Fundamentals of Machine Learning

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Task 3: LDA derivation from the Least Squares Error

Setting the derivatives of $\sum_{i=1}^{n} \left(w^T x_i + b - y_i\right)^2$ wrt. b, w to zero, we obtain

$$\frac{\partial}{\partial b} \sum_{i=1}^{n} \left(w^T x_i + b - y_i\right)^2 = 2 \sum_{i=1}^{n} \left(w^T x_i + b - y_i\right) \stackrel{!}{=} 0 \tag{1}$$

$$\frac{\partial}{\partial b} \sum_{i=1}^{n} \left(w^T x_i + b - y_i\right)^2 = 2 \sum_{i=1}^{n} \left(w^T x_i + b - y_i\right) x_i \stackrel{!}{=} 0 \tag{2}$$

Since we shall take the targets for class $k = 1$ to be n/n_1, where n_1 is the number of instances in class $k = 1$, and n the total number of instances. For class $k = 2$, we shall take the targets to be $-n/n_2$, where where n_2 is the number of instances in class $k = 2$. From equation 1 we obtain an expression for the bias in the form

$$b = -w^T \mu \tag{3}$$

where we have used

$$\sum_{i=1}^{n} y_i = n_1 \frac{n}{n_1} - n_2 \frac{n}{n_2} = 0 \tag{4}$$

and where μ is the mean of the total data set and is given by

$$\mu = \frac{1}{n} \sum_{i=1}^{n} x_i = \frac{1}{n} \left(n_1 \mu_1 + n_2 \mu_2\right) \tag{5}$$

By expanding equation 2

$$
\begin{aligned}
&\sum_{i=1}^{n} w^T x_i x_i + b \sum_{i=1}^{n} x_i - \sum_{i=1}^{n} y_i x_i \\
&= \sum_{i=1}^{n} x_i x_i^T w - w^T \mu \sum_{i=1}^{n} x_i - \left(\sum_{i \in k=1} y_i x_i + \sum_{i \in k=2} y_i x_i \right) \\
&= \sum_{i=1}^{n} x_i x_i^T w - w^T \mu \left(n\mu \right) - \left(\sum_{i \in k=1} \frac{n}{n_1} x_i - \sum_{i \in k=2} \frac{-n}{n_2} x_i \right) \\
&= \sum_{i=1}^{n} x_i x_i^T w - n w^T \mu\mu - n \left(\sum_{i \in k=1} \frac{1}{n_1} x_i - \sum_{i \in k=2} \frac{-1}{n_2} x_i \right) \\
&= \sum_{i=1}^{n} x_i x_i^T w - n w^T \mu\mu - n \left(\mu_1 - \mu_2 \right) \\
&= \left[\sum_{i=1}^{n} \left(x_i x_i^T \right) - n\mu\mu^T \right] w - n \left(\mu_1 - \mu_2 \right)
\end{aligned}
\tag{6}
$$

If we let the derivative equal to zero, we will see that:

$$
\left[\sum_{i=1}^{n} \left(x_i x_i^T \right) - n\mu\mu^T \right] w = n \left(\mu_1 - \mu_2 \right) \tag{7}
$$

Therefore, now we need to prove:

$$
\sum_{i=1}^{n} \left(x_i x_i^T \right) - n\mu\mu^T = S_W + \frac{n_1 n_2}{n} S_B \tag{8}
$$

Let's expand the left side of the equation above:

$$
\begin{aligned}
&\sum_{i=1}^{n} x_i x_i^T - n\left(\frac{n_1}{n}\mu_1 + \frac{n_2}{n}\mu_2\right)^2 \\
&= \sum_{i=1}^{n} x_i x_i^T - n\left(\frac{n_1^2}{n^2}||\mu_1||^2 + \frac{n_2^2}{n^2}||\mu_2||^2 + 2\frac{n_1 n_2}{n^2}\mu_1\mu_2^T\right) \\
&= \sum_{i=1}^{n} x_i x_i^T - \frac{n_1^2}{n}||\mu_1||^2 - \frac{n_2^2}{n}||\mu_2||^2 - 2\frac{n_1 n_2}{n}\mu_1\mu_2^T \\
&= \sum_{i=1}^{n} x_i x_i^T + \left(n_1 + \frac{n_1 n_2}{n} - 2n_1\right)||\mu_1||^2 \\
&\quad + \left(n_2 + \frac{n_1 n_2}{n} - 2n_2\right)||\mu_2||^2 - 2\frac{n_1 n_2}{n}\mu_1\mu_2^T \\
&= \sum_{i=1}^{n} x_i x_i^T + \left(n_1 - 2n_1\right)||\mu_1||^2 + \left(n_2 - 2n_2\right)||\mu_2||^2 + \frac{n_1 n_2}{n}||\mu_1 - \mu_2||^2 \\
&= \sum_{i=1}^{n} x_i x_i^T + n_1||\mu_1||^2 - 2\mu_1\left(n_1\mu_1^T\right) + n_2||\mu_2||^2 - 2\mu_2\left(n_2\mu_2^T\right) + \frac{n_1 n_2}{n}S_B \\
&= \sum_{i=1}^{n} x_i x_i^T + n_1||\mu_1||^2 - 2\mu_1\sum_{i\in k=1} x_i^T + n_2||\mu_2||^2 - 2\mu_2\sum_{i\in k=2} x_i^T + \frac{n_1 n_2}{n}S_B \\
&= \sum_{i\in k=1} x_i x_i^T + n_1||\mu_1||^2 - 2\mu_1\sum_{i\in k=1} x_i^T \\
&\quad + \sum_{i\in k=2} x_i x_i^T + n_2||\mu_2||^2 - 2\mu_2\sum_{i\in k=2} x_i^T + \frac{n_1 n_2}{n}S_B \\
&= \sum_{i\in k=1}\left(x_i x_i^T + ||\mu_1||^2 - 2\mu_1 x_i^T\right) + \sum_{i\in k=2}\left(x_i x_i^T + ||\mu_2||^2 - 2\mu_2 x_i^T\right) + \frac{n_1 n_2}{n}S_B \\
&= \sum_{i\in k=1}||x_i - \mu_1||^2 + \sum_{i\in k=2}||x_i - \mu_2||^2 + \frac{n_1 n_2}{n}S_B \\
&= S_W + \frac{n_1 n_2}{n}S_B
\end{aligned} \tag{9}
$$

Using, the definition of S_B, we note that $S_B w$ is always in the direction of $(\mu_2 - \mu_1)$. Thus we can write

$$
w \propto S_W^{-1}\left(\mu_2 - \mu_1\right) \tag{10}
$$