Chapter 3

Estimation in Generalized Linear Models

3.1 Introduction to Generalized Linear Models

3.1.1 Generalized Linear Normal Model

– Let us assume that random variable $Y_1, Y_2, \ldots Y_n$ are following the normal distribution $Y_i \sim N(\mu_i, \sigma^2)$.

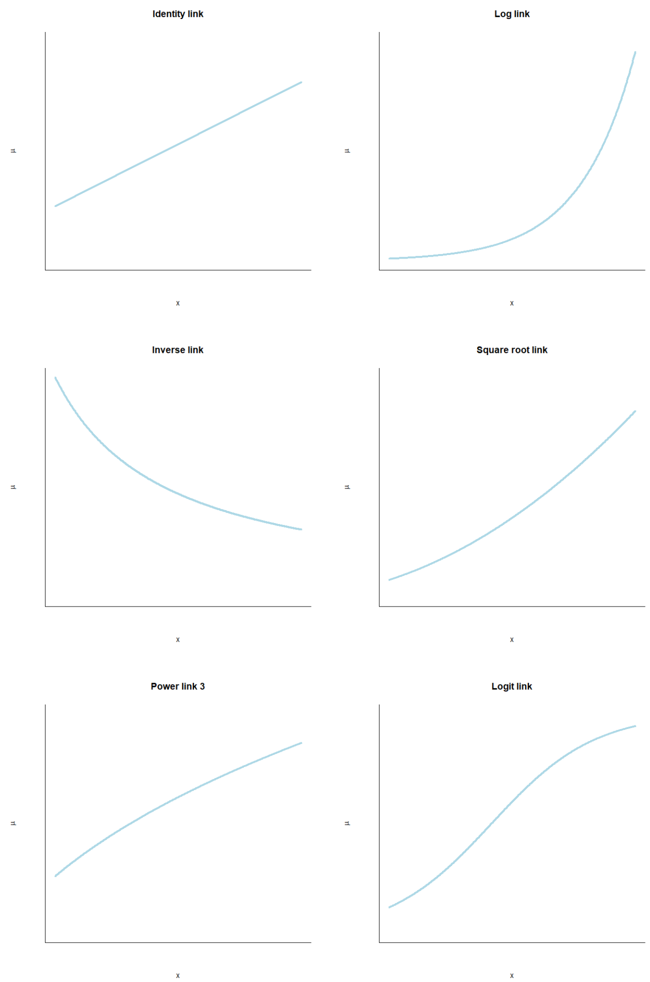
– In generalized linear models, the explanatory variables $X_1, X_2, \ldots, X_p$ are effecting to the expected value μ_i through the link function g:

$$g(\mu_i) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}. \tag{3.1}$$

– In practice, possible link functions $g(\mu_i)$ are

$$\mu_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{identity link}, \tag{3.2a}$$
$$\log(\mu_i) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \log\textit{-link}, \tag{3.2b}$$
$$\frac{1}{\mu_i} = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{inverse link}, \tag{3.2c}$$
$$\sqrt{\mu_i} = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{square root link}, \tag{3.2d}$$
$$\mu_i^k = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{Power link } k, \tag{3.2e}$$
$$\log\left(\frac{\mu_i}{1-\mu_i}\right) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{logit link}. \tag{3.2f}$$

– In case on nonlinear link functions, the models are nonlinear with respect to explanatory variables $X_1, X_2, \ldots, X_p$ with inverse function $\mu_i = g^{-1}(\mathbf{x}_i, \boldsymbol{\beta}) = h(\mathbf{x}_i, \boldsymbol{\beta})$ being:



$$\mu_i = \mathbf{x}_i'\boldsymbol{\beta}, \quad \textit{identity link}, \tag{3.3a}$$

$$\mu_i = e^{\mathbf{x}_i'\boldsymbol{\beta}}, \quad \text{log-}\textit{link}, \tag{3.3b}$$

$$\mu_i = \frac{1}{\mathbf{x}_i'\boldsymbol{\beta}}, \quad \textit{inverse link}, \tag{3.3c}$$

$$\mu_i = (\mathbf{x}_i'\boldsymbol{\beta})^2, \quad \textit{square root link}, \tag{3.3d}$$

$$\mu_i = (\mathbf{x}_i'\boldsymbol{\beta})^{\frac{1}{k}}, \quad \textit{Power link } k, \tag{3.3e}$$

$$\mu_i = \frac{e^{\mathbf{x}_i'\boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i'\boldsymbol{\beta}}}, \quad \textit{logit link.} \tag{3.3f}$$

– Polynomial models are often used models which are nonlinear with respect to explanatory variables. For example (in case of X_1, X_2), second degree polynomial model with interaction term (and with identity link) has the form

$$\mu_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i1}^2 + \beta_4 x_{i2}^2 + \beta_5 x_{i1} x_{i2}. \tag{3.4}$$

– So called *exponential model* has the forms

$$\mu_i = e^{\beta_0} x_{i1}^{\beta_1} x_{i2}^{\beta_2} * \cdots * x_{ip}^{\beta_p}, \tag{3.5a}$$

$$\log(\mu_i) = \beta_0 + \beta_1 \log(x_{i1}) + \beta_2 \log(x_{i2}) + \cdots + \beta_p \log(x_{ip}). \tag{3.5b}$$

Example 3.1.

Consider the research problem where there was interest to determine whether glucose had an effect on single-cell Tetrahymena cell size when cells were grown in cell culture on the growth medium. The cell size was measured by the (average) diameter of cells Y =diameter. In research, explanatory variables were the concentration of Tetrahymena cells X_1=conc and X_2=glucose which was coded in the following way:

$$x_{i2} = \begin{cases} \text{yes} = 1, & \text{when glucose was added to growth medium in experiment } i, \\ \text{no} = 2, & \text{when glucose was not added to growth medium in experiment } i. \end{cases}$$

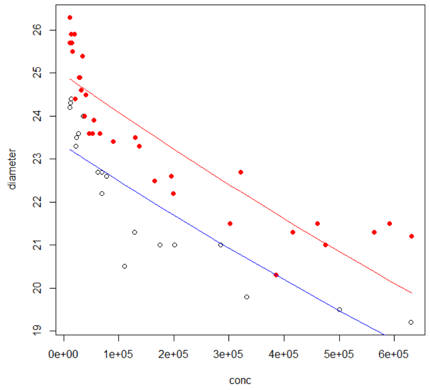
The dataset can be found on the file tetrahymena.txt.

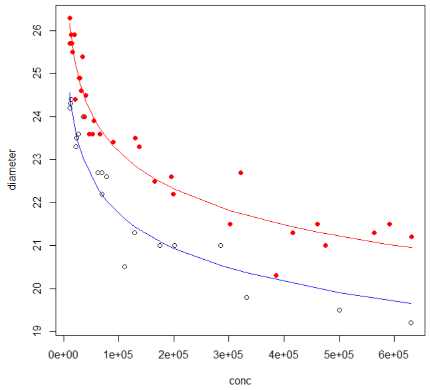
```
The data contains diameter and concentration of Tetrahymena cells with and without glucose
added to growth medium.
glucose: a numeric vector code, 1: yes, 2: no.
conc: a numeric vector, cell concentration (counts/ml).
diameter: a numeric vector, cell diameter (micrometre).

   glucose   conc diameter
1        1 631000     21.2
2        1 592000     21.5
.
50       2  13000     24.3
51       2  11000     24.2
```

Let us assume $Y_i \sim N(\mu_i, \sigma^2)$. Let us consider modeling the expected value μ_i by the following models

$$\mathcal{M}_{1|2_{\log}}: \quad \log(\mu_i) = \beta_0 + \beta_1 x_{i1} + \alpha_j, \qquad \mathcal{M}_{1|2_{\text{exponential}}}: \quad \mu_i = e^{\beta_0} x_{i1}^{\beta_1} e^{\alpha_j},$$

```
> model.log<-glm(diameter~conc+factor(glucose), family=gaussian(link="log"), data=data)
> summary(model.log)

Coefficients:
                     Estimate Std. Error t value Pr(>|t|)
(Intercept)         3.149e+00  9.424e-03 334.156  < 2e-16 ***
conc               -3.607e-07  2.964e-08 -12.170 2.80e-16 ***
factor(glucose)yes  6.836e-02  1.068e-02   6.398 6.18e-08 ***

(Dispersion parameter for gaussian family taken to be 0.6971037)

> model.exponential<-glm(diameter~log(conc)+factor(glucose), family=gaussian(link="log"),
> summary(model.exponential)

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)         3.711625   0.025437  145.91  < 2e-16 ***
log(conc)          -0.054908   0.002259  -24.31  < 2e-16 ***
factor(glucose)yes  0.063899   0.006013   10.63 3.33e-14 ***

(Dispersion parameter for gaussian family taken to be 0.2215944)
```





3.1.2 Gamma and Inverse Gaussian Generalized Linear Models

– If the random variable Y_i follow the Gamma distribution $Y_i \sim Gamma(\mu_i, \phi)$, then for realization y_i it holds that $y_i > 0$. Furthermore

$$
\begin{aligned}
f(y_i|\mu_i, \nu) &= \frac{1}{\Gamma(\nu)}\left(\frac{\nu}{\mu_i}\right)^{\nu} y_i^{\nu-1} e^{-\left(\frac{y_i\nu}{\mu_i}\right)}, \qquad y_i > 0 \\
\mathrm{E}(Y_i) &= \mu_i, \\
\mathrm{Var}(Y_i) &= \phi\mu_i^2,
\end{aligned}
$$

where $\phi = \nu^{-1}$.

– Gamma distribution is suitable in modeling situations when the considered response variable can have only positive values and when the variance increases (proportionally to rate μ_i^2) same time as the expected value μ_i increases.

– Under Gamma distribution, usually used link functions $g(\mu_i)$ are

$$\mu_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{identity link}, \tag{3.6a}$$

$$\log(\mu_i) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \log \textit{ link}, \tag{3.6b}$$

$$\frac{1}{\mu_i} = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{inverse link}. \tag{3.6c}$$

– If the random variable Y_i follow the Inverse Gaussian distribution $Y_i \sim IG(\mu_i, \phi)$, then for realization y_i it holds that $y_i > 0$. Furthermore

$$\begin{aligned} f(y_i|\mu_i,\gamma) &= \sqrt{\frac{\gamma}{2\pi y_i^3}} \exp\left(\frac{-\gamma(y_i-\mu_i)^2}{2\mu_i^2 y_i}\right), \qquad y_i > 0 \\ \mathrm{E}(Y_i) &= \mu_i, \\ \mathrm{Var}(Y_i) &= \phi\mu_i^3, \end{aligned}$$

where $\phi = \gamma^{-1}$.

– Inverse Gaussian distribution is suitable in modeling situations when the considered response variable can have only positive values and when the variance increases (proportionally to rate μ_i^3) same time as the expected value μ_i increases. Inverse Gaussian distribution is very much competing distribution for the Gamma distribution.

– Under Inverse Gaussian distribution, usually used link functions $g(\mu_i)$ are

$$\mu_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{identity link}, \tag{3.7a}$$

$$\log(\mu_i) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \log \textit{link}, \tag{3.7b}$$

$$\frac{1}{\mu_i} = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{inverse link}, \tag{3.7c}$$

$$\frac{1}{\mu_i^2} = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{canonical link}. \tag{3.7d}$$

Example 3.2.

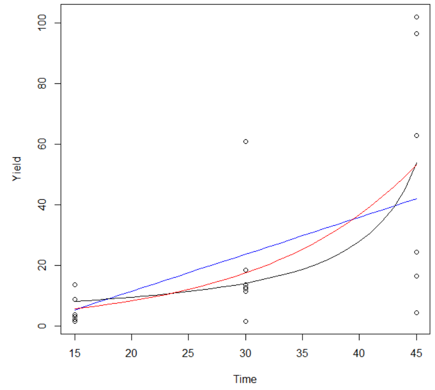
In biodiesel study, methyl ester was produced from waste canola oil. In experiments, it was measured what kind of effect the factors $X_1 = \text{Time}$ (15,30,45min), $X_2 = \text{Temperature}$ (240,255,270C), and level of Methanol/Oil weight ratio (1,1.5,2), $X_3 = \text{Methanol}$, have on yield of methyl ester, $Y = \text{Yield}$. Data obtained from experiments is available in a file canoladiesel.txt.

```
   Time Temp Methanol Yield
1    15  240      1.0   1.5
2    15  240      1.5   3.2
3    15  240      2.0   3.8
.
18   45  270      1.0  96.4
19   45  270      2.0 102.0

Source: S. Lee, D. Posarac, N. Ellis (2012). "An Experimental Investigation
of Biodiesel Synthesis from Waste Canola Oil Using Supercritical Methanol,"
Fuel, Vol. 91, pp. 229-237.
```

Let us assume $Y_i \sim Gamma(\mu_i, \phi)$, and let us consider the models

$$\mathcal{M}_{1_{\text{identity}}}: \quad \mu_i = \beta_0 + \beta_1 x_{i1}, \quad \mathcal{M}_{1_{\text{inverse}}}: \quad \frac{1}{\mu_i} = \beta_0 + \beta_1 x_{i1}, \quad \mathcal{M}_{1_{\log}}: \quad \log(\mu_i) = \beta_0 + \beta_1 x_{i1}.$$

```
> model.identity<-glm(Yield~Time, family=Gamma(link="identity"), data=data)
> coef(model.identity)
(Intercept)        Time
 -12.912377    1.219704
> model.inverse<-glm(Yield~Time, family=Gamma(link="inverse"), data=data)
> coef(model.inverse)
 (Intercept)         Time
 0.174318305 -0.003460192
> model.log<-glm(Yield~Time, family=Gamma(link="log"), data=data)
> coef(model.log)
(Intercept)        Time
 0.63975713  0.07409982
```



3.1.3 Beta Distribution Models

– If the random variable Y_i follow the beta distribution $Y_i \sim Beta(\mu_i, \phi)$, then for realization y_i it holds that $0 < y_i < 1$ and density function has the form

$$f(y|\mu_i, \phi) = \frac{\Gamma(\phi)}{\Gamma(\mu_i\phi)\Gamma((1-\mu_i)\phi)} y_i^{\mu_i\phi-1}(i - y_i)^{(1-\mu_i)\phi-1}, \tag{3.8}$$

where $0 < \mu_i < 1$ and $\phi > 0$.

– Furthermore

$$\mathrm{E}(Y_i) = \mu_i, \tag{3.9}$$

$$\mathrm{Var}(Y_i) = \mathrm{Var}(Y_i) = \frac{\mu_i(1-\mu_i)}{1+\phi}. \tag{3.10}$$

– Beta distribution is suitable in modeling situations when the considered response variable can naturally have values between some open interval (a, b).

– Since beta distribution is defined on interval $(0, 1)$, it is common that transformation $\frac{y-a}{b-a}$ is done on the original response variable.

– Most often used link function with beta distribution is the logit link function

$$\mathrm{logit}(\mu_i) = \log\left(\frac{\mu_i}{1-\mu_i}\right) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \mathrm{logit}\ \textit{link}. \tag{3.11}$$

Example 3.3.

The coffee company had developed a new dark coffee that the company wanted to explore its tastefulness with the help of sensory analysis. In the study, consumers were given a sample of coffee, after tasting, the consumers were asked to evaluate how tasteful the coffee was on the scale of 0 to 100. The consumers who were selected for the survey were also asked about what level of roasting they usually like their coffee to have. The dataset can be on the file coffeerating.txt.

	age	gender	flavor	rating
1	33	female	light	40
2	32	female	dark	87
3	49	female	medium	86
4	39	male	light	36
.				
324	46	female	medium	88
325	42	male	medium	71

By applying Beta model, $Y_i \sim Beta(\mu_i, \phi)$,

$$\operatorname{logit}(\mu_i) = \beta_0 + \beta_1 x_{i1} + \alpha_j + \gamma_h$$

we obtain the following parameter estimates.

```
> model.main<-betareg(Y~age+factor(gender)+factor(flavor), data=data, link=c("logit"))
> summary(model.main)
Call:
betareg(formula = Y ~ age + factor(gender) + factor(flavor), data = data,
    link = c("logit"))

Standardized weighted residuals 2:
    Min      1Q  Median      3Q     Max
-2.6086 -0.6613 -0.0303  0.5190  4.8256

Coefficients (mean model with logit link):
                      Estimate Std. Error z value Pr(>|z|)
(Intercept)           1.258107   0.066829   18.83   <2e-16 ***
age                   0.035037   0.001408   24.89   <2e-16 ***
factor(gender)male   -0.516011   0.021166  -24.38   <2e-16 ***
factor(flavor)light  -2.796063   0.038925  -71.83   <2e-16 ***
factor(flavor)medium -1.397279   0.038970  -35.85   <2e-16 ***

Phi coefficients (precision model with identity link):
      Estimate Std. Error z value Pr(>|z|)
(phi)   163.71      12.82   12.77   <2e-16 ***

Type of estimator: ML (maximum likelihood)
Log-likelihood: 663.2 on 6 Df
Pseudo R-squared: 0.9475
Number of iterations: 27 (BFGS) + 3 (Fisher scoring)
```

3.1.4 Count and Categorical Data Models

– In count data models, the random response variable Y_i can have a realization as an nonnegative integer $y_i = \{0, 1, 2, 3, 4, \dots\}$.

– In count data models, the random response variable Y_i is assumed to follow either *Poisson* distribution or *negative binomial* distribution.

– If the random variable Y_i follows the Poisson distribution $Y_i \sim Poi(\mu_i)$, then the realization will have non-negative integer value $y_i = \{0, 1, 2, 3, 4, \dots\}$, and $\mathrm{E}(Y_i) = \mu_i$ and $\mathrm{Var}(Y_i) = \mu_i$.

– Under Poisson distribution, possible link functions $g(\mu_i)$ are

$$\mu_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{identity link}, \tag{3.12a}$$

$$\log(\mu_i) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \log \textit{link}, \tag{3.12b}$$

$$\sqrt{\mu_i} = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}, \quad \textit{square root link}. \tag{3.12c}$$

– In categorical data models, the most simple situation is where the realization of the random variable Y_i can have only two different outcomes. Every binary outcome situations outcomes can be coded as values 0 and 1.

– The binary random variable Y_i is said to follow Bernoulli distribution $Y_i \sim Ber(\mu_i)$, where the probabilities $P(Y_i = 1)$ and $P(Y_i = 0)$ are denoted as

$$P(Y_i = 1) = \mu_i, \quad P(Y_i = 0) = 1 - \mu_i. \tag{3.13}$$

– When $Y_i \sim Ber(\mu_i)$, then the expected value and the variance of the random variable Y_i are

$$\mathrm{E}(Y_i) = \mu_i, \quad \mathrm{Var}(Y_i) = \mu_i(1 - \mu_i). \tag{3.14}$$

– Under the Bernoulli's distribution $Y_i \sim Ber(\mu_i)$, the most used link function is the logit link function

$$\mathrm{logit}(\mu_i) = \log\left(\frac{\mu_i}{1 - \mu_i}\right) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}. \tag{3.15}$$

– logit link is nonlinear link function by inducing the expected value to have a form

$$\mu_i = \frac{e^{\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}}}{1 + e^{\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}}}. \tag{3.16}$$

3.2 Maximum Likelihood Estimation

3.2.1 Exponential Family of Distributions

– The distribution of a random variable Y_i belongs to the exponential family if its probability density function can be written in the form

$$f(y_i|\Theta_i, \phi) = \exp\left(\frac{y_i\Theta_i - b(\Theta_i)}{a(\phi)} + c(y_i, \phi)\right), \tag{3.17}$$

where Θ_i is the natural or canonical parameter, ϕ is the dispersion parameter, and a, b and c are specific functions.

Example 3.4.

For the normal distribution $Y_i \sim N(\mu_i, \sigma^2)$ it holds that

$$f(y_i|\mu_i, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{1}{2}\cdot\frac{(y_i-\mu_i)^2}{\sigma^2}\right) = \exp\left(-\frac{1}{2}\cdot\frac{(y_i^2 - 2y_i\mu_i + \mu_i^2)}{\sigma^2} + \log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)\right)$$

$$= \exp\left(\frac{y_i\mu_i - \frac{1}{2}\mu_i^2}{\sigma^2} - \frac{y_i^2}{2\sigma^2} + \log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)\right) = \exp\left(\frac{y_i\Theta_i - b(\Theta_i)}{a(\phi)} + c(y_i, \phi)\right),$$

$$\Theta_i = \mu_i,\ \phi = \sigma^2,\ a(\phi) = \phi,\ b(\Theta_i) = \tfrac{1}{2}\Theta_i^2,\ c(y_i, \phi) = -\frac{y_i^2}{2\phi^2} + \log\left(\frac{1}{\sqrt{2\pi\phi^2}}\right).$$

– Let us consider now what kind properties the log-likelihood of the single random variable Y_i has when Y_i is belonging to the exponential family of distributions.

– Log-likelihood $l(\Theta_i, \phi) = \log(L(\Theta_i, \phi))$ for the random variable Y_i has when Y_i is belonging to the exponential family of distributions has the form

$$l(\Theta_i, \phi) = \log(f(y_i|\Theta_i, \phi)) = \frac{y_i\Theta_i - b(\Theta_i)}{a(\phi)} + c(y_i, \phi), \tag{3.18}$$

and the the partial derivative with respect to canonical parameter Θ_i is

$$\frac{\partial l(\Theta_i, \phi)}{\partial \Theta_i} = \frac{y_i - b'(\Theta_i)}{a(\phi)}. \tag{3.19}$$

– Generally, for any log-likelihood, the partial derivative with respect to unknown parameter Θ_i has the property

$$\frac{\partial l}{\partial \Theta_i} = \frac{\partial \log(L)}{\partial \Theta_i} = \frac{1}{L}\frac{\partial L}{\partial \Theta_i}, \tag{3.20}$$

and hence

$$\frac{\partial l}{\partial \Theta_i} \cdot L = \frac{\partial L}{\partial \Theta_i}. \tag{3.21}$$

– Thus the expected value of the partial derivative $\frac{\partial l}{\partial \Theta_i}$ is (under the certain regularity conditions holding in the case of the exponential family)

$$\begin{aligned}\mathrm{E}\left(\frac{\partial l}{\partial \Theta_i}\right) &= \int_{-\infty}^{\infty} \frac{\partial l}{\partial \Theta_i} \cdot f(y_i|\Theta_i, \phi)\, dy_i = \int_{-\infty}^{\infty} \frac{\partial l}{\partial \Theta_i} \cdot L\, dy_i = \int_{-\infty}^{\infty} \frac{\partial L}{\partial \Theta_i}\, dy_i \\ &= \frac{\partial}{\partial \Theta_i} \int_{-\infty}^{\infty} L\, dy_i = \frac{\partial}{\partial \Theta_i} \int_{-\infty}^{\infty} f(y_i|\Theta_i, \phi)\, dy_i = \frac{\partial}{\partial \Theta_i} \cdot 1 = 0. \end{aligned} \tag{3.22}$$

– By applying (3.22) to the exponential family of distributions, we get

$$\mathrm{E}\left(\frac{\partial l(\Theta_i, \phi)}{\partial \Theta_i}\right) = \frac{\mathrm{E}(Y_i) - b'(\Theta_i)}{a(\phi)} = 0, \tag{3.23}$$

and hence it must hold that

$$\mathrm{E}(Y_i) = \mu_i = b'(\Theta_i). \tag{3.24}$$

– Furthermore, the second partial derivative with respect to unknown parameter Θ_i has the property

$$\frac{\partial^2 l}{\partial \Theta_i^2} = \frac{\partial}{\partial \Theta_i}\left(\frac{1}{L}\frac{\partial L}{\partial \Theta_i}\right) = -\frac{1}{L^2}\left(\frac{\partial L}{\partial \Theta_i}\right)^2 + \frac{1}{L}\frac{\partial^2 L}{\partial \Theta_i^2} = -\left(\frac{\partial l}{\partial \Theta_i}\right)^2 + \frac{1}{L}\frac{\partial^2 L}{\partial \Theta_i^2}. \tag{3.25}$$

– Thus the variance of the partial derivative $\frac{\partial l}{\partial \Theta_i}$ is

$$\begin{aligned}
\mathrm{Var}\left(\frac{\partial l}{\partial \Theta_i}\right) = \mathrm{E}\left[\left(\frac{\partial l}{\partial \Theta_i}\right)^2\right] &= -\,\mathrm{E}\left(\frac{\partial^2 l}{\partial \Theta_i^2}\right) + \mathrm{E}\left(\frac{1}{L}\frac{\partial^2 L}{\partial \Theta_i^2}\right) = -\,\mathrm{E}\left(\frac{\partial^2 l}{\partial \Theta_i^2}\right) + \int_{-\infty}^{\infty} \frac{1}{L}\frac{\partial^2 L}{\partial \Theta_i^2} \cdot L\, dy_i \\
&= -\,\mathrm{E}\left(\frac{\partial^2 l}{\partial \Theta_i^2}\right) + \int_{-\infty}^{\infty} \frac{\partial^2 L}{\partial \Theta_i^2}\, dy_i = -\,\mathrm{E}\left(\frac{\partial^2 l}{\partial \Theta_i^2}\right) + \frac{\partial^2}{\partial \Theta_i^2}\int_{-\infty}^{\infty} L\, dy_i \\
&= -\,\mathrm{E}\left(\frac{\partial^2 l}{\partial \Theta_i^2}\right). \qquad (3.26)
\end{aligned}$$

– For the exponential family of distributions, we have

$$\frac{\partial^2 l(\Theta_i,\phi)}{\partial \Theta_i^2} = \frac{-b''(\Theta_i)}{a(\phi)}, \quad \text{and} \quad \left(\frac{\partial l(\Theta_i,\phi)}{\partial \Theta_i}\right)^2 = \frac{(y_i - b'(\Theta_i))^2}{a(\phi)^2}. \qquad (3.27)$$

– By applying the result of (3.26), i.e.,

$$\mathrm{E}\left[\left(\frac{\partial l(\Theta_i,\phi)}{\partial \Theta_i}\right)\right]^2 = -\,\mathrm{E}\left(\frac{\partial^2 l(\Theta_i,\phi)}{\partial \Theta_i^2}\right), \qquad (3.28)$$

we have

$$\frac{\mathrm{E}(Y_i - b'(\Theta_i))^2}{a(\phi)^2} = \frac{b''(\Theta_i)}{a(\phi)}. \qquad (3.29)$$

– Thus the variance of the random variable Y_i is

$$\mathrm{Var}(Y_i) = \mathrm{E}(Y_i - b'(\Theta_i))^2 = b''(\Theta_i)a(\phi). \tag{3.30}$$

– Above we have proved the following theorem.

Theorem 3.1. If the density function of the random variable Y_i has the form

$$f(y_i|\Theta_i, \phi) = \exp\left(\frac{y_i\Theta_i - b(\Theta_i)}{a(\phi)} + c(y_i, \phi)\right),$$

then the expected value of Y_i is

$$\mathrm{E}(Y_i) = \mu_i = b'(\Theta_i).$$

and the variance of Y_i is

$$\mathrm{Var}(Y_i) = \mathrm{E}(Y_i - b'(\Theta_i))^2 = b''(\Theta_i)a(\phi).$$

– In generalized linear models, the distribution of the random variable Y_i is assumed to be belonging to the exponential family of distributions and the canonical parameter Θ_i is the function of $\mathbf{x}_i$ and $\boldsymbol{\beta}$ through the expected value μ_i, i.e, $\Theta_i(\mu_i(\mathbf{x}_i, \boldsymbol{\beta}))$, where $g(\mu_i) = \eta_i = \mathbf{x}_i'\boldsymbol{\beta}$.

3.2.2 Newton–Raphson and Fisher Scoring Methods

– Let assume the random vector $\mathbf{y}$ is belonging to the exponential family of distributions, and let us consider the generalized linear model

$$g(\boldsymbol{\mu}) = \boldsymbol{\eta} = \mathbf{X}\boldsymbol{\beta}, \tag{3.31}$$

where $g(\boldsymbol{\mu}) = (g(\mu_1), g(\mu_2), \ldots, g(\mu_n))'$.

– Log-likelihood function of $\mathbf{y}$ then is

$$l(\boldsymbol{\Theta}(\boldsymbol{\beta}), \phi) = l(\boldsymbol{\beta}|\mathbf{y}) = \sum_{i=1}^{n} \log(f(y_i|\Theta_i, \phi)) = \sum_{i=1}^{n} \frac{y_i\Theta_i - b(\Theta_i)}{a(\phi)} + \sum_{i=1}^{n} c(y_i, \phi). \tag{3.32}$$

– To differentiate the log-likelihood function, we use the chain rule

$$\frac{\partial l(\boldsymbol{\beta}|y_i)}{\partial \beta_j} = \frac{\partial l(\boldsymbol{\beta}|y_i)}{\partial \Theta_i} \frac{\partial \Theta_i}{\partial \mu_i} \frac{\partial \mu_i}{\partial \eta_i} \frac{\partial \eta_i}{\partial \beta_j}. \tag{3.33}$$

– Since

$$\frac{\partial l(\boldsymbol{\beta}|y_i)}{\partial \Theta_i} = \frac{y_i - b'(\Theta_i)}{a(\phi)}, \quad \mu_i = b'(\Theta_i), \quad \frac{\partial \Theta_i}{\partial \mu_i} = \frac{1}{b''(\Theta_i)} \quad \mathrm{Var}(Y_i) = b''(\Theta_i)a(\phi), \quad \frac{\partial \eta_i}{\partial \beta_j} = x_{ij},$$

the partial derivatives $\frac{\partial l(\boldsymbol{\beta}|\mathbf{y})}{\partial \beta_j}$ simplifies to the form

$$\frac{\partial l(\boldsymbol{\beta}|\mathbf{y})}{\partial \beta_j} = \sum_{i=1}^{n} \frac{(y_i - \mu_i)}{\mathrm{Var}(Y_i)} \cdot x_{ij} \cdot \left(\frac{\partial \mu_i}{\partial \eta_i}\right), \qquad j = 0, 1, 2, \ldots, p. \tag{3.34}$$

– The partial derivative $\frac{\partial l(\boldsymbol{\beta}|\mathbf{y})}{\partial \beta_j}$ can be written as

$$\frac{\partial l(\boldsymbol{\beta}|\mathbf{y})}{\partial \beta_j} = \mathbf{x}'_{(j)}\mathbf{D}\mathbf{V}^{-1}(\mathbf{y}-\boldsymbol{\mu}), \qquad j = 0, 1, 2, \ldots, p, \tag{3.35}$$

where

$$\mathbf{D} = \begin{pmatrix} \frac{\partial \mu_1}{\partial \eta_1} & 0 & \ldots & 0 \\ 0 & \frac{\partial \mu_2}{\partial \eta_2} & \ldots & 0 \\ & & \vdots & \\ 0 & 0 & \ldots & \frac{\partial \mu_n}{\partial \eta_n} \end{pmatrix}, \qquad \mathbf{V} = \begin{pmatrix} \mathrm{Var}(Y_1) & 0 & \ldots & 0 \\ 0 & \mathrm{Var}(Y_2) & \ldots & 0 \\ & & \vdots & \\ 0 & 0 & \ldots & \mathrm{Var}(Y_n) \end{pmatrix}$$

and $\mathbf{x}_{(j)}$ is the jth column of the model matrix $\mathbf{X}$.

– When the partial derivatives $\frac{\partial l(\boldsymbol{\beta}|\mathbf{y})}{\partial \beta_j}$ are stacked as

$$\mathbf{u}_{\boldsymbol{\beta}} = \begin{pmatrix} \frac{\partial l(\boldsymbol{\beta})}{\partial \beta_0} \\ \frac{\partial l(\boldsymbol{\beta})}{\partial \beta_1} \\ \vdots \\ \frac{\partial l(\boldsymbol{\beta})}{\partial \beta_p} \end{pmatrix},$$

then the partial derivatives (the score function) can be written as

$$\mathbf{u}_{\boldsymbol{\beta}} = \frac{\partial l(\boldsymbol{\beta}|\mathbf{y})}{\partial \boldsymbol{\beta}} = \mathbf{X}'\mathbf{D}\mathbf{V}^{-1}(\mathbf{y}-\boldsymbol{\mu}). \tag{3.36}$$

– The score function $\mathbf{u}_{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{D}\mathbf{V}^{-1}(\mathbf{y} - \boldsymbol{\mu})$ depends on the parameters $\boldsymbol{\beta}$ implicitly through $\boldsymbol{\mu}$. If $\hat{\boldsymbol{\beta}}$ is a such estimator of $\boldsymbol{\beta}$ that the *likelihood equations*

$$\mathbf{u}_{\hat{\boldsymbol{\beta}}} = \mathbf{X}'\widehat{\mathbf{D}}\widehat{\mathbf{V}}^{-1}(\mathbf{y} - \hat{\boldsymbol{\mu}}) = \mathbf{0}, \tag{3.37}$$

are holding, then $\hat{\boldsymbol{\beta}}$ is the maximum likelihood estimator of $\boldsymbol{\beta}$.

– Usually no a close form solution for the likelihood equations $\mathbf{X}'\mathbf{D}\mathbf{V}^{-1}(\mathbf{y}-\boldsymbol{\mu}) = \mathbf{0}$ exists with respect to the parameter vector $\boldsymbol{\beta}$, and hence the maximum likelihood estimate $\hat{\boldsymbol{\beta}}$ needs to be numerically solved.

– Newton–Raphson and Fisher Scoring methods are numerical iterative algorithms to solve the maximum likelihood estimate of $\boldsymbol{\beta}$. Both methods are based on the second degree Taylor series expansion of the log-likelihood function:

$$l(\boldsymbol{\beta}|\mathbf{y}) \approx l(\boldsymbol{\beta}_t|\mathbf{y}) + \mathbf{u}_t'(\boldsymbol{\beta} - \boldsymbol{\beta}_t) + \frac{1}{2}(\boldsymbol{\beta} - \boldsymbol{\beta}_t)'\mathbf{H}_t(\boldsymbol{\beta} - \boldsymbol{\beta}_t), \tag{3.38}$$

where the subscript t denotes the approximation of the considered vector or matrix in the iterative process $t = 0, 1, 2, \ldots$, and the matrix $\mathbf{H}$ is the Hessian matrix

$$\mathbf{H} = \left(\frac{\partial^2 l(\boldsymbol{\beta}|\mathbf{y})}{\partial\boldsymbol{\beta}\partial\boldsymbol{\beta}'}\right) = \begin{pmatrix} \frac{\partial^2 l(\boldsymbol{\beta})}{\partial\beta_0\partial\beta_0} & \frac{\partial^2 l(\boldsymbol{\beta})}{\partial\beta_0\partial\beta_1} & \cdots & \frac{\partial^2 l(\boldsymbol{\beta})}{\partial\beta_0\partial\beta_p} \\ \frac{\partial^2 l(\boldsymbol{\beta})}{\partial\beta_1\partial\beta_0} & \frac{\partial^2 l(\boldsymbol{\beta})}{\partial\beta_1\partial\beta_1} & \cdots & \frac{\partial^2 l(\boldsymbol{\beta})}{\partial\beta_1\partial\beta_p} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial^2 l(\boldsymbol{\beta})}{\partial\beta_p\partial\beta_0} & \frac{\partial^2 l(\boldsymbol{\beta})}{\partial\beta_p\partial\beta_1} & \cdots & \frac{\partial^2 l(\boldsymbol{\beta})}{\partial\beta_p\partial\beta_p} \end{pmatrix}.$$

– In Newton–Raphson method, the partial derivatives $\frac{\partial l(\boldsymbol{\beta}|\mathbf{y})}{\partial \boldsymbol{\beta}}$ of the Taylor series approximation of the log-likelihood function is obtained and set to zero:

$$\frac{\partial l(\boldsymbol{\beta}|\mathbf{y})}{\partial \boldsymbol{\beta}} \approx \mathbf{u}_t + \mathbf{H}_t(\boldsymbol{\beta} - \boldsymbol{\beta}_t) = \mathbf{0}. \tag{3.39}$$

– After initial values $\boldsymbol{\beta}_0$, the next updated values in Newton–Raphson method are obtained from the equation

$$\boldsymbol{\beta}_{t+1} = \boldsymbol{\beta}_t - \mathbf{H}_t^{-1}\mathbf{u}_t. \tag{3.40}$$

– Iterative process in Fisher Scoring method is the same as in Newton–Raphson method except the Hessian matrix $\mathbf{H}$ is replaced by the Fisher information matrix $\mathbf{F} = -\operatorname{E}(\mathbf{H})$:

$$\boldsymbol{\beta}_{t+1} = \boldsymbol{\beta}_t + \mathbf{F}_t^{-1}\mathbf{u}_t, \tag{3.41}$$

– Both methods continue as long as the difference $\boldsymbol{\beta}_{t+1} - \boldsymbol{\beta}_t$ is sufficiently close to zero, which happens when the score function $\mathbf{u}_t$ is sufficiently close to zero. Then the maximum likelihood estimate of $\boldsymbol{\beta}$ is $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}_{t+1}$.

3.2.3 Weighted Least Squares Estimation

– Let $\hat{\boldsymbol{\beta}}$ be the maximum likelihood estimator for $\boldsymbol{\beta}$ in the generalized linear model $g(\boldsymbol{\mu}) = \boldsymbol{\eta} = \mathbf{X}\boldsymbol{\beta}$.

– Based on the Fisher Scoring method, we may assume that the difference between the true unknown parameter vector $\boldsymbol{\beta}$ and $\hat{\boldsymbol{\beta}}$ is (at least approximately) equal to

$$\hat{\boldsymbol{\beta}} - \boldsymbol{\beta} = \mathbf{F}_{\hat{\beta}}^{-1}\mathbf{u}_{\hat{\beta}}. \tag{3.42}$$

– Asymptotically as the sample size is increasing, we may assume that the estimated information matrix $\mathbf{F}_{\hat{\beta}}$ becomes a constant $\mathbf{F}_{\beta}$. Furthermore, as $n \to \infty$, the estimated score function becomes a zero vector $\mathbf{u}_{\hat{\beta}} = \mathbf{0}$.

– Hence, asymptotically, the expected value of the difference $\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}$ is

$$\mathrm{E}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) = \mathrm{E}(\mathbf{F}_{\boldsymbol{\beta}}^{-1}\mathbf{u}_{\hat{\beta}}) = \mathbf{F}_{\boldsymbol{\beta}}^{-1}\,\mathrm{E}(\mathbf{u}_{\hat{\beta}}) = \mathbf{F}_{\boldsymbol{\beta}}^{-1} \cdot \mathbf{0} = \mathbf{0}. \tag{3.43}$$

– Asymptotically it also holds

$$\begin{aligned}\mathrm{Cov}(\hat{\boldsymbol{\beta}}) = \mathrm{E}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})' &= \mathrm{E}(\mathbf{F}_{\boldsymbol{\beta}}^{-1}\mathbf{u}_{\hat{\beta}}\mathbf{u}_{\hat{\beta}}'\mathbf{F}_{\boldsymbol{\beta}}^{-1}) = \mathbf{F}_{\boldsymbol{\beta}}^{-1}\,\mathrm{E}(\mathbf{u}_{\hat{\beta}}\mathbf{u}_{\hat{\beta}}')\mathbf{F}_{\boldsymbol{\beta}}^{-1} \\ &= \mathbf{F}_{\boldsymbol{\beta}}^{-1}\mathbf{F}_{\hat{\beta}}\mathbf{F}_{\boldsymbol{\beta}}^{-1} = \mathbf{F}_{\boldsymbol{\beta}}^{-1}\mathbf{F}_{\beta}\mathbf{F}_{\boldsymbol{\beta}}^{-1} = \mathbf{F}_{\boldsymbol{\beta}}^{-1}.\end{aligned} \tag{3.44}$$

– Combining (3.43) and (3.44) together with fact that the maximum likelihood estimators are asymptotically generally following the normal distribution, the estimator $\hat{\boldsymbol{\beta}}$ follows asymptotically the normal distribution

$$\hat{\boldsymbol{\beta}} \sim N(\boldsymbol{\beta}, \mathbf{F}_{\boldsymbol{\beta}}^{-1}). \tag{3.45}$$

– Further, since $\mathbf{F}_{\boldsymbol{\beta}} = \mathrm{E}(\mathbf{u}_{\boldsymbol{\beta}}\mathbf{u}'_{\boldsymbol{\beta}})$, we have

$$\begin{aligned}
\mathbf{F}_{\boldsymbol{\beta}} &= \mathrm{E}\left(\mathbf{X}'\mathbf{D}\mathbf{V}^{-1}(\mathbf{y}-\boldsymbol{\mu})(\mathbf{y}-\boldsymbol{\mu})'\mathbf{V}^{-1}\mathbf{D}\mathbf{X}\right) && (3.46)\\
&= \mathbf{X}'\mathbf{D}\mathbf{V}^{-1}\,\mathrm{E}\left((\mathbf{y}-\boldsymbol{\mu})(\mathbf{y}-\boldsymbol{\mu})'\right)\mathbf{V}^{-1}\mathbf{D}\mathbf{X} && (3.47)\\
&= \mathbf{X}'\mathbf{D}\mathbf{V}^{-1}\mathbf{V}\mathbf{V}^{-1}\mathbf{D}\mathbf{X} = \mathbf{X}'\mathbf{D}\mathbf{V}^{-1}\mathbf{D}\mathbf{X} = \mathbf{X}'\mathbf{W}\mathbf{X}, && (3.48)
\end{aligned}$$

where

$$\mathbf{W} = \mathbf{D}\mathbf{V}^{-1}\mathbf{D} = \begin{pmatrix}
\frac{\left(\frac{\partial\mu_1}{\partial\eta_1}\right)^2}{\mathrm{Var}(Y_1)} & 0 & \cdots & 0 \\
0 & \frac{\left(\frac{\partial\mu_2}{\partial\eta_2}\right)^2}{\mathrm{Var}(Y_2)} & \cdots & 0 \\
 & & \vdots & \\
0 & 0 & \cdots & \frac{\left(\frac{\partial\mu_n}{\partial\eta_n}\right)^2}{\mathrm{Var}(Y_n)}
\end{pmatrix}$$

– Hence, asymptotically

$$\hat{\boldsymbol{\beta}} \sim N\left(\boldsymbol{\beta}, (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\right). \tag{3.49}$$

– The Fisher Scoring process $\boldsymbol{\beta}_{t+1} = \boldsymbol{\beta}_t + \mathbf{F}_t^{-1}\mathbf{u}_t$ can be written also as

$$\mathbf{F}_t\boldsymbol{\beta}_{t+1} = \mathbf{F}_t\boldsymbol{\beta}_t + \mathbf{u}_t. \tag{3.50}$$

– Since $\mathbf{F}_t = \mathbf{X}'\mathbf{W}_t\mathbf{X}$ and $\mathbf{u}_t = \mathbf{X}'\mathbf{D}_t\mathbf{V}^{-1}(\mathbf{y} - \boldsymbol{\mu}_t) = \mathbf{X}'\mathbf{W}_t\mathbf{D}_t^{-1}(\mathbf{y} - \boldsymbol{\mu}_t)$, we have

$$\begin{aligned} \mathbf{X}'\mathbf{W}_t\mathbf{X}\boldsymbol{\beta}_{t+1} &= \mathbf{X}'\mathbf{W}_t(\mathbf{X}\boldsymbol{\beta}_t + \mathbf{D}_t^{-1}(\mathbf{y} - \boldsymbol{\mu}_t)) \\ \mathbf{X}'\mathbf{W}_t\mathbf{X}\boldsymbol{\beta}_{t+1} &= \mathbf{X}'\mathbf{W}_t\mathbf{z}_t, \end{aligned} \tag{3.51}$$

where $\mathbf{z}_t = \mathbf{X}\boldsymbol{\beta}_t + \mathbf{D}_t^{-1}(\mathbf{y} - \boldsymbol{\mu}_t)$ is called as the *adjusted response variable*.

– Solving (3.51) with respect to $\boldsymbol{\beta}_{t+1}$ gives us the *weighted least squares estimate*

$$\boldsymbol{\beta}_{t+1} = (\mathbf{X}'\mathbf{W}_t\mathbf{X})^{-1}\mathbf{X}'\mathbf{W}_t\mathbf{z}_t. \tag{3.52}$$

– In weighted least squares estimation, iterative process is continued as long as the difference $\boldsymbol{\beta}_{t+1} - \boldsymbol{\beta}_t$ is sufficiently close to zero. The maximum likelihood estimate of $\boldsymbol{\beta}$ is $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}_{t+1}$.

– The maximum likelihood estimator $\hat{\boldsymbol{\beta}}$ follows approximately the normal distribution

$$\hat{\boldsymbol{\beta}} \sim N\left(\boldsymbol{\beta}, (\mathbf{X}'\widehat{\mathbf{W}}\mathbf{X})^{-1}\right), \tag{3.53}$$

where $\widehat{\mathbf{W}}$ is the estimate of $\mathbf{W}$.

3.2.4 Estimation of $\mathrm{Var}(Y_i)$

– In generalized linear models $g(\boldsymbol{\mu}) = \mathbf{X}\boldsymbol{\beta}$, the variance of the random variable Y_i has often the form

$$\mathrm{Var}(Y_i) = \phi \cdot v(\mu_i), \tag{3.54}$$

where ϕ is a positive unknown dispersion parameter and $v(\mu_i)$ is the function of unknown expected value μ_i.

– For example,

$$\begin{aligned}
\text{Normal distribution:} \quad & v(\mu_i) = 1, \\
\text{Gamma distribution:} \quad & v(\mu_i) = \mu_i^2, \\
\text{Inverse Gaussian distribution:} \quad & v(\mu_i) = \mu_i^3, \\
\text{Poisson distribution:} \quad & v(\mu_i) = \mu_i, \\
\text{Quasi-Poisson distribution:} \quad & v(\mu_i) = \mu_i, \\
\text{Bernoulli distribution:} \quad & v(\mu_i) = \mu_i(1-\mu_i), \\
\text{Quasi-Bernoulli distribution:} \quad & v(\mu_i) = \mu_i(1-\mu_i).
\end{aligned}$$

– For the Poisson and Bernoulli distribution, the dispersion parameter ϕ is equal to 1, but for all other distributions it needs to be estimated.

– The dispersion parameter ϕ is usually estimated by the Chisquared statistic

$$\tilde{\phi} = \frac{\sum_{i=1}^{n} \frac{(y_i - \hat{\mu}_i)^2}{v(\hat{\mu}_i)}}{n - \mathrm{rank}(\mathbf{X})} = \frac{X^2}{n - \mathrm{rank}(\mathbf{X})}. \tag{3.55}$$

– When $\mathrm{Var}(Y_i) = \phi v(\mu_i)$, the X^2 statistic has asymptotically the property

$$\sum_{i=1}^{n} \left(\frac{y_i - \hat{\mu}_i}{\sqrt{\phi v(\hat{\mu}_i)}} \right)^2 = \frac{1}{\phi} \sum_{i=1}^{n} \frac{(y_i - \hat{\mu}_i)^2}{v(\hat{\mu}_i)} = \frac{1}{\phi} X^2 \sim \chi^2_{(n - \mathrm{rank}(\mathbf{X}))}. \tag{3.56}$$

– Since

$$\mathrm{E}\left(\frac{1}{\phi} X^2 \right) = \frac{1}{\phi} \mathrm{E}\left(X^2 \right) = n - \mathrm{rank}(\mathbf{X}), \tag{3.57}$$

the estimator $\tilde{\phi}$ is the unbiased estimator of ϕ:

$$\mathrm{E}(\tilde{\phi}) = \frac{\mathrm{E}\left(X^2 \right)}{n - \mathrm{rank}(\mathbf{X})} = \phi. \tag{3.58}$$

– Note that, the estimate $\tilde{\phi}$ is calculated after the estimates $\hat{\mu}_i$ are obtained.

– The unbiased estimator of $\mathrm{Var}(Y_i)$ is

$$\widehat{\mathrm{Var}}(Y_i) = \tilde{\phi} v(\hat{\mu}_i). \tag{3.59}$$

Example 3.5.

Let us consider the model

$$\mathbf{y} \sim N(\boldsymbol{\mu}, \sigma^2 \mathbf{I}),$$
$$\log(\boldsymbol{\mu}) = \boldsymbol{\eta} = \mathbf{1}\beta_0.$$

The score function has the form

$$u_{\beta_0} = \frac{\partial l(\beta_0|\mathbf{y})}{\partial \beta_0} = \sum_{i=1}^{n} \frac{(y_i - \mu_i)}{\mathrm{Var}(Y_i)} \cdot x_{i0} \cdot \left(\frac{\partial \mu_i}{\partial \eta_i}\right) = \sum_{i=1}^{n} \frac{(y_i - e^{\beta_0})}{\phi} \cdot 1 \cdot e^{\beta_0}$$
$$= \frac{e^{\beta_0}}{\phi}\left[\sum_{i=1}^{n}(y_i - e^{\beta_0})\right] = \frac{e^{\beta_0}}{\phi}\left[\left(\sum_{i=1}^{n} y_i\right) - n \cdot e^{\beta_0}\right],$$

since

$$\mathrm{Var}(Y_i) = \sigma^2 = \phi, \qquad \frac{\partial \mu_i}{\partial \eta_i} = \frac{\partial e^{\eta_i}}{\partial \eta_i} = e^{\eta_i} = e^{\beta_0}.$$

The likelihood equations

$$u_{\beta_0} = \frac{\partial l(\beta_0|\mathbf{y})}{\partial \beta_0} = \frac{e^{\beta_0}}{\phi}\left[\left(\sum_{i=1}^{n} y_i\right) - n \cdot e^{\beta_0}\right] = 0$$

can hold only if $(\sum_{i=1}^n y_i) - n \cdot e^{\beta_0} = 0$ holds (for all $\beta_0 > -\infty$, $\phi < \infty$). Solving the equation $(\sum_{i=1}^n y_i) - n \cdot e^{\beta_0} = 0$ with respect to e^{β_0} gives us the maximum likelihood estimate of μ_i as the sample mean $\hat{\mu}_i = e^{\hat{\beta}_0} = \frac{\sum_{i=1}^n y_i}{n} = \bar{y}$, and furthermore, the maximum likelihood estimate of β_0 is $\hat{\beta}_0 = \log(\bar{y})$.

The estimate for ϕ is

$$\tilde{\phi} = \frac{\sum_{i=1}^n \frac{(y_i - \hat{\mu}_i)^2}{v(\hat{\mu}_i)}}{n - \text{rank}(\mathbf{X})} = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-1} = s_y^2,$$

and hence $\widehat{\text{Var}}(Y_i) = \tilde{\phi} = \tilde{\sigma}^2 = s_y^2$. The estimate of the matrix $\mathbf{W}$ is

$$\widehat{\mathbf{W}} = \begin{pmatrix} \frac{\left(\frac{\partial \hat{\mu}_1}{\partial \hat{\eta}_1}\right)^2}{\widehat{\text{Var}}(Y_1)} & 0 & \dots & 0 \\ 0 & \frac{\left(\frac{\partial \hat{\mu}_2}{\partial \hat{\eta}_2}\right)^2}{\widehat{\text{Var}}(Y_2)} & \dots & 0 \\ & & \vdots & \\ 0 & 0 & \dots & \frac{\left(\frac{\partial \hat{\mu}_n}{\partial \hat{\eta}_n}\right)^2}{\widehat{\text{Var}}(Y_n)} \end{pmatrix} = \begin{pmatrix} \frac{\bar{y}^2}{\tilde{\sigma}^2} & 0 & \dots & 0 \\ 0 & \frac{\bar{y}^2}{\tilde{\sigma}^2} & \dots & 0 \\ & & \vdots & \\ 0 & 0 & \dots & \frac{\bar{y}^2}{\tilde{\sigma}^2} \end{pmatrix} = \frac{\bar{y}^2}{\tilde{\sigma}^2}\mathbf{I},$$

and thus the estimate of the covariance matrix $\text{Cov}(\hat{\beta}_0)$ is

$$\widehat{\text{Cov}}(\hat{\beta}_0) = (\mathbf{1}'\widehat{\mathbf{W}}\mathbf{1})^{-1} = \left(\frac{\bar{y}^2}{\tilde{\sigma}^2}\mathbf{1}'\mathbf{1}\right)^{-1} = \left(\frac{\bar{y}^2 \cdot n}{\tilde{\sigma}^2}\right)^{-1} = \frac{1}{\bar{y}^2} \cdot \frac{\tilde{\sigma}^2}{n}.$$

3.3 Confidence and Prediction Intervals

3.3.1 Confidence Intervals in Generalized Linear Model

– The maximum likelihood estimator for the link function $g(\mu_{i_*}) = \eta_{i_*} = \mathbf{x}'_{i_*}\boldsymbol{\beta}$ is

$$\widehat{g(\mu_{i_*})} = \hat{\eta}_{i_*} = \mathbf{x}'_{i_*}\hat{\boldsymbol{\beta}}. \tag{3.60}$$

– Estimated variance for $\hat{\eta}_{i_*} = \mathbf{x}'_{i_*}\hat{\boldsymbol{\beta}}$ is

$$\widehat{\mathrm{Var}}\left(\mathbf{x}'_{i_*}\hat{\boldsymbol{\beta}}\right) = \mathbf{x}'_{i_*}\widehat{\mathrm{Cov}}(\hat{\boldsymbol{\beta}})\mathbf{x}_{i_*} = \mathbf{x}'_{i_*}(\mathbf{X}'\widehat{\mathbf{W}}\mathbf{X})^{-1}\mathbf{x}_{i_*}. \tag{3.61}$$

– Since approximately

$$\mathbf{x}'_{i_*}\hat{\boldsymbol{\beta}} \sim N(\mathbf{x}'_{i_*}\boldsymbol{\beta}, \mathbf{x}'_{i_*}(\mathbf{X}'\widehat{\mathbf{W}}\mathbf{X})^{-1}\mathbf{x}_{i_*}), \tag{3.62}$$

the $100(1-\alpha)\%$ confidence interval for the link function $\eta_{i_*} = \mathbf{x}'_{i_*}\boldsymbol{\beta}$ is

$$\left[\mathbf{x}'_{i_*}\hat{\boldsymbol{\beta}} - z_{\alpha/2}\sqrt{\mathbf{x}'_{i_*}\widehat{\mathrm{Cov}}(\hat{\boldsymbol{\beta}})\mathbf{x}_{i_*}}, \mathbf{x}'_{i_*}\hat{\boldsymbol{\beta}} + z_{\alpha/2}\sqrt{\mathbf{x}'_{i_*}\widehat{\mathrm{Cov}}(\hat{\boldsymbol{\beta}})\mathbf{x}_{i_*}}\right] = \left[L_{\alpha/2}, U_{\alpha/2}\right], \tag{3.63}$$

where $P(Z > z_{\alpha/2}) = \alpha/2$ as $Z \sim N(0,1)$.

– If $g(\mu_{i_*})$ is monotonically increasing function, then $100(1-\alpha)\%$ confidence interval for the expected value μ_{i_*} is

$$\left[g^{-1}(L_{\alpha/2}), g^{-1}(U_{\alpha/2})\right]. \tag{3.64}$$

3.3.2 Prediction Intervals in Generalized Linear Model

– The maximum likelihood predictor for the new observation Y_f (observable in future) with given values of the explanatory variables $\mathbf{x}_f$ is

$$\hat{Y}_f = g^{-1}(\mathbf{x}_f'\hat{\boldsymbol{\beta}}). \tag{3.65}$$

– By so called delta method, it can be shown that approximately

$$\mathrm{Var}(\hat{Y}_f) = \left(\frac{\partial \mu_f}{\partial \eta_f}\right)^2 \cdot \mathbf{x}_f' \,\mathrm{Cov}(\hat{\boldsymbol{\beta}})\mathbf{x}_f = \left(\frac{\partial \mu_f}{\partial \eta_f}\right)^2 \cdot \mathbf{x}_f'(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{x}_f. \tag{3.66}$$

– Since for the prediction error $e_f = Y_f - \hat{Y}_f$ it holds

$$\mathrm{Var}(e_f) = \mathrm{Var}(Y_f) + \mathrm{Var}(\hat{Y}_f) = \mathrm{Var}(Y_f) + \left(\frac{\partial \mu_f}{\partial \eta_f}\right)^2 \cdot \mathbf{x}_f' \,\mathrm{Cov}(\hat{\boldsymbol{\beta}})\mathbf{x}_f, \tag{3.67}$$

the estimated variance of the prediction error is

$$\widehat{\mathrm{Var}}(e_f) = \widehat{\mathrm{Var}}(Y_f) + \left(\frac{\partial \hat{\mu}_f}{\partial \hat{\eta}_f}\right)^2 \cdot \mathbf{x}_f'\widehat{\mathrm{Cov}}(\hat{\boldsymbol{\beta}})\mathbf{x}_f, \tag{3.68}$$

– Approximately $Y_f - \hat{Y}_f \sim N(0, \widehat{\mathrm{Var}}(e_f))$, and hence the $100(1-\alpha)\%$ prediction interval for the new observation Y_f is

$$\left[g^{-1}(\mathbf{x}_f'\hat{\boldsymbol{\beta}}) - z_{\alpha/2}\sqrt{\widehat{\mathrm{Var}}(e_f)},\, g^{-1}(\mathbf{x}_f'\hat{\boldsymbol{\beta}}) + z_{\alpha/2}\sqrt{\widehat{\mathrm{Var}}(e_f)}\right]. \tag{3.69}$$

– The prediction intervals for the new observation y_f (observable in future) with given values of the explanatory variables $\mathbf{x}_f$ can also be obtained by the bootstrap method.

Parametric bootstrap based method - Normal Distribution

1. Find the estimates $\hat{\eta}_f = \mathbf{x}'_f\hat{\boldsymbol{\beta}}$ and $\tilde{\phi} = \tilde{\sigma}^2$.
2. Simulate $\hat{\eta}_{f_*}$ from the distribution $\hat{\eta}_{f_*} \sim N\left(\hat{\eta}_f, \mathbf{x}'_f(\mathbf{X}'\widehat{\mathbf{W}}\mathbf{X})^{-1}\mathbf{x}_f\right)$.
3. Find the estimates $\hat{\mu}_{f_*} = g^{-1}(\hat{\eta}_{f_*})$.
4. Simulate y_{f_*} from the distribution $y_{f_*} \sim N(\hat{\mu}_{f_*}, \tilde{\sigma}^2)$.
5. Repeat M times the steps 2-4, and then determine $\alpha/2$ and $1-\alpha/2$ the quantiles of the simulated values y_{f_*} .

Parametric bootstrap based method - Gamma Distribution

1. Find the estimates $\hat{\eta}_f = \mathbf{x}'_f\hat{\boldsymbol{\beta}}$ and $\tilde{\phi}$.
2. Simulate $\hat{\eta}_{f_*}$ from the distribution $\hat{\eta}_{f_*} \sim N\left(\hat{\eta}_f, \mathbf{x}'_f(\mathbf{X}'\widehat{\mathbf{W}}\mathbf{X})^{-1}\mathbf{x}_f\right)$.
3. Find the estimates $\hat{\mu}_{f_*} = g^{-1}(\hat{\eta}_{f_*})$.
4. Simulate y_{f_*} from the distribution $y_{f_*} \sim Gamma(\hat{\mu}_{f_*}, \tilde{\phi})$. (Simulate y_{f_*} from the distribution $y_{f_*} \sim Gamma(a, s_*)$, where $a = \frac{1}{\tilde{\phi}}$ and $s_* = \tilde{\phi}\hat{\mu}_{f_*}$.)
5. Repeat M times the steps 2-4, and then determine $\alpha/2$ and $1-\alpha/2$ the quantiles of the simulated values y_{f_*} .

Parametric bootstrap based method - Inverse Gaussian Distribution

1. Find the estimates $\hat{\eta}_f = \mathbf{x}'_f\hat{\boldsymbol{\beta}}$ and $\tilde{\phi}$.
2. Simulate $\hat{\eta}_{f_*}$ from the distribution $\hat{\eta}_{f_*} \sim N\left(\hat{\eta}_f, \mathbf{x}'_f(\mathbf{X}'\widehat{\mathbf{W}}\mathbf{X})^{-1}\mathbf{x}_f\right)$.
3. Find the estimates $\hat{\mu}_{f_*} = g^{-1}(\hat{\eta}_{f_*})$.

4. Simulate y_{f_*} from the distribution $y_{f_*} \sim IG(\hat{\mu}_{f_*}, \tilde{\phi})$.
   (Simulate y_{f_*} from the distribution $y_{f_*} \sim IG\left(\hat{\mu}_{f_*}, \frac{1}{\tilde{\phi}}\right)$.)
5. Repeat M times the steps 2-4, and then determine $\alpha/2$ and $1-\alpha/2$ the quantiles of the simulated values y_{f_*} .

Example 3.6.

Consider the following data set related to genetic disorder cystic fibrosis:

```
  age sex height weight bmp fev1  rv frc tlc pemax
1   7   0    109   13.1  68   32 258 183 137    95
2   7   1    112   12.9  65   19 449 245 134    85
3   8   0    124   14.1  64   22 441 268 147   100
.
25  23   0    179   71.5  95   52 225 127 101   195
The cystfibr data frame has 25 rows and 10 columns. It contains lung function data for
cystic fibrosis patients (7-23 years old).

This data frame contains the following columns:
age - age in years.
sex - 0: male, 1:female.
height - height (cm).
weight - weight (kg).
bmp - body mass (percent of normal).
fev1 - forced expiratory volume.
rv - residual volume.
frc - functional residual capacity.
tlc - total lung capacity.
```

```
pemax - maximum expiratory pressure.

O'Neill et al. (1983), The effects of chronic hyperinflation, nutritional status,
and posture on respiratory muscle strength in cystic fibrosis,
Am. Rev. Respir. Dis., 128:1051-1054.
```

We denote variables as $Y = \mathsf{pemax},\ X_1 = \mathsf{height},\ X_2 = \mathsf{weight}\ X_3 = \mathsf{sex}.$ Further, we assume $Y_i \sim N(\mu_i, \sigma^2)$. We consider the model

$$\mu_i = e^{\beta_0} x_{i1}^{\beta_1} x_{i1}^{\beta_2} e^{\alpha_j},$$

and let us find confidence and prediction intervals for Y_f when

```
  age sex height weight bmp fev1  rv frc tlc
1   7   0    109   13.1  68   32 258 183 137
```

```
> data<-read.table("cysticfibrosis.txt", sep="\t", dec=".", header=TRUE)
> model.exponential<-glm(pemax~log(height)+log(weight)+factor(sex), family=gaussian(link="log"), data=data)
> newdata<-data[1,]
> pred<-predict(model.exponential, newdata=newdata, type="response")
> pred
       1
74.91101
> eta<-predict(model.exponential, newdata=newdata, type="link", se.fit=TRUE)
> link.lowerbound<-eta$fit-qnorm(0.975)*eta$se.fit
> link.upperbound<-eta$fit+qnorm(0.975)*eta$se.fit
> lower.mu<-exp(link.lowerbound)
> upper.mu<-exp(link.upperbound)
```

```
> lower.mu
       1
51.57218
> upper.mu
       1
108.8118

> pred<-predict(model.exponential, newdata=newdata, type="response")
> xf<-cbind(model.matrix(model.exponential)[1,])
> Var.Yf<-summary(model.exponential)$dispersion
> D.f<-pred
> Var.ef<-Var.Yf+(D.f^2)*t(xf)%*%vcov(model.exponential)%*%xf
> lower.yf<-pred-qnorm(0.9)*sqrt(Var.ef)
> upper.yf<-pred+qnorm(0.9)*sqrt(Var.ef)
> lower.yf
         [,1]
[1,] 35.30483
> upper.yf
         [,1]
[1,] 114.5172
```

Assignment 3.1.

Consider the normal distribution with the identity link function

$$\mathbf{y} \sim N(\boldsymbol{\mu}, \sigma^2 \mathbf{I}),$$
$$\boldsymbol{\mu} = \boldsymbol{\eta} = \mathbf{X}\boldsymbol{\beta}.$$

What kind of more simplified form the likelihood equations

$$\frac{\partial l(\boldsymbol{\beta}|\mathbf{y})}{\partial \boldsymbol{\beta}} = \mathbf{u}_{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{D}\mathbf{V}^{-1}(\mathbf{y} - \boldsymbol{\mu}) = \mathbf{0}$$

have in this case? Note that

$$\mathbf{D} = \begin{pmatrix} \frac{\partial \mu_1}{\partial \eta_1} & 0 & \dots & 0 \\ 0 & \frac{\partial \mu_2}{\partial \eta_2} & \dots & 0 \\ & & \vdots & \\ 0 & 0 & \dots & \frac{\partial \mu_n}{\partial \eta_n} \end{pmatrix}, \qquad \mathbf{V} = \begin{pmatrix} \mathrm{Var}(Y_1) & 0 & \dots & 0 \\ 0 & \mathrm{Var}(Y_2) & \dots & 0 \\ & & \vdots & \\ 0 & 0 & \dots & \mathrm{Var}(Y_n) \end{pmatrix}.$$

Can you obtain the maximum likelihood estimator $\hat{\boldsymbol{\beta}}$ directly by solving likelihood equations with respect to $\boldsymbol{\beta}$?

Assignment 3.2.

Consider the model

$$\begin{aligned} \mathbf{y} &\sim N(\boldsymbol{\mu}, \sigma^2\mathbf{I}), \\ \log(\boldsymbol{\mu}) &= \boldsymbol{\eta} = \mathbf{1}\beta_0. \end{aligned}$$

Construct the prediction intervals for the new observation Y_f.

Assignment 3.3.

In biodiesel study, methyl ester was produced from waste canola oil. In experiments, it was measured what kind of effect the factors $X_1 = \textsf{Time}$ (15,30,45min), $X_2 = \textsf{Temperature}$ (240,255,270C), and level of Methanol/Oil weight ratio (1,1.5,2), $X_3 = \textsf{Methanol}$, have on yield of methyl ester, $Y = \textsf{Yield}$. Data obtained from experiments is available in a file canoladiesel.txt.

```
   Time Temp Methanol Yield
1    15  240      1.0   1.5
2    15  240      1.5   3.2
3    15  240      2.0   3.8
.
18   45  270      1.0  96.4
19   45  270      2.0 102.0

Source: S. Lee, D. Posarac, N. Ellis (2012). "An Experimental Investigation
of Biodiesel Synthesis from Waste Canola Oil Using Supercritical Methanol,"
Fuel, Vol. 91, pp. 229-237.
```

Let us consider the models

$$\mathcal{M}_{1_{\text{inverse}}}: \quad \frac{1}{\mu_i} = \beta_0 + \beta_1 x_{i1}, \quad \mathcal{M}_{1_{\log}}: \quad \log(\mu_i) = \beta_0 + \beta_1 x_{i1}.$$

Create prediction intervals under different distributional assumptions.

Assignment 3.4.

The coffee company had developed a new dark coffee that the company wanted to explore its tastefulness with the help of sensory analysis. In the study, consumers were given a sample of coffee, after tasting, the consumers were asked to evaluate how tasteful the coffee was on the scale of 0 to 100. The consumers who were selected for the survey were also asked about what level of roasting they usually like their coffee to have. The dataset can be on the file coffeerating.txt.

```
    age gender flavor rating
1    33 female  light     40
2    32 female   dark     87
3    49 female medium     86
4    39   male  light     36
.
324  46 female medium     88
325  42   male medium     71
```

Let us assume $Y_i \sim Beta(\mu_i, \phi)$. Consider the model

$$\mathrm{logit}(\mu_i) = \beta_0 + \beta_1 x_{i1} + \alpha_j + \gamma_h + \tau_j x_{i1} + \omega_h x_{i1} + \psi_{jh}$$

Create prediction intervals by parametric bootstrap methods.