STAT347: Generalized Linear Models Lecture 5

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Today's topics:

- GLM computation
- Binary / Binomial data model
 - Data input
 - Link functions
 - R example
- Reading: Agresti Chapters 4.5, 5.1, Faraway Chapters 2.1, 3.1, 4.1-4.2

GLM computation

- Only discuss the case of $a(\phi) = 1$ to simplify notation
- If $a(\phi)$ is not a constant, one can get $\hat{\beta}$ from the score equations first, and then estimate ϕ from MLE with $\hat{\beta}$ plugged in

Score equation:

$$\dot{L}(\beta) = X^T D V^{-1}(y - \mu) = 0$$

where

$$L(\beta) = \sum [y_i \theta_i - b(\theta_i)]$$

- Newton's method
- Fisher scoring method
- Iteratively reweighted least squares (IRLS): equivalent to Fisher scoring

Newton's method

Second-order approximation of $L(\beta)$

$$L(\beta) \approx L(\beta^{(t)}) + \dot{L}(\beta^{(t)})^T (\beta - \beta^{(t)}) + \frac{1}{2} (\beta - \beta^{(t)})^T \ddot{L}(\beta^{(t)}) (\beta - \beta^{(t)})$$

at tth iteration. If $\ddot{L}(\beta^{(t)}) \leq 0$, then maximizing the second-order approximation is equivalent to solving

$$\dot{L}(\beta) \approx \dot{L}(\beta^{(t)}) + \ddot{L}(\beta^{(t)})(\beta - \beta^{(t)}) = 0$$

We have

$$\beta^{(t+1)} = \beta^{(t)} - \ddot{L}(\beta^{(t)})^{-1}\dot{L}(\beta^{(t)})$$

Newton's method

- Newton's method is a general algorithm for optimizing twice-differentiable functions.
- Generally, it converges to the global maximum if $L(\beta)$ is strongly concave
 - If $g(\cdot)$ is the canonical link, then $L(\beta)$ is concave in β

$$-\ddot{L}(\beta^{(t)}) = X^T W^{(t)} X = \frac{1}{a(\phi)} X^T V^{(t)} X = -\mathbb{E}\left(\ddot{L}(\beta^{(t)})\right) \succeq 0$$

- If $g(\cdot)$ is a general link, then $L(\beta)$ is NOT guaranteed to be concave in β
- If $-\ddot{L}(\beta^{(t)})$ is not non-negative, then step t does not maximize the quadratic approximation and Newton's method may not converge.

Fisher scoring method

- In lecture 2, we showed that $-\mathbb{E}(\ddot{L}(\beta)) \ge 0$ for any β .
- Instead of using the Hessian $\ddot{L}(\beta^{(t)})$ itself in the second order approximation, we use its expectation

$$J^{(t)} = \mathbb{E}\left(\ddot{L}(\beta^{(t)})\right) = -X^T W^{(t)} X$$

Each iteration becomes:

$$\beta^{(t+1)} = \beta^{(t)} - \left(J^{(t)}\right)^{-1} \dot{L}(\beta^{(t)})$$

- For the canonical link, Fisher scoring = Newton's method
- For a general link, Fisher scoring works better in practice

Iteratively reweighted least squares

• We can make a connection between the optimization for GLM and weighted least squares estimation.

Recall the score equation:

$$\dot{L}(\beta) = X^T D V^{-1}(y - \mu) = 0$$

where $V = \text{diag}(\text{Var}(y_1), \dots, \text{Var}(y_n))$ and $D = \text{diag}(g'(\mu_1), \dots, g'(\mu_n))^{-1}$, $y = (y_1, \dots, y_n)$ and $\mu = (\mu_1, \dots, \mu_n)$. Also in lecture 2, we used the notation $\eta_i = X_i^T \beta = g(\mu_i)$. Thus, $D = \text{diag}\left(\frac{\partial \mu_1}{\partial \eta_1}, \dots, \frac{\partial \mu_n}{\partial \eta_n}\right)$. We also defined the diagnoal matrix $W = D^2 V^{-1}$. Thus,

$$\dot{L}(\beta) = X^T D V^{-1}(y - \mu) = X^T W D^{-1}(y - \mu)$$

We can make a first order approximation of μ

$$\mu = \mu^{(t)} + D^{(t)}(\eta - \eta^{(t)})$$

then

$$\dot{L}(\beta) \approx X^T W^{(t)}(z^{(t)} - X\beta)$$

where

$$z^{(t)} = X\beta^{(t)} + \left(D^{(t)}\right)^{-1} \left(y - \mu^{(t)}\right)$$

is a linear approximation of η at the *t*th iteration.

Iteratively reweighted least squares (IRLS)

• At the t+1 th iteration, we solve the "approximated score equation":

$$X^T W^{(t)}(z^{(t)} - X\beta) = 0$$

which can be considered as a weighted linear regression with observations $z_i^{(t)}$ and weight w_i for each sample *i*.

- IRLS is equivalent to Fisher scoring. The *t*th step of Fisher scoring satisfy $(X^T W^{(t)} X) \beta^{(t+1)} = X^T W^{(t)} X \beta^{(t)} + X^T D^{(t)} (V^{(t)})^{-1} (y - \mu^{(t)})$ $= X^T W^{(t)} \left[X \beta^{(t)} + (D^{(t)})^{-1} (y - \mu^{(t)}) \right]$ $= X^T W^{(t)} z^{(t)}$
- Weight matrix $W^{(t)} \approx \operatorname{Var}\left(z^{(t)}\right)^{-1}$

Binary / binomial data model

If the observation y_i is binomial

 $y_i \sim \text{Binomial}(n_i, p_i)$

and probability function:

$$f(y_i) = \binom{n_i}{y_i} p_i^{y_i} (1 - p_i)^{n_i - y_i} = \binom{n_i}{y_i} \left(\frac{p_i}{1 - p_i}\right)^{y_i} (1 - p_i)^{n_i}$$

If $n_i = 1$, then y_i is a 0/1 binary data point (follows a Bernoulli distribution).

• Link function: $g(p_i) = X_i^T \beta$

• logistic regression:
$$log(\frac{p_i}{1-p_i}) = X_i^T \beta$$

Data input for binary model

If X_i are categorical variables, then we may have samples with the same Xi and we can group them together

- ungrouped data: each $n_i = 1$ and some samples have the same X_i , thus they share the same p_i
- a grouped sample \tilde{y}_k for group k where all observations in the group share the same X_i
 - Define n_k as the number of binary observations
 - The grouped response for group k is

$$\tilde{y}_k = \sum_{i \in I_k} y_i \sim \text{Binomial}(n_k, p_k)$$

 The grouped data follows the Binomial distribution because we assume that the samples are independent within each group

Likelihood for grouped and ungrouped data

• Let $N = \sum_{k} n_k$ The likelihood for the ungrouped data is:

$$f(y_1, y_2, \cdots, y_N) = \prod_i p_i^{y_i} (1 - p_i)^{1 - y_i}$$
$$= \prod_k \prod_{i \in I_k} p_k^{\tilde{y}_k} (1 - p_k)^{n_k - \tilde{y}_k}$$

The likelihood for the corresponding grouped data is:

$$f(\tilde{y}_1, \tilde{y}_2, \cdots, \tilde{y}_K) = \prod_k \binom{n_k}{y_k} \prod_{i \in I_k} p_k^{\tilde{y}_k} (1 - p_k)^{n_k - \tilde{y}_k}$$

• The likelihood is not the same between the grouped data and ungrouped data. However, the log-likelihood function only differs by a constant, thus the GLM solution does not change.

Link function for binary / binomial GLM

The expectation of each sample is $\mathbb{E}(y_i) = n_i p_i$ where n_i is a known constant. Thus we define the link function as a function of p_i

$$g(p_i) = X_i^T \beta$$

Equivalently,

$$p_i = g^{-1}(X_i^T \beta) \in [0, 1]$$

- If g is a one-to-one mapping and continuous function, then g⁻¹ should be monotone.
- one natural choice of g^{-1} is to make it as a cdf of some distribution.
- Denote $F(z) = g^{-1}(z)$ as some cdf function

• Let
$$\epsilon_i \overset{i.i.d.}{\sim} F(\cdot)$$

Latent variable threshold models

- Denote $F(z) = g^{-1}(z)$ as some cdf function
 - Let $\epsilon_i \overset{i.i.d.}{\sim} F(\cdot)$
 - Then

$$p_i = F(X_i^T \beta) = \mathbb{P}(\epsilon_i \le X_i^T \beta) = \mathbb{P}\left(X_i^T \beta - \epsilon_i > = 0\right)$$

- This is called a latent variable threshold models and $X_i^T \beta \epsilon_i$ are the "latent variables"
- It does not make any essential modeling difference choosing the cutoff to be 0 or any other value τ

Latent variable threshold models



Figure 5.1 Threshold latent variable model, for which we observe $y_i = 1$ when underlying latent variable $y_i^* > \tau$.

The probit link

• The probit link: F(z) is the cdf of a standard Gaussian distribution

$$p_i = \mathbb{P}\left(X_i^T \beta - \epsilon_i >= 0\right) = \mathbb{P}\left(X_i^T \beta + \epsilon_i >= 0\right)$$

where $\epsilon_i \sim N(0, 1)$. Let the hidden variable be $y_i^* = X_i^T \beta + \epsilon_i$, then it goes to the definition of the probit link that some of you may be more familiar with:

$$Y_i = \begin{cases} 1 & \text{if } y_i^{\star} >= 0\\ 0 & \text{else} \end{cases}$$

The logit link

• The logit link: F(z) is the cdf of a standard logistic distribution

$$F(z) = \frac{e^z}{1 + e^z}$$

- The link function is called the logit link: $g(p_i) = \text{logit}(p_i) = \log\left(\frac{p_i}{1-p_i}\right)$

- The logit link is the canonical link of the Binomial distribution

The identity link

- The identity link: F(z) is the cdf of a uniform [0,1] distribution and $p_i = X_i^T \beta$
 - The identity link corresponds to a uniform cdf only when $X_i^T \beta \in [0, 1]$ for all samples.
 - Because of the range issue, when using R to solve a binomial GLM with identity link, there can often be numerical problems (such as the error we saw in the earlier data example in Section 1.4, Data Example 1).

The log-log link

- All previous links assume a symmetric ϵ_i around 0
 - A corresponding restriction is that the response curve is symmetric at 0.5
 - We should use some other link functions if this assumption is severely violated
 - The log-log link: F(z) is the cdf of a standard double-exponential distribution (Gumbel distribution)

$$F(z) = e^{-e^{-z}}$$

- The link function is called the log-log link:

$$g(p_i) = -\log[-\log(p_i)] = X_i^T \beta$$

• With the log-log link, p_i approaches 0 sharply but approaches 1 slowly

The complementary log-log link

- With a complementary log-log link, p_i approaches 1 sharply but approaches 0 slowly

 $g(p_i) = \log[-\log(p_i)] = X_i^T \beta$



Figure 5.4 GLM for binary data using complementary log–log link function.

R data example for binary / binomial GLM (part I)

• Check Example3_1 R notebook