Generalized Linear Models and their Applications

STAT 431/STAT 831

Fall 2021 (1219)

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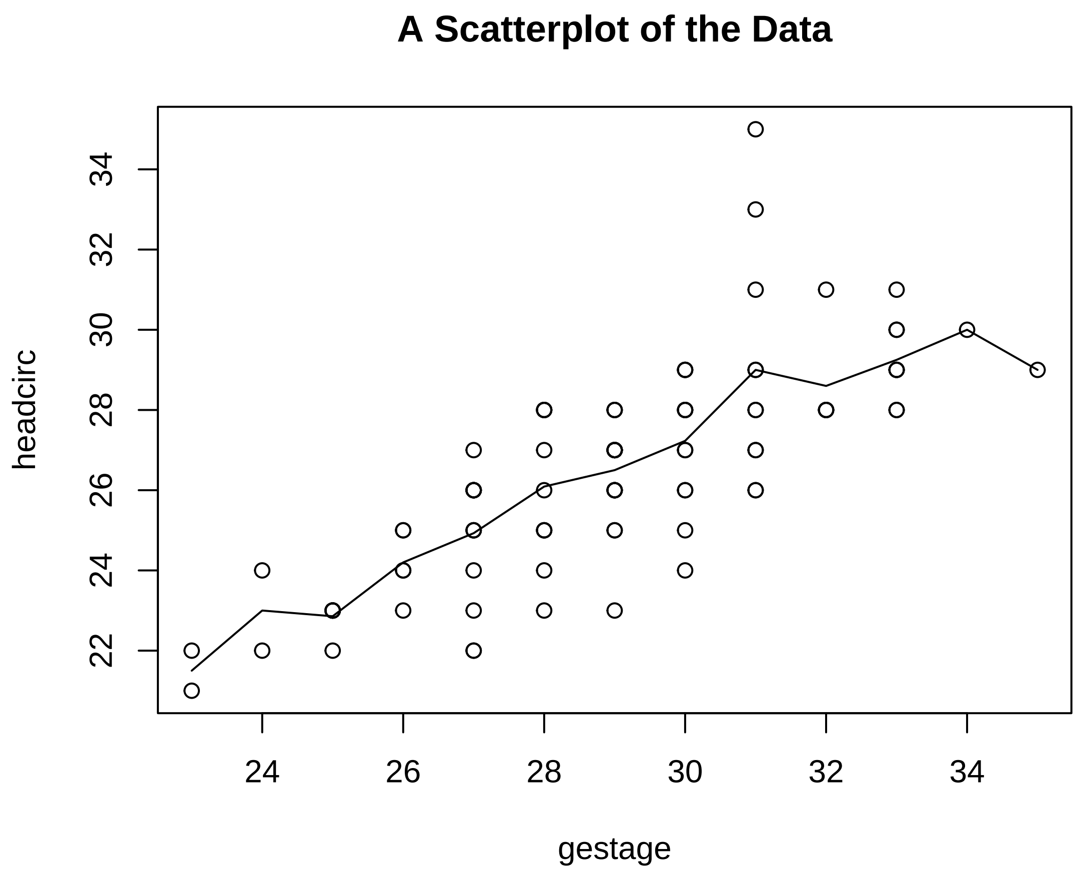
Contents

Topic 1a: Review of Linear Regression

Example: low birthweight infants study[1]

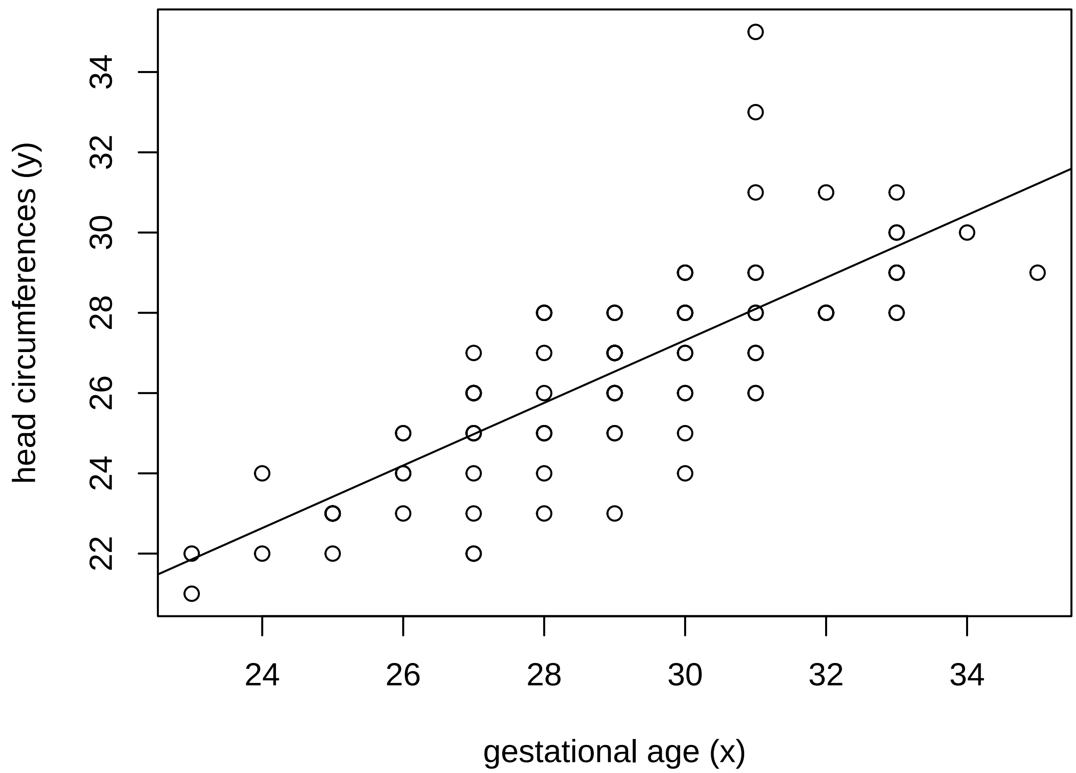
A study was conducted at two teaching hospitals in Boston, Massachusetts, where the head circumference, gestational age and some other variables are recorded for 100 low birth weight infants.

Question: what is the relationship between *gestational age* & head circumference?



We wish to model the relationship between *gestational age* and *head circumference* using a straight line!

[1]Principles of Biostatistics by Pagano and Gauvreau



The Model Fitting Process

1. Model Specification: select a probability distribution for the response variable and a linear equation linking the response to the explanatory variables.
2. Estimation: finding the equation (the parameters of the model).
3. Model checking: how well does the model fit the data?
4. Inference: interpret the fitted model, calculate confidence intervals, conduct hypothesis tests.

1. Model Specification

Notation

For each subject $i = 1, \ldots, n$ we have:

- Y_i = random variable representing the response, and
- $\mathbf{x}_i = (1, x_{i1}, \ldots, x_{ip})^\top$ a vector of explanatory variables.

Specification for Multiple Linear Regression

- Linear regression equation:

$$Y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \varepsilon_i \text{ where } \varepsilon_i \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2).$$

- Equivalently, Y_i's are independent $\mathcal{N}(\mu_i, \sigma^2)$ random variables or

$$\mu_i = \mathbb{E}[Y_i] = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}.$$

- For convenience, we often write linear regression models in matrix form as

$$\boldsymbol{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where

$$\boldsymbol{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1p} \\ 2 & x_{21} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

and

$$\boldsymbol{\varepsilon} \sim \text{MVN}(\mathbf{0}, \sigma^2\mathbf{I}).$$

2. Estimation

Least Squares

We wish to minimize a loss function:

$$\begin{aligned} S(\boldsymbol{\beta}) &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n} \big(y_i - (\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip})\big)^2 \\ &= (\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta})^\top (\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta}). \end{aligned}$$

The least squares estimators (LSE) are the solutions to the equations:

$$\frac{\partial S}{\partial \boldsymbol{\beta}} = \frac{\partial}{\partial \boldsymbol{\beta}} (\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta})^\top (\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta}) = 0.$$

Maximum Likelihood Estimation

The probability density function for Y_i is:

$$f(y_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2} \big(y_i - (\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip})\big)^2\right\}.$$

The log-likelihood function is therefore:

$$\begin{aligned} \ell(\boldsymbol{\beta}, \sigma^2) &= \log\left(\prod_{i=1}^{n} f(y_i)\right) \\ &= \sum_{i=1}^{n} \left(-\frac{1}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \big(y_i - (\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip})\big)\right) \\ &= -\frac{n}{2}\log(2\sigma^2) - \frac{1}{2\sigma^2} (\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta})^\top (\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta}). \end{aligned}$$

The maximum likelihood estimators (MLE) of $\boldsymbol{\beta}$ are obtained by solving:

$$\frac{\partial \ell}{\partial \boldsymbol{\beta}} = \frac{\partial}{\partial \boldsymbol{\beta}} \left[-\frac{1}{2\sigma^2} (\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta})^\top (\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta}) \right] = 0.$$

- Parameter Estimates: For linear regression LSE and MLE of $\boldsymbol{\beta}$ are the same

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{Y}.$$

- Fitted values: $\hat{\boldsymbol{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$.
- Residuals: $\hat{r}_i = (y_i - \hat{y}_i)$.
- Variance estimates:
  - An unbiased estimate of σ^2 is:

$$\hat{\sigma}^2 = \frac{1}{n - (p+1)} \sum_{i=1}^{n} \hat{r}_i^2.$$

  - An estimate of the variance of $\hat{\boldsymbol{\beta}}$ is:

$$\hat{\mathbb{V}}(\hat{\boldsymbol{\beta}}) = \hat{\sigma}^2 (\mathbf{X}^\top \mathbf{X})^{-1}.$$

Low Birthweight Infant Data Example

- For $n = 100$ infants, we have observed Y_i = head circumference and x_i = gestational age for baby i, $i = 1, \dots, 100$.
- Consider a simple linear regression model:

$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i.$$

- We can fit the model and obtain LSE/MSE using the `lm()` function in R.

```
lowbwt <- read.table("lowbwt.txt", header = T)
fit <- lm(headcirc ~ gestage, data = lowbwt)
summary(fit)

Call:
lm(formula = headcirc ~ gestage, data = lowbwt)

Residuals:
    Min      1Q  Median      3Q     Max 
-3.5358 -0.8760 -0.1458  0.9041  6.9041 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  3.91426    1.82915    2.14   0.0348 *  
gestage      0.78005    0.06307   12.37   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.59 on 98 degrees of freedom
Multiple R-squared:  0.6095,Adjusted R-squared:  0.6055 
F-statistic: 152.9 on 1 and 98 DF,  p-value: < 2.2e-16
```

- What is the interpretation of regression parameters β_0 and β_1?
  - β_0 (intercept): expected `headcirc` for a baby of a gestational age zero ($x = 0$).
  - β_1 (slope): expected change in `headcirc` associated with a one unit increase in gestational age.

3. Model Checking

Standardized Residuals:

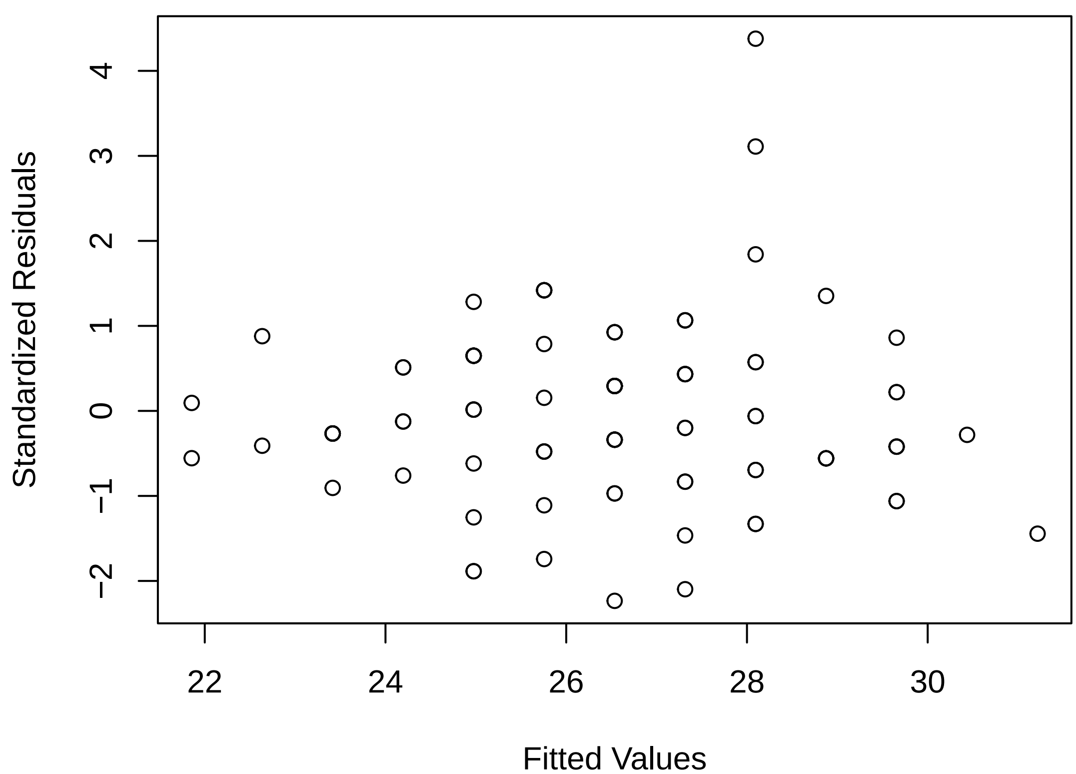
$$d_i = \frac{r_i}{\sqrt{\hat{\sigma}^2(1 - h_{ii})}},$$

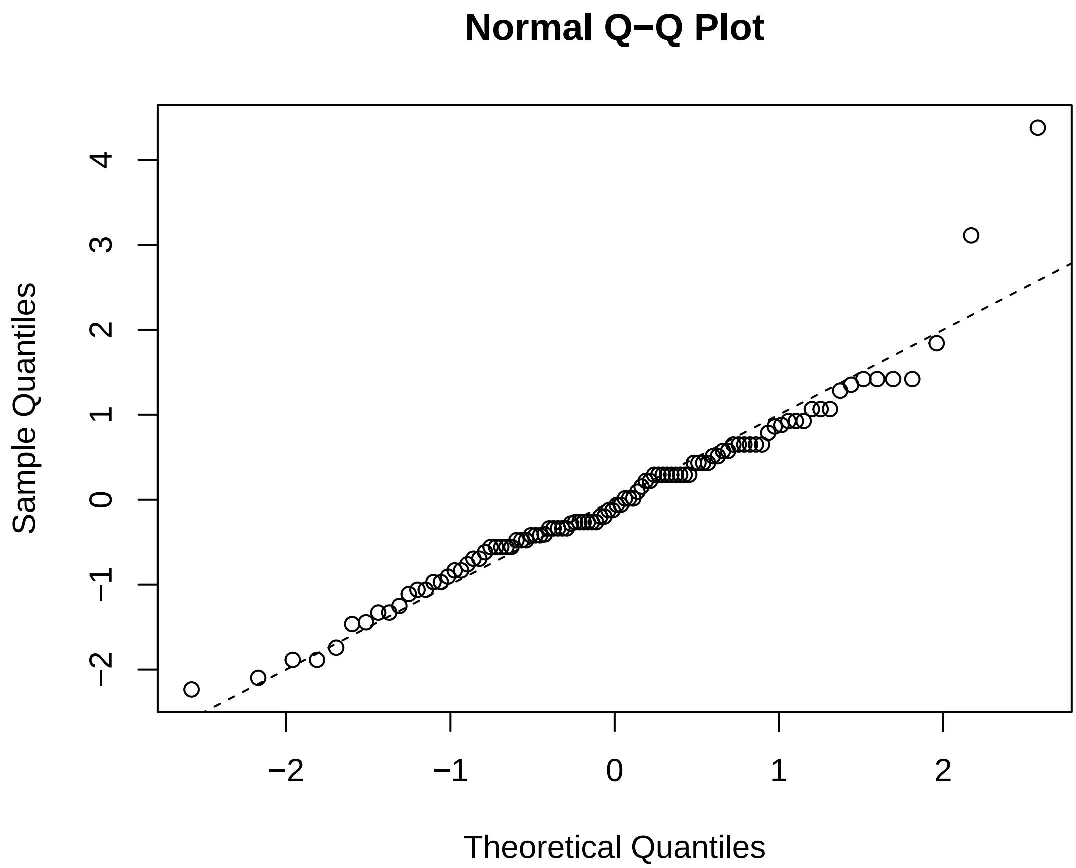
where h_{ii} is the (i, i) element of $\mathbf{H} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top$. By asymptotic theory, if the model provides a good fit to the data then we should expect that:

$$d_i \overset{\text{iid}}{\sim} \mathcal{N}(0, 1).$$

We visually check this by examining residual plots such as:

- Standardized residuals versus the fitted values.
- Standardized residuals versus the explanatory variable(s).
- Normal probability plot (QQ plot) of the standardized residuals.





4. Inference

- Under suitable assumptions, the fitted regression parameters are asymptotically normally distributed:

$$\hat{\boldsymbol{\beta}} \sim \mathrm{MVN}(\boldsymbol{\beta}, \sigma^2(\mathbf{X}^\top\mathbf{X})^{-1}),$$
$$\hat{\beta}_j \sim \mathcal{N}(\beta_j, \sigma^2 v_{jj}), \qquad \text{where } v_{jj} = \left[(\mathbf{X}^\top\mathbf{X})^{-1}\right]_{(j,j)}.$$

- Since σ^2 is generally unknown, we replace it with the unbiased estimate $\hat{\sigma}^2$, and obtain $\mathrm{se}(\hat{\beta}_j) = \sqrt{\hat{\sigma}^2 v_{jj}}$.
- The inference is then based on the t-distribution result:

$$\frac{\hat{\beta}_j - \beta_j}{\mathrm{se}(\hat{\beta}_j)} \sim t_{n-p-1}.$$

Low Birthweight Infant Data Example

- Is there a significant (linear) relationship between head circumference and gestational age?
  We wish to test H_0: $\beta_1 = 0$ vs H_A: $\beta_1 \neq 0$.

$$t = \frac{\hat{\beta}_1 - (0)}{\mathrm{se}(\hat{\beta}_1)} \sim t_{98},$$

  if H_0 is true, and we reject H_0 if $|t| > t_{98,0.975} = 1.985$. Here we have $t = 0.78/0.063 = 12.37 \gg 1.985$, so we reject H_0.

- What is the 95 % confidence interval for the expected increase in head circumference when the gestational age of a baby increases by 1 week?

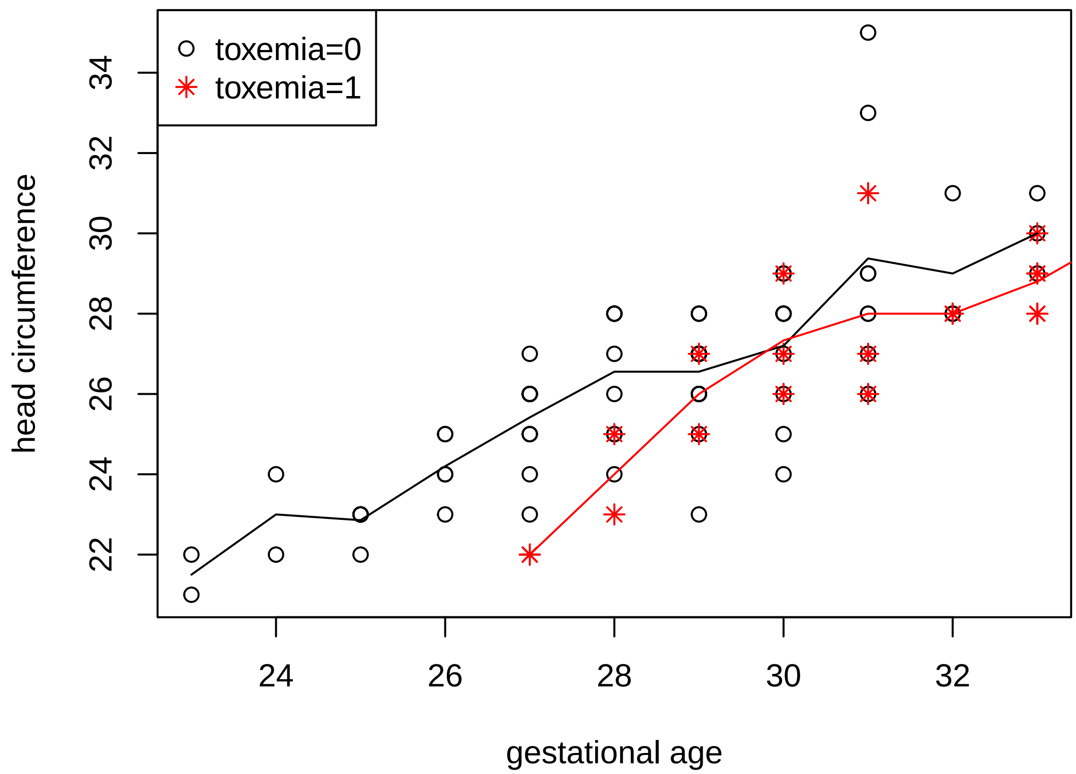
  A 95 % CI for β_1:

$$\hat{\beta}_1 \pm t_{98,0.975}\,\mathrm{se}(\hat{\beta}_1) = 0.78 \pm 1.985(0.063) = (0.665, 0.905).$$

Linear models with multiple predictors

Low Birthweight Infant Data Example

- *Toxemia*, a pregnancy complication characterized by high blood pressure and signs of damage to liver and kidneys, may also have an impact on the development of babies.



- Does *toxemia*, after adjustment for gestational age, also affect the head circumference?

```
fit <- lm(headcirc ~ gestage + factor(toxemia), data = lowbwt)
summary(fit)

Call:
lm(formula = headcirc ~ gestage + factor(toxemia), data = lowbwt)

Residuals:
    Min      1Q  Median      3Q     Max
-3.8427 -0.8427 -0.0525  0.8109  6.4092
```

```
Coefficients:
                 Estimate Std. Error t value Pr(>|t|)
(Intercept)       1.49558    1.86799   0.801  0.42530
gestage           0.87404    0.06561  13.322  < 2e-16 ***
factor(toxemia)1 -1.41233    0.40615  -3.477  0.00076 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.507 on 97 degrees of freedom
Multiple R-squared:  0.6528,Adjusted R-squared:  0.6456
F-statistic: 91.18 on 2 and 97 DF,  p-value: < 2.2e-16
```

What is the interpretation of β_2?

$\hat{\beta}_3 = -1.41233$. After adjustment of gestational age, the babies whose mothers had toxemia have smaller (by 1.41 cm) than those whose mothers did not. This difference is significant (test H_0: $\beta_2 = 0$, p-value $= 0.0076 < 0.05$).

- Is the rate of increase of head circumference with gestational age the same for infants whose mothers with toxemia as those whose mother without it?

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i1} x_{i2} + \varepsilon_i.$$

```
fit <- lm(headcirc ~ gestage * factor(toxemia), data = lowbwt)
summary(fit)

Call:
lm(formula = headcirc ~ gestage * factor(toxemia), data = lowbwt)

Residuals:
    Min      1Q  Median      3Q     Max
-3.8366 -0.8366 -0.0928  0.7910  6.4341

Coefficients:
                         Estimate Std. Error t value Pr(>|t|)
(Intercept)               1.76291    2.10225   0.839    0.404
gestage                   0.86461    0.07390  11.700   <2e-16 ***
factor(toxemia)1         -2.81503    4.98515  -0.565    0.574
gestage:factor(toxemia)1  0.04617    0.16352   0.282    0.778
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.515 on 96 degrees of freedom
Multiple R-squared:  0.6531,Adjusted R-squared:  0.6422
F-statistic: 60.23 on 3 and 96 DF,  p-value: < 2.2e-16
```

What is the interpretation of β_3?

β_3 is the differences in slopes between the two groups (`toxemia=1` vs `toxemia=0`). We want to test H_0: $\beta_3 = 0$, $t = 0.282$, p-value $= 0.778 > 0.05$. No evidence to reject H_0.

Limitations of Linear Regression

Linear regression models can be very useful but may not be appropriate to use when response Y is not continuous and can not be assumed to be normally distributed, e.g.,

- Binary data ($Y = 0$ or $Y = 1$),
- Count data ($Y = 0, 1, 2, 3, ...$).

Generalized Linear Models (GLM) extend the linear regression framework to address the above issue.

- Suitable for continuous and discrete data.
- Normal/Gaussian linear regression is a special case of GLM.
- Inference based on maximum likelihood methods (review next class — 431 Appendix, Stat 330 notes).

WEEK 2
13th to 17th September

Topic 1b: Review of Likelihood Methods

Distributions with a Single Parameter

Setup

- Suppose Y is a random variable with probability density (or mass) function $f(y; \theta)$, where $\theta \in \Omega$ is a continuous parameter.
- The true value of θ is unknown.
- We wish to make inferences about θ (i.e., we may want to estimate θ, calculate a 95 % CI or carry out tests of hypotheses regarding θ).

Likelihood Function

- The Likelihood function is any function which is proportional to the probability of observing the data one actually obtained, i.e.,
$$L(\theta; y) = cf(y; \theta) = c\,\mathbb{P}(Y = y; \theta),$$
where c is a *proportionality constant* that does not depend on θ.
- $L(\theta; y)$ contains all the information regarding θ from the data.
- $L(\theta; y)$ ranks the various parameter values in terms of their consistency with the data.
- Since $L(\theta; y)$ is defined in terms of the random variable y, it is itself a random variable.

Maximum Likelihood Estimator

- For the purposes of estimation we typically want to find θ value that makes the observed data the most likely (hence the term maximum likelihood).
- The maximum likelihood estimator (MLE) of θ is
$$\hat{\theta} = \arg\max_{\theta} L(\theta; y).$$
- Estimation becomes a simple optimization problem!

- It is often easier to work with the logarithm of the likelihood function, i.e., the log-likelihood function
$$\ell(\theta; y) = \log(L(\theta; y)).$$
- Equivalently, since the $\log(\cdot)$ function is monotonic, the value of θ that maximizes $L(\theta; y)$ also maximizes the log-likelihood $\ell(\theta; y)$.
- For simplicity, we drop the y and use $L(\theta) = L(\theta; y)$ and $\ell(\theta) = \ell(\theta; y)$.

A List of Important Functions

- Log-likelihood function: $\ell(\theta) = \log(L(\theta))$.
- Score function: $S(\theta) = \frac{\partial \ell(\theta)}{\partial \theta} = \ell'(\theta)$.
- Information function: $I(\theta) = -\frac{\partial^2 \ell(\theta)}{\partial \theta^2} = -\ell''(\theta)$.
- Fisher information function: $\mathcal{I}(\theta) = \mathbb{E}[I(\theta)]$.
- Relative likelihood function: $R(\theta) = L(\theta)/L(\hat{\theta})$.
- Log relative likelihood function: $r(\theta) = \log(L(\theta)/L(\hat{\theta})) = \ell(\theta) - \ell(\hat{\theta})$.

Maximum Likelihood Estimation

- Want θ that maximizes $\ell(\theta)$, or equivalently solves $S(\theta) = 0$.
- Sometimes $S(\theta) = 0$ can be solved explicitly (easy in this case), but often we must solve iteratively.
- Check that the solution corresponds to a maxima of $\ell(\theta)$ by verifying the value of the second derivative at $\hat{\theta}$ is negative, or
$$I(\hat{\theta}) = -\ell''(\hat{\theta}) > 0.$$
- Invariance property of MLEs: if $g(\theta)$ is any function of the parameter θ, then the MLE of $g(\theta)$ is $g(\hat{\theta})$.

> If $\hat{\theta}$ is the MLE of θ, then $e^{\hat{\theta}}$ is the MLE of e^{θ}.

Example: Binomial Distribution

Example: Binomial Distribution

- A study was conducted to examine the risk for hormone use in healthy postmenopausal women.
- Suppose a group of n women received a combined hormone therapy, and were monitored for the development of breast cancer during 8.5 years followup.
- Let
$$Y_i = \begin{cases} 1 & \text{, if woman } i \text{ developed breast cancer,} \\ 0 & \text{, otherwise,} \end{cases}$$
for $i = 1, \ldots, n$.
- Suppose $Y_i \overset{\text{iid}}{\sim} \text{Bernoulli}(\pi)$ where $\pi = \mathbb{P}(Y_i = 1)$, then the total number of woman developed breast cancer is:
$$Y = \sum_{i=1}^{n} Y_i \sim \text{Binomial}(n, \pi).$$
- We wish to find the MLE of unknown parameter π (probability of cancer).

- Likelihood function:
$$L(\pi; y) = c\,\mathbb{P}(Y = y; \pi) = \pi^y (1-\pi)^{n-y},$$
where we take $c = 1/\binom{n}{y}$ to simplify the likelihood.

- Log-likelihood function:
$$\ell(\pi) = y \log(\pi) + (n-y)\log(1-\pi).$$

- Score function:
$$S(\pi) = \frac{y}{\pi} - \frac{n-y}{1-\pi}.$$

- Maximum Likelihood Estimator:
$$S(\pi) = 0 \implies \hat{\pi} = \frac{\sum_{i=1}^n y_i}{n} = \bar{y}.$$

- Second derivative test using information function:
$$I(\pi) = -\ell'' = \frac{y}{\pi^2} + \frac{n-y}{(1-\pi)^2} > 0 \ \forall \pi \in (0,1).$$
Confirms that $\hat{\pi} = \bar{y}$ is the MLE.

Example: Hormone Therapy Data

- A group of $n = 8506$ postmenopausal women aged 50-79 received EPT and $Y = 166$ developed invasive breast cancer during the followup.
- Assume $Y \sim \text{Binomial}(n, \pi)$ with unknown parameter π.
- The maximum likelihood estimate of π is:
$$\hat{\pi} = \bar{y} = \frac{y}{n} = \frac{166}{8506} = 0.0195.$$

Example: Poisson Distribution

Suppose $y_1, \dots, y_n$ is an iid sample from a Poisson distribution with probability mass function:
$$f(y; \lambda) = \mathbb{P}(Y = y; \lambda) = \frac{\lambda^y e^{-\lambda}}{y!},\ \lambda > 0,\ y = 0, 1, 2, \dots.$$

- Likelihood function:
$$L(\lambda; y_1, \dots, y_n) = \prod_{i=1}^n f(y_i; \lambda) = \frac{\lambda^{\sum y_i} e^{-n\lambda}}{\prod_i y_i!}.$$

- Log-likelihood function:
$$\ell(\lambda) = \left(\sum_i y_i\right) \log(\lambda) - n\lambda - \sum_{i=1}^n \log(y_i!).$$

- Score function:
$$S(\lambda) = \frac{\sum_i y_i}{\lambda} - n = 0 \implies \hat{\lambda} = \frac{\sum_{i=1}^n y_i}{n} = \bar{y}.$$

Newton Raphson Algorithm For Finding MLE

- Sometimes, solving $S(\theta)=0$ can be challenging and closed form solutions may not be obtained, iterative method need to be used to find the MLE.
- Recall Taylor Series expansion of a differentiable function $f(x)$ about a point a:

$$f(x)=f(a)+\frac{f'(a)}{1!}(x-a)+\frac{f''(a)}{2!}(x-a)^2+\cdots.$$

- Now suppose we wish to find $\hat{\theta}$, the root of $S(\theta)=0$ and $\theta^{(0)}$ is a guess that is "close" to $\hat{\theta}$.
- Consider the Taylor series expansion of $S(\theta)$ about $\theta^{(0)}$:

$$S(\theta)=S(\theta^{(0)})+\frac{S'(\theta^{(0)})}{1!}(\theta-\theta^{(0)})+\frac{S''(\theta^{(0)})}{2!}(\theta-\theta^{(0)})^2+\cdots.$$

- For $|\theta-\theta^{(0)}|$ very small, the second and higher order terms can be dropped to a good approximation:

$$S(\theta)\simeq S(\theta^{(0)})+S'(\theta^{(0)})(\theta-\theta^{(0)}).$$
$$S(\theta)\simeq S(\theta^{(0)})-I(\theta^{(0)})(\theta-\theta^{(0)}).$$

- Then at $\theta=\hat{\theta}$,

$$\begin{aligned}S(\hat{\theta})&\simeq S(\theta^{(0)})-I(\theta^{(0)})(\hat{\theta}-\theta^{(0)})\\ I(\theta^{(0)})(\hat{\theta}-\theta^{(0)})&\simeq S(\theta^{(0)})\\ (\hat{\theta}-\theta^{(0)})&\simeq I^{-1}(\theta^{(0)})S(\theta^{(0)})\\ \hat{\theta}&\simeq \theta^{(0)}+I^{-1}(\theta^{(0)})S(\theta^{(0)}).\end{aligned}$$

- This suggests a revised guess for $\hat{\theta}$ is:

$$\theta^{(1)}=\theta^{(0)}+I^{-1}(\theta^{(0)})S(\theta^{(0)})$$

Newton Raphson Algorithm for finding the MLE

- Begin with an initial estimate $\theta^{(0)}$.
- Iteratively obtain updated estimate by using:

$$\theta^{(i+1)}=\theta^{(i)}+I^{-1}(\theta^{(i)})S(\theta^{(i)}).$$

- Iteration continues until $\theta^{(i+1)}\simeq\theta^{(i)}$ within a specified tolerance.
- Then set $\hat{\theta}=\theta^{(i+1)}$, check that $I(\hat{\theta})>0$.

Inference for Scalar Parameters θ

- So far we have discussed estimation of $\hat{\theta}$, next we want to conduct inference about θ, i.e., carry out hypothesis tests and construct confidence intervals of θ.
- Likelihood inference relies on the following asymptotic distribution results:

Useful asymptotic distributional results

- (log) Likelihood ratio statistic: $-2\log(R(\theta)) = -2r(\theta) \sim \chi^2_{(1)}$.
- Score statistic: $\big(S(\theta)\big)^2/I(\theta) \sim \chi^2_{(1)}$.
- Wald statistic: $(\hat\theta-\theta)^2 I(\hat\theta) \sim \chi^2_{(1)}$ or $(\hat\theta-\theta)\sqrt{I(\hat\theta)} \sim \mathcal{N}(0,1)$ since $Z \sim \mathcal{N}(0,1) \implies Z^2 \sim \chi^2_1$.

Confidence Interval (CI)

Suppose we want a $100(1-\alpha)\,\%$ confidence interval for θ.

- The Likelihood ratio (LR) based pivotal gives a confidence interval:

$$\{\theta : -2r(\theta) < \chi^2_1(1-\alpha)\},$$

  where $\chi^2_1(1-\alpha)$ is the upper α percentage point of the χ^2_1 distribution.

- The Wald-based pivotal gives an interval:

$$\Big\{\theta : (\hat\theta-\theta)^2 I(\hat\theta) < \chi^2_1(1-\alpha)\Big\},$$

  or equivalently

$$\hat\theta \pm Z_{1-\alpha/2}\big(I(\hat\theta)\big)^{-1/2},$$

  where $Z_{1-\alpha/2}$ is the upper $\alpha/2$ percentage point of the standard normal.

Example: Hormone Therapy Data

Likelihood Ratio based 95 % CI: $\{\theta : -2r(\theta) < \chi^2_1(0.95)\}$ where $r(\theta) = \ell(\theta) - \ell(\hat\theta)$.

- For the Binomial distribution: $\hat\theta = y/n$, and

$$r(\theta) = (y\log(\theta) + (n-y)\log(1-\theta)) - \left(y\log\Big(\frac{y}{n}\Big) + (n-y)\log\Big(1-\frac{y}{n}\Big)\right).$$

- To find the root of $-2r(\theta) = \chi^2_1(0.95)$:

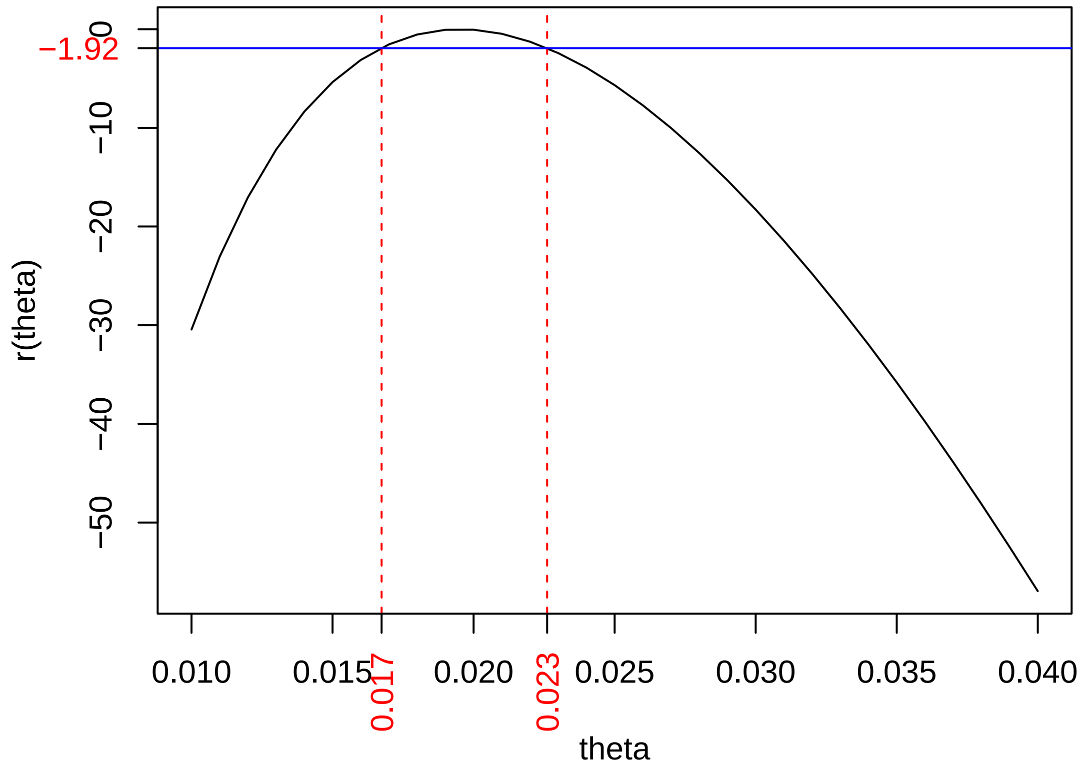
```
y = 166
n = 8506
LRCI = function(theta, y, n) {
  -2 * (y * log(theta) + (n - y) * log(1 - theta) - y * log(y/n) -
    (n - y) * log(1 - y/n)) - qchisq(0.95, 1)
}
mle = y/n
uniroot(LRCI, c(0, mle), y = y, n = n)$root

[1] 0.01673867

uniroot(LRCI, c(mle, 1), y = y, n = n)$root

[1] 0.02260709
```

- The likelihood ratio based 95 % CI is $(0.017, 0.023)$.



Wald based 95 % CI: $\hat{\theta} \pm Z_{0.975}\big(I(\hat{\theta})\big)^{-1/2}$.

- For Binomial distribution $\hat{\theta} = y/n$ and

$$I(\hat{\theta}) = \frac{y}{\hat{\theta}^2} + \frac{n-y}{(1-\hat{\theta})^2} = n^2\left(\frac{1}{y} + \frac{1}{n-y}\right).$$

- So we solve:

$$\begin{aligned}\hat{\theta} \pm 1.96\big(I(\hat{\theta})\big)^{-1/2} &= 0.0195 \pm 1.96(0.0015)\\ &= (0.017, 0.022).\end{aligned}$$

- The Wald based 95 % CI is: $(0.017, 0.022)$.

Hypotheses Test

Suppose we are interested in testing hypotheses:

$$\mathrm{H}_0\colon\ \theta = \theta_0 \text{ vs } \mathrm{H}_\mathrm{A}\colon\ \theta \neq \theta_0.$$

- Likelihood ratio (LR) test: p-value $= \mathbb{P}\big(\chi^2_1 > -2r(\theta_0)\big)$.
- Score test: p-value $= \mathbb{P}\Big(\chi^2_1 > \big(S(\theta)\big)^2 / I(\theta_0)\Big)$.

- Wald test:
$$p\text{-value} = \mathbb{P}\Big(\chi_1^2 > (\hat{\theta}-\theta_0)^2 I(\hat{\theta})\Big), \text{ or } p\text{-value} = \mathbb{P}\Big(|Z| > |\hat{\theta}-\theta_0|\sqrt{I(\hat{\theta})}\Big).$$

Example: Hormone Therapy Data

Suppose we wish to test if women received EPT would have a risk of breast cancer same as that of the general population, say about 1.5 %.
$$\mathrm{H}_0\colon\ \theta = 0.015 \text{ vs } \mathrm{H}_\mathrm{A}\colon\ \theta \neq 0.015.$$

- Likelihood Ratio based test:
$$\begin{aligned} r(\theta_0 = 0.015) &= \Big(y\log(0.015) + (n-y)\log(1-0.15)\Big) - \Big(y\log\Big(\frac{y}{n}\Big) + (n-y)\log\Big(1-\frac{y}{n}\Big)\Big) \\ &= -3.443. \end{aligned}$$

  Thus, the p-value for the test is given by:
$$p = \mathbb{P}\Big(\chi^2_{(1)} > -2r(0.015)\Big) = \mathbb{P}\Big(\chi^2_{(1)} > 6.886\Big) = 0.0087.$$

  Therefore, we *reject* H_0 and conclude that the risk of breast cancer for women received EPT is significantly different from 1.5 %.

Notes on Asymptotic Inference

- Asymptotic results: approximation improves as sample size increases.
- Results are exact for a Normal linear model if θ is the mean parameter and σ^2 is known.
- LR approach:
  - Need to evaluate (log) likelihood at two locations.
  - Not always a closed from solution for a CI.
  - Usually the best approach.
- Score approach:
  - Usually the least powerful test.
  - Don't actually need to find MLE to use.
- Wald's approach:
  - Always get a closed form solution for a CI.
  - May not behave well for skewed likelihoods (transform?).
- All three are asymptotically equivalent!

Likelihood Methods for Parameter Vectors

Suppose $\boldsymbol{\theta} \in \Omega$ is a continuous $p \times 1$ parameter vector indexing a probability density (or mass) function $f(\mathbf{y};\boldsymbol{\theta})$. The likelihood and log-likelihood functions are defined as before, but

- $\mathbf{S}(\boldsymbol{\theta}) = \frac{\partial \ell(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$ is the $p \times 1$ Score vector, i.e.,
$$\mathbf{S}(\boldsymbol{\theta}) = \begin{bmatrix} \frac{\partial \ell(\theta)}{\partial \theta_1} \\ \vdots \\ \frac{\partial \ell(\theta)}{\partial \theta_p} \end{bmatrix}.$$

- $\mathbf{I}(\boldsymbol{\theta}) = -\frac{\partial^2 \ell(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^\top \partial \boldsymbol{\theta}}$ is the $p \times p$ Information matrix, i.e.,

$$\mathbf{I}(\boldsymbol{\theta}) = \begin{bmatrix} -\frac{\partial^2 \ell(\theta)}{\partial \theta_1^2} & -\frac{\partial^2 \ell(\theta)}{\partial \theta_1 \partial \theta_2} & \cdots & \frac{\partial^2 \ell(\theta)}{\partial \theta_1 \partial \theta_p} \\ & -\frac{\partial^2 \ell(\theta)}{\partial \theta_2^2} & \cdots & \frac{\partial^2 \ell(\theta)}{\partial \theta_1 \partial \theta_p} \\ & & \ddots & \frac{\partial^2 \ell(\theta)}{\partial \theta_p^2} \end{bmatrix}.$$

- The Newton Raphson algorithm applies as before, but with vectors and matrices as follows:

$$\boldsymbol{\theta}^{(i+1)} = \boldsymbol{\theta}^{(i)} + \mathbf{I}^{-1}(\boldsymbol{\theta}^{(i)})\mathbf{S}(\boldsymbol{\theta}^{(i)}).$$

- Again, we apply iteratively until we obtain convergence, but now check to see if $\mathbf{I}(\hat{\boldsymbol{\theta}})$ is a positive definite matrix.

- Analogs to the LR, Score and Wald results apply based on partitioning the Information matrix by $\boldsymbol{\theta} = (\boldsymbol{\alpha}, \boldsymbol{\beta})^\top$, where $\boldsymbol{\alpha}$ is a $p \times 1$ vector of nuisance parameters and $\boldsymbol{\beta}$ is a $q \times 1$ vector of parameters of interest:

$$\mathbf{I} = \mathbf{I}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \begin{pmatrix} \mathbf{I}_{\boldsymbol{\alpha}\boldsymbol{\alpha}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) & \mathbf{I}_{\boldsymbol{\alpha}\boldsymbol{\beta}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) \\ \mathbf{I}_{\boldsymbol{\beta}\boldsymbol{\alpha}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) & \mathbf{I}_{\boldsymbol{\beta}\boldsymbol{\beta}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) \end{pmatrix},$$

  where $\mathbf{I}_{\boldsymbol{\alpha}\boldsymbol{\alpha}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\frac{\partial^2 \ell}{\partial \boldsymbol{\alpha} \partial \boldsymbol{\alpha}^\top}$ is $p \times p$, $\mathbf{I}_{\boldsymbol{\alpha}\boldsymbol{\beta}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\frac{\partial^2 \ell}{\partial \boldsymbol{\alpha} \partial \boldsymbol{\beta}^\top}$ is $p \times q$, $\mathbf{I}_{\boldsymbol{\beta}\boldsymbol{\alpha}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\frac{\partial^2 \ell}{\partial \boldsymbol{\beta} \partial \boldsymbol{\alpha}^\top}$ is $q \times p$, and $\mathbf{I}_{\boldsymbol{\beta}\boldsymbol{\beta}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\frac{\partial^2 \ell}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^\top}$ is $q \times q$.

Topic 2a: Formulation of Generalized Linear Models

The Exponential Family

Definition (Exponential Family)

Consider a random variable Y with probability density (or mass) function $f(y; \theta, \phi)$, we say that the distribution is a member of the exponential family if we can write

$$f(y; \theta, \phi) = \exp\left\{ \frac{y\theta - b(\theta)}{a(\phi)} + c(y; \phi) \right\},$$

for some functions $a(\cdot)$, $b(\cdot)$, and $c(\cdot)$.

- The parameter θ is called the canonical parameter, and it is unknown.
- The parameter ϕ is called the scale/dispersion parameter, is constant, and assumed to be known.

Many well known distributions (continuous/discrete) can be shown to be a member of the exponential family.

Examples

- Poisson Distribution: $Y \sim \text{Poisson}(\lambda)$,

$$f(y; \lambda) = \frac{\lambda^y e^{-\lambda}}{y!}, \ \lambda > 0, \ y = 0, 1, \ldots.$$

  Show that Poisson is a member of exponential family and identify the canonical parameter and the functions $a(\cdot)$, $b(\cdot)$, and $c(\cdot)$.

Solution. $f(y;\lambda) = \exp\{\log(f(y;\lambda))\} = \exp\{\frac{y\log(\lambda)-\lambda}{1} - \log(y!)\}$. Therefore,

$$\begin{aligned}
\theta &= \log(\lambda) \qquad \text{(canonical/natural parameter)},\\
b(\theta) &= \lambda = e^{\theta},\\
\phi &= 1,\\
a(\phi) &= 1,\\
c(y;\phi) &= -\log(y!).
\end{aligned}$$

- Normal Distribution: $Y \sim \mathcal{N}(\mu, \sigma^2)$ and σ^2 known,

$$f(y;\theta,\phi) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left\{-\frac{(y-\mu)^2}{2\sigma^2}\right\}.$$

Show that this Normal distribution is a member of the exponential family.

Solution.

$$\begin{aligned}
f(y;\mu,\sigma^2) &= \exp\left\{-\frac{y^2-2\mu y+\mu^2}{\sigma^2} - \frac{1}{2}\log(2\pi\sigma^2)\right\}\\
&= \exp\left\{\frac{y\mu-\mu^2/2}{\sigma^2} - \frac{y^2}{2\sigma^2} - \frac{1}{2}\log(2\pi\sigma^2)\right\}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\theta &= \mu,\\
\phi &= \sigma^2,\\
a(\phi) &= \phi = \sigma^2,\\
b(\theta) &= \frac{\mu^2}{2} = \frac{\theta^2}{2},\\
c(y;\phi) &= -\frac{y^2}{2\sigma^2} - \frac{1}{2}\log(2\pi\sigma^2).
\end{aligned}$$

Properties of Exponential Family

Consider a single observation y from the exponential family.

$$\begin{aligned}
L(\theta,\phi;y) = f(y;\theta,\phi) &= \exp\left\{\frac{y\theta-b(\theta)}{a(\phi)} + c(y;\phi)\right\}.\\
\ell(\theta,\phi;y) = \log\big(f(y;\theta,\phi)\big) &= \frac{y\theta-b(\theta)}{a(\phi)} + c(y;\phi).\\
S(\theta) &= \frac{\partial\ell}{\partial\theta} = \frac{y-b'(\theta)}{a(\phi)}.\\
I(\theta) &= -\frac{\partial^2\ell}{\partial\theta^2} = \frac{b''(\theta)}{a(\phi)}.\\
\mathcal{I}(\theta) &= \mathbb{E}\left[-\frac{\partial^2\ell}{\partial\theta^2}\right] = I(\theta).
\end{aligned}$$

Some General Results for Score and Information

Result # 1

The expectation of the score function is zero.

$$\mathbb{E}[S(\theta)] = 0.$$

Proof:

$$\begin{aligned}
\int f(y;\theta,\phi)\,\mathrm{d}y &= 1 \\
\frac{\partial}{\partial\theta}\int f(y;\theta,\phi)\,\mathrm{d}y &= 0 \\
\int \frac{\partial}{\partial\theta} f(y;\theta,\phi)\,\mathrm{d}y &= 0 \\
\int \left(\frac{\partial}{\partial\theta}\log(f(y;\theta,\phi))\right) f(y;\theta,\phi)\,\mathrm{d}y &= 0 \qquad (1) \\
\int S(\theta) f(y;\theta,\phi)\,\mathrm{d}y &= 0 \\
\mathbb{E}[S(\theta)] &= 0
\end{aligned}$$

Result # 2

The expectation of the score function squared is the expected information.

$$\mathbb{E}[S(\theta;y)^2] = \mathbb{E}[I(\theta;y)]$$

Proof: Differentiate (1) again,

$$\begin{aligned}
\int \left(\frac{\partial}{\partial\theta}\log(f(y;\theta,\phi))\right) f(y;\theta,\phi)\,\mathrm{d}y &= 0 \\
\int \left(\frac{\partial^2}{\partial\theta^2}\log(f(y;\theta,\phi))\right) f(y;\theta,\phi)\,\mathrm{d}y + \int \left(\frac{\partial}{\partial\theta}\log(f(y;\theta,\phi))\right) \frac{\partial}{\partial\theta} f(y;\theta,\phi)\,\mathrm{d}y &= 0 \\
\int \frac{\partial^2}{\partial\theta^2}\log(f(y;\theta,\phi)) f(y;\theta,\phi)\,\mathrm{d}y + \int \left(\frac{\partial}{\partial\theta} f(y;\theta,\phi)\right)^2 f(y;\theta,\phi)\,\mathrm{d}y &= 0 \\
\int -I(\theta) f(y;\theta,\phi)\,\mathrm{d}y + \int S(\theta)^2 f(y;\theta,\phi)\,\mathrm{d}y &= 0 \\
\mathbb{E}[-I(\theta;y)] + \mathbb{E}[S(\theta;y)^2] &= 0
\end{aligned}$$

Now for the exponential family, we apply above results and obtain:

$$\begin{aligned}
\mathbb{E}[S(\theta)] &= 0, \\
\mathbb{E}\left[\frac{Y - b'(\theta)}{a(\phi)}\right] &= 0, \\
\mathbb{E}[Y] &= b'(\theta),
\end{aligned}$$

$$\begin{aligned}
\mathbb{E}[S(\theta)^2] &= \mathbb{E}[I(\theta)], \\
\mathbb{E}\left[\left(\frac{Y - b'(\theta)}{a(\phi)}\right)^2\right] &= \mathbb{E}\left[\frac{b''(\theta)}{a(\phi)}\right], \\
\frac{1}{a(\phi)^2}\,\mathbb{E}\left[\big(Y - \mathbb{E}[Y]\big)^2\right] &= \frac{b''(\theta)}{a(\phi)}, \\
\mathrm{Var}(Y) &= b''(\theta)a(\phi).
\end{aligned}$$

Mean and Variance for the Exponential Family

- Mean: $\mathbb{E}[Y] = b'(\theta) = \mu$.
- Variance: $\mathrm{Var}(Y) = b''(\theta)a(\phi)$.

Note that:

- $b'(\theta) = \mu$ tells the relationship between *canonical* parameter θ and μ.
- $b''(\theta)$ is a function of θ and hence can be also expressed as a function of μ.
- Thus, we write $b''(\theta) = \mathbb{V}(\mu)$ and call $\mathbb{V}(\mu)$ the variance function.
- Subsequently, we have:
  $$\mathrm{Var}(Y) = b''(\theta)a(\phi) = \mathbb{V}(\mu)a(\phi),$$
  which is the mean-variance relationship for the exponential family.

Link Functions

Definition (Link Function)

The link function relates the linear predictor $\eta = \mathbf{x}^\top \boldsymbol{\beta}$ to the expected value μ of the random variable Y, i.e.,

$$g(\mu) = \eta = \mathbf{x}^\top \boldsymbol{\beta},$$

where $g(\,\cdot\,)$ is the link function.

Definition (Canonical Link Function)

When Y is a member of the exponential family we define the canonical link function to be:

$$g(\mu) = \theta = \eta = \mathbf{x}^\top \boldsymbol{\beta}$$

(i.e., the choice of $g(\,\cdot\,)$ that sets canonical parameter = linear predictor).

Examples

Recall that Poisson(λ) is a member of exponential family,

$$f(y;\lambda) = \frac{\lambda^y e^{-\lambda}}{y!} = \exp\left\{\frac{y\log(\lambda) - \lambda}{1} - \log(y!)\right\}$$

where $\theta = \log(\lambda)$, $\phi = 1$, $b(\theta) = \lambda = e^\theta$, and $a(\phi) = 1$. Now to find the mean, variance function, and canonical link function:

- Mean: $\mathbb{E}[Y] = b'(\theta) = e^\theta = \mu \implies \theta = \log(\mu)$.
- Variance Function: $\mathbb{V}(\mu) = b''(\theta) = e^\theta \implies \mathbb{V}(\mu) = \mu$.
- Variance: $\mathrm{Var}(Y) = \mathbb{V}(\mu)a(\phi) = \mu$ (mean-variance relationship).
- Canonical link: set $\theta = \eta$ using $\theta = \log(\mu) = \eta = \mathbf{x}^\top \boldsymbol{\beta}$, i.e., $g(\mu) = \log(\mu)$ where $\log(\,\cdot\,)$ is the canonical link.

Moving forward, we consider a log-linear model: $\log(\mu_i) = \mathbf{x}_i^\top \boldsymbol{\beta}$.

Remarks on Link Function

- We can choose any function $g(\,\cdot\,)$ as the link function in theory.
- The canonical link is a special link function, we often choose to use canonical link for its good statistical properties.
- Context and goodness of fit should motivate the choice of link function in practice.

Generalized Linear Models

Definition (Generalized Linear Model (GLM))

A Generalized Linear Model (GLM) is composed of three components:

- Random Component: The responses $Y_1, \dots, Y_n$ are independent random variables and each Y_i is assumed to come from a parametric distribution that is a member of the exponential family.
- Systematic Component (or linear predictor):

  $$\eta_i = \mathbf{x}_i^\top \boldsymbol{\beta},$$

  a linear combination of explanatory variables $\mathbf{x}_i$ and regression parameters $\boldsymbol{\beta}$.
- Link function:

  $$g(\mu_i) = \eta_i = \mathbf{x}_i^\top \boldsymbol{\beta},$$

  a function that relates the mean of response to the linear predictor.

Topic Summary

1. Definition of the Exponential Family.
   - Exponential form of the probability density (or mass) function.
   - Derivation of Score and Information.
   - Properties of exponential family, mean-variance relationship.
   - Definition of canonical link.
2. Definition of a Generalized Linear Model.

Next Topic: 2b Estimation for Generalized Linear Models.