Linear Regression

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Bayesian Methods and Modern Statistics: STA 360/601

Module 10

Setup

Let's assume that $D_i = (x_i, y_i)$ for all i.

Assume

$$Y_i \overset{iid}{\sim} N(w^T x_i, \sigma^2).$$

Assume σ^2 known and $\theta = w$.

What is the MLE?

$$\theta_{MLE} = \arg\max_{\theta \in \Theta} p(D \mid \theta)$$

What is the likelihood? (Want to get to the MLE).

Define $y = (y_1, \ldots, y_n)$. Note that $w^T x_i = x_i^T w$. Define $A = (x_1^T, \ldots, x_n^T)$. (A is often called the design matrix).

$$\begin{align}
p(D \mid \theta) &= p(y \mid x, \theta) \tag{1} \\
&= \prod_i p(y_i \mid x_i, \theta) \tag{2} \\
&= \prod_i \frac{1}{\sqrt{2\pi\sigma^2}} \exp\{-1/(2\sigma^2)(y_i - w^T x_i)^2\} \tag{3} \\
&= (\frac{1}{\sqrt{2\pi\sigma^2}})^n \exp\{-1/(2\sigma^2) \sum_i (y_i - w^T x_i)^2\} \tag{4} \\
&= (\frac{1}{\sqrt{2\pi\sigma^2}})^n \exp\{-1/(2\sigma^2)(y - Aw)^T (y - Aw)\} \tag{5}
\end{align}$$

Goal: minimize

$$(y - Aw)^T (y - Aw)$$

(Think about why we're minimizing).

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$$(y - Aw)^T(y - Aw)$$

Expand what we have above.

$$g := (y - Aw)^T(y - Aw) = y^T y - 2w^T A^T y + w^T A^T A w$$

Now take the gradient or derivative with respective to w.

$$\frac{\partial g}{\partial w} = -2A^T y + 2A^T A w =: 0.$$

This implies that

$$A^T y = A^T A w \implies \hat{\theta} = (A^T A)^{-1} A^T y$$

Why is $(A^T A)^{-1}$ invertible? (exercise). Hint: this also shows that $\hat{\theta}$ is unique!

Matrix Facts on previous slide

Note: We're using the fact above from matrix algebra that

$$\frac{\partial}{\partial w_j} a^T w = \sum_i a_i w_i = a_j.$$

The second fact we use is known as a quadratic form. Assume B is symmetric.

$$\frac{\partial}{\partial w_k} w^T B w = \frac{\partial}{\partial w_k} \sum_{i,j=1}^{n} w_i w_j b_{ij} \tag{6}$$

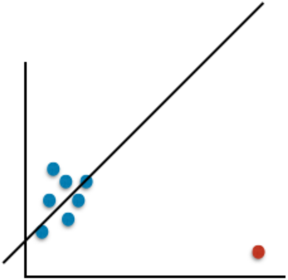
$$= \begin{cases} 2 w_i b_{ij}, \text{ if } i = j = k \\ w_i b_{ij} \text{ if } j = k, i \neq j \end{cases} \tag{7}$$

We picked up some nice tricks for working with gradients.
Also, we can identify that $\hat{\theta}$ is unbiased. (exercise).
What is the variance of $\hat{\theta}$? (exercise).

Bayesian linear regression

We derived the MLE. Why not use the MLE?

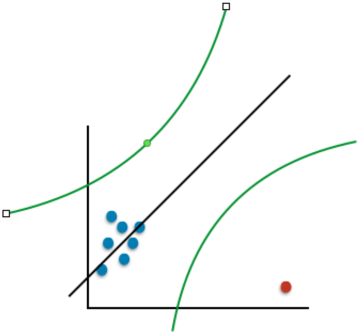
The MLE often overfits the data. Also, no notion of uncertainty.



Now suppose we want to predict a new point but what if this is the diagnostic for a patient. Or an investment for a stock portfolio.

How certain are you? (Let's put in error bars).

Bayesian linear regression



Now suppose we want to predict a new point but what if this is the diagnostic for a patient. Or an investment for a stock portfolio.

How certain are you? We're not certain at all!

Why Bayesian?

Bayesian approach allows you to say, I don't know!

We can tie back to decision theory and optimize a loss function by optimizing the predictive distribution

$$p(y \mid x, D)$$

Setup

$D = (x_i, y_i)$ for all i. Let $a = 1/\sigma^2$. Let $b = 1/\tau^2$.

$$
\begin{align}
y_i \mid w &\overset{ind}{\sim} N(w^T x_i, a^{-1}) \tag{8} \\
w &\sim MVN(0, b^{-1}, I) \tag{9} \\
& \tag{10}
\end{align}
$$

We assume that a,b are known. Here, $\theta = w$.
Recall: Look at the Multivariate model as these are needed to understand this module.

Computing the Posterior

What is the likelihood?

$$p(D \mid w) \propto P(D \mid w) \propto \exp\{-a/2(y - Aw)^T(y - Aw)\} \quad (11)$$

What is the posterior?

$$p(w \mid D) \propto p(D \mid w)p(w) \quad (12)$$
$$\propto \exp\{-a/2(y - Aw)^T(y - Aw)\} \times \exp\{-b/2w^T w)\} \quad (13)$$

Just like in the Multivariate modules, we just simplify. (Check these details on your own).

$$p(w \mid D) \propto MVN(w \mid \mu, \Lambda^{-1})$$

where $\Lambda = aA^T A + bI$ and $\mu = a\Lambda^{-1}A^T y$.

You can show (exercise that the Maximum a Posterior estimate of w is

$$a(aA^T A + bI)^{-1} A^T y = (A^T A + b/aI)^{-1} A^T y$$

How does this compare to the MLE estimate? Think about this on your own!
You will see more about Bayesian linear regression in lab. (For more on this, see Hoff).

The predictive distribution

$$
\begin{aligned}
& p(y \mid x, D) && (14) \\
& = \int p(y \mid x, D, w) p(w \mid x, D) dw && (15) \\
& = \int p(y \mid x, w) p(w \mid D) dw && (16) \\
& = \int N(y \mid w^T x, a^{-1}) N(w \mid \mu, \Lambda^{-1}) dw && (17) \\
& \propto \int \exp\{-a/2(y - w^T x)^2\} \exp\{-1/2(w - \mu)^T \Lambda (w - \mu)\} dw \\
& && (18) \\
& \propto \int \exp\{-a/2(y^2 - 2(w^T x)y + (w^T x)^2) \\
& - 1/2(w^T \Lambda w - 2w^T \Lambda \mu + \mu^T \Lambda \mu)\} && (19)
\end{aligned}
$$

$$
\begin{aligned}
&p(y \mid x, D) && (20)\\
&= \int N(y \mid w^T x, a^{-1}) N(w \mid \mu, \Lambda^{-1}) dw && (21)\\
&\propto \int \exp\{-a/2(y^2 - 2(w^T x)y + (w^T x)^2)\\
&- 1/2(w^T \Lambda w - 2w^T \Lambda \mu + \mu^T \Lambda \mu)\} && (22)
\end{aligned}
$$

Our goal is to make the above into

$$
\int N(w \mid -) g(y) dw = g(y) \propto N(y \mid -).
$$

How can you do this?

Exercise

1. First show that the above, can be written as $\int N(w \mid -)g(y)dw$ as give the parameters of the Gaussian.
2. Next, show trivially that $\int N(w \mid -)g(y)dw = g(y)$ with the parameters in 1.
3. Finally, show that $g(y) \propto N(y \mid -)$ and give the parameters for the normal of the predictive distribution.

To summarize, you should in the end find that

$$p(y \mid x, D) \propto \exp\{-\lambda/2(y-u)^2)$$

where $\lambda = a(1 - ax^T L^{-1} x), u = \lambda^{-1} a x^T L^{-1} \Lambda \mu$, $L = axx^T + \Lambda$. (You may assume that w has mean m).

Food for Thought

- When does $\hat{\theta}^B = \hat{\theta}^{MLE}$? (What does this mean in terms of the prior variance or precision)?
- Suppose $\hat{\theta}^B \neq \hat{\theta}^{MLE}$. What benefit are we getting from linear regression in this case over ordinary least squares? Explain.