

**INSY 7310 Introduction to Logistic Regression By S. Maghsoodloo**

The general form for the probability density function (pdf) of a logistic random variable,  $X \sim \text{Lg}$  (mean  $\mu$ , variance  $\sigma_x^2 = \sigma^2$ ), is given by

$$g(x; \mu, \sigma^2) = \frac{\pi}{\sigma\sqrt{3}} \frac{e^{-\pi(x-\mu)/\sigma\sqrt{3}}}{[1 + e^{-\pi(x-\mu)/\sigma\sqrt{3}}]^2}, \quad -\infty < X < \infty, -\infty < \mu < \infty, \sigma > 0 \quad (85)$$

Making the transformation  $Z = \frac{\pi(X - \mu_x)}{\sigma_x \sqrt{3}}$  in Eq. (85) and letting  $G(x)$  and  $F(z)$  represent the cdf (cumulative distribution function) of  $X$  and  $Z$ , respectively, the standard form of the logistic probability density function is obtained. As a result [letting  $\mu = \mu_x$ ,  $\sigma = \sigma_x = \sqrt{V(X)}$  & clearly  $x = \mu + z\sigma\sqrt{3} / \pi$ ], we obtain:

$$\begin{aligned} F(z) &= \Pr(Z \leq z) = \Pr\left(\frac{\pi(X - \mu)}{\sigma\sqrt{3}} \leq z\right) = \Pr(X \leq \mu + z\sigma\sqrt{3} / \pi) = G_x(\mu + z\sigma\sqrt{3} / \pi) \\ \rightarrow f(z) &= \frac{dF(z)}{dz} = \frac{dG_x(\mu + z\sigma\sqrt{3} / \pi)}{dz} = \frac{dG_x(\mu + z\sigma\sqrt{3} / \pi)}{dx} \times \frac{dx}{dz} = \frac{dG_x(x)}{dx} \times \frac{dx}{dz} \\ &= g(x) \times \frac{dx}{dz} = \frac{\pi}{\sigma\sqrt{3}} \frac{e^{-\pi(x-\mu)/\sigma\sqrt{3}}}{[1 + e^{-\pi(x-\mu)/\sigma\sqrt{3}}]^2} \times \frac{\sigma\sqrt{3}}{\pi} = \frac{e^{-z}}{(1 + e^{-z})^2} \end{aligned}$$

Thus, the standard form the logistic pdf is given by

$$f(z) = \frac{e^{-z}}{(1 + e^{-z})^2} = \frac{e^z}{(1 + e^z)^2} = \frac{1}{4} \text{sech}^2(z/2), \quad -\infty < z < \infty \quad (86)$$

where  $\text{Cosh}(z) = (e^z + e^{-z}) / 2$ ,  $\text{Sech}(z) = [(e^z + e^{-z}) / 2]^{-1} = 2 / (e^z + e^{-z})$ ,

$\text{Sinh}(z) = (e^z - e^{-z}) / 2$ , and  $\text{Tanh}(z) = (e^z - e^{-z}) / (e^z + e^{-z})$ . The expression

$$f(z) = \frac{1}{4} \text{sech}^2 \frac{z}{2} \text{ in Eq. (86) is obtained from the fact that } \text{Sech}(z) = \frac{2}{e^z + e^{-z}} = \frac{2e^z}{e^{2z} + 1} =$$

$$\frac{2e^z}{1+e^{2z}} \rightarrow \text{Sech}(z/2) = \frac{2e^{z/2}}{1+e^z} \rightarrow \frac{1}{2}\text{Sech}(z/2) = \frac{e^{z/2}}{1+e^z} \rightarrow \frac{1}{4}\text{Sech}^2(z/2) = \left[\frac{e^{z/2}}{1+e^z}\right]^2$$

$$\rightarrow \frac{1}{4}\text{Sech}^2(z/2) = \frac{e^z}{(1+e^z)^2} = f(z). \text{ Similarly, it can be verified that } \text{Cosh}(z) = 2\cosh^2(z/2) - 1,$$

or  $\text{Cosh}(2z) = 2\cosh^2(z) - 1$ ,  $\text{Cosh}^2(z) - \text{Sinh}^2(z) = 1$ ,  $\text{Sech}^2(z) = 1 - \text{Tanh}^2(z)$  and  $\text{Sinh}(2z) =$

$$2\text{Sinh}(z)\text{Cosh}(z). \text{ Further, } \int_{-\infty}^{\infty} \frac{e^{-z} dz}{(1+e^{-z})^2} = \left[ (1+e^{-z})^{-1} \right]_{-\infty}^{+\infty} = 1 \text{ shows that the integrand is a}$$

pdf over the range  $-\infty < z < \infty$ , and it can be verified from Eq. (86) that  $E(Z) = \int_{-\infty}^{\infty} \frac{ze^{-z} dz}{(1+e^{-z})^2} =$

$$0, V(Z) = \frac{\pi^2}{3} = \mu_2, \text{ the skewness } \alpha_3 = 0 \text{ and the kurtosis } \beta_4 = \frac{\mu_4}{(\mu_2)^2} - 3 = \alpha_4 - 3 = 1.20,$$

where  $\mu_4 = E(Z^4)$  and  $\mu_r = E\left[\left(\frac{X - \mu_x}{\sigma_x}\right)^r\right]$  represents the  $r^{\text{th}}$  central moment of a rv X. The

pdf in (86) is symmetrical about zero, i.e.,  $E(Z) = z_{0.50} = \text{The mode} = 0$ . Thus, the graph of the standard logistic pdf resembles the standard normal density but with thicker tails (normal kurtosis is zero) and less peaked in the middle because the height of the density at  $z = 0$  for the standard logistic is 0.25 while it is equal to  $1/\sqrt{2\pi} = 0.3989423$  for the  $N(0, 1)$  pdf. Note that the standard form of the logistic does not have a variance of 1 rather its variance is equal to  $\pi^2 / 3$  but its mean is zero. The cdf of Z is [for both forms of the pdf in Eq. (86)] given by

$$F(z) = \int_{-\infty}^z f(u)du = \int_{-\infty}^z \frac{e^{-u}}{(1+e^{-u})^2} du = \left[ (1+e^{-u})^{-1} \right]_{-\infty}^z = \frac{1}{1+e^{-z}}, \quad -\infty < z < \infty \quad (87)$$

Solving Eq. (87) for z in terms of the cdf, in order to obtain the inverse function, yields

$$1+e^{-z} = 1/F(z) \rightarrow e^{-z} = -1 + 1/F(z) \rightarrow -z = \ln[-1 + 1/F(z)] \rightarrow -z = \ln\left[\frac{1-F(z)}{F(z)}\right] \rightarrow$$

$$z = \ln\left[\frac{F(z)}{1-F(z)}\right] \rightarrow z_p = \ln\left[\frac{p}{1-p}\right] \quad (88a)$$

Eq. (88a) gives the percentile (or quantile) function of the standard form of the logistic density and again verifies that the 50<sup>th</sup> percentile ( $p = 0.50$ ) is equal to  $z_{0.50} = \ln(0.5/0.5) = 0$ ; the 95<sup>th</sup> percentile, with standard deviation  $\pi / \sqrt{3}$ , is equal to  $z_{0.95} = \ln(0.95/0.05) = 2.944439$  while  $Z_{N(0,1)}(0.95) = Z_{0.05} = 1.645$ . The reader is warned that the standard form of Logistic density as given in Eq. (86) does not have a variance of 1; further, the standardized form of the logistic density, i.e.,  $Lg(0, 1)$ , is given by  $f(\xi) = \pi(\sqrt{3})^{-1} \exp(-\pi\xi/\sqrt{3}) / (1 + e^{-\pi\xi/\sqrt{3}})^2$  with mean 0 and variance 1. However, this standardized form has no direct application in logistic regression. Further, it can be shown that inflection points of  $z$  with density in (86) is given by  $\mp \ln(2 + \sqrt{3})$ .

Now consider a dichotomous outcome variable with occurrence Pr of  $p$  when  $y = 1$  and failure Pr equal to  $(1 - p)$  when  $y = 0$ , where  $p$  is a function of a continuous variable  $x$  such as height, weight, age, length of time at a job, temperature, etc., and the dichotomous variable may be the presence ( $y = 1$ ) or absence ( $y = 0$ ) of coronary disease, or injured on the job ( $y = 1$ ) or not injured on the job ( $y = 0$ ), needs repair ( $y = 1$ ) or does not need repair ( $y = 0$ ). That is, in Logistic Regression the response variable is dichotomous (0 or 1) and further we assume that  $p = \text{Pr}(Y = 1)$  is a function of one (or more) continuous explanatory variable(s), i.e., in fact  $p = \text{Pr}(Y = 1|x)$ . For example, the probability  $p$  that a person has coronary disease is related to his/her age  $x$ , i.e.,  $p$  actually is  $p(x)$ , and in this case  $p(x)$  is an increasing function of  $x$ . As the age of a person increases, the chance that the person has coronary heart disease increases. In Logistic Regression literature the occurrence Pr of the dichotomous outcome is generally referred to as  $\pi(x)$ , but for simplicity of notation I will use  $p(x)$  to denote this Pr, i.e.,  $p(x)$  represents the Pr that a Bernoulli rv (success/failure; presence/absence; reliable/unreliable, etc) occurs with dependence on the continuous regressor  $x$ . As another example,  $p(x)$  may represent the Pr that a car needs warranty service ( $y = 1$ ) but the need of this service may well depend on the accumulated mileage  $x$ . Examining Eq. (88a) reveals that if  $p$  is a function of a regressor  $x$ , then the logistic quantile will also be a function of  $x$ , say  $h(x)$ , i.e.,

$$\ln\left[\frac{p(x)}{1-p(x)}\right] = h(x), \quad (88b)$$

where  $h(x)$  ranges from  $-\infty$  to  $\infty$ . In statistical literature  $\frac{p(x)}{1-p(x)} = \frac{p(x)}{q(x)}$  is called the Odds,

and  $\ln(\text{Odds})$  is called the logit transformation (i.e., logit means “log odds of event of interest occurring”). For example, if  $p(x)$  represents the Pr that a randomly selected individual has evidence of coronary heart disease (CHD) at the age 55 and it is known that the

$$\text{Odds}(55) = \frac{p(55)}{1-p(55)} = 2.5, \text{ then for that randomly-selected person having evidence of CHD at}$$

the age of 55 is 2&1/2 times more likely than not having coronary heart disease. Conversely, if  $p(x) = 0.80$ , then  $0.80/0.20 = 4$  implies that the odds are 4 to 1 in favor of the event of interest (or success). In general, if  $\text{Odds}(\text{against an event } A) = O(A)$  is 19 to 1, then its occurrence Pr is

$$1/(1+19) = 0.05, \text{ and } \text{Odds}(\text{against } A) = O(A) = \frac{Q(A)}{P(A)} = \frac{19/20}{1/20} = \frac{19}{1} \text{ (read as 19 to 1), where}$$

$Q(A) = 1-P(A)$  is the Pr that the event A will not occur. It is then said that the odds against the

$$\text{event } A \text{ is } O(A) = 19/1 \text{ (or 19 to 1), and the odds for the event } A \text{ is given by } \bar{O}(A) = \frac{P(A)}{Q(A)} =$$

$$\frac{0.05}{0.95} = \frac{1}{19} \text{ (read as 1 to 19). Note that Eq. (88b) can also be written as } \frac{p(x)}{1-p(x)} = e^{h(x)}.$$

$$\text{Rearranging the logit transformation in Eq. (88b) yields } h(x) = \ln\left[\frac{p(x)}{1-p(x)}\right] \rightarrow e^{h(x)} = \frac{p(x)}{1-p(x)}$$

$$\rightarrow e^{h(x)}[1-p(x)] = p(x) \rightarrow e^{h(x)} = p(x) + p(x)e^{h(x)} \rightarrow 1 = p(x)e^{-h(x)} + p(x) \rightarrow$$

$$p(x) = \frac{1}{1+e^{-h(x)}} = \frac{e^{h(x)}}{e^{h(x)}+1} = \frac{e^{h(x)}}{1+e^{h(x)}} = [1+e^{-h(x)}]^{-1} \quad (89)$$

If  $h(x)$  is a simple linear regression function, then  $\text{logit}(x) = h(x) = \beta_0 + \beta_1 x + \epsilon$ , and Eq. (89)

becomes the simplest form of logit regression function given below.

$$p(x) = \text{Pr}(Y=1|x) = \frac{e^{\beta_0 + \beta_1 x + \epsilon}}{1 + e^{\beta_0 + \beta_1 x + \epsilon}} = \frac{1}{1 + e^{-\beta_0 - \beta_1 x - \epsilon}} = \frac{1}{1 + e^{-h(x)}} = \frac{e^{h(x)}}{1 + e^{h(x)}} \quad (90a)$$

Or combining Eqs. (88b) and (90a) yields the logit (function)

$$\text{Logit}(x) = h(x) = \ln\left[\frac{p(x)}{1-p(x)}\right] = \ln(\text{Odds}) = \ln[p(x)] - \ln[q(x)] = \beta_0 + \beta_1 x + \epsilon \quad (90b)$$

$$\text{where from Eq. (89) we obtain } q(x) = 1 - p(x) = 1 - \frac{1}{1 + e^{-h(x)}} = \frac{1}{1 + e^{h(x)}} = [1 + e^{h(x)}]^{-1}.$$

If  $h(x)$  is a function of two regressors, then Eq. (90a) becomes

$$p(x) = \frac{e^{\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon}}{1 + e^{\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon}} \quad (90c)$$

Of course, at this point one could ask the logical question as to why we cannot model  $p(x)$  itself in a simple linear regression format, i.e., why can't we let  $p(x) = \beta_0 + \beta_1 x + \epsilon$ . The problem with such a model is that if we take the conditional expectation of  $Y$ , we obtain  $E(Y|x) = 1 \times p(x) + 0 \times [1 - p(x)] = \beta_0 + \beta_1 x + \epsilon$ , where  $p(x)$  must lie within the interval  $[0, 1]$  while  $\beta_0 + \beta_1 x$  cannot be constrained to lie in this interval  $[0, 1]$ . Therefore, the link function in logistic regression is the logit  $h(x) = \ln[p(x)/q(x)] = \beta_0 + \beta_1 x + \epsilon$ . If we could model  $p(x)$  directly as a simple linear regression of  $x$ , then the link would be the identity function. Further,  $p(x) = e^{h(x)} / [1 + e^{h(x)}]$  ranges from 0 to 1 just like  $p(x)$ .

So far we have established how to set up a logistic regression model, but the difficult part is parameter estimation and obtaining of 95% CIs. To better understand the difficulties, it is best to provide an example with a data set. The following example is borrowed from the text by J. L. Devore's 6<sup>th</sup> edition (2004) on his page 573 (Duxbury Press), which he refers to as Example 13.6. The data pertain to launch temperature and the failure incidence of O-rings in 24 space flights prior to the Challenger Disaster of January 1986.

**Table 6 (Example 13.6 on page 573 of J. L. Devore (2004);  $x$  = O-ring Temperature in Fahrenheit)**

$x$	53°F	56	57	63	66	67	67	67	68	69	70	70
Failure	Yes $y=1$	Yes $y=1$	Yes $y=1$	No $y=0$	No $y=0$	No $y=0$	No $y=0$	No $y=0$	No $y=0$	No $y=0$	No $y=0$	Yes $y=1$
$x$ =Temp°F	70	70	72	73	75	75	76	76	78	79	80	81
Failure	Yes	Yes	No	No	No	Yes	No	No	No	No	No	No

The above table shows that there were a total of 7 failures in  $n = 24$  independent trials, mostly occurring at lower temperatures  $x$ . Thus each launch was a Bernoulli trial that either failed ( $y =$

1) with probability  $p(x)$  or did not fail ( $y = 0$ ) with probability of  $1-p(x) = q(x)$ . Thus, the Bernoulli pmf (Pr Mass Function) of  $y$  is given by

$$\text{pmf}(y) = \begin{cases} p(x), & y=1 \\ 1-p(x), & y=0 \end{cases} = \begin{cases} p(x), & y=1 \\ q(x), & y=0 \end{cases} = p(x)^y \times q(x)^{1-y}, \quad y = 0, 1 \quad (91)$$

where  $x$  stands for O-ring Temperature, and  $q(x) = 1 - p(x)$  represents the Pr that the event of interest does not occur at  $x$ , and  $y =$  either 0, or 1.

Logistic Regression literature generally suggests three methods of estimation for fitting the occurrence Pr of the event of interest,  $p(x)$ , to the logistic regression model  $p(x) =$

$$e^{h(x)} / [1 + e^{h(x)}] = \frac{e^{\beta_0 + \beta_1 x + \epsilon}}{1 + e^{\beta_0 + \beta_1 x + \epsilon}} = \frac{1}{1 + e^{-\beta_0 - \beta_1 x - \epsilon}} : (1) \text{ Maximum Likelihood Estimation}$$

(MLE), (2) the method of Weighted Least-squares. (3) The discriminant analysis function is sometimes used but heavily depends on the normality assumption of the independent variable  $x$  in each of the two subgroups (0 & 1), and moderate departures of  $X$  from normality leads to very positively biased estimators of  $\beta_0$  &  $\beta_1$ . Further, the most commonly used estimation procedure in Logistic Regression literature (and statistical softwares) is the MLE.

### Maximum Likelihood Estimation (MLE) Procedure

Consider the regression logistic model

$$p(x) = \frac{e^{\beta_0 + \beta_1 x + \epsilon}}{1 + e^{\beta_0 + \beta_1 x + \epsilon}} = \frac{1}{1 + e^{-h(x)}} \quad (90a)$$

As illustrated in Table 6 we have  $n = 24$  pairs of  $(x_i, y_i) = (53, 1), (56, 1), (57, 1), (63, 0), \dots, (80, 0)$ . The likelihood function (LF) for Eq. (90a) and Table 6 is given by

$$L(\beta_0, \beta_1) = p(53) \times p(56) \times p(57) \times q(63) \times q(66) \times q(67) \dots \times q(80) \times q(81).$$

$$= \prod_{i=1}^{n=24} p(x_i)^{y_i} \times q(x_i)^{1-y_i}, \quad y_i = 0 \text{ or } 1. \quad (92a)$$

where we have made use of Eq. (91) and the fact that the 24 Bernoulli trials are independent. Because maximizing the log of a function also maximizes the function itself, it will be easiest to take the natural log of the LF in (92a) and attempt to maximize it. Further to simplify notation, we let  $p_i = p(x_i)$  and  $q_i = 1 - p(x_i)$ , and clearly the corresponding logit is  $h(x_i) = \beta_0 + \beta_1 x_i + \epsilon_i$ .

$$\begin{aligned}
L(\beta_0, \beta_1) &= \ln[L(\beta_0, \beta_1)] = \ln \prod_{i=1}^n p(x_i)^{y_i} \times q(x_i)^{1-y_i} = \sum_{i=1}^n [\ln p(x_i)^{y_i} + \ln q(x_i)^{1-y_i}] \\
&= \sum_{i=1}^n [y_i \ln p_i + (1-y_i) \ln q_i] = \sum_{i=1}^n [y_i (\ln p_i - \ln q_i) + \ln q_i] \quad (92b)
\end{aligned}$$

$$= \sum_{i=1}^n [y_i (\beta_0 + \beta_1 x_i) + \ln \left( \frac{1}{1 + e^{h(x_i)}} \right)] = \sum_{i=1}^n [y_i (\beta_0 + \beta_1 x_i) - \ln(1 + e^{h(x_i)})], \quad (92c)$$

where I have made use of Eqs. (90 a & b), leaving out  $\epsilon_i$  because partial differentiation will not be affected by  $\epsilon_i$ . The reader should be cognizant of the fact that Eq. (92b) stays in tact for all ungrouped binary Logistic-Regression models; the only variables that change are  $n$  and the form of  $h(x_i)$ . We first differentiate (92c) wrt  $\beta_0$ :

$$\begin{aligned}
\partial L(\beta_0, \beta_1) / \partial \beta_0 &= \sum_{i=1}^n [y_i (1) - \frac{\partial}{\partial \beta_0} \ln(1 + e^{h(x_i)})] = \sum_{i=1}^n [y_i - \frac{1}{1 + e^{h(x_i)}} \times \frac{\partial}{\partial \beta_0} (1 + e^{h(x_i)})] \\
&= \sum_{i=1}^n [y_i - \frac{e^{h(x_i)}}{1 + e^{h(x_i)}} \times \frac{\partial}{\partial \beta_0} h(x_i)] = \sum_{i=1}^n [y_i - p(x_i) \times (1)] = \sum_{i=1}^n [y_i - p(x_i)]
\end{aligned}$$

→ Set equal to 0 → Thus our first likelihood equation is  $\sum_{i=1}^n \hat{p}(x_i) = \sum_{i=1}^n y_i$  → this implies that

the sum of observed values of  $y$  must equal to the sum of the fitted values  $\hat{p}(x)$  as in the case of classical MLREG; for Table 6, we obtain

$$\sum_{i=1}^n \hat{p}(x_i) = \sum_{i=1}^n \left[ \frac{1}{1 + e^{-\hat{\beta}_0 - \hat{\beta}_1 x_i}} \right] = \sum_{i=1}^n \left[ \frac{1}{1 + e^{-\hat{h}(x_i)}} \right] = \sum_{i=1}^n [1 + e^{-\hat{h}(x_i)}]^{-1} = 7.0 = n_1,$$

where  $n_1$  represents the number of O-ring failures in  $n = 24$  Bernoulli trials.

We next differentiate the log-likelihood function in Eq. (92c) wrt  $\beta_1$ :

$$\partial L(\beta_0, \beta_1) / \partial \beta_1 = \sum_{i=1}^n [y_i x_i - \frac{\partial}{\partial \beta_1} \ln(1 + e^{h(x_i)})] = \sum_{i=1}^n [y_i x_i - \frac{e^{h(x_i)}}{1 + e^{h(x_i)}} \times \frac{\partial}{\partial \beta_1} h(x_i)] =$$

$\sum_{i=1}^n [y_i x_i - p(x_i) \times (x_i)] \xrightarrow{\text{Set equal to}} 0$  Thus our 2<sup>nd</sup> likelihood equation becomes

$$\sum_{i=1}^n x_i \hat{p}(x_i) = \sum_{i=1}^n y_i x_i : \text{ for Table 6 we have: } \sum_{i=1}^n \left[ \frac{x_i}{1 + e^{-\hat{\beta}_0 - \hat{\beta}_1 x_i}} \right] = \sum_{i=1}^n x_i \hat{p}(x_i) = \sum_{i=1}^n x_i y_i = 53 +$$

56 + 57 + 0 + ... + 75 = 451. I used the Excel solver and obtained the point estimates  $\hat{\beta}_0 = 10.87535$  and  $\hat{\beta}_1 = -0.17132 \rightarrow \hat{h}(x) = 10.87535 - 0.17132x$ ; in Minitab (Enter x and y pairs in columns C1 & C2 and go to Stat  $\rightarrow$  Regression  $\rightarrow$  Binary Logistic Regression, in the dialogue box select Response in Response/Frequency format, and for response put in y, and for model put in the variable name in C1) which verified my answers. Thus,  $\ln\left[\frac{\hat{p}(x)}{1 - \hat{p}(x)}\right] =$

$\ln(\hat{\text{Odds for } y=1}) = \hat{\beta}_0 + \hat{\beta}_1 x = \hat{h}(x) = 10.87535 - 0.17132x$ ; for example, when temperature is equal to 60°F, then  $\ln[\hat{\text{Odds}}(60^\circ\text{F})] = 10.87535 - 0.17132(60) = 0.596119 \rightarrow$

$\hat{\text{Odds of O-Ring failure}}(\text{at } 60^\circ\text{F}) = e^{0.596119} = 1.815061 \rightarrow$  then at 60 degrees Fahrenheit O-ring failure is 1.8151 times more likely than no failure, while at 61°F,  $\ln[\hat{\text{Odds}}(61^\circ\text{F})] = 0.42483$

$\rightarrow \hat{\text{Odds}}(61^\circ\text{F}) = 1.5293304114 \rightarrow$  this implies that for every one degree increase in temperature (°F) the odds of failure is diminished by a factor of  $1.5293304114/1.815061 = 0.8425515$ . Note that Minitab reports a value of 0.84 for this last factor which is called the Odds Ratio (OR, or ODR). That is, for every unit increase in x, the ODR diminishes by roughly

$$0.8426 \text{ because } \hat{\text{ODR}} = \hat{\text{Odds}}(x+1) / \hat{\text{Odds}}(x) = \frac{\hat{p}(x+1) / \hat{q}(x+1)}{\hat{p}(x) / \hat{q}(x)} = \frac{e^{\hat{h}(x+1)}}{e^{\hat{h}(x)}} =$$

$$e^{\hat{\beta}_0 + \hat{\beta}_1(x+1)} / e^{\hat{\beta}_0 + \hat{\beta}_1 x} = e^{\hat{\beta}_1} = e^{-0.17132} = 0.8425515. \text{ Thus, in general a one unit increase in } x$$

results in the estimated odds  $\hat{p}(x) / \hat{q}(x)$  multiplied by a factor of  $e^{\hat{\beta}_1}$ . Because  $\hat{\beta}_1 < 0$ , the relationship between  $p(x)$  and  $x$  is a decreasing one. The resulting logistic regression function

is given by:  $\hat{p}(x) = \frac{1}{1 + e^{-10.87535 + 0.17132x}}$ . This last logistic model implies that when  $x =$

$$60^\circ\text{F, the O-ring failure Pr is estimated as } \hat{p}(60) = \frac{1}{1 + e^{-10.87535 + 0.17132(60)}} = 0.64477,$$



while at  $x = 61^\circ\text{F}$ ,  $\hat{p}(61) = 0.60463$ . Note that  $\hat{\text{ODR}} = (0.60463 \times 0.35523) / [\hat{q}(61) \times \hat{p}(60)] = 0.8425515$  is always independent of  $x$  and depends only on the slope  $\beta_1$ .

### Computing the *se*'s of the Maximum Likelihood Estimators

It has been proven in statistical theory that the covariance matrix of the ML estimators (MLEs) asymptotically approaches the inverse of the Fisher's information matrix given below

$$\mathbf{I} = \begin{bmatrix} I_{11} & I_{12} \\ I_{21} & I_{22} \end{bmatrix} \quad (93)$$

where  $I_{ij} = E \left[ - \frac{\partial^2 L}{\partial \beta_i \partial \beta_j} \right] = I_{ji}$ ,  $L$  represents the natural log of the likelihood function and is

given in Eq. (92c) for the case of two parameters  $\beta_0$  and  $\beta_1$ . Further, from statistical theory, MLEs are generally biased but are asymptotically (as  $n \rightarrow \infty$ ) unbiased. We now proceed to compute the *se*'s of  $\hat{\beta}_0$  and  $\hat{\beta}_1$  for the data of Table 6. Note that if the occurrence Pr of the logistic event were a function of 2 regressors,  $x_1$  &  $x_2$  such that  $\text{logit}(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$ , then the Fisher's Information-Matrix will be a symmetric  $3 \times 3$  matrix.

$$\begin{aligned} \frac{\partial^2 L}{\partial \beta_0^2} &= \frac{\partial}{\partial \beta_0} \sum_{i=1}^n [y_i - p(x_i)] = - \sum_{i=1}^n \frac{\partial}{\partial \beta_0} p(x_i) = - \sum_{i=1}^n \frac{\partial}{\partial \beta_0} [1 + e^{-h(x_i)}]^{-1} = \\ &- \sum_{i=1}^n -[1 + e^{-h(x_i)}]^{-2} \frac{\partial}{\partial \beta_0} (1 + e^{-\beta_0 - \beta_1 x_i}) = \sum_{i=1}^n [1 + e^{-h(x_i)}]^{-2} \times [-e^{-h(x_i)}] = \\ &- \sum_{i=1}^n p^2(x_i) e^{-h(x_i)} \cong -3.73459135; \text{ similarly, } \frac{\partial^2 L}{\partial \beta_0 \partial \beta_1} = - \sum_{i=1}^n x_i p^2(x_i) e^{-h(x_i)} \cong - \end{aligned}$$

$$254.20087919, \text{ and } \frac{\partial^2 L}{\partial \beta_1^2} = - \sum_{i=1}^n x_i^2 p^2(x_i) e^{-h(x_i)} \cong -17446.21098707. \text{ Note that taking}$$

the expectation  $\frac{\partial^2 L}{\partial \beta_i \partial \beta_j}$  is mathematically intractable, at least to the ability of this author,

and thus I have approximated them by their sample values. Further,  $\frac{\partial^2 L}{\partial \beta_0^2} < 0$ ,  $\frac{\partial^2 L}{\partial \beta_1^2} < 0$  and

$$\frac{\partial^2 L}{\partial \beta_0^2} \times \frac{\partial^2 L}{\partial \beta_1^2} > \left( \frac{\partial^2 L}{\partial \beta_0 \partial \beta_1} \right)^2, \text{ implying that the response surface is strictly concave and hence}$$

there exists a global maximum. Thus, the fisher's information matrix is estimated by (recall

$$\text{that } I_{ij} = E \left[ - \frac{\partial^2 L}{\partial \beta_i \partial \beta_j} \right] \text{ by } \mathbf{I} = \begin{bmatrix} I_{11} & I_{12} \\ I_{21} & I_{22} \end{bmatrix} = \begin{bmatrix} 3.73459 & 254.20088 \\ 254.20088 & 17446.21099 \end{bmatrix} \rightarrow$$

$$\hat{\mathbf{I}}^{-1} = \begin{bmatrix} 32.52574 & -0.473918 \\ -0.473918 & 0.00696256 \end{bmatrix} \rightarrow se(\hat{\beta}_0) = \sqrt{32.52574} = 5.70313434 \text{ and } se(\hat{\beta}_1) =$$

$\sqrt{0.00696256} = 0.083442$ . These standard errors precisely match those of Minitab's.

Therefore, the 95% Confidence limits for  $\beta_0$  are  $\hat{\beta}_0 \mp Z_{0.025} \times se(\hat{\beta}_0) =$

$10.87535 \mp 1.959964 \times 5.703134 = (-0.3025886, 22.0532872)$ , where  $Z_{0.025}$  is the 0.975

quantile of  $N(0, 1) \rightarrow -0.3025886 \leq \beta_0 \leq 22.0532872$

Similarly, the 95% CI for  $\beta_1$  is given by  $\hat{\beta}_1 \mp Z_{0.025} \times se(\hat{\beta}_1) \rightarrow$

$$-0.3348638 \leq \beta_1 \leq -0.0077772$$

Note that in developing the above CI's I have used the fact that all ML estimators in the universe are asymptotically normally distributed. A larger sample size  $n$  leads to a more accurate normal approximation. The CI for the Odds ratio is obtained from  $ODR_L = e^{-0.3348638} = 0.7154356$  and  $ODR_U = e^{-0.0077772} = 0.9922529 \rightarrow 0.7154356 \leq ODR \leq 0.9922529$ . This last 95% CI also agrees with that of Minitab's to 2 decimals.

## The Method of Weighted Least-Squares

This method generally requires repeated observations at different levels of  $x$  so that a frequency distribution can be constructed. To illustrate the procedure, we use the data from the text by D. W. Hosmer and S. Lemeshow (*Applied Logistic Regression*, 2<sup>nd</sup> Ed., Wiley, ISBN:0-471-35632-8) in Table 1.1 on their page 3 where the variable  $x$  represents the age of an individual in the study and  $y$  represents the presence or absence of CHD (Coronary Heart

Disease). Because there were  $n = 100$  individuals in their sample, the authors proceeded to obtain a frequency distribution of the data in their Table 1.2, which except for minor modifications by me, is duplicated below. Note that in each age subgroup we have a binomial

**Table 1.2 on page 4 of Hosmer & Lemeshow (2000)**

Age Group $x$	$n_i$	CHD Present, i.e., Number of times that $y = 1$	$\hat{p}_i$	$\hat{q}_i$	$\hat{w}_i =$ $n_i \hat{p}_i \hat{q}_i$	$x_i =$ Mid- point
20-29 years	10	1	0.10	0.90	0.90	24.5
30-34	15	2	2/15	13/15	1.733333	32 years
35-39	12	3	0.25	0.75	2.25	37
40-44	15	5	1/3	2/3	3.333333	42
45-49	13	6	6/13	7/13	3.23077	47
50-54	8	5	5/8	3/8	1.875	52
55-59	17	13	13/17	4/17	3.05882	57
60-69	10	8	0.80	0.20	1.600	64.5
Totals	100	43	0.43	0.57	17.9813	= W

random variable with  $n_i$  Bernoulli trials and estimated success Pr of  $\hat{p}_i$ . The likelihood function for observing  $n_1$  successes (or  $y = 1$  events) in  $n$  trials for a grouped data is given by  $L(y_1, y_2, \dots,$

$$y_n; p) = \frac{n!}{n_1!(n - n_1)!} p^{n_1} (1 - p)^{n - n_1} = C p^{n_1} q^{n - n_1}, \text{ where } C = n! / [n_1!(n - n_1)!] = {}_n C_{n - n_1} \text{ is a}$$

constant (i.e., free of  $p$ ) and  $q = 1 - p$ . As a result,  $L(p) = \ln\left[\frac{n!}{n_1!(n - n_1)!} p^{n_1} (1 - p)^{n - n_1}\right] = \ln(C)$

$+ n_1 \ln(p) + (n - n_1) \ln(q)$ . Setting  $dL(p)/dp$  equal to zero results in the ML estimate of  $p$  as

$$\hat{p} = n_1 / n. \text{ Secondly, it can be shown that } d^2L(p)/dp^2 = -n/(pq) \text{ so that the } V(\hat{p} = n_1 / n) =$$

$pq/n$ . Because the variance of the Binomial rv is equal to  $npq$ , then the estimated variance at

each subgroup is  $n_i \hat{p}_i \hat{q}_i$ . We now regress  $\ln(\text{Odds})$  versus age  $x$ :  $\ln(\text{Odds for CHD}) = \ln\left(\frac{p_i}{1 - p_i}\right)$

$= \ln\left(\frac{p_i}{q_i}\right) = \beta_0 + \beta_1 x_i + \epsilon_i = \text{logit}(x_i) = y_i$ . In weighted regression we try to give less weight to the

subgroup with the larger variance and we assume that  $V(y|x_i)$  depends on the level of  $x$

through  $V(y|x_i) = \sigma_\epsilon^2/w_i$ , i.e., the weighted LSF is given by

$$\text{WLSF}(\beta_0, \beta_1) = \sum_{i=1}^C \epsilon_i^2 = \sum_{i=1}^C w_i (y_i - \beta_0 - \beta_1 x_i)^2 \quad (94)$$

where  $y_i = \ln\left(\frac{p_i}{1-p_i}\right)$  and  $C$  represents the number of categories (or subgroups) and is equal to

8 for Table 1.2 of Hosmer & Lemeshow reproduced above, and  $y_i = \ln\left(\frac{p_i}{1-p_i}\right) = \beta_0 + \beta_1 x_i + (\epsilon_i$

$/\sqrt{w_i})$ , or  $\sqrt{w_i} (y_i - \beta_0 - \beta_1 x_i) = \epsilon_i$  so that  $V(y|x_i) = \sigma_\epsilon^2/w_i$ . Differentiating Eq. (94) wrt to  $\beta_0$  and  $\beta_1$  and setting the resulting derivatives equal to zero leads to the following system of

weighted normal equations. 
$$\hat{\beta}_0 \sum_{i=1}^C w_i + \hat{\beta}_1 \sum_{i=1}^C w_i x_i = \sum_{i=1}^C w_i y_i \quad (95a)$$

$$\hat{\beta}_0 \sum_{i=1}^C w_i x_i + \hat{\beta}_1 \sum_{i=1}^C w_i x_i^2 = \sum_{i=1}^C w_i x_i y_i \quad (95b)$$

where  $w_i = n_i \hat{p}_i \hat{q}_i$ . Letting  $W = \sum_{i=1}^C w_i$  and solving the 1<sup>st</sup> normal equation (95a) for  $\hat{\beta}_0$  gives

$$\hat{\beta}_0 = \left( \sum_{i=1}^C w_i y_i - \hat{\beta}_1 \sum_{i=1}^C w_i x_i \right) / W = \bar{y} - \hat{\beta}_1 \bar{x} \quad (\text{where } \bar{y} = \sum w_i y_i / W)$$

Substituting the above expression for  $\hat{\beta}_0$  into (95b) results in

$$\hat{\beta}_1 = \frac{\sum_{i=1}^C w_i x_i y_i - \left( \sum_{i=1}^C w_i x_i \right) \left( \sum_{i=1}^C w_i y_i \right) / W}{\sum_{i=1}^C w_i x_i^2 - \left( \sum_{i=1}^C w_i x_i \right)^2 / W} = \frac{\sum_{i=1}^C w_i (y_i - \bar{y}) x_i}{\sum_{i=1}^C w_i (x_i - \bar{x})^2} = \frac{WS_{xy}}{WS_{xx}}$$

I used the Hosmer & Lemeshow's (2000) grouped data in their Table 1.2 and obtained  $W =$

$$17.98126, \sum_{i=1}^8 w_i x_i = 827.6658 \text{ (using subgroup midpoints for } x_i\text{'s)}, \sum_{i=1}^8 w_i y_i = -3.72119,$$

where  $y_i = \ln\left(\frac{\hat{p}_i}{\hat{q}_i}\right)$ ,  $\sum_{i=1}^{C=8} w_i x_i y_i = 34.19435$ ,  $\sum_{i=1}^8 w_i x_i^2 = 40076.7$ ,  $\hat{\beta}_1 = 0.103789$  and  $\hat{\beta}_0 = -4.98427$ . Hosmer & Lemeshow used the ML procedure and give the ML estimates as  $\hat{\beta}_1 = 0.111$  and  $\hat{\beta}_0 = -5.309$ . Note that as  $n$  increases, the values of weighted least-squares estimators approach those of the ML. Thus,  $\ln(\text{Odds for CHD}) = \ln\left(\frac{\hat{p}_i}{\hat{q}_i}\right) = -4.98427 + 0.103789x_i$ , and  $\hat{p}(x_i) = (1 + e^{4.98427 - 0.103789x_i})^{-1} \rightarrow \hat{p}(\text{at age 50}) = 0.551111 \rightarrow$  Thus, a randomly selected 50 year-old person has 0.5511 estimated Pr of having evidence of CHD. Using Hosmer & Lemeshow ML estimates, the same Pr at age 50 is equal to 0.55996.

Because ML estimates have nicer properties [1: they are asymptotically unbiased, (2) their SMD approaches normality, (3) if  $\hat{\theta}$  is the ML estimator of a parameter  $\theta$ , then  $h(\hat{\theta})$  is the ML estimator of  $h(\theta)$ ], I used the raw data in Table 1.1 of Hosmer & Lemeshow (2000) and proceeded to obtain their ML estimates. As before, the two likelihood equations with two

$$\text{unknowns are } \sum_{i=1}^n \hat{p}(x_i) = \sum_{i=1}^n \left[ \frac{1}{1 + e^{-\hat{\beta}_0 - \hat{\beta}_1 x_i}} \right] = \sum_{i=1}^n [1 + e^{-\hat{h}(x_i)}]^{-1} = 43 = \sum_{i=1}^n y_i = n_1$$

$$\sum_{i=1}^n x_i \hat{p}(x_i) = \sum_{i=1}^n y_i x_i \rightarrow \sum_{i=1}^n \left[ \frac{x_i}{1 + e^{-\hat{\beta}_0 - \hat{\beta}_1 x_i}} \right] = \sum_{i=1}^n x_i (1 + e^{-\hat{\beta}_0 - \hat{\beta}_1 x_i})^{-1} = 2205.$$

The Excel file on my website provides their raw data. The use of Excel solver yielded the solution set  $\hat{\beta}_0 = -5.30945332$  and  $\hat{\beta}_1 = 0.11092114$  (as compared to the reported values of  $-5.309$  &  $0.111$  on their page 10). Thus,

$$\hat{h}(x) = -5.30945332 + 0.11092114x = \ln\left[\frac{\hat{p}(x)}{1 - \hat{p}(x)}\right]$$

Note that Hosmer & Lemeshow (2000) use  $g(x)$  to represent  $\beta_0 + \beta_1 x + \epsilon$ , but I have used  $g(x)$  to denote the pdf of a Logistic random variable. A point estimate of the logit at  $x = 50$  years of age is given by  $\hat{h}(50) = 0.236603734$  so that a point estimate of the estimated odds is  $\hat{\text{Odds}}(\text{at age 50 for CHD}) = e^{0.236603734} = 1.266938973 \rightarrow$  this implies that a random 50-year old person is 1.267 times more likely to have evidence of CHD than not to have evidence of

CHD. Further, the point estimate of logistic Pr at age  $x = 50$  is  $\hat{p}(50) = 1/(1+e^{-0.236603734}) = 0.558876524$ , or  $\hat{p}(50) = 1.266938973/(1+1.266938973) = 0.558876524$  and  $\hat{q}(50) = 0.441123476$ . The corresponding Fisher's information matrix is

$$\mathbf{I} = \begin{bmatrix} I_{11} & I_{12} \\ I_{21} & I_{22} \end{bmatrix} = \begin{bmatrix} 17.92631205 & 826.1196216 \\ 826.1196216 & 39798.5425534 \end{bmatrix} \rightarrow \hat{\mathbf{I}}^{-1} =$$

$$\begin{bmatrix} 1.285173 & -0.02667702 \\ -0.02667702 & 0.0005788757 \end{bmatrix} \rightarrow se(\hat{\beta}_0) = \sqrt{1.285173} = 1.133655 \text{ and}$$

$se(\hat{\beta}_1) = \sqrt{0.0005788757} = 0.02406$ . These standard errors precisely match those of the authors' to 4 decimals.

### 95% CI for the Fitted Logistic Regression $p(x)$

$$\text{Because } p(x) = \frac{e^{h(x)}}{1 + e^{h(x)}} = \frac{e^{\beta_0 + \beta_1 x + \epsilon}}{1 + e^{\beta_0 + \beta_1 x + \epsilon}} = [1 + e^{-h(x)}]^{-1}, \text{ then we first need to}$$

obtain the requisite CI for  $h(x)$  and this in turn will give us the 95% CI for  $p(x)$ . Therefore, we need to compute the  $se$  of the estimated logit  $\hat{h}(x)$ , which requires computing the  $V[\hat{h}(x)]$  first followed by taking its square root. Proceeding with applying the variance operator to  $\hat{h}(x)$  we obtain

$$V[\hat{h}(x)] = V(\hat{\beta}_0 + \hat{\beta}_1 x) = V(\hat{\beta}_0) + x^2 V(\hat{\beta}_1) + 2x[\text{Cov}(\hat{\beta}_0, \hat{\beta}_1)] \quad (96)$$

where  $\hat{\beta}_0$  and  $\hat{\beta}_1$  are correlated estimators because the information in Eq. (93) is not a diagonal matrix. The last term on the RHS of Eq. (96) gives the covariance between  $\hat{\beta}_0$  and  $\hat{\beta}_1$  which is defined as

$$\text{COV}(\hat{\beta}_0, \hat{\beta}_1) = E\{[(\hat{\beta}_0 - E(\hat{\beta}_0))] \times [(\hat{\beta}_1 - E(\hat{\beta}_1))]\} = E(\hat{\beta}_0 \hat{\beta}_1) - E(\hat{\beta}_0) \times E(\hat{\beta}_1)$$

Note that all ML estimators are only asymptotically unbiased, i.e.,  $E(\hat{\beta})$  is in general different from the vector parameter  $\beta$  for  $n \leq 50$ . For the Example by Hosmer & Lemeshow (their Table

1.1) we have  $\hat{\mathbf{I}}^{-1} = \begin{bmatrix} 1.285173 & -0.02667702 \\ -0.02667702 & 0.0005788757 \end{bmatrix}$ , which shows from Eq. (96) that

$$\hat{V}[\hat{h}(x)] = 1.285173 + x^2(0.0005788757) + 2x(-0.02667702) \quad (97)$$

Thus, for a person of age  $x = 50$ , Eq. (97) gives  $\hat{V}[\hat{h}(50)] = 1.285173 + (50)^2(0.0005788757) + 100(-0.02667702) = 0.06466025 \rightarrow se[\hat{h}(50)] = 0.2542838 \rightarrow h_L(50) = 0.236603680 - 1.96 \times 0.2542838 = -0.2617925644$ , and  $h_U(50) = 0.236603680 + 1.96 \times 0.2542838 = 0.7350$ .

Thus, the lower 95% confidence limit for the fitted  $p(x)$  at age 50 is  $p_L(50) = (1 + e^{0.2617926})^{-1} = 0.43492311$  and  $p_U(50) = (1 + e^{-0.735})^{-1} = 0.67590153 \rightarrow 0.434923 \leq p(50) \leq 0.675902 \rightarrow$  the Pr that a randomly-selected 50-year old person will have evidence of CHD, before that person is selected, lies within the random interval  $[p_L(50), p_U(50)]$  is 95%, where the CI end points and CI length change for one random sample of size 100 to the next. Put differently, in repeated sampling, say 100000 samples each of size  $n = 100$ , roughly 95000 of the CIs (of differing end points) will contain the true mean proportion  $p(50)$ .

### The Likelihood Ratio Statistic for Testing $H_0 : \beta_1 = 0$

In the field of statistics, the likelihood ratio statistic for testing  $H_0 : \beta_1 = 0$  is defined as

$$LRS = \frac{\text{Max } L(x|H_0)}{\text{Max } L(x|\hat{\beta})} \quad (98a)$$

where  $\hat{\beta} = [\hat{\beta}_0 \quad \hat{\beta}_1]^T$  for the case of simple LREG. Some authors in statistical literature use  $\lambda$  for LRS and others denote LRS by  $\Lambda$ . For simplicity, I will just use LRS to denote the likelihood ratio statistic. The denominator of LRS,  $L(x|\hat{\beta})$  is the value of the likelihood function [see Eq. (98a)] when all the parameters in the density function are replaced by their corresponding ML estimates, i.e.,  $L(x|\hat{\beta})$  is maximized wrt all parameters, while the numerator is the maximum of LF wrt only some of the parameters while the remaining parameters are restricted under  $H_0$ . Because the denominator of (98a) maximizes  $L(x|\beta)$  wrt to all parameters while the numerator wrt to only some of the parameters, then the

numerator can never exceed the denominator and hence the likelihood ratio statistic is restricted to the interval  $0 \leq \text{LRS} \leq 1$ . Thus for our simple logistic regression of testing  $H_0: \beta_1 =$

$$0, \text{ the LRS reduces to: } \text{LRS} = \frac{\text{Max } L(x|\hat{\beta}_0)}{\text{Max } L(x|\hat{\beta}_0, \hat{\beta}_1)} \quad (98b)$$

Note that the numerator assumes that  $\beta_1$  is set equal to zero as stated under  $H_0$ . Further, when the values of numerator and dominator of (98b) are close to each other, then the value of  $\hat{\beta}_1$  must be close to zero in agreement with  $H_0$ . However, when the denominator is much larger than numerator, then  $\hat{\beta}_1$  must be far from zero leading to the rejection of  $H_0: \beta_1 = 0$ . Therefore, the 5% rejection region for testing  $H_0: \beta_1 = 0$  corresponds to small values of LRS having a Pr of at most 0.05. Fortunately, although the exact sampling distribution (SMD) of LRS in (98b) is difficult to obtain, and intractable when the underlying distribution is unknown, from statistical theory the SMD of  $-2 \times \ln(\text{LRS})$  approaches a  $\chi^2_v$  as  $n \rightarrow \infty$ , where the degrees of freedom  $v$  is equal to the number of parameters hypothesized under  $H_0$  (in this case  $v = 1$ ). That is,  $-2 \times \ln(\text{LRS}) \rightarrow \chi^2_1$  as  $n$  increases towards infinity for testing  $H_0: \beta_1 = 0$ . For the sake of

$$\text{illustration, I will compute } -2 \times \ln(\text{LRS}) = -2 \times \ln \left[ \frac{\text{Max } L(x|\hat{\beta}_0)}{\text{Max } L(x|\hat{\beta}_0, \hat{\beta}_1)} \right] = -2 \times \ln [L(x|\hat{\beta}_0)] +$$

$2 \times \ln [L(x|\hat{\beta}_0, \hat{\beta}_1)] = D_0 - D_1$ , which Hosmer & Lemeshow (2000) denote it by  $G$ , i.e.,

$$G = -2 \times \ln(\text{LRS}) = -2 \times \ln \left[ \frac{\text{Max } L(x|\hat{\beta}_0)}{\text{Max } L(x|\hat{\beta}_0, \hat{\beta}_1)} \right] = D_0 - D_1 \quad (99a)$$

where  $D_0 = -2 \times \ln [L(x|\hat{\beta}_0)]$  is called the deviance with  $\beta_1 = 0$  (i.e., deviance under  $H_0: \beta_1 = 0$ ),

$D_1 = -2 \times \ln [L(x|\hat{\beta}_0, \hat{\beta}_1)]$  is the deviance with  $\beta_1 \neq 0$  (or deviance under  $H_1$ ), and  $G$  has an

approximate  $\chi^2$  distribution with  $v = 1$  *df*. For the data of Table 1.1 of Hosmer & Lemeshow (listed on my website) the value of  $D_1$  from Eq. (92b), on p. 107 of these notes, is given by

$$D_1 = -2 \times \ln [\text{Max } L(x|\hat{\beta}_0, \hat{\beta}_1)] = -2 \times \sum_{i=1}^n [y_i \ln \hat{p}_i + (1 - y_i) \ln \hat{q}_i] \quad (99b)$$



$$= -2 \times (-53.6765463) = 107.3530927$$

In order to compute  $D_0$ , we let  $h(x) = \beta_0 + \epsilon$ , i.e., we assume  $H_0: \beta_1 = 0$  is true.  $\rightarrow L(\beta_0, \beta_1 = 0) =$

$$\sum_{i=1}^n [y_i \beta_0 - \ln(1 + e^{\beta_0})] \rightarrow \partial L(\beta_0) / \partial \beta_0 = \sum_{i=1}^n [y_i - \frac{e^{\beta_0}}{1 + e^{\beta_0}}] \xrightarrow{\text{Set Equal to}} 0 \rightarrow$$

$$\hat{\beta}_0 | H_0 \text{ is true} = \ln\left(\frac{\bar{y}}{1 - \bar{y}}\right) = \ln(0.43/0.57) = -0.281851152 \rightarrow \text{Max } L(x | H_0: \beta_1 = 0 \text{ is true}) =$$

$$\sum_{i=1}^n [y_i \hat{\beta}_0 - \ln(1 + e^{\hat{\beta}_0})] = \hat{\beta}_0 \sum_{i=1}^n y_i - n \times \ln(1 + e^{\hat{\beta}_0}) = -68.3314914 \rightarrow D_0 = -2 \times \text{Max}$$

$$\ln[L(x | \hat{\beta}_0)] = 136.662983 \rightarrow G = -2 \times \ln(\text{LRS}) = 136.662983 - 107.3530927 = 29.30989; \text{ this}$$

compares exactly to 2 decimals with Hosmer & Lemeshow's answer of  $G = 29.31$  atop their

page 15. Lastly, we compute the Pr level for testing  $H_0: \beta_1 = 0$ , which is given by  $\hat{\alpha} = P\text{-value} = p$

$$= \Pr(\chi_1^2 \geq 29.30989) = 0.0000000616801 = 0.07616801 \rightarrow \text{Very strongly reject } H_0: \beta_1 = 0 \rightarrow \text{the}$$

age of a person is a strong predictor of evidence of CHD.

### Score Test (ST) Statistic for Testing $H_0: \beta_1 = 0$

Besides the Z-statistic,  $\hat{\beta}_1 / se(\hat{\beta}_1)$ , and the LRS,  $G$ , there is one other statistic, called the Score Test (ST), for testing  $H_0: \beta_1 = 0$ . This is based on the value of  $\partial L(\beta_0, \beta_1) / \partial \beta_1$  given that  $H_0: \beta_1 = 0$  and  $\partial L(\beta_0, \beta_1) / \partial \beta_0 = 0$  are true. Recall that the ML estimate of  $\beta_1$  is obtained by setting both  $\partial L(\beta_0, \beta_1) / \partial \beta_0$  and  $\partial L(\beta_0, \beta_1) / \partial \beta_1$  equal to zero and solving the resulting system of the two likelihood equations for the ML estimates of  $\beta_0$  and  $\beta_1$ . Under the null hypothesis  $H_0: \beta_1 = 0$ , the

$$1^{\text{st}} \text{ likelihood equation } \partial L(\beta_0, \beta_1) / \partial \beta_0 = 0 \text{ yields } \sum_{i=1}^n \hat{p}(x_i) = \sum_{i=1}^n y_i = n_1 \rightarrow \sum_{i=1}^n \left[ \frac{1}{1 + e^{-\hat{\beta}_0}} \right] =$$

$$\sum_{i=1}^n y_i \rightarrow n \left[ \frac{1}{1 + e^{-\hat{\beta}_0}} \right] = \sum_{i=1}^n y_i \rightarrow 1 + e^{-\hat{\beta}_0} = 1 / \bar{y} \rightarrow e^{-\hat{\beta}_0} = -1 + 1 / \bar{y} \rightarrow -\hat{\beta}_0 = \ln\left(\frac{1 - \bar{y}}{\bar{y}}\right) \rightarrow \hat{\beta}_0$$

$$= \ln\left(\frac{\bar{y}}{1 - \bar{y}}\right) = \ln\left(\frac{n_1 / n}{1 - n_1 / n}\right) \rightarrow \hat{\beta}_0 = \ln\left(\frac{n_1}{n - n_1}\right) = \ln\left(\frac{n_1}{n_0}\right), \hat{p}(x_i) = \bar{y} = n_1 / n, \text{ and } n_0 = n - n_1.$$

Because the ML estimate of  $\beta_1$  is obtained from  $\partial L(\beta_0, \beta_1) / \partial \beta_1 = 0$ , and thus, if  $\partial L(\beta_0, \beta_1) / \partial \beta_1$  is

far away from zero, its large distance from zero will be in contradiction with the null hypothesis  $H_0: \beta_1 = 0$ . Therefore, we must compute  $\partial L(\beta_0, \beta_1)/\partial \beta_1$  assuming that  $H_0$  and  $\partial L(\beta_0, \beta_1)/\partial \beta_0 = 0$  are true and assess if it is significantly different from zero. Assuming  $H_0$  is true, we obtain  $\partial L(\beta_0,$

$$\beta_1)/\partial \beta_1 = \sum_{i=1}^n [y_i x_i - x_i \hat{p}(x_i)] = \sum_{i=1}^n [y_i x_i - \bar{y} \times x_i] = \sum_{i=1}^n x_i (y_i - \bar{y}).$$

It is assumed that this last partial derivative is approximately Gaussian with mean zero under  $H_0$  and conditional variance, keeping  $x_i$  fixed, which is computed below.

$$V[\sum_{i=1}^n x_i (y_i - \bar{y})] = V[\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})] = V[\sum_{i=1}^n (x_i - \bar{x})y_i] = \sum_{i=1}^n (x_i - \bar{x})^2 V(y_i) =$$

$$\sum_{i=1}^n (x_i - \bar{x})^2 pq = S_{xx} \times pq \rightarrow \text{Thus, the estimate of the } V[\sum_{i=1}^n x_i (y_i - \bar{y})] \text{ is } \sum_{i=1}^n (x_i - \bar{x})^2 \hat{p}\hat{q} =$$

$$S_{xx} \times \bar{y}(1 - \bar{y}). \text{ As a result, the Score Test Statistic is given by } ST = \frac{\sum_{i=1}^n x_i (y_i - \bar{y})}{\sqrt{\bar{y}(1 - \bar{y})S_{xx}}}, \text{ which is}$$

approximately normally distributed with zero mean and STDEV equaling 1. For Table 1.1 of

Hosmer and Lemeshow (2000), we have:  $\bar{y} = 43/100 = 0.43$ ,  $1 - \bar{y} = 0.57$ ,  $S_{xx} = 210560 -$

$$4438^2/100 = 13601.5600, \sum_{i=1}^n x_i y_i = 2205, \bar{y} \sum_{i=1}^n x_i = 0.43 \times 4438 = 1908.34 \rightarrow$$

$$\sum_{i=1}^n x_i (y_i - \bar{y}) = 2205 - 1908.34 = 296.66 \rightarrow ST = \frac{296.66}{\sqrt{0.43 \times 0.57 \times 13601.56}} = 5.137987 \rightarrow$$

$P$ -value = Pr Level of the Test =  $\hat{\alpha} = 2\Pr(Z_{N(0,1)} \geq 5.137987) = 2.78198 \times 10^{-7} \rightarrow$  Strongly reject

$H_0: \beta_1 = 0$ . Note that  $ST^2 = 5.137987^2 = 26.39891$  is fairly close to  $G = 29.30989$ , as expected

because  $Z_{N(0,1)}^2 \sim \chi_1^2$  distributed. The discrepancy is due to the fact that  $G = -2 \times \ln(\text{LRS})$  is

only approximately  $\chi_1^2$  distributed.

## Goodness-of-Fit (GOF) Tests in Logistic Regression

Minitab reports three GOF statistics to ascertain how well the logistic model fits a

binary data set. (1) Pearson Chi-Square Statistic, (2) Deviance, and (3) Hosmer-Lemeshow Test. The last (H&L) is a contingency type of GOF test using 10 subgroups (based on 10 deciles), and in my opinion should not be used unless  $n > 50$ . Even, for  $50 < n \leq 100$ , some of the expected frequencies may turn out to be less than 5 and thus the SMD of the GOF statistic

$\sum_{i=1}^{10} \frac{(f_j - E_j)^2}{E_j}$  would not closely resemble  $\chi_8^2$ , where there are  $C = 10$  subgroups with two

constraints  $\partial L(\beta_0, \beta_1)/\partial \beta_0 = 0$  and  $\partial L(\beta_0, \beta_1)/\partial \beta_1 = 0$ . Therefore, I will discuss only the first two GOF tests, starting with Deviance.

Recall that the observed values of  $y$  can equal to either 1 (when success occurs) or zero (when the event of interest does not occur). When  $y = 1$  at an  $x$  that is not repeated, then the fit is excellent iff  $\hat{p}(x)$  is close to 1 because  $p(x) = \Pr(Y = 1 | x)$ , and thus,  $\ln[1/\hat{p}(x)] = -\ln[\hat{p}(x)]$  is a measure of goodness-of-fit of the logistic regression model at  $y = 1$  because a large value of  $\ln[1/\hat{p}(x)]$  implies that  $\hat{p}(x)$  must be close to zero and the model does not fit  $y = 1$  at this  $x$ -value. Thus, the  $y = 1$  deviance residual is defined as  $d[1, \hat{p}(x)] = \{2 \times \ln[1/\hat{p}(x)]\}^{1/2} = \sqrt{-2 \times \ln[\hat{p}(x)]}$  iff  $x$  is not repeated. Similarly, when  $y = 0$  at an  $x$  that is not repeated, the fit is excellent iff  $\hat{q}(x)$  is close to 1, but the case  $y = 0$  creates the problem that  $\ln[(0/\hat{q}(x))]$  is not defined; further, we have to define the  $y = 0$  deviance residual in such a manner that it is always negative because the  $y = 1$  deviance residual is always positive when  $x$  is not repeated. For this reason, the  $y = 0$  logistic residual is basically defined as  $\ln[\hat{q}(x)] < 0 \rightarrow 2 \times \ln[\hat{q}(x)] < 0 \rightarrow \sqrt{2 \times \ln[\hat{q}(x)]}$  is imaginary and hence the  $y = 0$  deviance residual is defined as  $d[0, \hat{q}(x)] = -\sqrt{-2 \times \ln \hat{q}(x)}$ . Note that when  $y = 0$  at an  $x$  that is distinct from all other subjects, a negative value of  $\ln[\hat{q}(x)]$  close to zero is a measure of goodness-of-fit. Thus, for the portion of the data where  $x$  is not repeated the total deviance residual is given by  $DR_1 =$

$\sum_{\text{All } x \text{'s are different}} \{d[1, \hat{p}(x)] + d[0, \hat{q}(x)]\}$ . If there are at least two subjects with the same

value of  $x_j$ , there cannot be but one fitted value  $\hat{p}_j$  for all the subjects with the same  $x_j$ . For example, for the Challenger data on my website,  $x = 70^\circ\text{F}$  is replicated 4 times with the results

$y = 1$  three times and  $y = 0$  once but with the same logistic Pr equal to  $\hat{p}(70) =$

$$\frac{1}{1 + e^{-10.87535 + 0.17132(70)}} = 0.24655. \text{ For such a case, the deviance residual is a weighed}$$

average of the  $d[1, \hat{p}(x)]$  and  $d[0, \hat{q}(x)]$  given below:

$$DRES_i(y_j, p_j) = \pm \sqrt{2 \left[ y_j \ln\left(\frac{y_j}{n_j \hat{p}_j}\right) + (n_j - y_j) \ln\left(\frac{n_j - y_j}{n_j \hat{q}_j}\right) \right]} \quad (100)$$

where  $n_j$  = total number of subjects with the same  $x_j$ ,  $y_j$  = number of positive responses (i.e., number times that  $y = 1$ ), and the sign of  $d(y_j, p_j)$  is positive iff  $(y_j - n_j p_j) > 0$ . For the Challenger data at  $x = 70^\circ\text{F}$ ,  $n_9 = 4$ ,  $y_9 = 3$ ,  $\hat{p}_9 = 0.24655$ ,  $\hat{q}_9 = 0.75345$  and  $(y_j - n_j p_j) = 3 - 4 \times 0.24655 = 2.0138$

$$> 0. \text{ Hence, } DRES(y_9, 0.24655) = \sqrt{2 \left[ 3 \ln\left(\frac{3}{0.98621}\right) + (4 - 3) \ln\left(\frac{4 - 3}{3.013791}\right) \right]} = 2.11390607,$$

which is the same as that of Minitab's to 7 decimals. Note that when  $n_j = 1$  and  $y_j = 1$ , then Eq. (100) reduces to  $d[1, \hat{p}(x)]$ , and when  $y_j = 0$ , Eq. (100) reduces to  $d[0, \hat{q}(x)]$  and always  $\sum_{\text{all } x \text{'s}} n_j = n$ ; further, unlike residuals for most statistical models, the deviance residuals

do not usually sum identically to zero, i.e., their sum is generally different from zero but is usually close to zero. For the Challenger data  $\sum_{\text{all } x \text{'s}} d(y_j, p_j) = -3.41409357$ . The deviance in

$$\text{logistic regression is defined as } D = \sum_{\text{all Distinct } x \text{'s}} [d(y_j, p_j)]^2 = SS_{DRES} \quad (101)$$

and for the Challenger data  $D = 15.75918096$ . The statistic  $D$  in Eq. (101) is asymptotically chi-square with  $df = \text{number of distinct } x_j \text{'s} - 2$  constraints. For the Challenger data there are 17

distinct  $x$  values and hence the  $P\text{-value} = \hat{\alpha} = \Pr(\chi_{15}^2 \geq 15.75918096) = 0.39823473$ , which again implies that the logistic model fits the data well. Note that there are 17 squared terms in Eq. (101) and that is why there must be only one residual when there are replications at an  $x_j$  so that the  $df$  would be  $17 - 2$ . Further, the larger the  $P\text{-value}$  is, the better is the fit.

## The Pearson Chi-Square Statistic

The residual for this statistic is defined as  $(y_j - \hat{y}_j)$ , where again there are two possibilities: (1)  $x_j$  is not repeated (i.e., only a single value of  $x_j$ ), (2) At least two or more

subjects with the same value of  $x_j$ . When there is only one subject at  $x_j$ , then the rv  $y_j$  has a Bernoulli distribution with success  $Pr, p_j = p(x_j)$ ,  $E(x_j) = p_j$  and variance  $p_j q_j$ . Hence, the residual  $e_j = y_j - \hat{Y}_j = y_j - \hat{p}_j$ . When an  $x_j$  ( $n_j > 1$ ) is replicated, say  $n_j$  times, then at that  $x_j$ , the rv  $y_j$  has a binomial pmf with success  $Pr, p_j$ ,  $E(y_j) = n_j \times p_j$ ,  $V(y_j) = n_j \times p_j \times q_j$  so that  $e_j = y_j - \hat{Y}_j = y_j - n_j \times \hat{p}_j$ . For the Challenger data, there are  $n_9 = 4$  replicates at  $x = 70^\circ\text{F}$  but  $y_j = 3$  successes, and hence  $e_9 = 3 - 4 \times 0.24655 = 2.01379114$  and the corresponding studentized residual is given by  $r_9 = 2.01379114 / \sqrt{4 \times 0.24655 \times 0.75345} = 2.33616437$ . Further, like in the case of deviance residuals, the sum of Pearson's residuals does not add to zero but is close to zero.

My calculations for Table 6 of my website show that the Pearson's GOF statistic is  $\chi_{15}^2 \cong$

$$\sum_{j=1}^{17} \frac{(y_j - n_j \hat{p}_j)^2}{n_j \times \hat{p}_j \times \hat{q}_j} = 14.0485605 \rightarrow P\text{-value} = p = \hat{\alpha} = \Pr(\chi_{15}^2 \geq 14.0485605) = 0.52184944; \text{ this}$$

matches the *Pr* level reported by Minitab to 3 decimals. It seems that, in general, the Deviance provides a more powerful test (i.e., smaller *P-value*) than the Pearson's GOF statistic.

**Exercise 32.** The ICU (Intensive Care Unit) data from Hosmer & Lemeshow (2000) has many features versus a patient's age,  $x$ . The primary objective was to use logistic regression to predict survival  $Pr$  at the time of hospital discharge. One important dichotomous rv was Vital Status (STA) where 0 denoted Lived and 1 indicated that the patient died. The STA data for  $n = 200$  patients are provided on my website. First arrange the data in ascending order of age. (a) Use MS Excel to obtain the ML estimates of  $\beta_0$  &  $\beta_1$  and give the estimate of the logit  $h$ (at age  $x = 60$ ). Compute the odds for a random patient of age 60 and interpret its value. (b) Obtain the 95% CI's for  $\beta_0$ ,  $\beta_1$  & the odds ratio; note that the ODR is independent of  $x$ . (c) Obtain the 95% CI for the logit at  $x = 60$  and for  $p$ (60 years old) and interpret. (d) Test  $H_0: \beta_1 = 0$  using the Z-statistic, LRS = G, and the ST by computing their *P-values*. State your decision regarding  $H_0$  at the 5% level. (e) Use Excel to compute the Deviance residual and that of Pearson's only at  $x = 36$  and 40 years and check against those of Minitab's. Then, use Minitab's Residuals to compute the statistics D and Pearson's GOF, and use their *P-values* to determine the model's GOF.