

Lecture 18: Mean and Variance

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This is some warmup discussion before the first section.

1 Recap

Consider the following equation:

$$y = w^\top \phi(x) + \epsilon$$

This is our standard regression model, with $\phi(x)$ being the $d \times 1$ feature vector.

$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

is the noise in the model, modelled as a Gaussian with 0 mean and variance σ^2 .

$$w \sim \mathcal{N}(0, \Sigma_p)$$

is the $d \times 1$ weight vector, drawn from a Gaussian distribution.

A Gaussian process is a collection of random variables which have a joint Gaussian distribution.

Given N observations $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$, for a new observation (x^*, y^*) , we have:

$$y^* / x^*, D \sim \mathcal{N}(\mu, \Sigma)$$

$$D = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$$

We want to find out μ and Σ in the above equation.

We have seen that

$$\mathbf{E}(y^* / x^*, D) = \Phi(x^*)^\top \Sigma_p \Phi(\Phi^\top \Sigma_p \Phi + \sigma^2 \mathbf{I})^{-1} y \quad (1)$$

Here $\Phi^\top \Sigma_p \Phi$ may be invertible only if $d \rightarrow \infty$.

2 Analysing the mean further

Suppose $x^* \in D$. Without loss of generality, let $x^* = x_1$. If $\epsilon = 0$ (which implies $\sigma = 0$), we expect y^* to be exactly equal to y_1 . If the noise was present even for an $x_i \in D$, the measured y can be different from y_i . Let us try to verify this.

Putting $x^* = x_1$ and $\sigma = 0$ in (1), we have:

$$\mathbf{E}(y_1 / x_1, D, \sigma = 0) = \Phi(x_1)^\top \Sigma_p \Phi(\Phi^\top \Sigma_p \Phi)^{-1} y \quad (2)$$

Now $\Phi(x_1)^\top \Sigma_p \Phi$ is the first row of $\Phi^\top \Sigma_p \Phi$.

If B is an invertible matrix and $B_{1,\cdot}$ is its first row, then

$$(AB)_{1,\cdot} = A_{1,\cdot} B$$

We can write:

$$BB^{-1} = \mathbf{I} \implies B_{1,\cdot} B = \mathbf{I}_{1,\cdot} = [1, 0, \dots, 0]_{1 \times n}$$

So if we take the matrix $\Phi^\top \Sigma_p \Phi$ as B above we obtain the same row vector as above. (Note that we have assumed $\Phi^\top \Sigma_p \Phi$ to be invertible, which may not always be the case). Finally, multiplying with y which is a $n \times 1$ column vector, we obtain y_1 on the RHS of (2).

Now let's investigate what happens if $\sigma \neq 0$.

Again, taking $B = \Phi^\top \Sigma_p \Phi$ and B_1 as its first row, we have the RHS of (2) as

$$B_1(B + \sigma^2 I)^{-1} y = B_1(B + \sigma^2 B B^{-1}) y = B_1(\mathbf{I} + \sigma^2 B^{-1})^{-1} B^{-1} y = y_1 - \sigma^2 B_1 B^{-1} y$$

Here $(\mathbf{I} + \sigma^2 B^{-1})^{-1}$ was expanded as $\mathbf{I} - \sigma^2 B^{-1}$ using Taylor's theorem, under the assumption that σ is small enough for the expansion to be valid.

3 Variance

$$y = w^T \cdot \phi(x) + \epsilon \sim \mathcal{N}(0, \sigma^2)$$

$$w \sim \mathcal{N}(0, \epsilon_P)$$

What would the value of $\text{var}(y|D)$ be? Where $\mathbf{D} = (x_i, y_i)_{i=1}^N$ $\mathbf{P}(y^*|x^*, \mathbf{D})$

$$\begin{aligned} \text{var}(y|D) &= \text{var}(w^T \phi(x)) + \sigma^2 \\ &= \mathbb{E}(\phi(x^*)^T (w - \bar{w})(w - \bar{w})^T \phi(x^*) | D) + \sigma^2 \end{aligned}$$

Here w is kind of stochastic.

$$= \phi(x^*)^T \mathbb{E}((w - \bar{w})(w - \bar{w})^T | D) \phi(x^*) + \sigma^2$$

For now, we rather focus on $\mathbf{P}(w|\mathbf{D})$. The problem of finding the variance of y^* reduces to finding the covariance matrix of w .

If we know w , we can easily find the distribution of \mathbf{D} .

$$P(w|D) = \frac{P(D|w) \cdot P(w)}{P(D)}$$

$$\implies P(w|D) \propto P(D|w) \cdot P(w)$$

Now,

$$P(D|w) \cdot P(w) = \exp\left[-\frac{(\vec{y} - \phi^T w)^T (\vec{y} - \phi^T w)}{2\sigma^2}\right] \cdot \exp\left[-w^T \epsilon_p^{-1} w / 2\right]$$

$$z^{-1} = \phi\phi^T/\sigma^2 + \epsilon_P^{-1}$$

Confirming \overline{w} is the same that we found earlier.

$$\overline{w} = \frac{z \sum_{i=1}^N \phi(x_i)(y_i)}{\sigma^2} = \frac{Z\phi \cdot y}{\sigma^2}$$

$$\mathcal{E}(x^*, y^* | D) = \phi(x^*)^T [\phi\phi^T/\sigma^2 + \epsilon_P^{-1}] \frac{\phi \cdot y}{\sigma^2}$$