{m+2})}]$. By linear algebra knowledge we know that $m + 2$ vectors $\in \mathbb{R}^{m+1}$, are always linearly dependent (i.e. $x_1^\top, \dots, x_{m+2}^\top$ are linearly dependent). Hence $x_1^\top W, \dots, x_{m+2}^\top W$ should also be linearly dependent, which results in a contradiction. This contradiction proves that there are no $m+2$ points $\in \mathbb{R}^m$ which can be shattered by hyperplanes in m dimension. Thus, the VC dimension of \mathcal{H} is $m + 1$. [University of Pennsylvania, CIS250 wiki, 2018]

Problem 2.

The log likelihood of our model is:

$$\log p(\mathbf{y}|\mathbf{X}, \mathbf{w}) = \sum_{i=1}^N \log p(y_i|\mathbf{x}_i, \theta)$$

But since the noise ϵ is Gaussian, the likelihood is just:

$$\begin{aligned} \log p(\mathbf{y}|\mathbf{X}, \mathbf{w}) &= \sum_{i=1}^N \log N(y_i; \mathbf{x}_i \mathbf{w}, \sigma^2) \\ &= \sum_{i=1}^N \log \frac{1}{\sqrt{2\pi\sigma_e^2}} \exp\left(-\frac{(y_i - \mathbf{x}_i \mathbf{w})^2}{2\sigma_e^2}\right) \\ &= -\frac{N}{2} \log 2\pi\sigma_e^2 - \sum_{i=1}^N \frac{(y_i - \mathbf{x}_i \mathbf{w})^2}{2\sigma_e^2} \end{aligned}$$

So:

$$\begin{aligned} \mathbf{w}_{MLE} &= \operatorname{argmax}_w - \sum_{i=1}^N (y_i - \mathbf{x}_i \mathbf{w})^2 \\ &= \operatorname{argmin}_w \frac{1}{N} \sum_{i=1}^N (y_i - \mathbf{x}_i \mathbf{w})^2 \\ &= \operatorname{argmin}_w MSE_{train} \end{aligned}$$

That is, the parameters \mathbf{w} chosen to maximise the likelihood are exactly those chosen to minimise the mean-squared error.

Problem 3.

We assume that the likelihood function (\mathcal{L}) is the Gaussian itself.

$$\begin{aligned}\mathcal{L} &= p(\mathbf{X}|\theta) = \mathcal{N}(\mathbf{X}|\theta) \\ &= \mathcal{N}(\mathbf{X}|\mu, \Sigma)\end{aligned}$$

Therefore, for MLE of a Gaussian model, we will need to find good estimates of both parameters: μ and Σ :

$$\begin{aligned}\mu_{MLE} &= \operatorname{argmax}_{\mu} \mathcal{N}(\mathbf{X}|\mu, \Sigma) \\ \Sigma_{MLE} &= \operatorname{argmax}_{\Sigma} \mathcal{N}(\mathbf{X}|\mu, \Sigma)\end{aligned}$$

For simplicity we will use log likelihood (the $\log()$ function is monotonically increasing). Now we want to get the best parameters $\theta = [\mu, \Sigma]$ for a dataset \mathbf{X} evaluating on a Gaussian distribution.

$$\theta_{MLE} = \operatorname{argmax}_{\theta} \log(\mathcal{N}(\mathbf{X}|\theta))$$

$$\begin{aligned}\mathcal{LL} &= \log(\mathcal{N}(\mathbf{X}|\theta)) = \sum_{n=1}^N \log(\mathcal{N}(\mathbf{x}_n|\theta)) \\ &= \sum_{n=1}^N \log(\mathcal{N}(\mathbf{x}_n|\mu, \Sigma)) \\ &= \sum_{n=1}^N \log(\mathcal{N}(\mathbf{x}_n|\mu, \sigma^2)) \\ &= \sum_{n=1}^N \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp^{-\frac{1}{2}\left(\frac{(x_n-\mu)^2}{\sigma^2}\right)}\right) \\ &= \sum_{n=1}^N \left(\log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) + \log\left(\exp^{-\frac{1}{2}\left(\frac{(x_n-\mu)^2}{\sigma^2}\right)}\right)\right) \\ &= \sum_{n=1}^N \left(\log(1) - \log(\sqrt{2\pi\sigma^2}) + \log\left(\exp^{-\frac{1}{2}\left(\frac{(x_n-\mu)^2}{\sigma^2}\right)}\right)\right)\end{aligned}$$

$$\begin{aligned}
&= \sum_{n=1}^N \left(\log(1) - \log(\sqrt{2\pi\sigma^2}) + \left(-\frac{1}{2} \left(\frac{(x_n - \mu)^2}{\sigma^2} \right) \cdot \log(e) \right) \right) \\
&= \sum_{n=1}^N \left(-\log(\sqrt{2\pi\sigma^2}) + \left(-\frac{1}{2} \left(\frac{(x_n - \mu)^2}{\sigma^2} \right) \right) \right) \\
&= \sum_{n=1}^N \left(-\frac{1}{2} \cdot \log(2\pi\sigma^2) - \frac{1}{2} \left(\frac{(x_n - \mu)^2}{\sigma^2} \right) \right) \\
&= -\frac{N}{2} \log(2\pi\sigma^2) + \sum_{n=1}^N -\frac{1}{2} \left(\frac{(x_n - \mu)^2}{\sigma^2} \right) \\
&= -\frac{N}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2
\end{aligned}$$

So, now we're going to solve the problem for each variable one-by-one:

$$\begin{aligned}
&\underset{\mu}{\operatorname{argmax}} \mathcal{LL}(X|\mu, \sigma^2) \\
&\underset{\sigma^2}{\operatorname{argmax}} \mathcal{LL}(X|\mu, \sigma^2)
\end{aligned}$$

MLE of μ :

$$\begin{aligned}
\mathcal{LL} &= -\frac{N}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \\
\underset{\mu}{\operatorname{argmax}} \mathcal{LL}(X|\mu, \sigma^2) &:= \frac{\partial \mathcal{LL}}{\partial \mu} = 0 \\
\frac{\partial \mathcal{LL}}{\partial \mu} &= \frac{\partial}{\partial \mu} \left(-\frac{N}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= \frac{\partial}{\partial \mu} \left(-\frac{N}{2} \log(2\pi\sigma^2) \right) + \frac{\partial}{\partial \mu} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= 0 + \frac{\partial}{\partial \mu} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= \frac{\partial}{\partial \mu} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right)
\end{aligned}$$

$$\begin{aligned}
&= \frac{\partial}{\partial \mu} \left(\sum_{n=1}^N -\frac{1}{2\sigma^2} (x_n - \mu)^2 \right) \\
&= \sum_{n=1}^N \frac{\partial}{\partial \mu} \left(-\frac{1}{2\sigma^2} (x_n - \mu)^2 \right) \\
&= \sum_{n=1}^N \left(\frac{\partial}{\partial \mu} \left(-\frac{1}{2\sigma^2} \right) \cdot (x_n - \mu)^2 + \left(-\frac{1}{2\sigma^2} \right) \cdot \frac{\partial}{\partial \mu} (x_n - \mu)^2 \right) \\
&= \sum_{n=1}^N \left(0 + \left(-\frac{1}{2\sigma^2} \right) \cdot \frac{\partial}{\partial \mu} (x_n - \mu)^2 \right) \\
&= -\frac{1}{2\sigma^2} \sum_{n=1}^N \frac{\partial}{\partial \mu} (x_n - \mu)^2 \\
&= -\frac{1}{2\sigma^2} \sum_{n=1}^N 2(x_n - \mu) \cdot -1 \\
&= \frac{1}{\sigma^2} \sum_{n=1}^N (x_n - \mu) = 0 \\
0 &= \sum_{n=1}^N (x_n - \mu) \\
0 &= \sum_{n=1}^N x_n - \sum_{n=1}^N \mu \\
0 &= \sum_{n=1}^N x_n - N \cdot \mu \\
N \cdot \mu &= \sum_{n=1}^N x_n \\
\mu &= \frac{1}{N} \sum_{n=1}^N x_n
\end{aligned}$$

MLE of σ^2 :

$$\begin{aligned}
\frac{\partial \mathcal{LL}}{\partial \sigma^2} &= \frac{\partial}{\partial \sigma^2} \left(-\frac{N}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= \frac{\partial}{\partial \sigma^2} \left(-\frac{N}{2} \log(2\pi\sigma^2) \right) + \frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= \frac{\partial}{\partial \sigma^2} \left(-\frac{N}{2} \right) \cdot \log(2\pi\sigma^2) + \left(-\frac{N}{2} \right) \cdot \frac{\partial}{\partial \sigma^2} (\log(2\pi\sigma^2)) + \frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= 0 + \left(-\frac{N}{2} \right) \cdot \frac{\partial}{\partial \sigma^2} (\log(2\pi\sigma^2)) + \frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= -\frac{N}{2} \cdot \frac{\partial}{\partial \sigma^2} (\log(2\pi\sigma^2)) + \frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= -\frac{N}{2} \cdot \frac{1}{2\pi\sigma^2} \cdot 2\pi + \frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= -\frac{N}{2} \cdot \frac{1}{\sigma^2} + \frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(\frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} (x_n - \mu)^2 \right) \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(\frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \right) \cdot (x_n - \mu)^2 + \left(-\frac{1}{2\sigma^2} \right) \cdot \frac{\partial}{\partial \sigma^2} (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(\frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \right) \cdot (x_n - \mu)^2 + 0 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(\frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2\sigma^2} \right) \cdot (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(\frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2} \cdot \sigma^{-2} \right) \cdot (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(\frac{\partial}{\partial \sigma^2} \left(-\frac{1}{2} \right) \cdot \sigma^{-2} + \left(-\frac{1}{2} \right) \cdot \frac{\partial}{\partial \sigma^2} \sigma^{-2} \right) \cdot (x_n - \mu)^2
\end{aligned}$$

$$\begin{aligned}
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(0 + \left(-\frac{1}{2} \cdot \frac{\partial}{\partial \sigma^2} \sigma^{-2} \right) \cdot (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(-\frac{1}{2} \cdot \frac{\partial}{\partial \sigma^2} \sigma^{-2} \cdot (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(-\frac{1}{2} \cdot \frac{\partial}{\partial \sigma^2} ((\sigma^2)^{-1}) \cdot (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(-\frac{1}{2} \cdot -1 \cdot (\sigma^2)^{-2} \cdot 1 \cdot (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(\frac{1}{2} \cdot (\sigma^2)^{-2} \cdot (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \sum_{n=1}^N \left(\frac{1}{2\sigma^4} \cdot (x_n - \mu)^2 \right) \\
&= -\frac{N}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{n=1}^N (x_n - \mu)^2 \\
&= \frac{1}{2\sigma^2} \left(-N + \frac{1}{\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
0 &= \frac{1}{2\sigma^2} \left(-N + \frac{1}{\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right) \\
0 &= -N + \frac{1}{\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \\
N\sigma^2 &= \sum_{n=1}^N (x_n - \mu)^2 \\
\sigma^2 &= \frac{1}{N} \sum_{n=1}^N (x_n - \mu)^2
\end{aligned}$$

To conclude:

$$\begin{aligned}
\mu_{MLE} &= \frac{1}{N} \sum_{n=1}^N x_n \\
\sigma_{MLE}^2 &= \frac{1}{N} \sum_{n=1}^N (x_n - \mu)^2
\end{aligned}$$

Problem 4.

A) Using the least squares method we want to find parameter values that minimizes the residual sum of squares (RSS):

$$\begin{aligned} RSS &= \sum_{i=1}^n r_i^2 = \sum_{i=1}^n (y_i - x_i W)^2 \\ &= \|y - XW\|^2 \quad \text{where } X \in \mathbb{R}^{n \times (p+1)} \quad \text{and } y \in \mathbb{R}^n, W \in \mathbb{R}^{p+1} \\ &= (y - XW)^\top (y - XW) \end{aligned}$$

which leads to:

$$\hat{W} = \underset{W}{\operatorname{argmin}} (y - XW)^\top (y - XW)$$

Differentiate RSS this with respect to β :

$$\begin{aligned} RSS &= (y - XW)^\top (y - XW) \\ &= (y^\top - W^\top X^\top)(y - XW) \\ &= y^\top y - y^\top XW - W^\top X^\top y + W^\top X^\top XW \end{aligned}$$

$$\begin{aligned} \frac{\partial RSS}{\partial W} &= \frac{\partial (y^\top y - y^\top XW - W^\top X^\top y + W^\top X^\top XW)}{\partial W} \\ &= 0 - X^\top y - X^\top y + (X^\top X + (X X^\top)^\top)W \\ &= -2X^\top y + 2X^\top XW \end{aligned}$$

This first derivative should equal to 0. So,

$$\begin{aligned} -2X^\top y + 2X^\top XW &= 0 \\ X^\top XW &= X^\top y \\ W &= (X^\top X)^{-1} X^\top y \end{aligned}$$

B) L2 regularization:

$$\begin{aligned}
\hat{W} &= \underset{W}{\operatorname{argmin}} (y - XW)^\top (y - XW) + \lambda W^\top W \\
\frac{\partial RSS}{\partial W} &= \frac{\partial (y^\top y - y^\top XW - W^\top X^\top y + W^\top X^\top XW + \lambda W^\top W)}{\partial W} \\
&= 0 - X^\top y - X^\top y + (X^\top X + (XX^\top)^\top)W + 2\lambda W \\
&= -2X^\top y + 2X^\top XW + 2\lambda W
\end{aligned}$$

This first derivative should equal to 0. So,

$$\begin{aligned}
-2X^\top y + 2X^\top XW + 2\lambda W &= 0 \\
(X^\top X + \lambda I)W &= X^\top y \\
W &= (X^\top X + \lambda I)^{-1} X^\top y
\end{aligned}$$