

Lecture 8: Generalized Linear Models

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8.1 GLM Theory

Random structure:

$$Y_i \stackrel{\text{ind}}{\sim} \text{Exponential Family}(\theta_i, \phi)$$

$$f(y_i) = \exp \left\{ \frac{y_i \theta_i - b(\theta_i)}{a_i(\phi)} + c(y_i, \phi) \right\}$$

Recall from the last lecture that

$$\mu_i \triangleq \mathbb{E}[Y_i] = b'(\theta_i)$$

and

$$\text{Var}[Y_i] = b''(\theta_i) a_i(\phi)$$

Systematic structure:

$$\eta_i = x_i^T \beta, \text{ "linear predictor"}$$

$$\eta_i = g(\mu_i), \text{ "link function"}$$

8.1.1 Canonical Link Function

Set $\eta_i = \theta_i$. Therefore,

$$\mu_i = b'(\theta_i) = b'(\eta_i)$$

$$\eta_i = (b')^{-1}(\mu_i)$$

and the canonical link function is

$$g(\cdot) = (b')^{-1}(\cdot)$$

With a canonical link function $g(\cdot)$, the log likelihood of β becomes

$$l(\beta) \stackrel{\text{ind}}{=} \sum_{i=1}^n \log f(Y_i)$$

$$\stackrel{\text{canonical}}{=} \sum_{i=1}^n \frac{y_i \eta_i - b(\eta_i)}{a_i(\phi)} + c(y_i, \phi)$$

$$\stackrel{\eta_i = x_i^T \beta}{=} \sum_{i=1}^n \frac{y_i x_i^T \beta - b(x_i^T \beta)}{a_i(\phi)} + c(y_i, \phi)$$

Question: what is $\underset{\beta}{\operatorname{argmax}} l(\beta)$?

8.2 Review: Optimization Methods

Problem: $f: \mathbb{R}^p \rightarrow \mathbb{R}$. Find x^* such that $f(x^*) \geq f(x)$ for all $x \in \mathbb{R}^p$.

8.2.1 Newton-Raphson Method (the most general method)

Notation

Gradient: $\nabla f(x)$ is a p -dimensional vector, the same dimension as x , and

$$\nabla f(x) = \left(\frac{\partial f}{\partial x_1}(x), \dots, \frac{\partial f}{\partial x_p}(x) \right)^T$$

Hessian: $H_f(x)$ is a $p \times p$ matrix, and

$$[H_f(x)]_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}(x)$$

- If f is strictly concave, $H_f(x)$ is negative definite
- If f is smooth (has derivatives on both sides), $H_f(x)$ is symmetric

N-R for multidimensional optimization

Using 1st order Taylor expansion to approximate $\nabla f(x)$, we have

$$\nabla f(x) \approx \nabla f(x_0) + H_f(x_0)(x - x_0)$$

If x^* is a local maxima, then

$$\nabla f(x_0) + H_f(x_0)(x^* - x_0) \approx \nabla f(x) = 0$$

Therefore,

$$x^* = x_0 - (H_f(x_0))^{-1} \nabla f(x_0)$$

N-R algorithm (iterative)

- Start at an arbitrary value $x^{(0)}$.
- At the k^{th} iteration, $x^{(k+1)} = x^{(k)} - H_f(x^{(k)})^{-1} \nabla f(x^{(k)})$.
- Repeat the above step until convergence.

8.2.2 Fisher Scoring Method

- Fisher scoring figures out a very nice form of Hessian of log likelihood.
- It takes expectation of first and second derivatives since the likelihood is random due to its property of including the samples and responses in its formula.

- $l(\beta; Y_1, Y_2, \dots, Y_n) \stackrel{\text{ind}}{=} \sum_{i=1}^n \log f(Y_i|\beta)$ is the log likelihood to be maximized.
- In the following calculations, we take derivatives of likelihood functions with respect to β .

Gradient (score function)

$$S(\beta) = \nabla l(\beta) = \sum_{i=1}^n \frac{\nabla f(Y_i; \beta)}{f(Y_i; \beta)}$$

Note that the score function $S(\beta)$ is a $p \times 1$ random vector.

Property: $\mathbb{E}[S(\beta)] = 0$

Proof:

$$\begin{aligned} \mathbb{E}[S(\beta)] &= \sum_{i=1}^n \mathbb{E} \left[\frac{\nabla f(Y_i; \beta)}{f(Y_i; \beta)} \right] \\ &= \sum_{i=1}^n \int \frac{\nabla f(y_i; \beta)}{f(y_i; \beta)} f(y_i; \beta) dy_i \\ &\stackrel{\nabla \leftrightarrow \int}{=} \sum_{i=1}^n \nabla \int f(y_i; \beta) dy_i \\ &= \sum_{i=1}^n \nabla 1 \\ &= 0 \end{aligned}$$

Hessian $H_l(\beta)$

$$H_l(\beta) = \sum_{i=1}^n \frac{f(Y_i; \beta) H_f(\beta) - \nabla f(Y_i; \beta) \cdot (\nabla f(Y_i; \beta))^T}{f^2(Y_i; \beta)}$$

Fisher proposed to simplify $H_l(\beta)$ as $\mathbb{E}[H_l(\beta)]$.

Notice that $\forall i$

$$\begin{aligned} \mathbb{E} \left[\frac{f(Y_i; \beta) H_f(\beta)}{f^2(Y_i; \beta)} \right] &= \int \frac{f(y_i; \beta) H_f(\beta)}{f^2(y_i; \beta)} f(y_i; \beta) dy_i \\ &= \int H_f(\beta) dy_i \\ &= \nabla^2 1 \\ &= 0 \end{aligned}$$

Therefore,

$$\begin{aligned}
 \mathbb{E}[H_l(\beta)] &= -\mathbb{E}\left[\sum_{i=1}^n \frac{\nabla f(Y_i; \beta) \cdot (\nabla f(Y_i; \beta))^T}{f^2(Y_i; \beta)}\right] \\
 &= -\sum_{i=1}^n \mathbb{E}[S_i(\beta) \cdot (S_i(\beta))^T] && \text{where } S_i(\beta) = \frac{\nabla f(Y_i; \beta)}{f(Y_i; \beta)} \\
 &= -\sum_{i=1}^n \text{Cov}(S_i(\beta)) && \text{since } \mathbb{E}[S_i(\beta)] = 0 \\
 &= -I(\beta)
 \end{aligned}$$

where $I(\beta)$ is Fisher's information.

Note: $(I(\beta))^{-1}$ is the asymptotic covariance matrix of $\hat{\beta}_{MLE}$.

Optimization algorithm

- NR update: $\beta^{(k+1)} = \beta^{(k)} - H_l(\beta^{(k)})^{-1} S(\beta^{(k)})$
- FS update: $\beta^{(k+1)} = \beta^{(k)} + I(\beta^{(k)})^{-1} S(\beta^{(k)})$

Example: logistic regression

$$\begin{aligned}
 l(\beta) &= \sum_{i=1}^n \left[Y_i \log\left(\frac{\pi_i}{1 - \pi_i}\right) + \log(1 - \pi_i) \right] \\
 &\stackrel{\log \frac{\pi_i}{1 - \pi_i} = x_i^T \beta}{=} \sum_{i=1}^n \left[Y_i x_i^T \beta + \log(1 + e^{x_i^T \beta}) \right]
 \end{aligned}$$

Therefore,

$$\begin{aligned}
 S(\beta) &= \nabla l(\beta) = \sum_{i=1}^n \left[Y_i x_i - \frac{e^{x_i^T \beta} x_i}{1 + e^{x_i^T \beta}} \right] \\
 H_l(\beta) &= -\sum_{i=1}^n \left[\frac{e^{x_i^T \beta}}{(1 + e^{x_i^T \beta})^2} x_i \cdot x_i^T \right]
 \end{aligned}$$

Thus,

$$\mathbb{E}[H_l(\beta)] = H_l(\beta)$$

That is, Fisher's Scoring Method is identical to Newton-Raphson Method in this scenario.

8.2.3 Iteratively Reweighted Least Squares (IRLS) Based on FS

$$l(\beta) = \sum_{i=1}^n \frac{Y_i \theta_i - b(\theta_i)}{a_i(\phi)} + c(Y_i, \phi) \triangleq \sum_{i=1}^n l_i$$

To get $\nabla l(\beta)$, we look at ∇l_i first and we have

$$\frac{\partial l_i}{\partial \beta_j} = \frac{\partial l_i}{\partial \theta_i} \frac{\partial \theta_i}{\partial \mu_i} \frac{\partial \mu_i}{\partial \eta_i} \frac{\partial \eta_i}{\partial \beta_j}$$

Notice:

$$\begin{aligned}\frac{\partial l_i}{\partial \theta_i} &= \frac{Y_i - b'(\theta_i)}{a_i(\phi)} = \frac{Y_i - \mu_i}{a_i(\phi)} \\ \frac{\partial \theta_i}{\partial \mu_i} &= \frac{1}{b''(\theta_i)} \text{ since } \mu_i = b'(\theta_i), \frac{\partial \mu_i}{\partial \theta_i} = b''(\theta_i) \\ \frac{\partial \eta_i}{\partial \beta_j} &= x_{ij} \text{ since } \eta_i = x_i^T \beta = \sum_{j=1}^p x_{ij} \beta_j\end{aligned}$$

Therefore,

$$\frac{\partial l_i}{\partial \beta_j} = \frac{Y_i - \mu_i}{a_i(\phi)} \frac{1}{b''(\theta_i)} \frac{\partial \mu_i}{\partial \eta_i} x_{ij}$$

Now, define

$$w_i = \frac{\left(\frac{\partial \mu_i}{\partial \eta_i}\right)^2}{a_i(\phi) b''(\theta_i)}$$

and we have

$$\begin{aligned}\frac{\partial l_i}{\partial \beta_j} &= (Y_i - \mu_i) w_i \frac{\partial \eta_i}{\partial \mu_i} x_{ij} \\ \frac{\partial l}{\partial \beta_j} &= \sum \frac{\partial l_i}{\partial \beta_j}\end{aligned}$$

Therefore,

$$S(\beta) = \nabla l(\beta) = X^T W (Y - \mu) \frac{d\eta}{d\mu}$$

where

$$W = \begin{bmatrix} w_1 & & \\ & \ddots & \\ & & w_n \end{bmatrix}_{n \times n}$$

and

$$(Y - \mu) \frac{d\eta}{d\mu} = \begin{bmatrix} (Y_1 - \mu_1) \frac{d\eta_1}{d\mu_1} \\ \vdots \\ (Y_n - \mu_n) \frac{d\eta_n}{d\mu_n} \end{bmatrix}$$

To get $H_l(\beta)$, we have

$$\frac{\partial^2 l_i}{\partial \beta_j \partial \beta_k} = (Y_i - \mu_i) \frac{\partial(w_i \frac{\partial \eta_i}{\partial \mu_i} x_{ij})}{\partial \beta_k} + \frac{\partial(Y_i - \mu_i)}{\partial \beta_k} w_i \frac{\partial \eta_i}{\partial \mu_i} x_{ij}$$

$$\begin{aligned}\mathbb{E} \left[\frac{\partial^2 l_i}{\partial \beta_j \partial \beta_k} \right] &= \mathbb{E} \left[(Y_i - \mu_i) \frac{\partial(w_i \frac{\partial \eta_i}{\partial \mu_i} x_{ij})}{\partial \beta_k} \right] + \mathbb{E} \left[\frac{\partial(Y_i - \mu_i)}{\partial \beta_k} w_i \frac{\partial \eta_i}{\partial \mu_i} x_{ij} \right] \\ &= 0 - \mathbb{E} \left[\frac{\partial \mu_i}{\partial \beta_k} w_i \frac{\partial \eta_i}{\partial \mu_i} x_{ij} \right] \\ &= -\mathbb{E} \left[\frac{\partial \eta_i}{\partial \beta_k} w_i x_{ij} \right] \\ &= -x_{ik} w_i x_{ij}\end{aligned}$$

So

$$I(\beta) = -\mathbb{E}[H_l(\beta)] = \underset{(p \times n)(n \times n)(n \times p)}{X^T W X}$$

Therefore, by FS,

$$\begin{aligned} \beta^{(k+1)} &= \beta^{(k)} + (I(\beta^{(k)}))^{-1} S(\beta^{(k)}) \\ &= \beta^{(k)} + (X^T W^{(k)} X)^{-1} X^T W^{(k)} (Y - \mu^{(k)}) \frac{d\eta^{(k)}}{d\mu^{(k)}} \end{aligned}$$