

SIMULTANEOUS INFERENCE IN GENERALIZED
LINEAR MODEL SETTINGS

By

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CHAPTER 1

INTRODUCTION

Modern epidemiological and medical research routinely employs generalized linear modeling. These models can be helpful in understanding what behaviors or traits can influence the incidence of a particular disease or characteristic. For example, logistic regression models provide a means of relating the incidence of some trait or disease to a set of possible predictor variables, while loglinear models help us understand associations between a trait and predictor variables.

After building a generalized linear model (GLM), one typically wishes to estimate particular quantities of interest such as response probabilities, odds ratios, or relative risks. Customarily, these are reported via confidence intervals or confidence bounds using some pre-specified level of significance for each inference. For example, using a loglinear model, one could report $100(1 - \alpha)\%$ confidence intervals for each relative risk resulting from the model. Using one-at-a-time intervals is appropriate when the investigators are not making overall conclusions about the quantities of interest. For example, if the aforementioned loglinear model was estimated and $100(1 - \alpha)\%$ confidence intervals for the relative risks were reported, conclusions about each individual relative risk could be made, but any statements comparing these relative risks would inflate the assumed α error rate. Research on simultaneous estimation procedures for quantities from generalized linear models has received little attention beyond very routine treatments, such as making Bonferroni adjustments to the usual confidence interval or constructing Scheffé intervals. However, recent advances made in simultaneous inference for linear models may be applied in the generalized linear

model setting. Additionally, further improvements may be made by utilizing some unique properties of the estimated parameters from generalized linear models. I plan to present the justification for employing these simultaneous inference methods in the generalized linear model setting and, via simulation, compare their performance. Thus, the objective of this study is to develop simultaneous interval based procedures that will estimate functions of linear combinations of the parameters of a generalized linear model. Specifically, this includes simultaneously estimating the expected response function, odds ratios, and relative risks from generalized linear models.

Overall, attention is focused on quantities that are estimated from a GLM, not the estimation of the GLM itself. Obviously, the performance of any of these procedures will be influenced by how well the model is estimated, but this dissertation will assume the model is well estimated. Additionally, all of the procedures developed in this paper involve constructing interval estimates. Often, procedures that account for multiplicity employ hypothesis tests to make overall conclusions about a set of data. It is more appropriate in the applications I will discuss to use simultaneous intervals instead of stepwise procedures, since I wish to not only detect statistical differences between quantities, but also to assess the practical significance of these differences. Thus, all methods discussed are interval-based procedures.

Before presenting the details of generalized linear models, a practical example of the implementation of a GLM may provide a frame of reference. A 2003 study from the *American Journal of Epidemiology* explored the relationship between maternal stress and preterm birth [1]. Several previously identified sources of maternal stress, such as high incidence of life events, increased anxiety, living in a dangerous neighborhood, and increased perception of stress, were explored for any association with preterm births. Specifically, the study focused on predicting the prevalence of preterm birth among pregnant women aged 16 or older from two prenatal clinics in central North Carolina. Upon admission to the study, women were asked to complete

Table 1.1: Maternal Stress Relative Risks and 95% Confidence Intervals

Life Events Stress	RR	95% CI
No Stress	1.00	
Med-Low Stress	1.5	(1.0, 2.2)
Med-High Stress	1.4	(0.9, 2.1)
High Stress	1.8	(1.2, 2.7)

questionnaires in addition to completing a psychological instrument. Also, several blood, urine, and genital tract tests were conducted in order to assess the physical health of the candidates. In all, 2,029 women were eligible, recruited, and completed the preliminary tests in order to participate in the study. Of these participants, 231 delivered preterm, less than 37 weeks gestation. A loglinear model was employed to assess the relationship between the sources and levels of maternal stress and preterm birth. As a result, the authors considered the resulting model relative risks for each individual stress factor or level of a stress factor and its association with preterm birth. Additionally, 95% confidence intervals were computed for each relative risk. The relative risk will be discussed in detail later, but note that for this study each relative risk is the risk of preterm birth for an individual with one particular maternal stress factor relative to the risk of preterm birth for an individual with none of the other identified sources of maternal stress present. Thus a large relative risk for a particular source of maternal stress indicates a strong association between that stress factor and preterm birth. In general, other quantities derived from the generalized linear model may also be of interest. Table 1.1 contains results from the preterm birth study discussed, though these results have been simplified from the actual implemented model for ease of presentation. In particular, the relative risks for different levels of stress due to general life events is presented. As previously discussed, note

that the 95% confidence intervals for each relative risk presented in Table 1.1 estimate the risk of preterm birth for each individual subject to a particular level of a maternal stress factor (life event stress) with reference to the control (the case with no identified source of maternal stress). For this scenario, one-at-a-time inferences are reasonable if the researcher wishes to answer questions such as, “how does the presence of one source of maternal stress affect the risk of preterm birth?” Note that this question is only concerned with the presence of a particular stress factor and how it affects the incidence of preterm births. If one wishes to make any overall conclusions comparing how the multiple sources of maternal stress affect the risk of preterm birth, then another estimation procedure that accounts for multiplicity needs to be implemented. For instance, in the preterm birth study, the researchers reported the above relative risks and confidence intervals, and then remarked that “(w)omen in the highest negative life events impact quartile had the highest risk (RR=1.8, 95% CI: 1.2, 2.7); however, the middle categories did not show increasing risk with increasing measures of stress.” This kind of conclusion is inappropriate given that the researchers only computed one-at-a-time 95% confidence intervals for the relative risks. Therefore, this is a case that would benefit from simultaneous inference on the relative risks.

As another example where simultaneous inference would be appropriate, consider the case where the researcher wishes to identify the set of the sources and levels of maternal stress that are significantly associated with preterm birth. In this case the one-at-a-time intervals are again inappropriate. In order to make this kind of conclusion, the researcher needs to determine which groups of relative risks are significantly different from 1. If the researcher additionally wants to determine the practical significance of the differences between the varying sources and levels of maternal stress and the control, then confidence intervals with a multiplicity adjustment are required. Stepwise procedures are not adequate as they only determine where statistically significant differences exist, but do not provide a way to estimate the scale of these

differences. Additionally, it is often desirable to make conclusions such as “if the subject has one level of a predictor variable, then he is twice as likely to have the disease than if he has any other level of that predictor variable”. Many other examples of similar conclusions could be given, but generally, these conclusions are comparing one parameter to another and the desired outcome is to somehow relate these parameters. Thus, if one wishes to make any comparisons of these parameters, it is desirable to control the overall type I error rate by accounting for the multiplicity of inferences.

In the following chapters, I will present the motivation for simultaneous inference of certain parameters and outline both the current methodologies and my proposed methodologies. Additionally, the simulation results of the proposed methods are presented and analyzed. Specifically, in chapter two, I present the generalized linear model and the typical quantities that are estimated from the model, and discuss why simultaneous inference of these quantities is essential in some situations. Additionally, I review some methods for computing one-at-a-time confidence intervals on various quantities resulting from generalized linear models. In chapter three, I outline the current methodologies used for simultaneously estimating various functions resulting from generalized linear models, and I propose four new methods to estimate these parameters from GLMs. In chapter four, I summarize how I evaluated these new methods using simulation and present the simulation results. Finally, I propose some future research questions regarding simultaneous estimation of a GLM and present some applications of the new methods in the concluding chapter.

CHAPTER 2

The GLM and Estimated Quantities

There are several generalized linear models (GLM) that permit estimates, such as the odds ratio or relative risk, where multiplicity adjustments often seem warranted. Some of these models include the logistic regression model, loglinear model, Poisson regression model, and the probit or complementary log-log model. In general, a GLM can be expressed as

$$Y_i = g^{-1}(\mathbf{x}'_i \boldsymbol{\beta} + \epsilon_i), \quad i = 1, \dots, n \quad (2.1)$$

or alternatively,

$$\phi_i = g(E(Y_i|\mathbf{x}_i)) = \mathbf{x}'_i \boldsymbol{\beta}, \quad i = 1, \dots, n \quad (2.2)$$

where g links the expected response, $E(Y_i|\mathbf{x}_i)$, to ϕ_i , with \mathbf{x}_i the vector of covariates corresponding to Y_i , $\boldsymbol{\beta}$ the $k \times 1$ vector of regression parameters, and ϵ_i independently and identically distributed random variables. In the later sections, $\mathbf{Y} = (Y_1, \dots, Y_n)'$ is the vector of responses and $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)'$ is the full rank matrix of predictor variables. Each GLM corresponds to a particular link function g , typically called the canonical link when it transforms the mean to the natural parameter. In general, the maximum likelihood estimate (MLE) of the regression parameters is denoted $\hat{\boldsymbol{\beta}} = (\hat{\beta}_1, \dots, \hat{\beta}_k)$. The MLE is asymptotically multivariate normal with mean $\boldsymbol{\beta}$ and covariance matrix

$$\mathbf{V} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \quad (2.3)$$

where \mathbf{W} is a diagonal matrix with diagonal elements $w_i = (\partial\mu_i/\partial\phi_i)^2/\text{var}(Y_i)$ for $\mu_i = E(Y_i|\mathbf{x}_i)$ and ϕ_i in (2.2). Thus,

$$\hat{\boldsymbol{\beta}} \sim N_k(\boldsymbol{\beta}, \mathbf{V}). \quad (2.4)$$

We can estimate the covariance matrix, \mathbf{V} , by

$$\hat{\mathbf{V}} = \hat{c}\hat{v}(\hat{\boldsymbol{\beta}}) = (\mathbf{X}'\hat{\mathbf{W}}\mathbf{X})^{-1} \quad (2.5)$$

with $\hat{\mathbf{W}} = \mathbf{W}|_{\boldsymbol{\beta}=\hat{\boldsymbol{\beta}}}$. Further results will require the estimated covariance of $\mathbf{x}'_i\boldsymbol{\beta}$ for a given \mathbf{x}_i vector with k known elements. This is given by

$$\hat{\sigma}_{GLM}^2(\mathbf{x}_i) = \sqrt{\mathbf{x}'_i\hat{\mathbf{V}}\mathbf{x}_i}, \quad i = 1, \dots, n. \quad (2.6)$$

At times I will need to refer to a linear model in this proposal. A linear model is generally given by

$$Y_i = \mathbf{x}'_i\boldsymbol{\theta} + \epsilon_i, \quad i = 1, \dots, n \quad (2.7)$$

or alternatively,

$$E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\theta} \quad (2.8)$$

where $\boldsymbol{\theta}$ is the vector of regression parameters, \mathbf{Y} and \mathbf{X} are as previously defined, and $\epsilon_i \sim iid N(0, \sigma_{LM}^2)$. The MLEs for $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k)$ are denoted $\hat{\boldsymbol{\theta}}$ and

$$\hat{\boldsymbol{\theta}} \sim N_k(\boldsymbol{\theta}, \sigma_{LM}^2\mathbf{F}) \quad (2.9)$$

where σ_{LM}^2 is the variance of the model residuals for a linear model and $\mathbf{F} = (\mathbf{X}'\mathbf{X})^{-1}$. Whenever a linear model is referenced in this paper, the notation presented above will be utilized.

As discussed previously, the objective of this research is not to merely estimate a GLM, but to simultaneously estimate quantities derived from a GLM. There are many natural quantities that can be of interest when modeling data with a GLM. These include measures such as the expected mean response, the odds ratio, the relative

risk, and possibly others. While the focus of this paper is on the estimation of these quantities from GLMs, it should be mentioned that they may be estimated directly from the data. I will first present these measures in general, and then discuss them specifically in the context of generalized linear models.

2.1 The Expected Mean Response

The expected mean response is a generic term for either the response probability or the mean response. Depending on the sampling distribution of the data, either one or the other is of interest. For example, if we assume binomial sampling, the expected mean response function is the probability of a success for a given level of the predictor variables, or the response probability. When a Poisson sampling scheme is assumed, the expected mean response is the average for a particular cell in the contingency table, or the mean response.

A response probability is the proper quantity of interest if one wishes to understand the probability of developing a disease or another characteristic for a given set of predictor variables that are believed to be associated with the disease. For example, a response probability could be used to inform a particular patient of their probability of developing a particular disease given their history and profile. With respect to the preterm birth example, if a doctor has a patient known to be experiencing a major life event, such as a death in the family, then she could ascertain that patient's risk of preterm birth and take appropriate measures.

Conversely, the mean response might be used in a situation where a clinician has recorded a host of risk factors for a particular disease and wishes to predict how many of the subjects will develop the disease. This communicates how many patients on average will or will not develop a certain characteristic. In the context of the preterm birth example, the Poisson mean response could be used to estimate how many subjects out of the total sample size will experience a preterm birth. The

Poisson mean response is simply estimated directly from the frequencies given in a contingency table when it is not estimated from a model.

In general, a one-at-a-time $100(1 - \alpha)\%$ confidence interval for the response probability is given by

$$\hat{\pi}_i \pm z_{\alpha/2}(v\hat{a}r(\hat{\pi}_i))^{1/2} \quad (2.10)$$

where $var(\hat{\pi}_i) = \frac{\pi_i(1-\pi_i)}{m_i}$ and $v\hat{a}r(\hat{\pi}_i) = \frac{\hat{\pi}_i(1-\hat{\pi}_i)}{m_i}$. (Note that confidence intervals on the mean response for Poisson sampling distribution models are not typically computed.) This one-at-a-time confidence interval for π_i is often employed to estimate an expected mean response for binomial or multinomial sampling scenarios. If the researcher simply wants to know how a particular level of the predictor variables affects the incidence of disease, this is all that needs to be calculated. First, consider the case where the predictor variable is categorical, as in the preterm birth example. Suppose a clinician wishes to estimate the risk of preterm birth for a particular patient in her clinic. Then the one-at-a-time interval would be adequate. Alternatively, consider a scenario where a researcher wants to make some kind of overall conclusion about the relationship between all the sources and levels of maternal stress and preterm birth. For example, suppose the researcher wishes to compare the risk of preterm birth for all the maternal stress factors and their levels. In order to simultaneously estimate these differences, the researcher would need to employ some kind of procedure that accounts for the multiple inferences being made. Additionally, it would be of practical interest to identify a group of maternal stress factors and levels that are “most associated” with preterm birth and another group of maternal stress factors and levels that are “least associated” with preterm births. This too would necessitate a procedure that adjusts for multiplicity while also providing interval estimates of the response probabilities for each stress factor. Finally, consider the case where the researcher would want to compare the probability of preterm birth for each maternal stress factor or level with the probability of preterm birth for a control or reference

level. In this example, the reasonable reference level would be subjects that have no identified sources of maternal stress. Again the appropriate procedure would adjust for multiplicity.

Now consider the case where the predictor variable is continuous. Often, with a continuous predictor variable, a specific range of the domain is of particular interest. For example, if we added a continuous measure of each patient's prepregnancy body mass index (BMI) in the preterm birth study, we might have particular interest in BMI's less than 19.8 (underweight), 19.8 to 26.0 (normal weight), 26.0 to 29.0 (overweight), and over 29.0 (obese). It may be of interest to compare the expected number of preterm birth cases for subjects within these BMI groups within a particular maternal stress factor group. In order to make conclusions such as the obese patients have the largest number of preterm birth cases, interval estimates need to be used that account for the multiple inferences being made. The methods I propose will adjust for this kind of multiplicity.

2.2 The Odds Ratio

The odds ratio is a widely used measure in epidemiological and medical applications. The odds ratio is generally defined as the ratio of the odds of a characteristic (or disease) occurring in one group to the odds of it occurring in another group. With reference to the preterm birth study, odds ratios could have been computed that would estimate the relative odds of preterm birth for a particular level of a maternal stress factor to the odds for those mothers with no identifiable stress factors. Thus, an odds ratio of 2.11 for mothers who live in a neighborhood perceived to be dangerous, would be interpreted as: the odds of delivering a preterm infant when living in a neighborhood that is perceived to be dangerous is 2.11 times greater than the odds of having a preterm infant when a subject is not exposed to any identifiable sources of maternal stress.

Table 2.1: Sample Contingency Table

	$X = x_1$	$X = x_2$	
$Y = 1$	a	b	m_1
$Y = 0$	c	d	m_2
	n_1	n_2	n

The sample odds ratio can easily be computed from the raw data and is given by $\hat{\eta} = \frac{ad}{bc}$ for counts as given in Table 2.1 irrespective of which sampling model (binomial, multinomial, or Poisson) is assumed for the cell counts. For large samples, again under all sampling models, the log odds ratio, $\log(\hat{\eta})$ is asymptotically normal with mean $\log(\eta)$ and estimated standard error $\hat{\sigma}_{\log\hat{\eta}} = (\frac{1}{a} + \frac{1}{b} + \frac{1}{c} + \frac{1}{d})^{1/2}$. Thus, a $100(1 - \alpha)\%$ one-at-a-time large sample confidence interval for the log odds ratio is given by

$$\log(\hat{\eta}) \pm z_{\alpha/2} \hat{\sigma}_{\log(\hat{\eta})}. \quad (2.11)$$

Exponentiating the lower and upper bounds of this interval yields confidence bounds for the odds ratio.

It is common to see one-at-a-time confidence intervals for odds ratios reported along with their point estimates. Suppose a researcher wants to report the estimated odds ratio for a particular patient profile with confidence limits. For example, in the preterm birth example, she may want to report the odds ratio of preterm birth for those exposed to a particular maternal stress factor compared to those with no identifiable maternal stress factors. In this case, the one-at-a-time intervals are appropriate. Alternatively, consider the case where the researcher wants to identify which, if any, of the maternal stress factors or levels of a stress factor are statistically associated with a preterm birth or to identify a set of stress factors or level of a stress

factor whose association with preterm birth is larger than that for no stress factors present. The one-at-a-time intervals will not suffice for these kinds of questions as there are multiple inferences being made. In order to control the type I error rate, a simultaneous estimation procedure should be utilized. Additionally, the researcher may wish to compare the odds of preterm birth for any maternal stress factor to the odds of preterm birth for all other sources of maternal stress. In order to do this, a multiple comparison procedure must also be utilized as the researcher actually wants to compare the probabilities of preterm birth across all the possible sources of maternal stress. It is tempting to make overall conclusions about the odds ratios when reporting estimated odds ratios via one-at-a-time confidence intervals. However, the error rate associated with these overall conclusions based on multiple one-at-a-time intervals is not controlled, or even known. In this case, a method that simultaneously estimates the parameters is warranted.

2.3 Other Quantities

Another quantity frequently reported is the relative risk. The relative risk communicates the risk of developing a disease at one level of the predictor variable relative to another level of the predictor variable. An example of a study employing relative risks is the preterm birth study. In Table 2, the estimated relative risk would be given by $\hat{\gamma} = \frac{a/n_1}{b/n_2}$ where the counts are as in Table 2.1. Suppose a researcher reports that the estimated relative risk of preterm birth is 1.75, given the subject lives in a neighborhood perceived to be dangerous. Thus the proportion of those that experience a preterm birth among those that live in the dangerous neighborhood is estimated to be 1.75 times the proportion of those who experience a preterm birth among those with no identified sources of stress. Again, the log scale is often utilized and large sample derivations show that the log of the sample relative risk, $\log(\hat{\gamma})$ is asymptotically normal with mean $\log(\gamma)$ and estimated standard error $\hat{\sigma}_{\log(\gamma)} = \left(\frac{1-\hat{\pi}_1}{\hat{\pi}_1 n_1} + \frac{1-\hat{\pi}_2}{\hat{\pi}_2 n_2}\right)^{1/2}$

where $\hat{\pi}_i$ for $i = 1, 2$ is the estimated probability of disease among those in group i and n_i is the sample size for group $i = 1, 2$. Thus, the $100(1 - \alpha)\%$ confidence interval for the log relative risk is

$$\log(\hat{\gamma}) \pm z_{\alpha/2} \hat{\sigma}_{\log(\hat{\gamma})}. \quad (2.12)$$

These resulting bounds may be exponentiated in order to obtain confidence limits on the relative risk.

It is sufficient to report an estimated relative risk via a one-at-a-time confidence interval when a researcher only needs to understand how one level of the predictor variable affects the incidence of disease. The preterm birth study reported relative risks and the associated confidence intervals, thus only individual inferences about each source of maternal stress or level of a maternal stress factor relative to the case with no source of stress can be made. However, suppose a researcher wishes to pick out which risk factor or level of a risk factor contributes most to a disease or condition, or obtain ranking information for the sources and levels of maternal stress with respect to risk of disease or condition. As estimation is still also of interest, multiplicity adjustments need to be made to the confidence intervals.

In addition to the relative risk, other quantities should be considered as well. For example, many epidemiological researchers find the attributable proportion a useful measure. Suppose we have a disease and several risk factors for that disease. Then the attributable proportion would be the probability that a diseased individual in the given risk factor has the disease because of that risk factor [2]. This is of interest when there are multiple risk factors for a disease. Thus, this measure is of particular interest in case-control studies where the incidence of disease is related to several risk factors as it allows the researcher to understand how much the disease could be reduced by eliminating a particular risk factor.

One-at-a-time confidence intervals can also be utilized to estimate the attributable proportions. Model-based confidence interval formulas can be computed on the usual

attributable proportion. Often transformations of the relative risk are utilized to compute bounds on the attributable proportion since they can be more efficient asymptotically. However, the MLE-based interval performs adequately [3] and is more easily adjusted for simultaneous inference in the sequel. Thus, a one-at-a-time confidence interval for the attributable proportion, denoted κ , is given by,

$$\hat{\kappa} \pm z_{\alpha/2} \times \text{var}(\hat{\kappa})^{1/2} \quad (2.13)$$

where $z_{\alpha/2}$ is the z critical value that gives $100(1 - \alpha)\%$ confidence. (Details for computing $\text{var}(\hat{\kappa})$ are given in [4].)

Again, this interval is all that is required in many applications. However, if the researcher wishes to compare the attributable proportions for a group of risk factors, an adjustment for multiplicity would be necessary. This might be necessary if, for example, one wished to understand which risk factor should be focused on most for prevention of the disease. Here we would want to identify the largest attributable proportion and focus on disease prevention via reducing the effect of that risk factor.

2.4 Interval Estimation from GLMs

Though we have introduced notation for both linear models and GLMs, the rest of this section focuses on the particular GLMs utilized to illustrate the results in this paper. While the methods derived apply to any GLM, particular attention will be devoted to the logistic and Poisson models due to their applicability and popularity.

2.4.1 Logistic Regression Model

The logistic regression model is widely used in epidemiological and health science applications. The predictor variable in a logistic regression model can be either a single variable or a vector of variables. Thus, let $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ik})$ be a vector of predictor variables for $i = 1, \dots, n$ where n is the total number of observations, and k

is the number of predictor variables. Thus, \mathbf{x}_i is the i^{th} vector of predictor variables. Recall that for qualitative covariates, the \mathbf{x}_i 's would be defined as appropriate indicator variables. For example, in the preterm birth study \mathbf{x}_i could be the maternal stress vector of predictor variables with binary elements indicating the presence of a particular source or level of a source of maternal stress. Thus, if the i^{th} case is a patient exposed only to dangerous neighborhoods as a source of maternal stress, we would code $\mathbf{x}_i = (1, 1, 0, 0, 0, \dots, 0)$ where the first element has a 1 for the intercept term, the second place has a 1 to indicate the presence of stress in the form of a dangerous neighborhood, and the other elements of the vector are 0 indicating the patient was not exposed to the other sources of maternal stress. A logistic regression model assumes that the probability of a success for the i^{th} observation is $\pi(\mathbf{x}_i)$ where

$$\pi(\mathbf{x}_i) = P[Y_i = 1] = \frac{e^{\mathbf{x}_i' \boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i' \boldsymbol{\beta}}} = \frac{e^{\beta_1 x_{i1} + \dots + \beta_k x_{ik}}}{1 + e^{\beta_1 x_{i1} + \dots + \beta_k x_{ik}}}, \quad i = 1, \dots, n. \quad (2.14)$$

The matrix \mathbf{X} , as previously defined, contains information relating to the predicted value, \mathbf{Y} , for the model. Alternatively, we can express this model as

$$\phi(\mathbf{x}_i) = \text{logit}[\pi(\mathbf{x}_i)] = \ln\left[\frac{\pi(\mathbf{x}_i)}{1 - \pi(\mathbf{x}_i)}\right] = \mathbf{x}_i' \boldsymbol{\beta}, \quad i = 1, \dots, n. \quad (2.15)$$

Now let the MLE of $\pi(\mathbf{x}_i)$ be denoted $\hat{\pi}(\mathbf{x}_i)$. We will make the usual assumption that the Y_i random variables are independent and binomially distributed with parameters m_i (assumed known) and $\pi(\mathbf{x}_i)$ given by (2.14), $i = 1, \dots, n$. Thus, $\mathbf{W} = \text{diag}[m_i \pi(\mathbf{x}_i)(1 - \pi(\mathbf{x}_i))]$, $i = 1, \dots, n$ and the asymptotic distribution of the MLE of $\boldsymbol{\beta}$ is given by (2.4). For $\hat{\mathbf{W}} = \text{diag}[m_i \hat{\pi}(\mathbf{x}_i)(1 - \hat{\pi}(\mathbf{x}_i))]$, $i = 1, \dots, n$, the estimated covariance matrix of $\hat{\boldsymbol{\beta}}$ is given by (2.5).

When it is assumed that a logistic regression model is appropriate, the typical quantities of interest are the coefficients of the regression model, or the log odds ratios, β_i , $i = 1, \dots, k$, and the response probabilities, $\pi(\mathbf{x}_i)$. These quantities relate to what was generally referred to as the expected response function. In particular, the

expected response function for a logistic regression model is the response probability since this model assumes binomial sampling.

When considering response probabilities for single experimental units, one-at-a-time confidence intervals seem appropriate. (Confidence intervals provide additional information about the precision of the estimated response probability, so are often preferable to point estimates.) An appropriate confidence interval on the $\text{logit}(\pi(\mathbf{x}_i)) = \mathbf{x}'_i\boldsymbol{\beta}$ is computed by

$$\mathbf{x}'_i\hat{\boldsymbol{\beta}} \pm z_{1-\alpha/2}\hat{\sigma}_{GLM}(\mathbf{x}_i) \quad (2.16)$$

where $z_{1-\alpha/2}$ is a z-percentile and $\hat{\sigma}_{GLM}(\mathbf{x}_i)$ is given by (2.6) with $\hat{\mathbf{W}}$ as previously defined. Let the upper and lower limits of (2.16) be denoted by U_{LOGIT} and L_{LOGIT} , respectively. Then we can apply the anti-logit and obtain bounds on the response probability. Thus, a $100(1 - \alpha)\%$ confidence interval for the response probability is given by

$$\left(\frac{\exp(L_{LOGIT})}{1 + \exp(L_{LOGIT})}, \frac{\exp(U_{LOGIT})}{1 + \exp(U_{LOGIT})} \right). \quad (2.17)$$

Another quantity of interest from a logistic regression model is the odds ratio. One-at-a-time large sample confidence intervals can easily be constructed on the log odds ratios, as they are linear functions of the k logistic regression coefficients, $\boldsymbol{\beta}$. Thus we may utilize the asymptotic multivariate normal distribution of the maximum likelihood estimates of these k logistic regression coefficients, given by (2.4), to obtain large sample confidence intervals for the appropriate odds ratios. For illustration, suppose a particular odds ratio is given by $\exp(\mathbf{c}_i\boldsymbol{\beta})$ for $\mathbf{c}_i = (c_{i1}, \dots, c_{ik})$, a vector of appropriate constants. Then a one-at-a-time large sample confidence interval for this particular odds ratio is given by

$$\left(\exp\{\mathbf{c}_i\hat{\boldsymbol{\beta}} - z_{\alpha/2}\hat{\sigma}_{GLM}(\mathbf{c}_i)\}, \exp\{\mathbf{c}_i\hat{\boldsymbol{\beta}} + z_{\alpha/2}\hat{\sigma}_{GLM}(\mathbf{c}_i)\} \right) \quad (2.18)$$

where $\hat{\sigma}_{GLM}(\mathbf{c}_i)$ is given by (2.6). Typically, in epidemiological applications, the logistic regression model employed for computing the model-based odds ratios utilizes

reference coding. When reference coding, as explained below, is utilized, special care must be taken in interpreting the model-based odds ratios.

2.4.2 Reference Coding for Logistic Regression

If a logistic regression model is employed for a categorical predictor variable, the design coding typically used necessitates that one of the levels of \mathbf{x} be a reference level. Then odds ratios that result from the model coefficients are observed and compared to that reference level. Most often the reference level is a true control, but at times the reference level is arbitrary. When the reference level is informative, we may wish to: (1) estimate all the odds ratios relative to the reference level simultaneously, thereby allowing the researcher to assess the practical significance of any observed difference from the reference level while also providing the ability to evaluate which non-reference levels are significantly greater than or less than the reference level and (2) make comparisons for a pre-specified set of contrasts of the odds ratios. If the reference level is arbitrary, it seems reasonable to simultaneously compute all odds ratios or all odds ratio differences and then emulate one of the two scenarios described above. Again, if we wish to assess the practical significance of any estimates we need to estimate these quantities simultaneously rather than utilize a stepwise procedure. Note that for both above cases, when there is only one categorical predictor variable \mathbf{x} , then all inference procedures performed on the odds ratios resulting from the logistic regression model are equivalent to any similar analysis performed on the crude data in contingency table format. Differences will occur in models with multiple covariates.

The standard method for computing the odds ratios resulting from a logistic regression model using reference coding for the design matrix is to exponentiate the appropriate linear combinations of the estimated regression coefficients. For example, if we have a logit model such as (2.15), where there are k levels for our single predictor variable, then we can utilize the explanatory variables x_1, \dots, x_{k-1} with the covariate

Table 2.2: Examples of Estimated Odds Ratios

$e^{\hat{\beta}_1}$	The odds comparing the first non-reference level to the reference level
$e^{\hat{\beta}_2}$	The odds comparing the second non-reference level to the reference level
\vdots	\vdots
$e^{\hat{\beta}_2 - \hat{\beta}_1}$	The odds comparing the second non-reference level to the first non-reference level
\vdots	\vdots
$e^{\hat{\beta}_k - \hat{\beta}_{k-1}}$	The odds comparing the k^{th} non-reference level to the $(k - 1)^{th}$ non-reference level

vector at the reference level of our predictor variable equal to $\mathbf{0}$, that is, $x_1 = \dots = x_{k-1} = 0$. Thus, x_1, \dots, x_{k-1} would be defined as indicator variables for the $k - 1$ non-reference levels of our predictor variable. When this model is assumed, then we can interpret $e^{\hat{\beta}_1}$ as follows: the odds that $Y = 1$ for the first non-reference level is $e^{\hat{\beta}_1}$ times greater than that for the reference level. Table 2.2 illustrates other estimated odds ratios and their corresponding interpretations. The estimated odds ratios defined in Table 2.2 could then be utilized to construct confidence intervals that would aid in interpreting the model.

2.4.3 Loglinear or Poisson Model

Another model often employed in epidemiological studies is the loglinear model. The loglinear model relates the counts of a Poisson or multinomial distribution to a set of covariates. It may assume the total sample size is random or fixed, depending on whether the model assumes Poisson or multinomial sampling, respectively. For an

$I \times J$ contingency table let $N = I \times J$. Note that the number of cells in a contingency table, N , is distinct from the sample size or number of observations, denoted n , although they can be equal. Whenever the number of observations, n , is fixed, we have multinomial sampling for Y_i , $i = 1, \dots, N - 1$. However, when the sample size n is not fixed, we usually assume Poisson sampling for Y_i , $i = 1, \dots, N$. For ease in notation let $n^* = N - 1$ for multinomial sampling and N for Poisson. Then the loglinear model is

$$\log(\mu(\mathbf{x}_i)) = \mathbf{x}_i' \boldsymbol{\beta}, \quad i = 1, \dots, n^* \quad (2.19)$$

where $E(\mathbf{Y}) = \boldsymbol{\mu} = (\mu(\mathbf{x}_1), \dots, \mu(\mathbf{x}_{n^*}))'$ is the vector of expected counts of the respective cells of the contingency table, \mathbf{x}_i is a $1 \times k$ vector of covariates as described in (2.2), and $\boldsymbol{\beta}$ is a k -dimensional vector of model parameters. A loglinear model may also be expressed as

$$\log(\mu(\mathbf{x}_i)) = \sum_{j=1}^k \beta_j x_{ij}, \quad i = 1, \dots, n^*, \quad (2.20)$$

where each x_{ij} is the covariate value corresponding to β_i for the i^{th} level of \mathbf{Y} , $i = 1, \dots, n^*$, and $j = 1, \dots, k$. Recall the assumption that Y_i is a Poisson or multinomial random variable. Thus, the expectation of any Y_i is a positive value, $\mu(\mathbf{x}_i)$ for $i = 1, \dots, n^*$.

The derivation of the large sample distribution of the model parameters depends on the sampling assumptions. When n is not fixed, we assume Poisson sampling. Then the MLE of $\hat{\boldsymbol{\beta}}$ is asymptotically normal with mean $\boldsymbol{\beta}$ and covariance matrix $\mathbf{V} = (\mathbf{X}' \text{diag}(\boldsymbol{\mu}) \mathbf{X})^{-1}$. Notice that $\mathbf{W} = \text{diag}[\boldsymbol{\mu}]$. Thus, the estimated covariance matrix of $\hat{\boldsymbol{\beta}}$ is given by $\hat{\mathbf{V}} = \text{cov}(\hat{\boldsymbol{\beta}}) = [\mathbf{X}' \text{diag}(\hat{\boldsymbol{\mu}}) \mathbf{X}]^{-1}$. For Poisson sampling, we have,

$$\hat{\boldsymbol{\beta}} \sim N(\boldsymbol{\beta}, (\mathbf{X}' \text{diag}(\boldsymbol{\mu}) \mathbf{X})^{-1}). \quad (2.21)$$

Alternatively, when n , the overall sample size, is fixed we assume multinomial sampling. Typically, under multinomial sampling, we have interest in cell probabilities,

$\hat{\boldsymbol{\pi}} = \hat{\boldsymbol{\mu}}/n$. Here the $\hat{\boldsymbol{\pi}}$ are multivariate normal with mean $\boldsymbol{\pi}$ and covariance matrix $\mathbf{V} = cov(\hat{\boldsymbol{\beta}}) = \{\mathbf{X}'[diag(\boldsymbol{\mu}) - (\boldsymbol{\mu}\boldsymbol{\mu}'/n)]\mathbf{X}\}^{-1} = \{n\mathbf{X}'[diag(\boldsymbol{\pi}) - \boldsymbol{\pi}\boldsymbol{\pi}']\mathbf{X}\}^{-1}$. Notice that $\mathbf{W} = diag(\boldsymbol{\mu}) - (\boldsymbol{\mu}\boldsymbol{\mu}'/n)$. Additionally, the estimated covariance matrix for the regression parameters is given by $\hat{\mathbf{V}} = cov(\hat{\boldsymbol{\beta}}) = \{\mathbf{X}'[diag(\hat{\boldsymbol{\mu}}) - (\hat{\boldsymbol{\mu}}\hat{\boldsymbol{\mu}}'/n)]\mathbf{X}\}^{-1} = \{\mathbf{X}'[diag(\hat{\boldsymbol{\pi}}) - \hat{\boldsymbol{\pi}}\hat{\boldsymbol{\pi}}']\mathbf{X}/n\}^{-1}$ when we have one multinomial sample. Thus for multinomial sampling,

$$\hat{\boldsymbol{\beta}} \sim N(\boldsymbol{\beta}, (\mathbf{X}'[diag(\boldsymbol{\mu}) - (\boldsymbol{\mu}\boldsymbol{\mu}'/n)]\mathbf{X})^{-1}). \quad (2.22)$$

Notice that the asymptotic normality of the parameters holds for both Poisson and multinomial sampling. When Poisson sampling is assumed, the expected response function is the mean cell count, $\boldsymbol{\mu}$. Alternatively, when multinomial sampling is assumed, the expected response function is $\boldsymbol{\pi}$. All inferences on the model parameters or any functions of the model parameters can be made via the asymptotic distributions previously stated. I will focus on the case where Poisson sampling is assumed as it is the customary assumption. Additionally, when Poisson sampling is assumed, the loglinear model is often referred to as a Poisson model. Intervals for response probabilities from multinomial loglinear models could be formed in a manner similar to that described for logistic regression, but this is rarely done with loglinear models. Instead, focus is usually on the estimated relative risks.

When utilizing a loglinear model the relative risk yields point estimates that are often more applicable to clinical situations than the odds ratio; thus we consider relative risk here. The use of the relative risk is very common in epidemiological applications, thus discussion of the relative risk will focus on these types of scenarios. Estimating the relative risk from a loglinear model is a particularly easy implementation since it may be shown that the estimated relative risk is simply $exp(\hat{\beta}_1)$ where $\hat{\beta}_1$ is the slope coefficient for x_1 , the predictor variable indicating presence of the intervention. Other models, such as the logistic model, could be used similarly to estimate the relative risk, although other models do not always yield simple formulas.

Consider for instance, the case where we are estimating the relative risk from a loglinear model. The estimated relative risks would be of the form $exp(\hat{\beta}_j)$ where $\hat{\beta}_j$ is the estimated slope coefficient for the covariate x_j , $j = 1, \dots, k$. Let \mathbf{c}_i be a vector with the j^{th} element equal to 1 and all other elements equal to 0. A confidence band is formed by

$$\left(exp\{\hat{\beta}_j - z_{\alpha/2} \times \hat{\sigma}_{GLM}(\mathbf{c}_j)\}, exp\{\hat{\beta}_j + z_{\alpha/2} \times \hat{\sigma}_{GLM}(\mathbf{c}_j)\} \right)$$

where $\hat{\sigma}_{GLM}(\mathbf{c}_j)$ is given by (2.6) and \mathbf{W} for Poisson sampling is given previously in by equation 2.21.

Other models using alternative canonical links could also be considered. For example, other GLMs are formed by utilizing the probit link, where $g = \Phi^{-1}(\pi(x))$, and the complementary log-log link, where $g = \log(-\log(1 - \pi(x)))$. These both assume a binomial sampling scenario and the usual focus is on the resulting probability of success, $\pi(x)$.

CHAPTER 3

Inferences on Quantities Estimated from a GLM

When utilizing GLMs, several quantities may be of interest. For example, the expected response, odds ratio, or relative risk may be estimated via the GLM. This section focuses on the case where the expected response function is of primary concern. All the methods discussed utilize the fact that GLMs may be expressed as

$$g(E(Y_i|\mathbf{x}_i)) = \mathbf{x}_i'\boldsymbol{\beta} \quad (3.1)$$

where Y_i is the response for the i^{th} observation, $\mathbf{x}_i = (x_{i1}, \dots, x_{ik})$ is the vector of appropriate covariate values for the i^{th} observation, $\boldsymbol{\beta} = (\beta_1, \dots, \beta_k)$ is the vector of parameters, and g is the canonical link. (Specific assumptions and details on this model are given in equations (2.1) and (2.2).)

3.1 Inference on the Mean Response

This section will focus on the response probability or estimated mean response, $\pi(\mathbf{x}_i) = E(Y_i|\mathbf{x}_i)$, $i = 1, \dots, n$ in a GLM assuming binomial or multinomial sampling. Alternatively, if we assume Poisson sampling, we would have interest in the expected cell counts, $\mu(\mathbf{x}_i) = E(Y_i|\mathbf{x}_i)$, $i = 1, \dots, n$. This general methodology can be extended to the Poisson sampling scheme provided our inferences are on $\mu(\mathbf{x}_i)$, rather than $\pi(\mathbf{x}_i)$. Suppose we have a covariate \mathbf{X} with k -dimensional domain \mathcal{J} in a GLM of the form $g(E(Y|\mathbf{x}_i)) = \mathbf{x}_i'\boldsymbol{\beta}$, $i = 1, \dots, n$. Then let $\mathcal{X} \subset \mathcal{J}$ be a compact subset of the domain which is of special interest. The intention of this section is to bound the expected response function, $E(Y|\mathbf{x}_i)$, for all $\mathbf{x}_i \in \mathcal{X}$ using confidence bounds on a

GLM. The subset \mathcal{X} can be a set of the domain that is of special interest or it may be selected to answer a particular question. Discussion is restricted to the case where there is one covariate, but the methodologies may be extended to cases with many covariates. Even in the single covariate case, \mathbf{X} may be a matrix if, for example, the model employs reference coding.

3.1.1 Previous Methods

Two primary approaches for simultaneously estimating the mean response function are discussed. The first is a conventional approach utilizing bounds similar to the well-known Scheffé bounds. The second is a modern approach utilizing solutions referred to as tube-formulas for constructing simultaneous intervals.

Scheffé bounds are a well-known methodology in simultaneous inferences, and are widely applied in linear models and generalized linear models. Some of the regularity conditions necessary for applying Scheffé bounds include that the sample size is sufficiently large and that the domain for the predictor variable is fixed [5]. Under these suitable regularity conditions, the maximum likelihood estimates (MLEs) of a linear model are multivariate normal with mean vector $\boldsymbol{\beta}$ and covariance matrix equal to the inverse of the Fisher information matrix $\sigma_{LM}^2 \mathbf{F}$ where $\mathbf{F} = (\mathbf{X}'\mathbf{X})^{-1}$. (See (2.8) for details on model assumptions.) In a standard regression model, Scheffé bounds are often utilized to obtain simultaneous intervals. These bounds are simultaneous for all $\mathbf{x}_i \in \mathbb{R}^k$ and thus are conservative for any finite set of such comparisons. Alternatively, Casella and Strawderman [6] derived Scheffé-type bounds for a regression model with restrictions assumed on the domain. These intervals are exact for this restricted domain. The advantage of assuming these restrictions is that the usual Scheffé bounds are conservative when the entire domain is not used. Piegorsch and Casella [7] utilized the Casella and Strawderman (CS) method to obtain simultaneous bounds on a logistic regression model. Specifically, they obtained Scheffé-type bounds

on the $\mathbf{x}'_i\boldsymbol{\beta}$ in a logistic regression utilizing a restricted predictor variable domain of rectangular form. The method originally developed by Casella and Strawderman, and later extended by Piegorsch and Casella, is less conservative than the usual Scheffé bounds as it restricts the predictor variable space.

It is desirable at this point to reparameterize the model so that it is in the so-called diagonalized form (Casella and Strawderman [6]). This will simplify the calculations used hereafter. By the Spectral Theorem for symmetric matrices [8], the matrix \mathbf{F} may be decomposed, given that \mathbf{F} is symmetric. Thus, a linear model may be diagonalized by noting that $\mathbf{F} = \mathbf{U}\mathbf{D}\mathbf{U}'$ where $\mathbf{D} = \text{diag}(\lambda_i)$, a diagonal $k \times k$ matrix of the ordered eigenvalues of \mathbf{F} , and $\mathbf{U} = (\mathbf{u}_1, \dots, \mathbf{u}_k)$ is the $k \times k$ matrix of corresponding orthonormal eigenvectors. Now define $\mathbf{Z}_{n \times k} = \mathbf{X}\mathbf{U}\mathbf{D}^{-1/2}$ and $\boldsymbol{\eta}_{k \times 1} = \mathbf{D}^{1/2}\mathbf{U}'\boldsymbol{\theta}$ where $\mathbf{U}\mathbf{U}' = \mathbf{I}$ since each row, \mathbf{u}_i , is orthonormal. Thus,

$$\mathbf{Z}\boldsymbol{\eta} = [\mathbf{X}\mathbf{U}\mathbf{D}^{-1/2}][\mathbf{D}^{1/2}\mathbf{U}'\boldsymbol{\theta}] = \mathbf{X}\mathbf{U}\mathbf{U}'\boldsymbol{\theta} = \mathbf{X}\mathbf{I}\boldsymbol{\theta} = \mathbf{X}\boldsymbol{\theta}$$

where the model may be written as $\mathbf{Y} = \mathbf{Z}\boldsymbol{\eta} + \boldsymbol{\epsilon}$. Note that $\hat{\boldsymbol{\eta}} = \mathbf{D}^{1/2}\mathbf{U}'\hat{\boldsymbol{\theta}}$ is distributed $N_k(\boldsymbol{\eta}, \sigma_{LM}^2\mathbf{I})$, given that (2.4) holds.

The authors Casella and Strawderman [6] consider bounding linear models of the form $Y_i = \mathbf{x}_i\boldsymbol{\theta} + \epsilon_i$ with the usual restrictions on $\boldsymbol{\epsilon}$ (see (2.7)) and with a domain for \mathbf{x}_i of the form $\Omega_{\mathbf{x}_i} = \{\mathbf{x}_i : \sum_{j=1}^r x_{ij}^2 \geq q^2 \sum_{j=r+1}^k x_{ij}^2\}$ where q is a fixed constant. When $r = 1$ these regions are cone-shaped regions, and if $r > 1$ there is no easy visualization of the space. Casella and Strawderman achieve exact results for bounding linear models for domains of this general form. Alternatively, both Casella and Strawderman [6] and Piegorsch and Casella [7] consider a more defined set of interval constraints on \mathbf{X} which are of the form

$$R_{\mathbf{x}_i} = \{a_{11} < x_{i1} < a_{12}, a_{21} < x_{i2} < a_{22}, \dots, a_{k1} < x_{ik} < a_{k2}\} \subset \Omega_{\mathbf{x}_i}$$

for a specified q . These intervals would be of particular interest in many experimental settings and thus are assumed for the remainder of this section.

The goal of the restricted-Scheffé procedure developed by Casella and Strawderman is to bound the regression function for all $\mathbf{x}_i \in \Omega_{\mathbf{x}_i}$. Thus, keeping in mind the objective of inference on $E(Y_i|\mathbf{x}_i) = \mathbf{x}_i'\boldsymbol{\theta}$, consider

$$S(\Omega_{\mathbf{x}_i}) = \{\boldsymbol{\theta} : (\mathbf{x}_i'\hat{\boldsymbol{\theta}} - \mathbf{x}_i'\boldsymbol{\theta})^2 \leq d^2\sigma_{LM}^2\mathbf{x}_i'\mathbf{F}^{-1}\mathbf{x}_i \forall \mathbf{x}_i \in \Omega_{\mathbf{x}_i}\} \quad (3.2)$$

where d is an arbitrary constant. Casella and Strawderman derive a procedure to calculate the value of d that yields,

$$P[S(\Omega_{\mathbf{x}_i})] = 1 - \alpha. \quad (3.3)$$

Their derivation involves considering a domain for \mathbf{Z} similar to $\Omega_{\mathbf{x}_i}$,

$$\Omega_{\mathbf{z}_i} = \{\mathbf{z}_i : \sum_{j=1}^r z_{ij}^2 \geq q^2 \sum_{j=r+1}^k z_{ij}^2\}$$

where q is a fixed constant. Thus, Casella and Strawderman prove that for a specified d

$$P[S(\Omega_{\mathbf{z}_i})] = P\{\boldsymbol{\eta} : (\mathbf{z}_i'\hat{\boldsymbol{\eta}} - \mathbf{z}_i'\boldsymbol{\eta})^2 \leq d^2\sigma_{LM}^2\mathbf{z}_i'\mathbf{z}_i \forall \mathbf{z}_i \in \Omega_{\mathbf{z}_i}\} = 1 - \alpha \quad (3.4)$$

where $\hat{\boldsymbol{\eta}}$ is the MLE under spectral decomposition. Notice that the only difference between the sets $S(\Omega_{\mathbf{x}_i})$ and $S(\Omega_{\mathbf{z}_i})$ is the space we are operating in. Recall the form assumed about the domain of interest, $R_{\mathbf{x}_i}$. This is a convex set in \mathbb{R}^k . Thus, the image of this set, $R_{\mathbf{z}_i}$, will also be convex, since a linear map preserves convexity. Note that for $\boldsymbol{\gamma} = \frac{\hat{\boldsymbol{\eta}} - \boldsymbol{\eta}}{\sigma_{LM}}$, the quantity

$$S(\Omega_{\mathbf{z}_i}) = \{\boldsymbol{\gamma} : (\boldsymbol{\gamma}\mathbf{z}_i)^2 \leq d^2\mathbf{z}_i'\mathbf{z}_i \quad \forall \mathbf{z}_i \in \Omega_{\mathbf{z}_i}\}. \quad (3.5)$$

Assume this form of $S(\Omega_{\mathbf{z}_i})$ henceforth. Since we have a domain of the form $\Omega_{\mathbf{z}_i}$ and wish to obtain a Scheffé-type probability band, then via Theorem 1 in [6] we have

$$P(S(\Omega_{\mathbf{z}_i})) = P(\chi_k^2 \leq d^2) + P(E_{r,s}(b, d^2)) \quad (3.6)$$

where $E_{r,s}(b, d^2) = \{(\chi_r^2, \chi_s^2) : \chi_r^2 + \chi_s^2 \geq d^2, (a\chi_r + b\chi_s)^2 \leq d^2, \chi_r^2 \leq q^2\chi_s^2\}$, $a^2 + b^2 = 1$, and χ_r^2 and χ_s^2 are independent chi-square random variables. Also note that q is a

fixed constant determined by $\Omega_{\mathbf{z}_i}$ and b , r , and s are determined by the value of d and the parameters of the problem. (For specific details see Casella and Strawderman [6].) A solution for the quantity d which yields appropriate simultaneous intervals may be found by setting the right hand side of (3.6) equal to $1 - \alpha$ and solving for d . Casella and Strawderman applied this theorem to a linear model achieving exact results for all $\mathbf{x}_i \in \Omega_{\mathbf{x}_i}$, thus yielding a conservative solution for all $\mathbf{x}_i \in R_{\mathbf{x}_i} \subset \Omega_{\mathbf{x}_i}$. The details of the derivation of the appropriate $\Omega_{\mathbf{z}_i}$ (and hence $\Omega_{\mathbf{x}_i}$) are given by Casella and Strawderman [6]. The resulting restricted-Scheffé intervals are of the form $\hat{Y} \pm d\hat{\sigma}(\mathbf{x}_i)$ where d is a critical value determined by an algorithm which is described in Appendix C.

Piegorsch and Casella applied this procedure specifically to logistic regression. However, it has not been applied for use in a generic GLM, and it is unclear how these bounds will perform for other generalized linear models. Note that although this method is still conservative, it is less conservative than the conventional Scheffé bounds, as it is not applicable for the entire predictor variable space.

As another alternative to the Scheffé-type bounds, Sun, Loader, and McCormick (2000) [9] (SLM) proposed a solution for simultaneously estimating the mean response for the general class of GLMs with all \mathbf{x}_i in a compact set. This general method of bounding a regression function, called simultaneous confidence regions (SCR), can account for a variety of linear and nonlinear models. Specifically, the SCR bounds can be applied when there are heteroscedastic and non-additive error terms, as is the case for many GLMs. The SCR bounds utilize error expansions to approximate the non-coverage probability for a GLM. They are far less conservative than Scheffé solutions and perform exceptionally well for moderate sample sizes.

The SCR bounds are based on applying the so-called tube formula due to Naiman [10] with various possible adjustments. The tube formula provides a lower bound for the coverage probability of a confidence band of a regression function over a specified

closed set. However, the tube-formula assumes the error distribution of the model is normal. Clearly, this is not a valid assumption if we have a GLM, although it does provide a starting point for constructing confidence bounds, as the large sample error distribution is approximately normal. Obviously, this assumption will be problematic for smaller sample sizes.

The basic tube-formula methodology is described by Naiman in his 1986 paper (Naiman [10]). This paper outlines a solution for constructing simultaneous confidence bands on polynomial regression models of the form

$$Y_i = \sum_{j=1}^k \theta_j f_j(x_i) + e_i, \quad i = 1, \dots, n, \quad x_i \in I. \quad (3.7)$$

Here it is assumed that I is a closed interval in \mathbb{R} , that $e_i \sim iidN(0, \sigma_{LM}^2)$ with σ_{LM}^2 unknown, and that θ_j ($j = 1, \dots, k$) are unknown constants. The vector

$$\mathbf{f}(x_i) = (f_1(x_i), \dots, f_k(x_i))'$$

maps from I to \mathbb{R}^k . Naiman's intent is to provide simultaneous confidence bounds on $E(Y_i|x_i) = \boldsymbol{\theta}'\mathbf{f}(x_i)$ for all $\mathbf{x}_i \in \mathbf{I}$ where an estimate $\hat{\boldsymbol{\theta}} = (\hat{\theta}_1, \dots, \hat{\theta}_k)'$ is available such that $\hat{\boldsymbol{\theta}}$ is distributed $N(\boldsymbol{\theta}, \sigma_{LM}^2 \mathbf{F})$ with σ_{LM}^2 unknown, \mathbf{F} known and s_{LM}^2 an independent estimator of σ_{LM}^2 such that $\frac{\nu s_{LM}^2}{\sigma_{LM}^2} \sim \chi_\nu^2$ ($\nu = n - k$).

In order to understand how Naiman derives these bounds, consider alternatively another mapping, γ , from I to the unit sphere S^{k-1} centered at the origin of \mathbb{R}^k , such that γ is piecewise differentiable and

$$\Lambda(\gamma) = \int_I \|\gamma'(x)\| \partial x \quad (3.8)$$

is finite. Since γ maps \mathbf{I} to the unit sphere, S^{k-1} , it will be considered in place of the primary mapping $\mathbf{f}(x_i)$. Specifically, it is the projection of $\mathbf{f}(x_i)$ on S^{k-1} . Note that $\gamma(x) = \|\mathbf{P}\mathbf{f}(x_i)\|^{-1} \mathbf{P}\mathbf{f}(x_i)$ for $x_i \in I$ where \mathbf{P} is a $k \times k$ matrix such that $\mathbf{F} = \mathbf{P}'\mathbf{P}$. The quantity $\Lambda(\gamma)$ is called the path length, as it measures the length of the path, γ , a continuous mapping essentially connecting the points in the image of \mathbf{f} . The

image of the path in S^{k-1} is then denoted by $\Gamma(\gamma) = \{\gamma(x) : x \in I\}$. The goal is to bound Γ with a tube via bounding the $\Lambda(\gamma)$, which equivalently bounds the regression function, $\mathbf{f}(x_i)$, on I as they share the same domain.

Regarding the image of the path function, $\Gamma(\gamma)$, Naiman demonstrates that

$$\mu(\Gamma(\gamma)_{(g)}) \leq \min(F_{k-2,2}[\frac{2(g^{-2}-1)}{k-2}] \times \frac{\Lambda}{2\pi} + \frac{1}{2}F_{k-1,1}[\frac{g^{-2}-1}{k-1}], 1) \quad (3.9)$$

where $g \in [0, 1]$ such that $\Gamma_g = \{\mathbf{u} \in S^{k-1} : c_\Gamma(\mathbf{u}) \geq g\}$ (a set of points in S^{k-1} that surround Γ) with $c_\Gamma(\mathbf{u}) = \sup\{\mathbf{u}'\mathbf{v} : \mathbf{v} \in \Gamma\}$ for any $\mathbf{u} \in S^{k-1}$ and μ is the uniform measure. Naiman then applies these results to obtain confidence bands of the form $\hat{\boldsymbol{\theta}}'\mathbf{f}(x_i) \pm d(\hat{\sigma}_{LM})(\mathbf{f}(x_i)'\mathbf{F}\mathbf{f}(x_i))$. The intervals are formed utilizing the critical value d which is determined by setting

$$1 - \int_0^{1/d} \min(F_{k-2,2}[\frac{2(dt^{-2}-1)}{k-2}] \times \frac{\Lambda}{\pi} + \frac{1}{2}F_{k-1,1}[\frac{dt^{-2}-1}{k-1}], 1) f_T(t) \partial t \quad (3.10)$$

equal to $1 - \alpha$ and solving for d . Here $f_T(t)$ is the density of a random variable T where $rT^2 \sim F_{\nu,r}$.

Utilizing these tube-formula bounds, SLM form simultaneous bounds on the expected response function for a GLM. Recall that Naiman derived these bounds assuming normally distributed residuals. Clearly, generalized linear models only have normally distributed residuals asymptotically. Thus, the tube-formulas were originally applied directly via the asymptotic normality of the residuals to obtain asymptotic simultaneous confidence bands. Modifications were then made to the usual tube-based bounds to improve them for small to moderate sample sizes.

The following description outlines how to apply the tube-formula bounds to GLMs. Let the maximum likelihood estimate (MLE) of a predicted response for a GLM at \mathbf{x}_i be denoted by \hat{Y}_i . Ultimately, the interval desired is of the form

$$I_d(\mathbf{x}_i) = (g^{-1}(\mathbf{x}'_i\hat{\boldsymbol{\beta}} - d\hat{\sigma}_{GLM}(\mathbf{x}_i)), g^{-1}(\mathbf{x}'_i\hat{\boldsymbol{\beta}} + d\hat{\sigma}_{GLM}(\mathbf{x}_i))) \quad \forall \mathbf{x}_i \in \mathcal{X}$$

where $[\hat{\sigma}_{GLM}(\mathbf{x}_i)]^2$ is the asymptotic variance of $\mathbf{x}'_i\hat{\boldsymbol{\beta}}$ and \mathcal{X} is a particular compact

subset of the domain. The tube formulas will enable us to find a value d such that

$$P[g(E(Y_i|\mathbf{x}_i)) \in I_d(\mathbf{x}_i), \text{ for all } \mathbf{x}_i \in \mathcal{X}] \geq 1 - \alpha. \quad (3.11)$$

Applying the tube formula directly to solve for d , yields what SLM term a naive SCR. We will utilize the notation d_{TUBE} to indicate a critical value calculated in this manner. This solution performs adequately when the asymptotic distribution of the residuals is nearly normal. However, this method will not attain the desired confidence level when the sample size is relatively small, as typically the residuals are nonnormal discrete random variables for GLMs. In order to improve the small sample performance, the authors consider some modifications to the tube-formula.

They begin by approximating the sampling distribution of the residual via construction of expansions on the estimated model. This approximation of the sampling distribution will be utilized to obtain a critical point for the confidence interval formula that is adjusted with respect to the bias introduced by the MLEs. Consider the random process $W_n(\mathbf{x}_i) = \frac{g(\hat{Y}_i) - g(E(Y_i|\mathbf{x}_i))}{\hat{\sigma}_G(\mathbf{x}_i)}$ where $\mathbf{x}_i = (x_{i1}, \dots, x_{ik})$ is the i^{th} vector of $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)'$ and $[\hat{\sigma}_G(\mathbf{x}_i)]^2$ is the asymptotic variance of $g(\hat{Y}_i)$. This converges in distribution to a Gaussian random field. Let $W(\mathbf{x}_i)$ be a random variable with the same distribution as the limiting distribution of $W_n(\mathbf{x}_i)$. Then the bias behaves like $|W_n(\mathbf{x}_i) - W(\mathbf{x}_i)|$. This equivalent expression of the bias may be bounded via inverse Edgeworth expansions. SLM propose three corrections that can aid in correcting the bias introduced from estimating the regression parameters in a GLM with MLEs. These three solutions are based on the inverse Edgeworth expansion of the random process given by,

$$|W_n(\mathbf{x}_i)| = |W(\mathbf{x}_i)| - p_2(\mathbf{x}_i, W_n(\mathbf{x}_i)) \quad (3.12)$$

where the term subtracted can be thought of as a correction for the bias of the process. It is based on the centered moments of the process $W_n(\mathbf{x}_i)$ denoted κ_i for $i = 1, 2, 3, 4$

and is given by,

$$\begin{aligned}
p_2(\mathbf{x}_i, Z) = & -Z\left\{\frac{1}{2}[\kappa_2(\mathbf{x}_i) - 1 + \kappa_1^2(\mathbf{x}_i)]\right. \\
& + \frac{1}{24}[\kappa_4(\mathbf{x}_i) + 4\kappa_1(\mathbf{x}_i)\kappa_3(\mathbf{x}_i)](Z^2 - 3) \\
& \left. + \frac{1}{72}\kappa_3^2(\mathbf{x}_i)(Z^4 - 10Z^2 + 15)\right\} = O(n^{-1}). \tag{3.13}
\end{aligned}$$

The κ_i 's may be computed as detailed by Hall(1992, [11]). Details are provided in Appendix D.

The inverse Edgeworth expansions (3.13) are then also utilized to account for the bias typically observed in the MLEs of generalized linear models. A first version of a corrected SCR, denoted SCR1, is a solution where the bias term, $p_2(\mathbf{x}_i, W_n(\mathbf{x}_i))$, is bounded. First consider the supremum of the bias term, $R'_p = \sup_{\mathbf{x}_i \in \mathcal{X}} \{p_2(\mathbf{x}_i, W_n(\mathbf{x}_i))\} = O_p(1/n)$. We want to find a positive constant R'_p such that $P[R'_p \leq r'_p] = 1 - \alpha$ as $n \rightarrow \infty$. Details are given in Sun, Loader, and McCormick [9] and Hall [11]. Additionally, specific calculation procedures are described in Appendix D.

These r'_p values are then used to correct the bias in the choice of d via the tube-formula method. Namely, our new interval is given by

$$\left(g^{-1}(\mathbf{x}'_i \hat{\boldsymbol{\beta}} - d_{SCR1} \hat{\sigma}_{GLM}(\mathbf{x}_i)), g^{-1}(\mathbf{x}'_i \hat{\boldsymbol{\beta}} + d_{SCR1} \hat{\sigma}_{GLM}(\mathbf{x}_i))\right) \tag{3.14}$$

where the new critical point, d_{SCR1} is equal to $d_{TUBE} - |r'_p|$ where d_{TUBE} is the aforementioned solution.

Another version of the corrected SCR, SCR2, considers the modified process, $W_n^0(\mathbf{x}_i) = \frac{W_n(\mathbf{x}_i) - \kappa_1(\mathbf{x}_i)}{\sqrt{\kappa_2(\mathbf{x}_i)}}$, such that $|W_n^0(\mathbf{x}_i)| = |W(\mathbf{x}_i)| - q_2(\mathbf{x}_i, W_n^0(\mathbf{x}_i))$ with q_2 similar to p_2 . The tube formula is then applied to $W_n^0(\mathbf{x}_i)$. Bounding this normalized process, $W_n^0(\mathbf{x}_i)$, further corrects the bias. Doing this results in confidence bounds on the $E(Y_i|\mathbf{x}_i)$ which are an improvement of the tube method applied directly to $W_n(\mathbf{x}_i)$. It is of interest to note that this method corrects the bias via a first level approximation. The resulting confidence region is of the form,

$$\left(g^{-1}(\mathbf{x}'_i \hat{\boldsymbol{\beta}} - d_{SCR2} \hat{\sigma}_{GLM}(\mathbf{x}_i)), g^{-1}(\mathbf{x}'_i \hat{\boldsymbol{\beta}} + d_{SCR2} \hat{\sigma}_{GLM}(\mathbf{x}_i))\right) \tag{3.15}$$

where d_{SCR2} is this bias-corrected solution for the critical value. Note that this is just a critical value, like d , that is corrected for the bias. SLM term this a two-sided corrected SCR. Recall that it utilizes the modified Gaussian process that corrects the bias inherit in the MLE estimates and finds a critical value that adjusts for that bias.

A last solution, called the centered SCR (SCR3), begins by estimating the mean and variance of the Gaussian process $W_n(\mathbf{x}_i)$. These are the centered moments and are given by $\hat{\kappa}_1(\mathbf{x}_i)$ and $\hat{\kappa}_2(\mathbf{x}_i)$, respectively. These essentially move and rescale the confidence region so it is no longer biased. The tube-based critical value d_{TUBE} is again involved, so the final interval is

$$\left(g^{-1}((\mathbf{x}'_i \hat{\boldsymbol{\beta}})^* - d_{TUBE} \hat{\sigma}_i^*), g^{-1}((\mathbf{x}'_i \hat{\boldsymbol{\beta}})^* + d_{TUBE} \hat{\sigma}_i^*) \right) \quad (3.16)$$

where $(\mathbf{x}'_i \hat{\boldsymbol{\beta}})^* = \mathbf{x}'_i \hat{\boldsymbol{\beta}} - \hat{\kappa}_1(\mathbf{x}_i) \hat{\sigma}_{GLM}(\mathbf{x}_i)$ and $\hat{\sigma}_i^* = \hat{\sigma}_{GLM}(\mathbf{x}_i) \sqrt{\hat{\kappa}_2(\mathbf{x}_i)}$. These formulas are given in Appendix D.

3.1.2 Proposed Methods

Expanding on the methodologies presented in the previous section, I have developed two new approaches for estimating a mean response function over a specified compact set via confidence regions.

The first proposed method is based on the restricted-Scheffé bounds developed by Casella and Strawderman and further refined by Piegorsch and Casella. In Piegorsch and Casella [7], the authors derive and implement conservative simultaneous bounds on the response probabilities of logistic regression models for rectangular domains. I have generalized these bounds on the expected response function for any GLM. Outlined below is the method by which these bounds may be computed.

For any GLM, let the anti link function be g^{-1} so that

$$E(Y_i | \mathbf{x}_i) = g^{-1}(\mathbf{x}'_i \boldsymbol{\beta}), \quad i = 1, \dots, n \quad (3.17)$$

where $E(Y_i | \mathbf{x}_i)$ denotes the response probability (logistic regression) or the mean

response (loglinear models or Poisson regression) for the specified covariate levels given by \mathbf{x}_i (Complete model specifications are given in (2.2)). Recall that the MLE of $\boldsymbol{\beta}$, $\hat{\boldsymbol{\beta}}$, is asymptotically normal with mean $\boldsymbol{\beta}$ and $k \times k$ covariance matrix \mathbf{V} where $\mathbf{V} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}$ with \mathbf{W} defined in (2.3).

Applying the restricted-Scheffé procedure of Casella and Strawderman to GLMs yields appropriate conservative simultaneous confidence intervals for the mean response. Casella and Strawderman assumed that the MLEs of the regression parameters were normally distributed with a specified mean vector and covariance matrix. For our case we only have asymptotic normality of the MLEs and therefore, the probability in (3.6) is not exactly $1 - \alpha$ but instead converges to $1 - \alpha$ as $n \rightarrow \infty$. We will also require a slightly different definition for $S(\Omega_{\mathbf{x}_i})$ and $S(\Omega_{\mathbf{z}_i})$. Recall $S(\Omega_{\mathbf{x}_i}) = \{\boldsymbol{\theta} : (\mathbf{x}'_i\hat{\boldsymbol{\theta}} - \mathbf{x}'_i\boldsymbol{\theta})^2 \leq d^2\sigma_{LM}^2\mathbf{x}'_i\mathbf{F}^{-1}\mathbf{x}_i \ \forall \mathbf{x}_i \in \Omega_{\mathbf{x}_i}\}$ for linear models. Here however $S(\Omega_{\mathbf{x}_i}) = \{\boldsymbol{\beta} : (\mathbf{x}'_i\hat{\boldsymbol{\beta}} - \mathbf{x}'_i\boldsymbol{\beta})^2 \leq d^2\mathbf{x}'_i\mathbf{V}^{-1}\mathbf{x}_i \ \forall \mathbf{x}_i \in \Omega_{\mathbf{x}_i}\}$. Notice that the inequalities in both sets have an upper bound given by the variance of $\mathbf{x}'_i\hat{\boldsymbol{\beta}}$ or $\mathbf{x}'_i\hat{\boldsymbol{\theta}}$, respectively. $S(\Omega_{\mathbf{z}_i})$ will have a similar definition for GLMs and the diagonalization described in section 4.1 applies with $\mathbf{F} = \mathbf{V}$. Thus, for any $S(\Omega_{\mathbf{z}_i})$ of the form (3.5) generalized appropriately for a GLM,

$$P(S(\Omega_{\mathbf{z}_i})) \rightarrow P(\chi_k^2 \leq d^2) + P(E_{r,s}(b, d^2)) \quad (3.18)$$

as $n \rightarrow \infty$ where

$$E_{r,s}(b, d^2) = \{(\chi_r^2, \chi_s^2) : \chi_r^2 + \chi_s^2 \geq d^2, (a\chi_r + b\chi_s)^2 \leq d^2, \chi_r^2 \leq q^2\chi_s^2\}, \quad (3.19)$$

where $a^2 + b^2 = 1$ and χ_r^2 and χ_s^2 are independent chi-square random variables. Note that q is a fixed constant determined by the particular $\Omega_{\mathbf{x}_i}$. (Recall we will choose the smallest $\Omega_{\mathbf{x}_i} \supset R_{\mathbf{x}_i}$.) Additionally, the constants b , r , and s are determined by the value of d and the parameters of the problem. (Details of the computation of b , r , and s specifically for GLMs are given in Appendix C.) Notice that the coverage probability of the set $S(\Omega_{\mathbf{z}_i})$ is the sum of the usual coverage probability of the Scheffé

set ($P(\chi_p^2 \leq d^2)$) and a probability that adjusts for the restricted domain. Recall that these bounds are derived assuming a domain of the form $\Omega_{\mathbf{x}_i}$. If a set of the form $R_{\mathbf{x}_i}$ is of interest, an approximate answer may still be found as in Piegorsch and Casella. In order to find a bound for a domain of the form $R_{\mathbf{x}_i}$, the smallest set of the form $\Omega_{\mathbf{x}_i}$ is established such that $\Omega_{\mathbf{x}_i}$ contains $R_{\mathbf{x}_i}$. (This procedure is detailed in Appendix C.) We may consider sets on either the \mathbf{X} domain, $\Omega_{\mathbf{x}_i}$ and $R_{\mathbf{x}_i}$, or their equivalent sets on the \mathbf{Z} domain, $\Omega_{\mathbf{z}_i}$ and $R_{\mathbf{z}_i}$.

Recall that the method of Casella and Strawderman provides simultaneous bounds on a linear model for a transformed domain of the form $\Omega_{\mathbf{z}_i}$, and thus equivalently for $\Omega_{\mathbf{x}_i}$. The adapted method of Piegorsch and Casella computes these bounds for domains of the form $R_{\mathbf{x}_i}$ in logistic regression models. I propose extending these bounds for use in any generalized linear model with a canonical link. The simultaneous bounds may be transformed from $\mathbf{x}'_i \boldsymbol{\beta}$, $\mathbf{x}_i \in R_{\mathbf{x}_i}$, to the expected response function via the anti-link function.

In order to apply the Casella-Strawderman results to GLMs, we must first show that the probability of the set $S(\Omega_{\mathbf{x}_i})$ converges to $1 - \alpha$.

Corollary 3.1 *If $\hat{\boldsymbol{\beta}}$ is asymptotically normal with mean vector $\boldsymbol{\beta}$ and covariance matrix \mathbf{V} , then*

$$P(S(\Omega_{\mathbf{z}_i})) \rightarrow P(\chi_k^2 \leq d^2) + P(E_{r,s}(b, d^2)) \quad \text{as } n \rightarrow \infty. \quad (3.20)$$

with $E_{r,s}(b, d^2)$ given by (3.19) where q is determined by the particular $\Omega_{\mathbf{z}_i}$ considered and appropriate constants b , r , and s .

Proof: Recall $\Omega_{\mathbf{z}_i} = \{\mathbf{z}_i : \sum_{j=1}^r z_{ij}^2 \geq q^2 \sum_{j=r+1}^k z_{ij}^2\}$ for a specified constant q . Here \mathbf{z}_i is the diagonalized form of \mathbf{x}_i . Theorem 1 from Casella and Strawderman [6] gave exact equality of the same probabilities in (3.20) under exact normality for $\hat{\boldsymbol{\beta}}$. Consequently, under asymptotic normality we have (3.20). \square

Unfortunately (3.20) requires \mathbf{V} known. Consider the following corollary to the Casella and Strawderman theorem, that holds for GLMs.

Corollary 3.2 *If $\hat{\boldsymbol{\beta}}$ is asymptotically normal with mean vector $\boldsymbol{\beta}$ and covariance matrix \mathbf{V} , estimated by $\hat{\mathbf{V}}$, then for $S(\Omega_{\mathbf{z}_i})$ utilizing $\hat{\mathbf{V}}$ instead of \mathbf{V} (3.20) still holds.*

Proof: Let $\hat{\mathbf{V}} = (\mathbf{X}'\hat{\mathbf{W}}\mathbf{X})^{-1}$ then since $\hat{\boldsymbol{\beta}} \xrightarrow{p} \boldsymbol{\beta}$ we have $\hat{\mathbf{W}} = \mathbf{W}|_{\boldsymbol{\beta}=\hat{\boldsymbol{\beta}}} \xrightarrow{p} \mathbf{W}$. Thus $\hat{\mathbf{V}} = (\mathbf{X}'\hat{\mathbf{W}}\mathbf{X})^{-1} \xrightarrow{p} \mathbf{V} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}$. Consequently the convergence in (3.20) also holds when \mathbf{V} is estimated by $\hat{\mathbf{V}}$. \square

Now let d_{CS} be the value of d such that the probability on the right-hand side of (3.20) is $1 - \alpha$. Then

$$P(g^{-1}(\mathbf{x}'_i\hat{\boldsymbol{\beta}} - |d_{CS}|\hat{\sigma}_i^*) \leq E(Y_i|\mathbf{x}_i) \leq g^{-1}(\mathbf{x}'_i\hat{\boldsymbol{\beta}} + |d_{CS}|\hat{\sigma}_i^*)) \rightarrow 1 - \alpha \quad \text{as } n \rightarrow \infty \quad (3.21)$$

where $\hat{\sigma}_i^* = (\mathbf{x}'_i\hat{\mathbf{V}}^{-1}\mathbf{x}_i)^{1/2}$.

We have theoretically demonstrated that the restricted-Scheffé bounds of Casella and Strawderman may be applied to GLMs, but the computational details remain unclear. A detailed computational algorithm to compute the restricted-Scheffé bounds for any GLM is given in Appendix C.

As an alternative to the restricted-Scheffé bounds, we can also apply an estimate of $\boldsymbol{\beta}$, $\hat{\boldsymbol{\beta}}^*$ to the simultaneous confidence regions (SCRs) developed by SLM [9] and the restricted-Scheffé bounds for GLMs. Recall that SLM derived four SCR bounds. First, the tube-based bounds were applied to the maximum likelihood estimators by appealing to their asymptotic normal distribution (d_{TUBE}). Second, the bias was bounded and then the tube-formula solution was applied (d_{SCR1}). Third, the SCR bounds were derived for a modified process which accounts for the bias in the distribution of the MLE (d_{SCR2}). And fourth, the random process was centered and rescaled to correct the bias before applying the tube-based bounds (centered SCR). The vari-

ous solutions all attempt to correct the bias of the maximum likelihood estimates for GLMs. In particular, when the sample size is small the MLEs are highly nonnormal, and the adjustments to the tube formulas are especially helpful. I propose estimating simultaneous SCR bounds, and restricted-Scheffé bounds, that are not based on the MLE, but on an alternative to the MLE, the penalized maximum likelihood estimator (pMLE). The pMLE is a bias-corrected estimate that is closely related to the usual MLE. The tube-formula bounds can then be applied utilizing the pMLE estimates rather than the MLEs. In particular, the naive SCR and centered SCR (SCR3) bounds can easily be applied. The difference between the proposed method and the methods of Sun et al. (2000) [9] is that utilizing the pMLE estimates doesn't merely "correct" the bias, but prevents the bias from occurring (in the first order) a priori. No additional bias correcting procedures will be necessary since the pMLE estimate has little bias from the start. Additionally, this method eliminates inestimable model parameters (0 or ∞) due to zero cell counts in GLMs. This difficulty was not resolved by the methodologies presented by SLM, and can be particularly troublesome with small to moderate sample sizes. Also, recall that the bias corrections employed in some of the SCR bounds were only bias-reducing asymptotically. This procedure is bias-reducing for any sample size.

The penalized maximum likelihood estimate (pMLE) was developed by David Firth [12] as an alternative to the MLE. Firth developed these estimators for use in models, such as GLMs, where the typical MLE is known to be a biased estimate. Specifically, all of the derivations depend on the model belonging to the general exponential class. These distributions have the general form

$$f(t, \theta) = \exp\{[(t\theta - K(\theta))/a(\phi) + c(t, \phi)]\}, \quad (3.22)$$

where when ϕ , the dispersion parameter, is known, this simplifies to

$$f(t, \theta) = \exp\{(t\theta - K(\theta))\}$$

[13]. Although this is an unusual form for an exponential class model, it lends itself quite well to a derivation later in the section, and this form can be shown to be equivalent to the standard form under the correct reparameterization. The general pMLE procedure involves penalizing the score function via the Jeffreys invariant prior for the particular parameter of interest. This penalty yields estimates of the regression parameters that are unbiased in the first-order. Typically, when computing an MLE, the first derivative of the log likelihood, often called the score function, is computed and set equal to 0, yielding the MLE as the solution. For estimating a set of parameters $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k)$, let the usual vector of score functions be denoted $\mathbf{U}(\boldsymbol{\theta}) = (U_1(\boldsymbol{\theta}), \dots, U_k(\boldsymbol{\theta}))'$. Note that $U_r(\boldsymbol{\theta})$ is the derivative of the log-likelihood (score function) with respect to the r^{th} parameter. Firth proposes shifting the score function to correct the bias present in most MLE estimates for GLMs. The shift is determined by the estimated bias, $b(\boldsymbol{\theta})$ and information matrix, $i(\boldsymbol{\theta})$. Then the shifted or penalized score function, $\mathbf{U}^*(\boldsymbol{\theta}) = \mathbf{U}(\boldsymbol{\theta}) - i(\boldsymbol{\theta})b(\boldsymbol{\theta}) = (U_1^*(\boldsymbol{\theta}), \dots, U_k^*(\boldsymbol{\theta}))'$ is set equal to $\mathbf{0}$ and a penalized MLE is the solution. Thus, the pMLE, $\boldsymbol{\theta}^*$, is the solution to $\mathbf{U}^*(\boldsymbol{\theta}) = \mathbf{0}$. The details of estimating the bias are given in Firth [12], but as previously noted, the calculations are based on utilizing a Jeffreys prior for the parameters of interest, $\boldsymbol{\theta}$. Firth applies this estimator to the logistic regression model, but the methodology can be applied to any exponential class model, specifically any GLM. Firth states that for a GLM with a canonical link the modified score function is given by

$$U_r^*(\boldsymbol{\theta}) = U_r(\boldsymbol{\theta}) + \frac{1}{2\phi} \sum_{i=1}^n \left(\frac{\kappa_{3i}}{\kappa_{2i}} \right) h_i x_{ir}, \quad (r = 1, \dots, k), \quad (3.23)$$

where $U_r(\boldsymbol{\theta})$ is the derivative of the log likelihood function for the r^{th} parameter, n is the number of observations Y_i , ϕ is the dispersion parameter in (3.22), and h_i is the i^{th} diagonal of the hat matrix (the leverage). The leverage, or the i^{th} diagonal of the hat matrix, is a measure of the distance between each observation, x_{ir} , and the mean, \bar{x} . (See McCullough and Nelder [13] for an explicit definition.) Additionally, κ_{ti} is the

t^{th} ($t = 2, 3$) cumulant, or t^{th} central moment, of Y_i , $i = 1, \dots, n$. The cumulants may be calculated using the cumulant generating function $K_i(s) = \log(M_i(s))$ where $M_i(s)$ is the moment generating function for the distribution of the dependent variable, Y_i . Each cumulant is found by taking the derivative of $K_i(s)$ with respect to s and then letting $s = 0$. For example, $\kappa_{2i} = K_i^{(2)}(0)$ where $K_i^{(2)}(s)$ is the second derivative of the cumulant generating function. Note that the third cumulant, κ_{3i} , estimates the bias. Justification for this formula is outlined by McCullough and Nelder (1989) [13] in section 15 of *Generalized Linear Models*. Specifically, assume a binomial logit model has a response variable $Y_i \sim BIN(m_i, \pi_i)$, $i = 1, \dots, n$ where m_i , $i = 1, \dots, n$ are assumed known and the Y_i variables are independent. Notice that in this scenario $k = n$. Thus, the moment generating function is given by $M_i(s) = (\pi_i e^s + (1 - \pi_i))^{m_i}$. Moreover, the cumulant generating function would be $K_i(s) = m_i \log(\pi_i e^s + (1 - \pi_i))$. Thus, the first, second, and third derivatives of the cumulant generating function are given by

$$K_i'(s) = \frac{m_i \pi_i e^s}{\pi_i e^s + (1 - \pi_i)},$$

$$K_i^{(2)}(s) = \frac{m_i \pi_i e^s}{\pi_i e^s + (1 - \pi_i)} - \frac{m_i \pi_i^2 e^{2s}}{(\pi_i e^s + (1 - \pi_i))^2},$$

and

$$K_i^{(3)}(s) = \frac{m_i \pi_i e^s}{\pi_i e^s + (1 - \pi_i)} - \frac{3m_i \pi_i^2 e^{2s}}{(\pi_i e^s + (1 - \pi_i))^2} + \frac{m_i \pi_i^3 e^{3s}}{(\pi_i e^s + (1 - \pi_i))^3},$$

respectively. Consequently, the second and third cumulants are $\kappa_{2i} = m_i \pi_i (1 - \pi_i)$ and $\kappa_{3i} = m_i \pi_i (1 - \pi_i) (1 - 2\pi_i)$. Additionally, the likelihood function is given by $L(\pi_i) = \pi_i^{y_i} (1 - \pi_i)^{m_i - y_i}$, $i = 1, \dots, n$. Thus, the usual score function, the first derivative of the log likelihood is given by $U_r(\boldsymbol{\pi}) = \sum_{i=1}^n (y_i - m_i \pi_i) x_{ir}$, $r = 1, \dots, n$.

Therefore, the penalized score function is

$$U_r^*(\boldsymbol{\pi}) = \sum_{i=1}^n (y_i - m_i \pi_i) x_{ir} + \frac{1}{2\phi} \sum_{i=1}^n (1 - 2\pi_i) h_i x_{ir}, \quad r = 1, \dots, n. \quad (3.24)$$

In the case of a single binomial trial, the dispersion parameter is $\phi = 1/1 = 1$ (McCullough and Nelder (1989) [13]). Thus, (3.24) simplifies to,

$$U_r^*(\boldsymbol{\pi}) = \sum_{i=1}^n \left\{ \left(y_i + \frac{h_i}{2} \right) - (h_i + m_i) \pi_i \right\} x_{ir}$$

for $r = 1, \dots, n$.

Note that in models with no bias present in the MLE, such as a simple linear regression model, the score function will not be penalized as the third cumulant will be zero.

Now we may apply the tube-formula confidence bounds to the penalized MLEs, rather than the MLEs. All calculations will follow the previous SCR interval descriptions since the information matrix of the pMLEs is the usual information matrix of the MLEs (See Firth (1993) [12]). Consequently no alteration of the methodology is necessary. We are simply replacing $\hat{\boldsymbol{\beta}}$ with the pMLE of $\hat{\boldsymbol{\beta}}$, $\hat{\boldsymbol{\beta}}^*$. We do not need to consider the first two SCR methods as they were adjusting for the bias. Rather, we will simply consider the critical value d_{TUBE} applied to the pMLE $\hat{\boldsymbol{\beta}}^*$. Additionally, the centered SCR could be applied with possible improvement as this interval is re-centered and re-scaled. The CS bounds can also be calculated utilizing $\hat{\boldsymbol{\beta}}^*$ instead of $\hat{\boldsymbol{\beta}}$. We refer to this as the pCS bounds in the sequel. No other modifications will be necessary.

We will refer to our SCR bounds utilizing the pMLEs as bias prevented SCRs, or pSCRs. The first of these is given by

$$(g^{-1}(\mathbf{x}'_i \hat{\boldsymbol{\beta}}^* - d_{TUBE} \hat{\sigma}(\mathbf{x}_i)), g^{-1}(\mathbf{x}'_i \hat{\boldsymbol{\beta}}^* + d_{TUBE} \hat{\sigma}(\mathbf{x}_i))), \quad i = 1, \dots, n \quad (3.25)$$

where $\hat{\boldsymbol{\beta}}^*$ is a penalized maximum likelihood estimate, $\hat{\sigma}(\mathbf{x}_i)$ is given by (2.6), and d_{TUBE} is obtained as described in section 3.1.1. The Casella-Strawderman results

could also be applied to an interval of the form (3.25) with d_{TUBE} replaced by d_{CS} , where d_{CS} is obtained as described in section 3.1.1. Finally, the centered SCR may be utilized to yield the second pSCR. This interval is of the form

$$\left(g^{-1}((\mathbf{x}'_i \hat{\boldsymbol{\beta}})^* - d_{pSCR2}), g^{-1}((\mathbf{x}'_i \hat{\boldsymbol{\beta}})^* + d_{pSCR2}) \right), \quad i = 1, \dots, n \quad (3.26)$$

for $(\mathbf{x}'_i \hat{\boldsymbol{\beta}})^* = \mathbf{x}'_i \hat{\boldsymbol{\beta}}^* - \hat{\kappa}_1^*(\mathbf{x}_i) \sqrt{\mathbf{x}'_i \hat{\mathbf{V}} \mathbf{x}_i}$ and $d_{pSCR2} = d_{TUBE} \sqrt{\mathbf{x}'_i \hat{\mathbf{V}} \mathbf{x}_i \hat{\kappa}_2^*(\mathbf{x}_i)}$ where $\hat{\kappa}_1^*(\mathbf{x}_i)$ and $\hat{\kappa}_2^*(\mathbf{x}_i)$ are now based on the estimator $\hat{\boldsymbol{\beta}}^*$. The formulas for these moments of the Gaussian field are given in Appendix D.

Since $\hat{\boldsymbol{\beta}}^*$ attempts to eliminate the bias, it is reasonable to expect that the confidence regions based on this estimator will attain the desired level of confidence for smaller sample sizes than the SCR bounds of SLM. The pSCR bounds for moderate to large samples should be very similar to SLM's corrected and centered SCR bounds.

3.2 Bounds for Simultaneously Estimating Functions of Model

Parameters

Often an estimate of something other than the expected response, whether a probability or a mean, is desired. In previous sections, quantities such as the odds ratio, relative risk, and attributable proportion were discussed. Odds ratios or relative risks have immediate clinical application and are often easier for non-statisticians to understand than expected responses. As discussed previously, all of these quantities may be estimated directly from the data. However, it is preferable at times to estimate these quantities via generalized linear models. Specifically, these quantities may all be expressed as functions of the parameters of GLMs. Consequently, it is possible to utilize all of the methodologies discussed in section 3.1 to simultaneously estimate quantities such as the odds ratio or relative risk. In this section I propose methods that utilize these simultaneous bounds for GLMs to estimate quantities such as odds ratios, thereby accounting for multiplicity of inference. Since the odds ratio, relative

risk, and attributable proportion were described previously, I will not review these quantities. Rather we begin by reviewing some relevant methods for simultaneous estimation.

3.2.1 Previous Methods

When quantities such as the odds ratios or relative risks are of interest, we are often utilizing discrete random variables to predict a binary response variable. While it is possible to have continuous predictors and compute quantities such as the odds ratio, the use and application of the odds ratio in these situations is less obvious and the need for multiplicity is less apparent. Consequently, attention will first focus on the case of categorical predictors.

Researchers have previously explored simultaneous estimation of various sets of the parameters. For example, in 1996, McCann and Edwards [14] proposed a procedure to simultaneously estimate p contrasts of k unknown parameters. This method utilizes Naiman's Inequality, discussed previously, to obtain conservative simultaneous confidence regions for the p contrasts of interest. These new bounds outperform the existing competing conservative bounds for many scenarios. However, the McCann-Edwards (ME) method applied only to linear models in general. I propose adapting the SCR and related bounds from section 3.1 to simultaneously bound p contrasts of k unknown parameters from generalized linear models in an analogous manner. First, I will review the ME method for linear models, and then detail the proposed method for GLMs.

Assume we have a regression model of the form,

$$\mathbf{Y} = \mathbf{X}'\boldsymbol{\theta}$$

where \mathbf{Y} is a $n \times 1$ vector of responses, \mathbf{X} is a $k \times n$ matrix of predictor variables, and $\boldsymbol{\theta}$ is a $k \times 1$ vector of regression parameters as described by (2.7). Assume that

the MLE for $\boldsymbol{\theta}$, $\hat{\boldsymbol{\theta}}$, is asymptotically multivariate normal with mean $\boldsymbol{\theta}$ and covariance matrix $\sigma_{LM}^2 \mathbf{F}$ with \mathbf{F} assumed known and full rank. Also assume that an estimate for σ_{LM}^2 exists and is given by $\hat{\sigma}_{LM}^2$ where $\hat{\sigma}_{LM}^2$ is independent of $\hat{\boldsymbol{\theta}}$ and is such that $\frac{\nu \hat{\sigma}_{LM}^2}{\sigma_{LM}^2} \sim \chi_\nu^2$. Thus, we have k unknown parameters to estimate via the usual MLE, $\hat{\boldsymbol{\theta}} = (\hat{\theta}_1, \hat{\theta}_2, \dots, \hat{\theta}_k)$. Now suppose p linear combinations of the regression parameters are of interest. Let \mathbf{C} be a $p \times k$ matrix of constants such that $\mathbf{C}\boldsymbol{\theta}$ is a vector of these linear combinations of $\boldsymbol{\theta}$. Now, given the distributional assumptions on $\hat{\boldsymbol{\theta}}$, $\mathbf{C}\hat{\boldsymbol{\theta}}$ is multivariate normal with mean $\mathbf{C}\boldsymbol{\theta}$ and covariance matrix $\sigma_{LM}^2 \mathbf{CFC}'$. Thus, if a single contrast is given by $\mathbf{c}'_j \boldsymbol{\theta}$ where $\mathbf{C} = (\mathbf{c}_1, \dots, \mathbf{c}_p)'$ and each $\mathbf{c}'_j = (c_{j1}, \dots, c_{jk})$, then we can form exact simultaneous interval estimates for each contrast via the following formula:

$$\mathbf{c}'_j \hat{\boldsymbol{\theta}} \pm d \hat{\sigma}_j, \quad j = 1, \dots, p \quad (3.27)$$

where $\hat{\sigma}_j = \hat{\sigma}_{LM} (\mathbf{c}'_j \mathbf{F} \mathbf{c}_j)^{1/2}$ and d is a p -dimensional multivariate t quantile with ν degrees of freedom and correlation matrix \mathbf{R} , with \mathbf{R} the correlation matrix corresponding to \mathbf{CFC}' . The path length inequality proposed by McCann and Edwards provides a conservative solution for d that outperforms the existing conservative solutions in many cases. Note that their solution only provides conservative intervals, as obtaining the multivariate- t quantile providing an exact interval is generally an intractable problem. The following theorem given by McCann and Edwards (1996) in [14] details this solution.

Theorem 3.1 *Let \mathbf{T} have a p -dimensional multivariate- t distribution with degrees of freedom ν and underlying correlation matrix \mathbf{R} of rank r . The probability*

$$P(|T_j| \leq d, \quad j = 1, \dots, p)$$

is bounded below by the expression

$$1 - \int_0^{1/d} \min(F_{r-2,2}[(s((dt)^{-2} - 1))/(r-2)] \times (\Lambda/\pi) + F_{r-1,1}[(dt)^{-2} - 1]/(r-1), 1) f_{\mathbf{T}}(t) dt,$$

with

$$\Lambda = \sum_{j=1}^{p-1} \cos^{-1}(|r_{j,j+1}|),$$

where $F_{m,n}$ is the distribution function of an F random variable with m and n degrees of freedom and f_T is the density function of a random variable T such that $rT^2 \sim F_{\nu,r}$. If d is such that the foregoing expression is at least $1 - \alpha$, then the intervals (3.27) will be conservative simultaneous $(1 - \alpha)100\%$ confidence intervals.

This inequality determines a value of d that depends on the correlation structure \mathbf{R} and the path length Λ . The path length also depends on the ordering of the indices $1, 2, \dots, p$ and yields the smallest value of d for the optimum ordering. ME recommend estimating the optimum ordering via the nearest neighbor algorithm (Townsend, 1987) as no exact solution exists and this method often provides the optimum ordering. It is noted that as the path length function approaches either infinity or zero the value of d becomes $(rF_{\alpha,r,\nu})^{1/2}$ (Scheffé's critical value) or $t_{\alpha/2,\nu}$ (the one-at-a-time critical value), respectively. Simulations show that when the degrees of freedom are low and the number of comparisons are high, the ME method outperforms other existing conservative solutions. Note that the ME method has simply applied Naiman's inequality to an interval and parameterization carefully chosen to contain the quantities of interest.

However, the ME method is only strictly valid for linear models. I propose adapting the SCR bounds and their counterparts for generalized linear models in an analogous manner in order to make simultaneous inference on linear combinations of the parameters from GLMs, such as odds ratios or relative risks.

3.2.2 Proposed Methods

In order to estimate the linear combinations of the GLM parameters, I propose applying the SCR and PC methodologies in a fashion similar to the ME bounds. Recall that the only requirement for applying the SCR-type bounds is normality of the

regression parameter estimates, which is true asymptotically for GLMs. Application of these bounds to various quantities of interest are outlined in detail below.

3.2.2.1 A General Set of Comparisons of the Model Parameters

Consider the general setup and estimators for GLMs presented in Chapter 2. In section 3.1 the SCR bands were applied to GLMs to estimate the expected response function simultaneously over a closed set \mathcal{X} . Now these bounds, along with the pSCR, CS, and pCS bounds, may be applied to simultaneously estimate a set of p linear combinations of the regression parameters from a GLM. These linear combinations will each be of the form $\mathbf{c}'_j\boldsymbol{\beta}$ where \mathbf{c}_j is a $k \times 1$ vector for $j = 1, \dots, p$. Let $\mathbf{C} = (\mathbf{c}_1, \dots, \mathbf{c}_p)'$ be a $p \times k$ matrix. Thus $\mathbf{C}\boldsymbol{\beta}$ is a vector of the p linear combinations of interest. Utilizing the SCR methodologies, we have that the expected response function is simultaneously estimated by bounds with at least $100(1 - \alpha)\%$ coverage $\forall \mathbf{x}_i \in \mathcal{X}$. As the results detailed in section 3.1 can be applied to simultaneously estimate the expected response function, they can be applied to \mathcal{X} to obtain simultaneous intervals on $g^{-1}(\mathbf{c}'_j\boldsymbol{\beta})$ provided $\mathbf{c}_j \in \mathcal{X}$ for $j = 1, \dots, p$. This interval may then be transformed to obtain simultaneous bounds on the $\mathbf{c}'_j\boldsymbol{\beta}$ via the link g . Generally, the bounds will be of the form

$$\mathbf{c}'_j\hat{\boldsymbol{\beta}} \pm d \times \hat{\sigma}_{GLM}(\mathbf{c}_j), \quad j = 1, \dots, p \quad (3.28)$$

where $\hat{\sigma}_{GLM}(\mathbf{c}_j)$ is given by (2.6). The following theorems detail the use of the aforementioned critical values to obtain $100(1 - \alpha)\%$ coverage for a fixed set of p linear combinations of the parameters. Note that we will have eight possible solutions for confidence bands on a fixed set of p linear combinations of the parameters since the usual CS, the pCS, the four SCR, and the two pSCR intervals may all be applied.

Recall the domains, denoted $R_{\mathbf{x}_i}$, presented in section 3.1 pertaining to the CS method for linear models. Let $R_{\mathbf{x}_i}^*$ be the smallest hyper-rectangle of the CS form

that contains the \mathbf{c}_j , $\forall j = 1, \dots, p$. A set of this form will be utilized in the following theorem.

Theorem 3.2 *Under the GLM setting described in (2.1), the asymptotic simultaneous coverage probability of the bands (3.28) has a lower bound of $1 - \alpha$ for $d = d_{CS}$ when d_{CS} is computed for $R_{\mathbf{x}_i} = R_{\mathbf{x}_i}^*$. The same holds for the bands (3.28) when $\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}^*$, the p MLE of $\boldsymbol{\beta}$.*

Proof: Note that this result holds for any $\mathbf{x}_i \in \Omega_{\mathbf{x}_i}$ and that $\Omega_{\mathbf{x}_i} \supset R_{\mathbf{x}_i} = R_{\mathbf{x}_i}^*$ where the vectors $\mathbf{c}_j = (c_{j1}, \dots, c_{jp})$, $j = 1, \dots, p$, are embedded in the hyper-rectangle $R_{\mathbf{x}_i}^*$. Thus \mathbf{c}_j , $j = 1, \dots, p$ is contained in $\Omega_{\mathbf{x}_i}$ and consequently, utilizing $d = d_{CS}$ in (3.28) guarantees at least $100(1 - \alpha)\%$ simultaneous coverage asymptotically for the p intervals of interest. Also note that the limiting distributions of $\hat{\boldsymbol{\beta}}^*$ and $\hat{\boldsymbol{\beta}}$ are identical. Thus the asymptotic coverage of the bands (3.28) based on $\hat{\boldsymbol{\beta}}^*$ is the same as those based on $\hat{\boldsymbol{\beta}}$. \square

Now let \mathcal{X}^* be the smallest compact subset of the domain where $\mathbf{c}_j \in \mathcal{X}^*$, $\forall j = 1, \dots, p$.

Theorem 3.3 *Under the GLM setting described in (2.1), the asymptotic simultaneous coverage probability of the bands (3.28) has a lower bound of $1 - \alpha$ for $d = d_{TUBE}$, $d = d_{SCR1}$ and $d = d_{SCR2}$ where these critical values are computed for $\mathcal{X} = \mathcal{X}^*$. For $\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}^*$, the p MLE of $\boldsymbol{\beta}$, the same holds for $d = d_{TUBE}$.*

Proof: Note that this result holds for any $\mathbf{x}_i \in \mathcal{X} = \mathcal{X}^*$. The vectors $\mathbf{c}_j = (c_{j1}, \dots, c_{jk})$, $j = 1, \dots, p$, are embedded in the set \mathcal{X}^* . Thus, $\mathbf{c}_j \in \mathcal{X} = \mathcal{X}^* \quad \forall j$ and consequently, utilizing $d = d_{TUBE}$, $d = d_{SCR1}$ or d_{SCR2} in (3.28) guarantees at least $100(1 - \alpha)\%$ simultaneous coverage asymptotically for the intervals. Moreover, since the limiting distributions of $\hat{\boldsymbol{\beta}}^*$ and $\hat{\boldsymbol{\beta}}$ are identical, then the asymptotic coverage of the bands (3.28) based on $\hat{\boldsymbol{\beta}}^*$ is the same as those based on $\hat{\boldsymbol{\beta}}$. \square

Theorem 3.4 *Under the GLM setting described in (2.1), the asymptotic simultaneous coverage probability of the band*

$$\mathbf{c}'_j \hat{\boldsymbol{\beta}} - \hat{\kappa}_1(\mathbf{c}_i) \hat{\sigma}_{GLM}(\mathbf{c}_i) \pm d_{TUBE} \hat{\sigma}_{GLM}(\mathbf{c}_i) \sqrt{\hat{\kappa}_2(\mathbf{c}_i)} \quad (3.29)$$

where $\hat{\sigma}_{GLM}(\mathbf{c}'_j)$ is given by (2.6), has a lower bound of $1 - \alpha$ with $\hat{\kappa}_1(\mathbf{c}_j)$ and $\hat{\kappa}_2(\mathbf{c}_j)$ defined as stated in section 3.1 and $\mathcal{X} = \mathcal{X}^*$. The same holds for $\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}^*$, the pMLE of $\boldsymbol{\beta}$ with $\hat{\kappa}_1(\mathbf{c}_j)$ and $\hat{\kappa}_2(\mathbf{c}_j)$ defined appropriately for $\hat{\boldsymbol{\beta}}^*$ and \mathcal{X} again equal to \mathcal{X}^* .

Proof: Note that this result holds for any $\mathbf{x}_i \in \mathcal{X}^*$. The vectors $\mathbf{c}_j = (c_{j1}, \dots, c_{jk})$, $j = 1, \dots, p$, are embedded in the set \mathcal{X}^* . Thus, $\mathbf{c}_j \in \mathcal{X} = \mathcal{X}^* \quad \forall j$ and consequently the intervals in (3.29) utilizing $\hat{\boldsymbol{\beta}}$, the usual MLE for $\boldsymbol{\beta}$, guarantee at least $100(1 - \alpha)\%$ simultaneous coverage asymptotically for the intervals. Since the limiting distributions of $\hat{\boldsymbol{\beta}}^*$ and $\hat{\boldsymbol{\beta}}$ are identical, then the asymptotic coverage of the bands (3.28) based on $\hat{\boldsymbol{\beta}}^*$ is the same as those based on $\hat{\boldsymbol{\beta}}$. \square

3.2.2.2 Illustrations of Simultaneous Procedures for Particular Scenarios

The simultaneous procedures for estimating any specified combination of the model parameters from a GLM include the following: SCR (all four forms), PC (restricted-Scheffé), pPC (pMLE restricted-Scheffé), and both pSCR bounds. The relevant bounding procedures will be demonstrated for the odds ratio, relative risk, and attributable proportion, but note that other quantities of interest could also be estimated.

Since we have assumed the model estimated is a GLM, it is possible to apply any of the proposed eight confidence bounds to the general expected response function. Following the procedure described in section 3.1, one could find the bounds for any GLM on a restricted domain and then apply the link function. For example, a GLM is generally given by

$$g(E(Y_i|\mathbf{x}_i)) = \mathbf{x}'_i \boldsymbol{\beta}, \quad i = 1, \dots, n.$$

We will outline the procedure for some common link functions, *log* and *logit*. Note that it is possible to simultaneously estimate any specified set of linear combination of the regression parameters for a specified GLM using any of the eight methods described in previously in this chapter.

As an example, recall the preterm birth study discussed in Chapter 1. This study employed a loglinear model where the reference level was the case with no apparent source of maternal stress. Recall the model was given by (2.14), thus let $\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_k)$ be the $(k + 1) \times 1$ parameter vector, for this example $k = 3$. In this study, the relative risks for each level of the source of maternal stress compared back to the cases with no identified maternal stress factor were of primary interest and, as discussed previously, the overall conclusions made in the study merits simultaneous estimation of these relative risks. We focused specifically on the variable indicating “Life Event” stress (see Table 1.1). This factor had four overall levels for the independent variable indicating the presence of any “Life Event” maternal stress. To utilize the procedure outlined in section 3.2.2.1, we need to define the matrix $\mathbf{C}_{3 \times 4} = (\mathbf{c}_1, \dots, \mathbf{c}_3)'$. Specifically, let $\mathbf{c}_j = (c_{j1}, c_{j2}, \dots, c_{j4})$, where $c_{j,i} = 0$ for $i \neq j + 1$ and $c_{j,j+1} = 1$, $i = 1, \dots, 4$; $j = 1, \dots, 3$. Since β_j is the log of the relative risk for the j^{th} level of the independent variable, then $\mathbf{C}\boldsymbol{\beta} = (\beta_1, \beta_2, \beta_3)'$, is the vector of log relative risks for “Life Event” stress in the preterm birth study. The \mathbf{C} matrix that yields $\mathbf{C}\boldsymbol{\beta}$ equal to the log relative risks for other reference-coded Poisson models would be defined similarly. Notice that in our example \mathcal{X} will be the three dimensional subspace where $x_1 = 0$ and $\sum_{i=2}^4 x_i \leq 1$. (Note that \mathbf{c}_j , $j = 1, \dots, 3$, is contained in this \mathcal{X} .)

Asymptotic simultaneous $100(1 - \alpha)\%$ confidence bands for the log relative risks of interest in the preterm birth study can now be formed by utilizing (3.28) or (3.29) with an appropriate critical value and $\hat{\boldsymbol{\beta}}$ or $\hat{\boldsymbol{\beta}}^*$ as warranted. To obtain asymptotic simultaneous confidence bands on the relative risks, the bands on the log relative risks

would be exponentiated. These intervals will allow us to make overall conclusions with a specified asymptotic error rate.

Alternatively, now suppose relative risks are of interest using a slightly different model. Specifically, model-based relative risks can be estimated utilizing a Poisson regression on a proportion. Thus, assume a simple model of the form,

$$\log(\pi(\mathbf{x}_i)) = \beta_0 + \mathbf{x}_i' \boldsymbol{\beta} = \mathbf{x}_i^* \boldsymbol{\beta}^*$$

for $i = 1, \dots, n$ where $\boldsymbol{\beta}_{(k+1) \times 1}^* = (\beta_0, \beta_1, \dots, \beta_k)'$ and $\mathbf{x}_i^* = (1, x_{i1}, \dots, x_{ik})'$ is a predictor vector of dimension $k + 1$. Then the relative risk is easily estimated by exponentiating any one of the regression parameters, e^{β_i} ($i = 1, \dots, k$). Thus, in order to estimate the i^{th} relative risk, let the matrix \mathbf{C} be defined as described in 5.2.1 with each $c_{ij} = 0$ when $i \neq j + 1$ and $c_{j,j+1} = 1$, $i = 1, \dots, k + 1$; $j = 1, \dots, p$. Again we can obtain asymptotic simultaneous $100(1 - \alpha)\%$ confidence bands for the relative risks by utilizing (2.12) or (3.29) with an appropriate critical value and $\hat{\boldsymbol{\beta}}$ or $\hat{\boldsymbol{\beta}}^*$ as warranted. Here \mathcal{X} would be similar to that for the skin cancer study. To complete the calculations, the resulting bounds would be exponentiated, as they were for the odds ratio calculations.

Once relative risks are estimated from a Poisson regression model, it may be helpful to additionally estimate the attributable proportions. Recall that the point estimate of a relative risk is given by $\gamma_i = \exp(\mathbf{c}_j' \boldsymbol{\beta})$ for $j = 1, \dots, p$. As the attributable proportion is a one-to-one increasing function of the relative risk, the following holds, $\kappa_i = 1 - \frac{1}{\gamma_i} = \frac{\gamma_i - 1}{\gamma_i}$, $i = 1, \dots, n$ where κ is the attributable proportion and γ is the relative risk. Suppose the relative risk interval has lower and upper limits denoted L_{RR} and U_{RR} , respectively. Then the limits on the attributable proportion are given by

$$\left(\frac{L_{RR} - 1}{L_{RR}}, \frac{U_{RR} - 1}{U_{RR}} \right). \quad (3.30)$$

If (L_{RR}, U_{RR}) were obtained with simultaneous coverage for a specified set, then the

same simultaneous coverage properties will hold for the equivalent set of attributable proportions.

Note that all the previous examples assumed the estimated quantities should refer back to the reference level. However, this general methodology can be extended to make other kinds of comparisons between the estimated quantities. For example, if we consider a logistic model with reference coding, we could consider an alternative set of odds ratios for joint estimation. Recall that every e^{β_i} is the odds ratio for the i^{th} level compared to the reference level (or control). Alternatively, suppose it was of interest to estimate the odds ratio comparing the first nonreference level of the covariate to every other nonreference level. Then these odds ratios could be estimated via $e^{\beta_1 - \beta_j}$ for $j = 2, \dots, k$. Thus, the contrast matrix, \mathbf{C} , would have rows that appear something like,

$$\mathbf{c}_j = (0, 1, 0, \dots, 0, -1, 0, \dots, 0).$$

Then via (3.28) or (3.29) we could estimate the log odds ratios simultaneously for an appropriate d and $\hat{\beta}$ or $\hat{\beta}^*$ as warranted. Simply exponentiating the results would give simultaneous bands for this particular set of odds ratios.

CHAPTER 4

Simulations

In order to evaluate the performance of the proposed restricted Scheffé bounds, pMLE Scheffé bounds, and the pMLE SCR bounds, I conducted Monte Carlo simulations. I ran two main simulation studies; simulations for the simultaneous estimation of the expected response function and simulations for the simultaneous estimation of a linear function of the regression parameters which easily gives simultaneous intervals on the odds ratios, relative risks, or attributable proportions via transformation. Some recommendations are provided on the choice of intervals for various scenarios. Additionally, an example of this kind of transformation is given in section 5.2.

4.1 Expected Response Function Simulations

These simulations assume only one predictor variable so that the vector of parameter estimates is of the general form $\boldsymbol{\beta} = (\beta_0, \beta_1)'$. The estimated coverage, or alternatively, the estimated error was recorded for each scenario simulated. I simulated scenarios for various values of the parameter $\boldsymbol{\beta}$, the sample size, n , and the predictor variable, x . Simulations focused on the most commonly utilized GLMs, logistic regression and Poisson models, although other models could be investigated. Simulations included the following scenarios. Regression parameters as follows: (1) $\boldsymbol{\beta} = (-1, -0.5)$, (2) $\boldsymbol{\beta} = (0, 1)$, (3) $\boldsymbol{\beta} = (2, 4)$, and (4) $\boldsymbol{\beta} = (-0.5, -1)$. The sample sizes were $n=10, 25$, and 50 . The domain, \mathcal{X} , for both logit and Poisson models is continuous. For the logit model, I generated points equally spaced over wide and narrow intervals. First appropriate values of π were chosen that would determine either a wide

or narrow range for the domain. For a wide domain $\pi_L=0.1$ and $\pi_U=0.9$ and for a narrow domain $\pi_L=0.25$ and $\pi_U=0.75$. The \mathbf{X} interval endpoints were then determined by inverting the GLM so that $x = (\text{logit}(\pi) - \beta_0)/\beta_1$ where β_0 and β_1 are the parameters. Thus, for the logit model, $x_L = (\text{logit}(\pi_L) - \beta_0)/\beta_1$ and $x_U = (\text{logit}(\pi_U) - \beta_0)/\beta_1$ are the endpoints of the domain. Then let $x_1 = x_L$ and $x_n = x_U$ and let the remaining points be equally spaced between x_1 and x_n . Thus, $\mathbf{X} = (x_1, x_2, \dots, x_n)$ is a vector of a countable set of points contained in $\mathcal{X} = \{x : x_L \leq x \leq x_U\}$. In order to simulate the response, a set of $Y_i, i = 1, \dots, n$ response variables was generated in the following manner. First, we generated Uniform(0,1) random variables, $U_i, i = 1, \dots, n$. Then we let the response variable Y_i be 1 if $U_i < \pi(\mathbf{x}_i)$ and 0 otherwise when generating data for a logit model. Note that $\pi(\mathbf{x}_i) = \frac{1}{1+e^{\beta_0+\beta_1\mathbf{x}_i}}$ for $i = 1, \dots, n$. For the Poisson model, I generated a set of uniform random variables for the \mathbf{X} values. The wide domain was distributed Uniform(0,1), while the narrow domain was distributed Uniform(0,0.5). To generate the response variable for a Poisson regression model, Y_i is a Poisson random variable generated to have mean $\mu(\mathbf{x}_i) = e^{\beta_0+\beta_1\mathbf{x}_i}$ for each $i = 1, \dots, n$. For both models, I then used this set of Y_i values and the $\mathbf{X} \in \mathcal{X}$ data set to compute the estimated parameter values and estimated covariance matrix. These were also utilized to obtain the equations for the bounds over \mathcal{X} for each method evaluated. Note that we are not generating binomial, multinomial or Poisson random variables and fitting the model to the generated observations. Rather, we are assuming the model holds exactly. For situations where the logistic and Poisson models do not work well, these methods could perform quite poorly. For each sample I will note whether the estimated bounds cover the true response function \mathbf{X} , a finite set contained in \mathcal{X} . I will then estimate the simultaneous coverage with the empirical coverage of my simulated samples.

Additionally, in order to determine the number of simulated samples required to estimate the error to within ± 0.005 we calculated a lower bound on the number of

simulations. If we are willing to tolerate 5% type I error ($\alpha = 0.05$), a lower bound on the number of simulations may be determined via $[(0.05)(0.95)/\rho]^{1/2} < 0.005$ where ρ is the number of simulations [7]. This yields $\rho > 1900$. Thus we ran 5000 simulations to reduce error.

4.1.1 Expected Response Function Simulation Results

The most significant distinction among all the competing intervals with regard to the empirical confidence level, was the estimator used, MLE or pMLE. See Figure 4.1 for a plot comparing two MLE intervals to two pMLE intervals. Generally, the

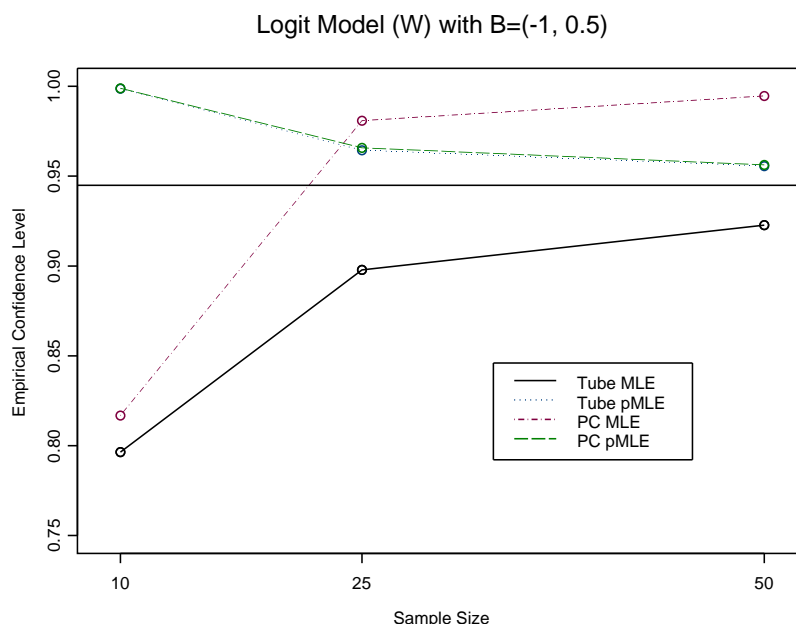


Figure 4.1: MLE and PMLE SCR Intervals with wide range

pMLE based intervals achieved the desired level of confidence at all sample sizes. In contrast, the MLE based intervals as a group only reached the desired level of confidence for some cases of $n=25$ or 50 . Clearly, the ability of the pMLE intervals to achieve the desired level of α at any sample size is an improvement over any of the usual MLE intervals. Though we see this improvement in the reliability of the pMLE

based intervals, the pMLE based intervals are extremely conservative, particularly at small sample sizes. Again, see Figure 4.1 for an example. This could be due to the computation of the biasing constant used to shift the likelihood equations for solving for the pMLE. At the larger sample sizes the pMLE bias adjustment is more precise while at small sample sizes this adjustment is more conservative.

Recall that we applied the pMLE estimator to the restricted-Scheffé, naive SCR, and SCR3 intervals. Interestingly, the reshifted and rescaled SCR interval (SCR3) does not perform as well as the naive tube-based SCR interval or any of the other intervals. See Figure 4.2 for an example. Similar behavior was observed to Figure 4.2 for other parameter sets. Clearly, when using a bias-preventing estimator, trying

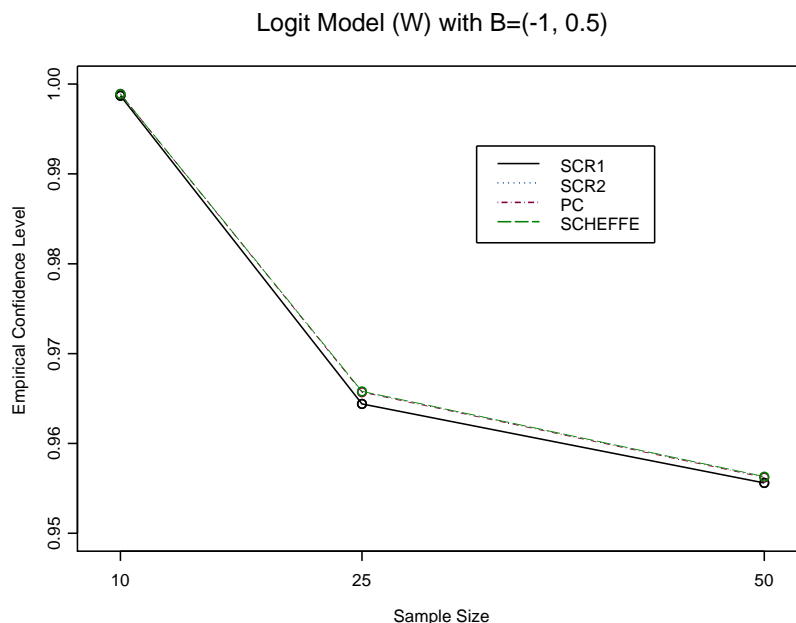


Figure 4.2: pMLE Intervals Logit-Wide Range B=1

to correct the remaining bias is not helpful, and in fact is often detrimental. Though the pMLE SCR3 intervals are not usually a good idea as an alternative to any MLE based intervals, the other pMLE intervals (restricted-Scheffé and naive SCR) perform far better than the MLE intervals in all cases. See both Figure 4.1 and Figure 4.2 for

examples.

As the sample size increases to moderately large sizes ($n=25, 50$ or 100), the MLE based intervals as a whole do reach the desired level of confidence and the pMLE based estimators's empirical confidence level decreases to a level much closer to the intended level of confidence (see Figure 4.1), and in many cases the pMLE based intervals (either PC or naive SCR) are actually less conservative than the usual MLE based intervals. While the pMLE based intervals were intended to address poor coverage at small sample sizes, these intervals also appear to improve the conservative nature of the usual MLE based intervals at the moderate sample sizes. Thus, at these moderate to large sample sizes the pMLE based intervals still attain the desired level of confidence but, in general, do not over-reach the desired confidence level as the usual MLE based intervals often do.

Note that so far I have presented only one parameter case for the logit model. Recall that I investigated four sets of parameters for the logit model and three sets of parameters for the Poisson model. The plots comparing the two superior pMLE intervals to the corresponding MLE intervals are displayed in Figures 4.3 to 4.15 in this section. Generally, for the logit model simulations, we see very similar behavior to the plots analyzed previously. However, for some choices of the regression parameters, a sample size of 100 was required to achieve the desired confidence level with the naive tube MLE interval. See Figures 4.3 to 4.5.

In regard to the domain used in the estimation of the interval, when a wide domain was assumed for estimation of the GLM, the MLE based intervals needed larger sample sizes to attain the desired level of confidence than when the domain width was narrow. This held for the logit model in particular (see Figure 4.3). However, this trend did not translate to the pMLE based intervals in general, where the domain of interest really only affected how conservative the intervals were.

The choice of the four parameter sets did not change the overall trends observed

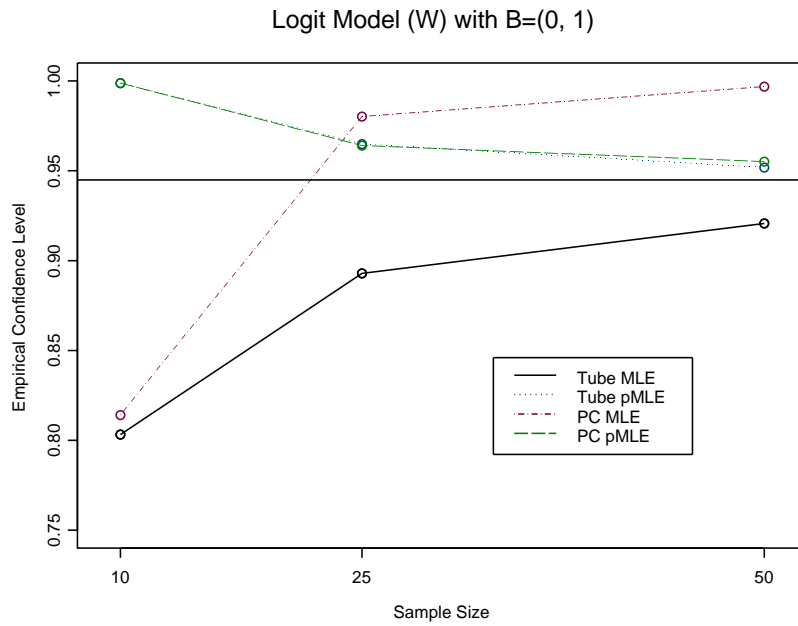


Figure 4.3: MLE and PMLE SCR Intervals with wide range

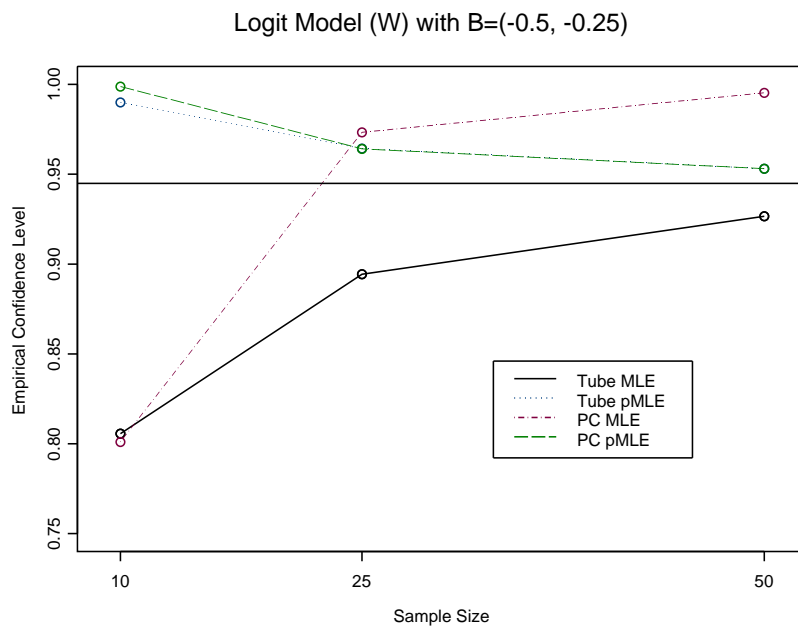


Figure 4.4: MLE and PMLE SCR Intervals with wide range

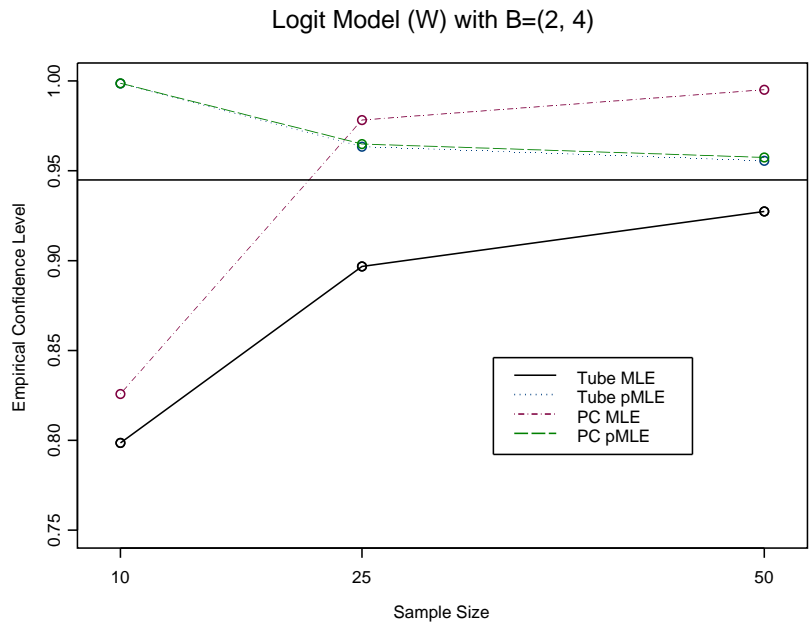


Figure 4.5: MLE and PMLE SCR Intervals with wide range

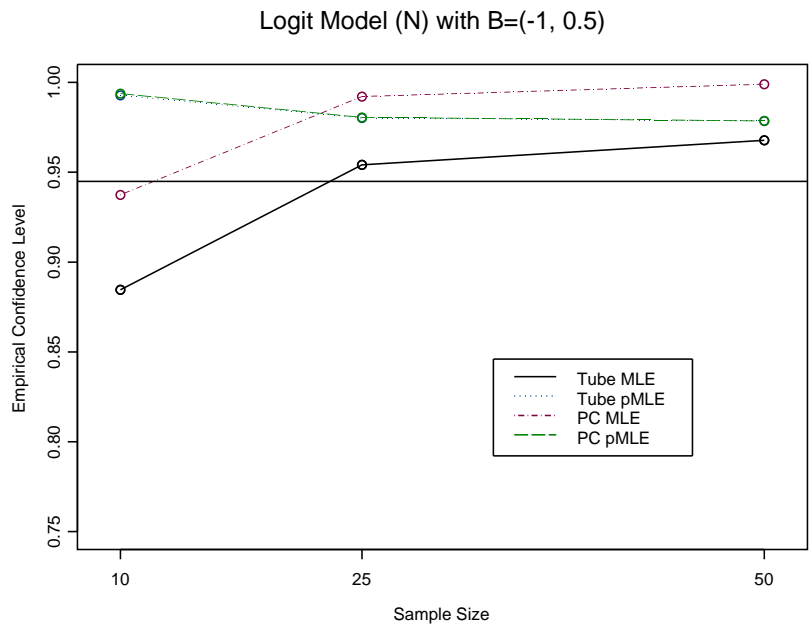


Figure 4.6: MLE and PMLE SCR Intervals with narrow range

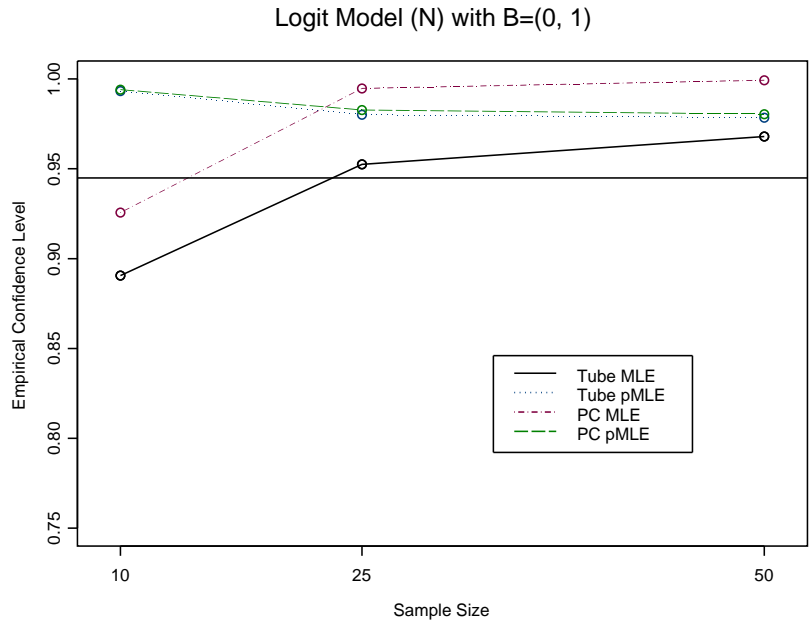


Figure 4.7: MLE and PMLE SCR Intervals with narrow range

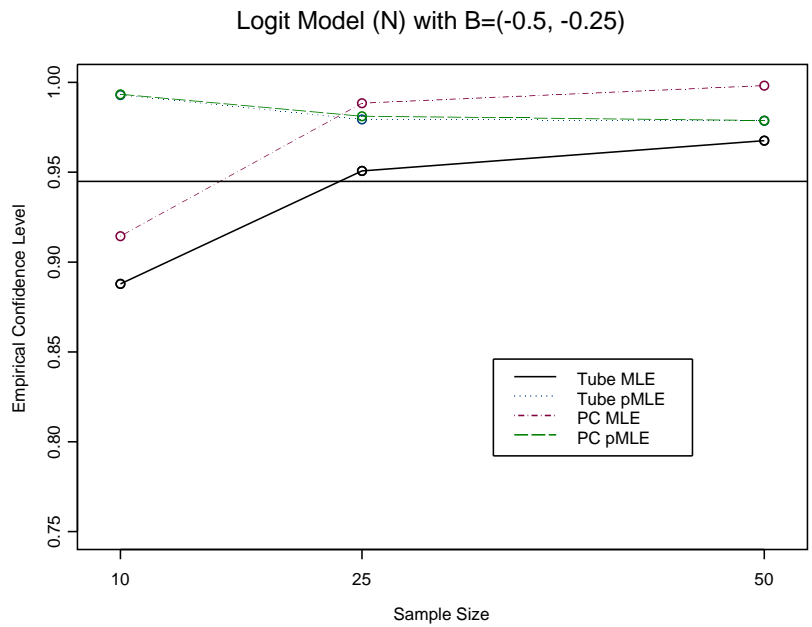


Figure 4.8: MLE and PMLE SCR Intervals with narrow range

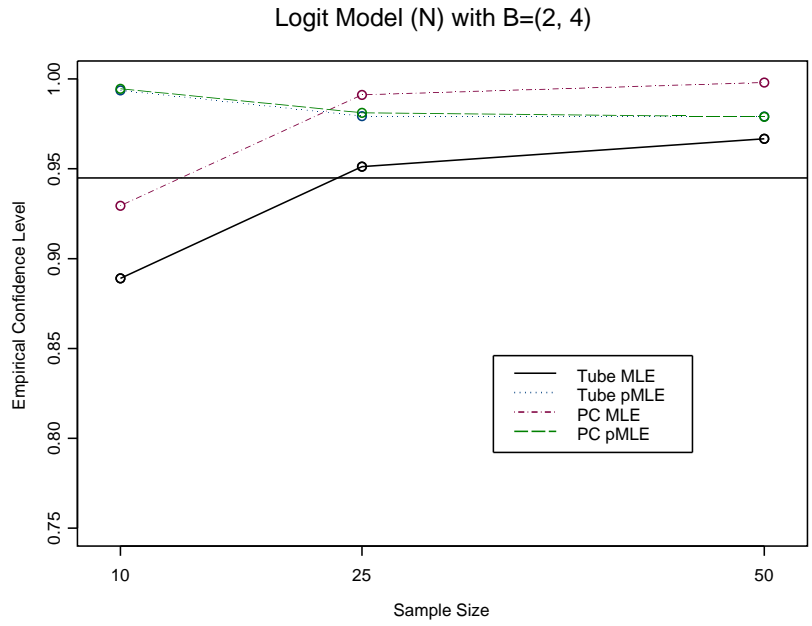


Figure 4.9: MLE and PMLE SCR Intervals with narrow range

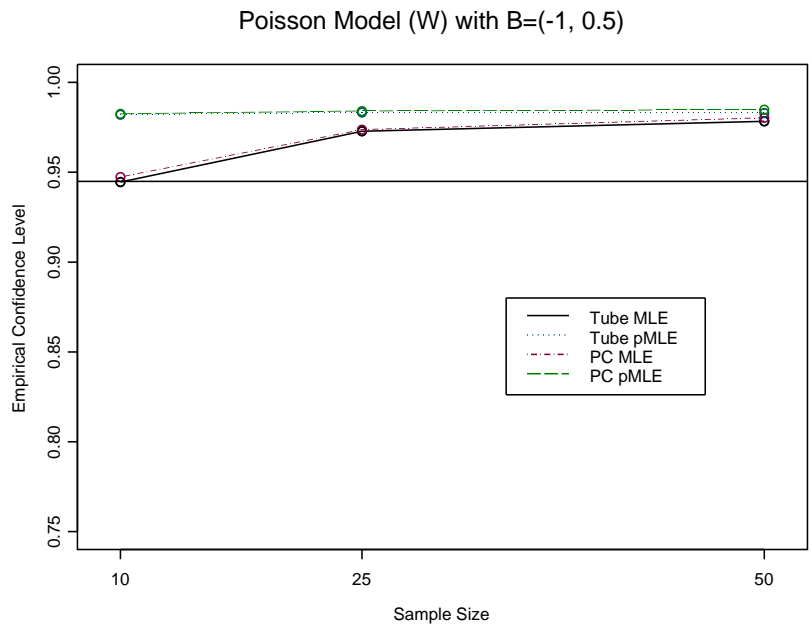


Figure 4.10: MLE and PMLE SCR Intervals with narrow range

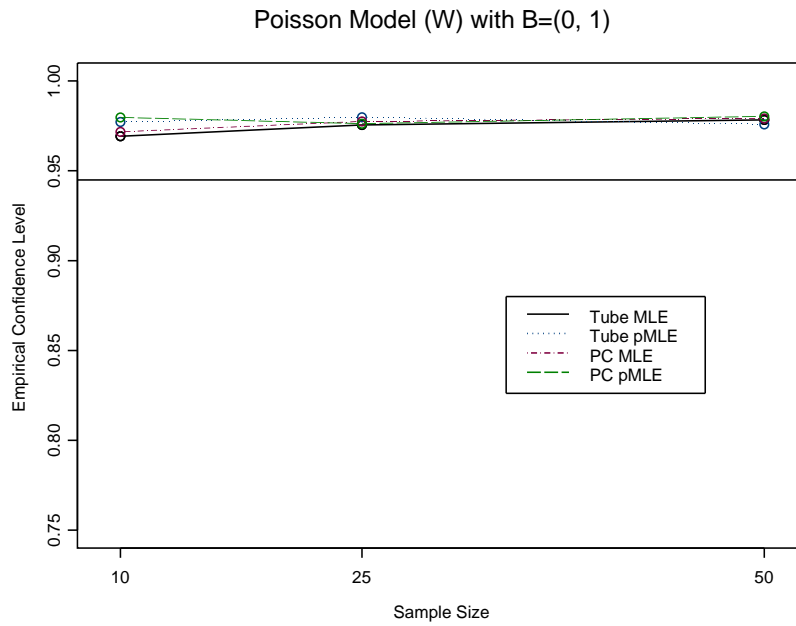


Figure 4.11: MLE and PMLE SCR Intervals with narrow range

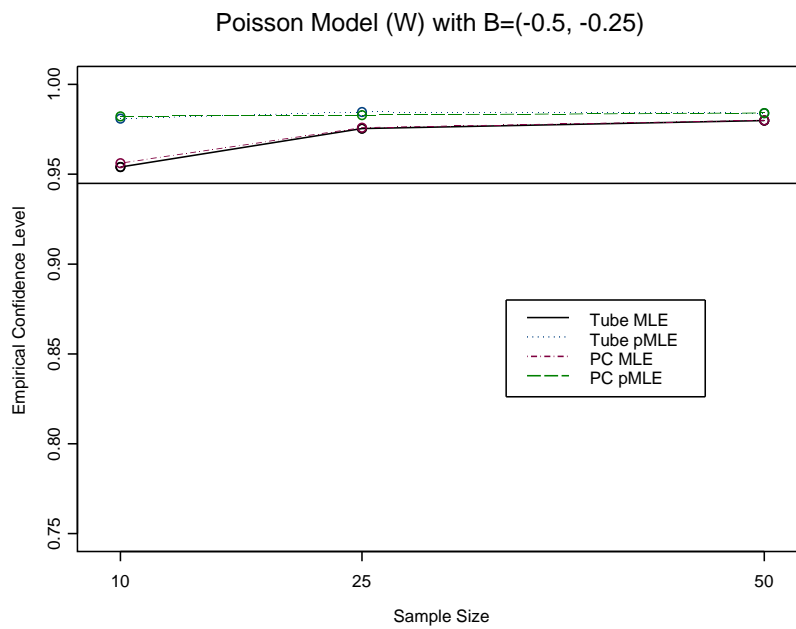


Figure 4.12: MLE and PMLE SCR Intervals with narrow range

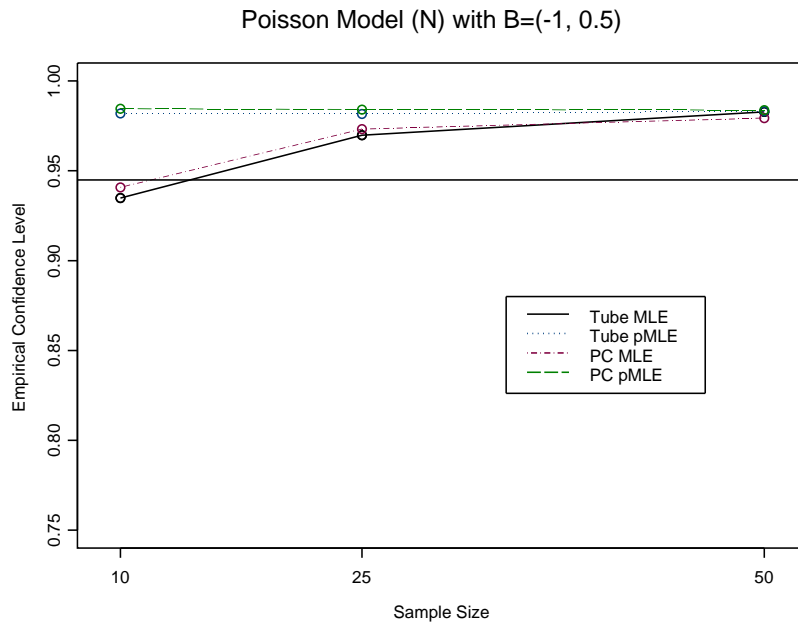


Figure 4.13: MLE and PMLE SCR Intervals with narrow range

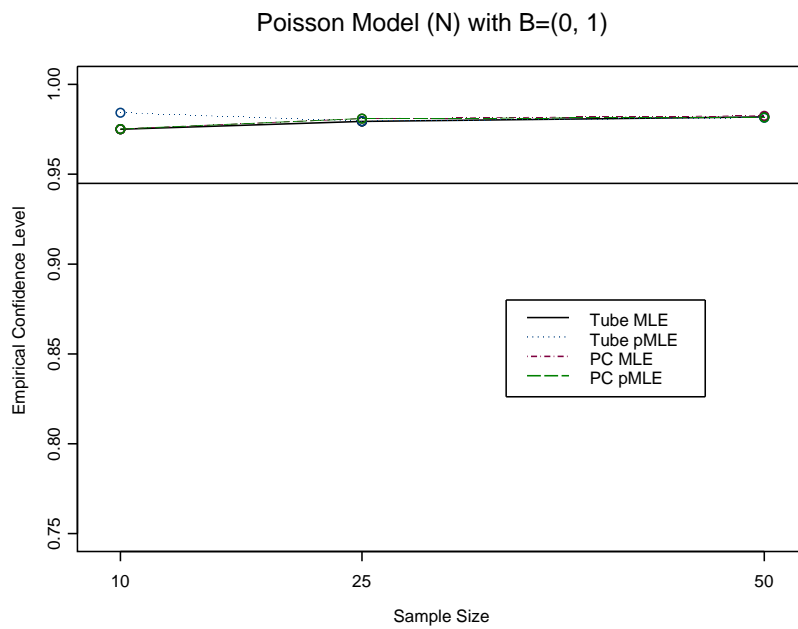


Figure 4.14: MLE and PMLE SCR Intervals with narrow range

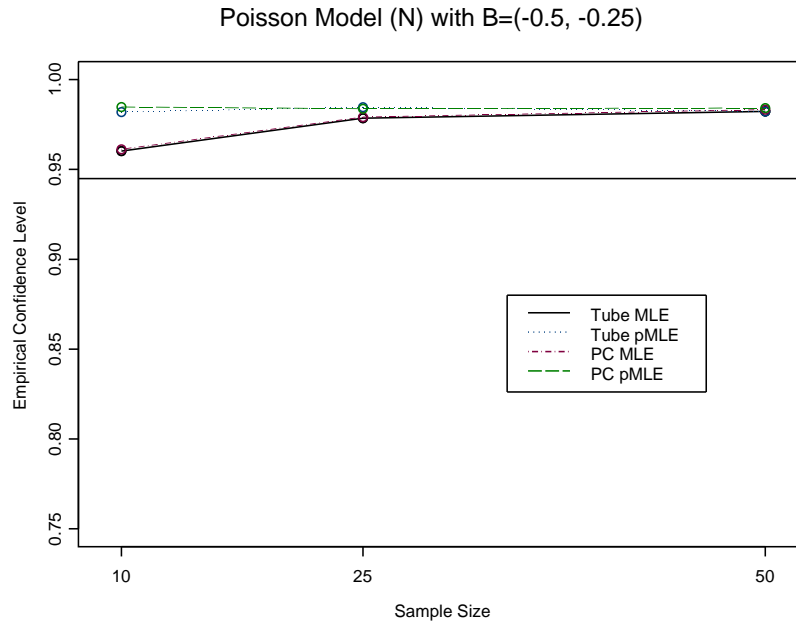


Figure 4.15: MLE and PMLE SCR Intervals with narrow range

for the competing intervals significantly. In contrast, the choice of the link function did. The logistic models were in general less conservative than the Poisson models (compare Figures 4.1 and 4.10). The performance of the MLE and competing pMLE intervals was most distinct when investigating the logistic regression model. Conversely, the Poisson model empirical confidence levels did not vary greatly across the sample sizes when the pMLE based intervals were utilized. Even the MLE based intervals were conservative at times for this link function and attained the desired level of confidence even at the smallest sample sizes for many cases (see Figure 4.10 as an example). Thus, many of the comments made about the logistic regression models do not apply when considering Poisson regression models. In general, little distinction can be made among the competing intervals. At times, the MLE based intervals appear to be a little less conservative than the pMLE based intervals, but often that difference is negligible. I believe that the conservative nature of all the methods for estimating the mean response of a Poisson model needs to be addressed.

This conservative behavior may be due to the tendency of Poisson regression models to overestimate the variance of the regression parameters (see [15] and [16]). A sandwich estimator of the variance should be studied to potentially correct this problem [17]. A sandwich variance estimator, along with generalized estimating equations (GEE's) for estimating the model parameters, can correct a misspecified variance function for Poisson models. The sandwich estimator is a robust variance estimator that consistently estimates the true variance when the parametric model fails to hold. Since the parameters estimated from GEE's have asymptotic normality when utilizing the sandwiched covariance matrix, we may directly apply the usual MLE based interval methods.

Though the MLE intervals are not of primary concern, it should be noted that among the MLE methods, as expected, the Scheffé is the most conservative of all. Yet little distinction can be made among the other methods except that the SCR3 intervals tend to not reach the desired level of confidence as quickly as the other SCR intervals. See Appendix A for examples. However, these trends do not translate to the intervals utilizing the pMLE estimator since: 1) not all SCR intervals are employed using this estimator and thus cannot be compared, and 2) the bias-preventing estimate does drastically change the behavior of each interval overall.

4.2 Functions of the Parameters Simulations

In order to estimate the error associated with the confidence regions for estimating the set of regression parameters, and hence, odds ratios, relative risks or attributable proportions, I will again assume only one predictor variable. In general, the single predictor variable is assumed to be categorical. However, using reference cell coding for one categorical predictor entails utilizing several binary predictor variables. This will be taken into account in the simulations. When evaluating the odds ratio we also need to consider what type of multiple comparisons could be of interest. I will

consider only contrasts corresponding to comparisons with a control. For example, comparisons with a control would require simultaneously estimating the odds ratio for each nonreference level with the reference level from a logistic regression model when reference cell coding is utilized. This entails simultaneously estimating all slope parameters. Recall that the control is the reference level, thus if we have $k+1$ regression parameters, there will be k comparisons or k odds ratios to be simultaneously estimated. Thus we are simultaneously estimating e^{β_i} for every $i = 1, \dots, k$. Similarly, the relative risks for each level of a predictor variable with reference to the control could be investigated for a Poisson regression model. The attributable proportion also could be observed for both a Poisson regression model and a logistic regression model. These too are one-to-one functions of the k slope parameters.

We investigated both logistic and Poisson regression models for evaluating the limits on the estimated odds ratios, relative risks, or attributable proportions. In this scenario the generation of the \mathcal{X} data set and $Y_i, i = 1, \dots, n$ was identical to that described in section 4.1. However, in this case we evaluated the estimated coverage of the simultaneous confidence bounds for the discrete set of interest only. This coverage was estimated in an analogous manner to that for the expected response. Namely, the data were generated, the model was estimated, and finally the intervals for the slope parameters were constructed. Each time the interval captured the true parameter value, a success was recorded and the number of captures out of all k comparisons was recorded. This was repeated 5000 times and the average empirical confidence level was recorded. For the purpose of the simulations, I considered $k = 4$, where k is the number of estimated parameters (slope parameters in this special case). The sample sizes considered are $n=50, 100, 200,$ and 300 and $\alpha = 0.05$. Also, as in 4.1, I recorded the empirical confidence level for each method considered.

At times, the estimated covariance matrix was near-singular. This means that the covariance matrix was estimated to be a quantity such that when the calculations for

computing the inverse of the matrix were begun, an error occurs in the LU factorization. An error is returned in this case by the Fortran compiler. Additionally, the model is ill-fitting if the response vector is either all 1's or all 0's. Thus, cases where the response vector is all 0 or 1 or the covariance matrix is singular or near-singular were recorded and data were regenerated. When $n=50$, there were 252 cases that were thrown out and the data regenerated. When $n=100$, 200, or 300, no cases of near-singular matrices or all 0's or 1's response vectors occurred.

4.2.1 Functions of the Parameters Simulation Results

As with the intervals on the mean response, performance of the intervals on the parameters was most affected by the estimator utilized, MLE or pMLE. In general, when the pMLE estimator was used for any interval method, the desired level of confidence was reached at any sample size (see Figure 4.16 or Figure 4.17).

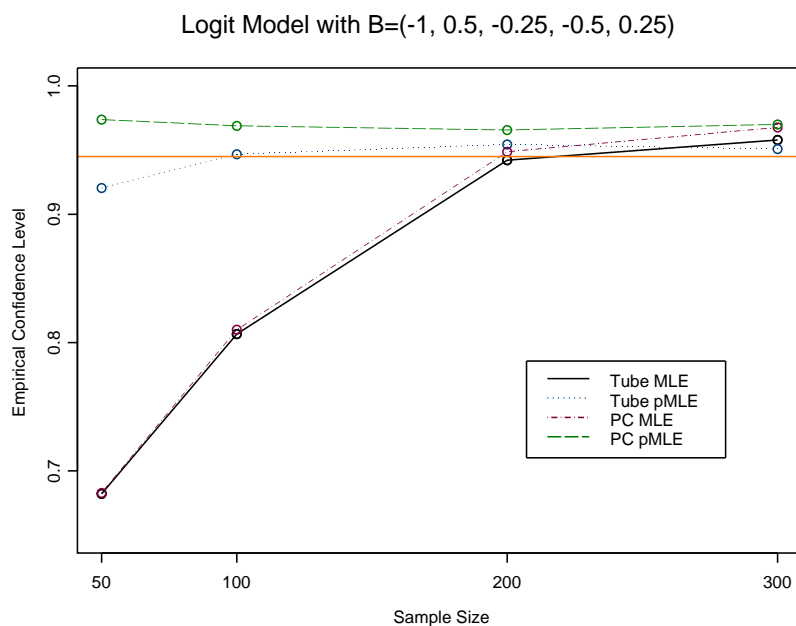


Figure 4.16: MLE and PMLE SCR Intervals for the Parameters

In contrast, the MLE based intervals did not in general attain the desired confi-

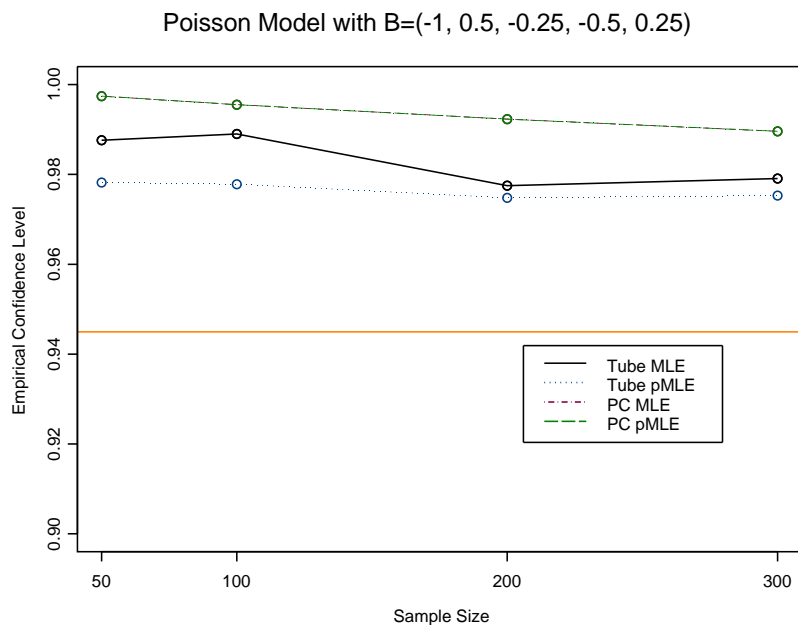


Figure 4.17: MLE and PMLE SCR Intervals for the Parameters

dence level until either $n = 200$ or $n = 300$ for most cases studied. At the smallest sample size ($n = 50$), the pMLE based interval attained the desired level of confidence and was not overly conservative (see Figure 4.16 or Figure 4.17). As the sample size increased, the pMLE based interval's empirical confidence level slowly approaches the desired confidence level, just as we saw with the mean response simulations. At the largest sample size simulated ($n = 300$), the pMLE based interval had an empirical confidence level between the various MLE intervals. In general, only the MLE Scheffé and PC intervals are more conservative than the two pMLE intervals, while all the MLE SCR intervals are a little less conservative. Thus, whether a practitioner utilizes the MLE or pMLE based intervals makes little difference at these larger sample sizes.

CHAPTER 5

CONCLUSIONS

5.1 Application of Proposed Methods

Using practical examples with emphasis placed on implementation of the procedures and the interpretation of the results, I will now illustrate how to utilize the proposed intervals. One example focuses on estimating the mean response of a GLM while the other utilizes a GLM with reference coded binary predictors to estimate a set of odds ratios.

5.1.1 Diabetes among Pima Women

Diabetes is a common disease among females of the Pima culture in Arizona. A study was conducted to better understand the incidence of diabetes in the population of Pima women [18]. One explanatory variable that is believed to be associated with diabetes in young Pima women, age 24 and younger, is the plasma glucose concentration. The glucose concentration was measured with an oral glucose tolerance test on the 51 Pima women aged 24 or younger. A binary variable indicates presence of diabetes in the young women (0=no diabetes and 1=diabetes), thus a simple logistic regression model is reasonable. Table 5.1 contains the estimated probability of diabetes for women with high glucose readings (140 and above). Individual 95% confidence intervals were calculated for each proportion as well as naive tube or SCR1 intervals with the restriction that the glucose was greater than 140. Note that each proportion in Table 5.1 uses the notation $\pi_{glucoselevel}$ with the estimated proportion giving the probability of diabetes for an individual Pima women with that glucose

Table 5.1: Intervals for Proportion of Pima Women with Diabetes

Point Estimate for π	95% MLE Individual Confidence Intervals for π	95% pMLE SCR1 Simultaneous Confidence Intervals for π
$\hat{\pi}_{140}=0.268$	(0.109,0.523)	(0.101,0.561)
$\hat{\pi}_{142}=0.297$	(0.120,0.567)	(0.108,0.598)
$\hat{\pi}_{143}=0.312$	(0.125,0.589)	(0.111,0.616)
$\hat{\pi}_{148}=0.391$	(0.155,0.693)	(0.128,0.703)
$\hat{\pi}_{151}=0.443$	(0.175,0.748)	(0.140,0.750)
$\hat{\pi}_{154}=0.495$	(0.197,0.796)	(0.151,0.792)
$\hat{\pi}_{177}=0.831$	(0.417,0.971)	(0.259,0.962)
$\hat{\pi}_{188}=0.914$	(0.540,0.990)	(0.322,0.984)
$\hat{\pi}_{199}=0.958$	(0.658,0.996)	(0.391,0.994)

level. A discussion of the results follows the presented interval estimates in Table 5.1. First note that, as expected, the individual confidence intervals are narrower than the simultaneous intervals. Thus, using the individual confidence intervals, it will be easier to reject certain proportions as the true value. Note that the proportion estimates given in Table 5.1 are from the pMLE estimated model. The MLE model was $logit(\hat{\pi}) = -10.840 + 0.0703X$ while the pMLE model was $logit(\hat{\pi}) = -10.826 + 0.0701X$. The change in the length and center of the intervals could lead to very different conclusions given certain research questions.

5.1.2 Depression in Adolescents

A study was conducted on the classification of depression (high or low) among adolescents between the ages of 12 to 18 with either learning disabilities (LD) or with serious emotional disturbances (SED) [19]. Six risk factors for high levels of

depression were considered (as a combination of the age (12-14,15-16,17-18) factor and group (LD and SED) factor). Thus, there were a total of 6 levels for a single categorical predictor variable. In the text, Epidemiological Research Methods [19], it is suggested that a logistic regression model is appropriate for these data. The estimated odds ratios are provided to ascertain any differences in the level of depression for the different groups. Simultaneous estimation of the odds ratio from the logistic regression model should be considered here since it is reasonable to make conclusions about the group with the highest or lowest odds of high levels of depression. As suggested in the text [19], the group with the lowest risk of high levels of depression (17-18,SED) was the referent or control category. The reference coding takes this into account so that every log odds ratio refers back to that baseline category. The estimated log odds ratios for the 5 estimated slope coefficients are given in table 5.2. Note that $\beta_{age,condition}$ and $\theta_{age,condition}$ refer to the parameter or odds ratio respectively for an adolescent of a particular age group and condition. Additionally, Table 5.2 contains the estimated model odds ratios comparing the odds of high levels of depression for each risk category with reference to the 17-18,SED category and the individual and restricted-Scheffé or PC simultaneous intervals. All point estimates utilize the pMLE estimated model. Note that the 95% individual confidence intervals demonstrated an odds ratio significantly different than 1 for the case where the adolescent was age 12-14 and learning disabled. Once simultaneous adjustments are made, the significant association no longer exists. This would be an example of a case where the one-at-a-time intervals and simultaneous intervals would contradict and care should be taken about which methodology is appropriate. For instance, in order to say that the odds of high levels of depression is highest among the group aged 12 to 14 and with serious emotional disorders, simultaneous intervals would need to be computed. Clearly, that conclusion should not be made for this study since that is not supported via the simultaneous intervals.

Table 5.2: Intervals for Odds Ratio for Depression in Adolescents

Point Estimate for Odds Ratio	95% MLE Individual Confidence Interval for θ	95% pMLE PC Simultaneous Confidence Interval for θ
$\hat{\theta}_{12-14,LD}=1.939$	(0.812,4.627)	(0.384,8.926)
$\hat{\theta}_{12-14,SED}=4.683$	(1.642,13.383)	(0.671,29.874)
$\hat{\theta}_{15-16,LD}=1.616$	(0.651,4.102)	(0.300,8.053)
$\hat{\theta}_{15-16,SED}=1.458$	(0.520,4.088)	(0.222,9.189)
$\hat{\theta}_{17-18,LD}=1.844$	(0.696,4.884)	(0.307,10.381)
$\hat{\beta}_{17-18,SED}=1.00$		

5.2 Overall Conclusions

The proposed pMLE based intervals, including the pScheffé, pMLE restricted-Scheffé, and pSCR1 intervals, did improve small sample estimation over the usual MLE based intervals. As demonstrated, the usual MLE based intervals often could not attain the desired level of confidence for what was considered a small sample size for the varying models. In contrast, the pMLE did attain the desired level of confidence. However, the penalty with using the pMLE based intervals is that these intervals are very conservative at these small sample sizes. As the sample size increases to moderate levels, the distinction between the MLE and pMLE based intervals lessens, but the pMLE intervals, as a whole, tend to be less conservative than the MLE based intervals.

5.2.1 Recommendations for Estimating the Mean Response

When selecting an interval method for a set of comparisons, attention should be paid to what the set of predictor variables are. For instance, when there are

many comparisons and interest is focused on the entire estimation space, the Scheffé intervals would ensure the desired level of confidence. However, if a restricted interval of the predictor variable is of interest or a finite number of discrete points embedded in a continuous domain is of interest, then the restricted-Scheffé or one of the SCR methods, respectively, is most advantageous.

In summary, recommendations are to use pMLE intervals for all small to moderate sample sizes. Specifically, the pMLE SCR1 intervals were the least conservative of all the pMLE based intervals and are thus the best choice. However, for ease of computation, the restricted-Scheffé pMLE intervals are a good second choice with far more computational ease. Then, for moderate and larger sample sizes, the pMLE based intervals are again recommended, though the behavior of these intervals have not been studied for any sample size greater than 50. Again, the SCR1 pMLE interval is the overall best choice. Though even less distinction may be made between the pMLE intervals at the larger sample sizes.

5.2.2 Recommendations for Estimating the Parameters

Overall, for small to moderate sample sizes, the SCR1 pMLE attains the desired level of confidence while not being as conservative as the PC pMLE interval. Thus, for most cases where the sample size is greater than 50, I recommend utilizing a naive tube critical point with the pMLE estimators. For sample sizes smaller than 50, the cautious choice would be the PC pMLE interval. This is a slightly conservative interval, yet it attains the desired level of confidence, unlike any other competing interval. I would not recommend using the MLE based intervals at smaller sample sizes. If the sample size is moderate to large ($n=200$ or 300) there is little observed difference between the pMLE and MLE intervals and thus, for convenience, the MLE intervals may justifiably be utilized.

5.3 Future Research

There are many avenues to explore in the future that are related to this research topic. Some of these include performing in-depth simulations of these methods for more complex GLMs. Namely, if a GLM has a predictor matrix, given by \mathbf{X} , that is a mix of categorical and continuous predictors, then nothing is known about how the aforementioned simultaneous procedures would behave. There are a host of other issues to explore as well when we have a predictor matrix such as \mathbf{X} . For instance, what multiple comparison techniques are applicable, what should we compare, and how do we adjust for the other variables in the model? Additionally, for the single predictor variable case, other configurations of the contrast matrix \mathbf{C} should be considered. For example, these other forms of \mathbf{C} could be utilized to assess how the methods perform for all-pairwise types of comparisons. Also, GLMs with interaction and quadratic terms need to be explored. This entails describing what the odds ratios and relative risks are for the interaction and quadratic terms as well as evaluating and determining the appropriate simultaneous estimation techniques for these more complex models. Other estimation methods for the Poisson models should also be explored. As demonstrated in the simulation studies, the Poisson models may have over-estimated the standard errors associated with the parameters. Thus, sandwich variance estimators via generalized estimating equations as described in section 4.1.1 would be a reasonable solution to this problem. Finally, pMLE based parameter estimates for improving GLM estimation should be explored, particularly in cases where the sample size is typically quite small. For example, a natural application is dose-response models. These models typically have 10 or less replications per dose and there are frequent problems with bias in the parameters estimates. Additionally, when at least one dose has either all success's or all failure's for the response variable, the usual MLE estimates fail. The pMLE estimates would be a reasonable solution to this problem and some simulation studies to assess the accuracy of these estimators

would be beneficial.

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APPENDIX A

FIGURES

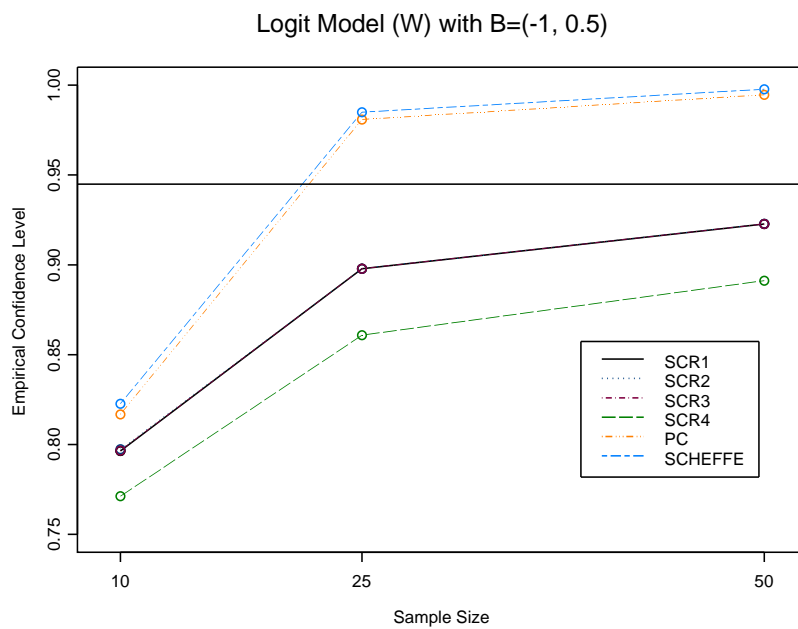


Figure A.1: MLE Intervals Logit-Wide Range $B=1$

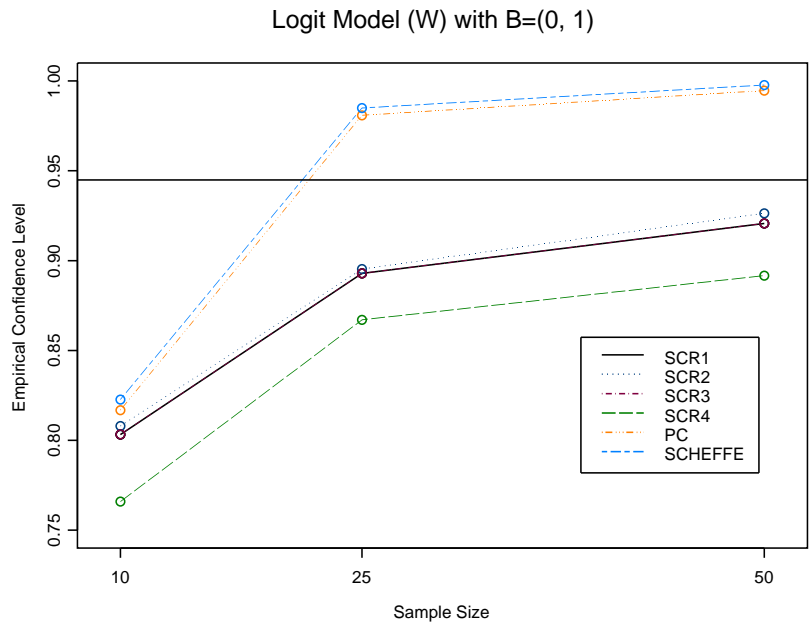


Figure A.2: MLE Intervals Logit-Wide Range B=2

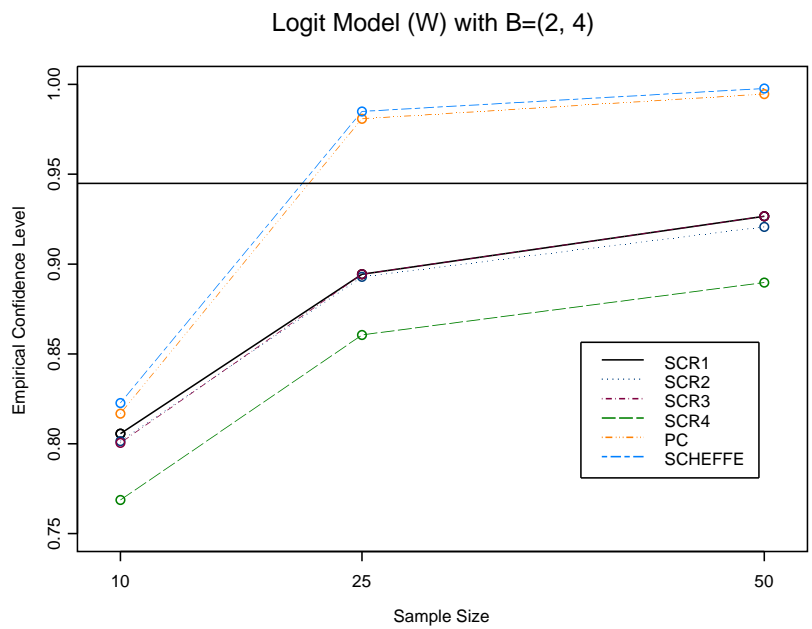


Figure A.3: MLE Intervals Logit-Wide Range B=3

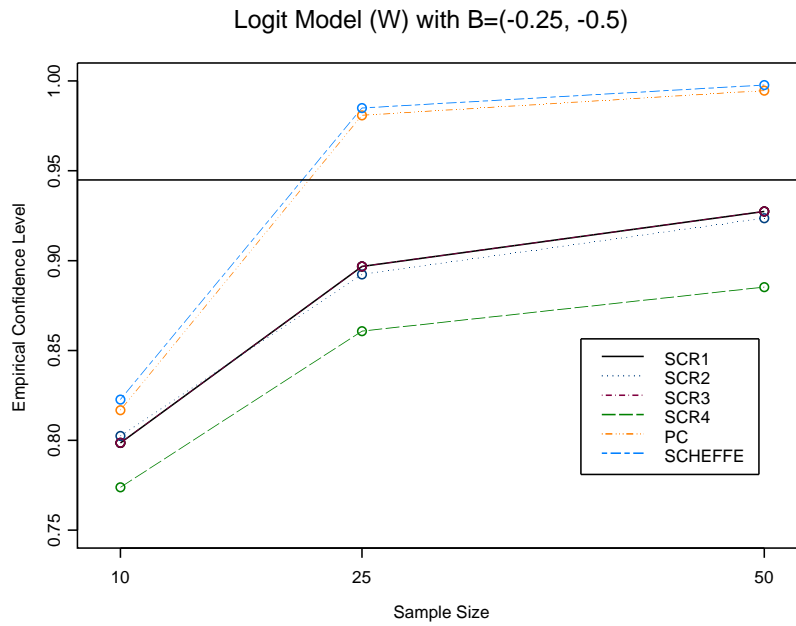


Figure A.4: MLE Intervals Logit-Wide Range $B=4$

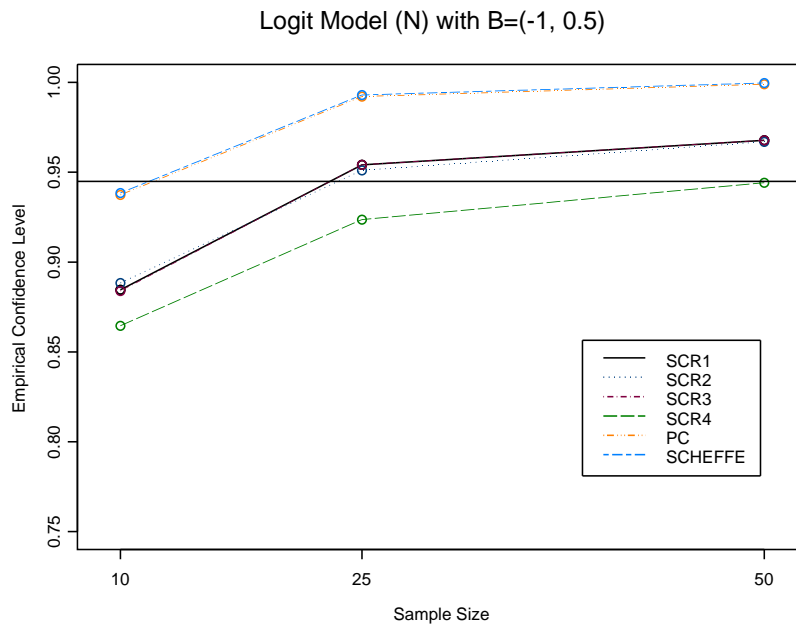


Figure A.5: MLE Intervals Logit-Narrow Range $B=1$

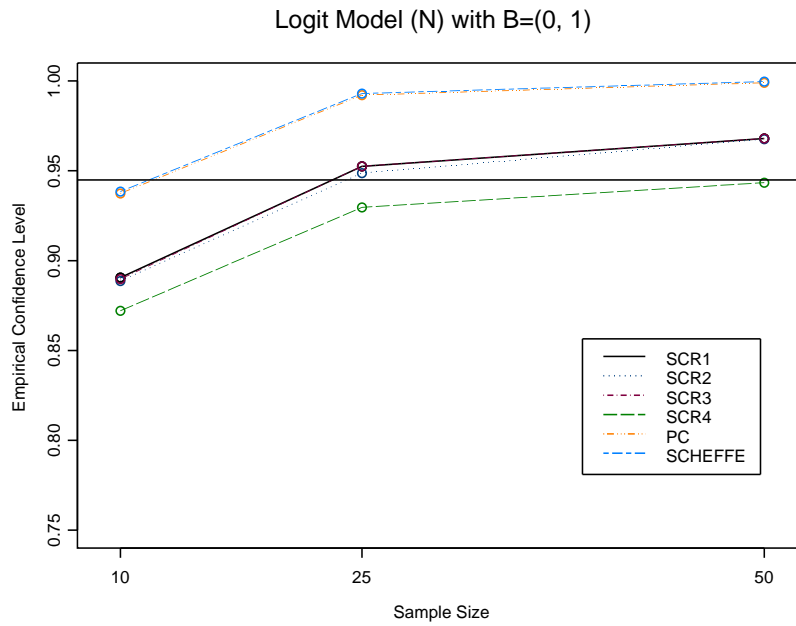


Figure A.6: MLE Intervals Logit-Narrow Range B=2

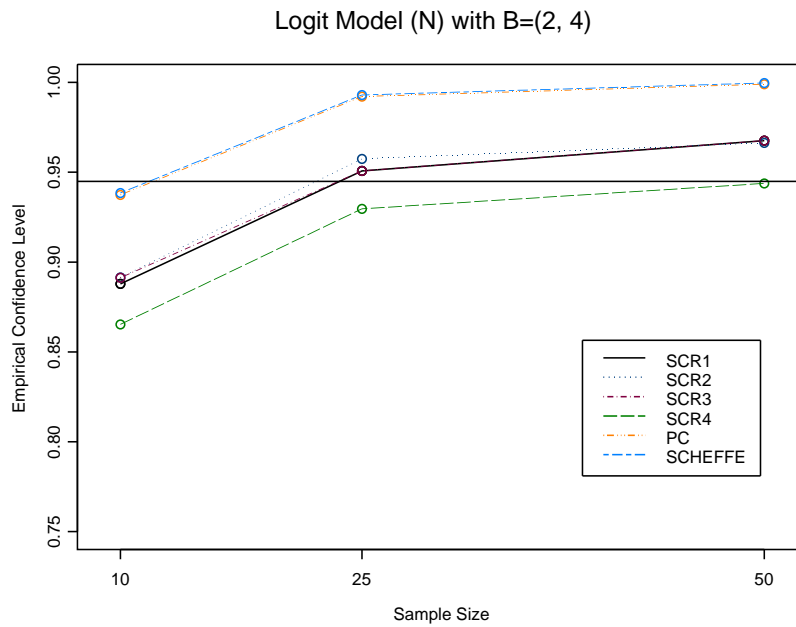


Figure A.7: MLE Intervals Logit-Narrow Range B=3

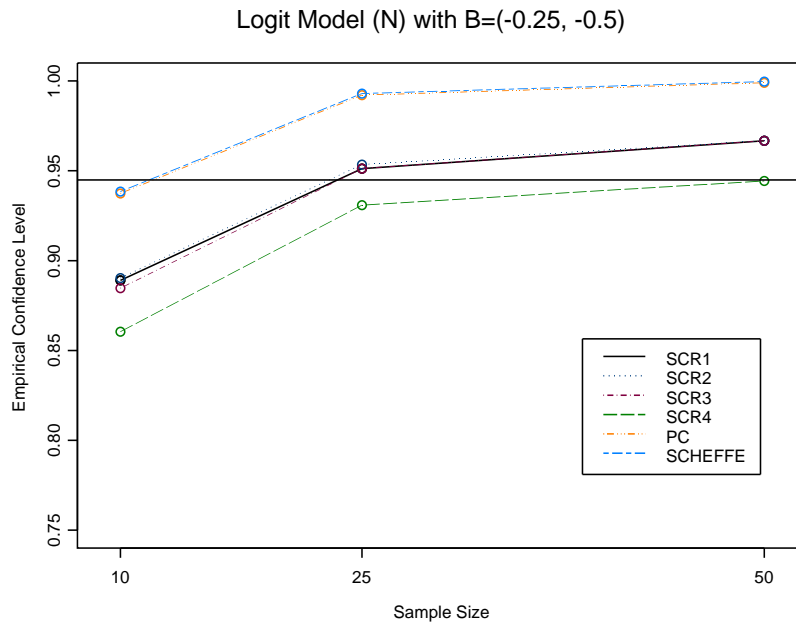


Figure A.8: MLE Intervals Logit-Narrow Range $B=4$

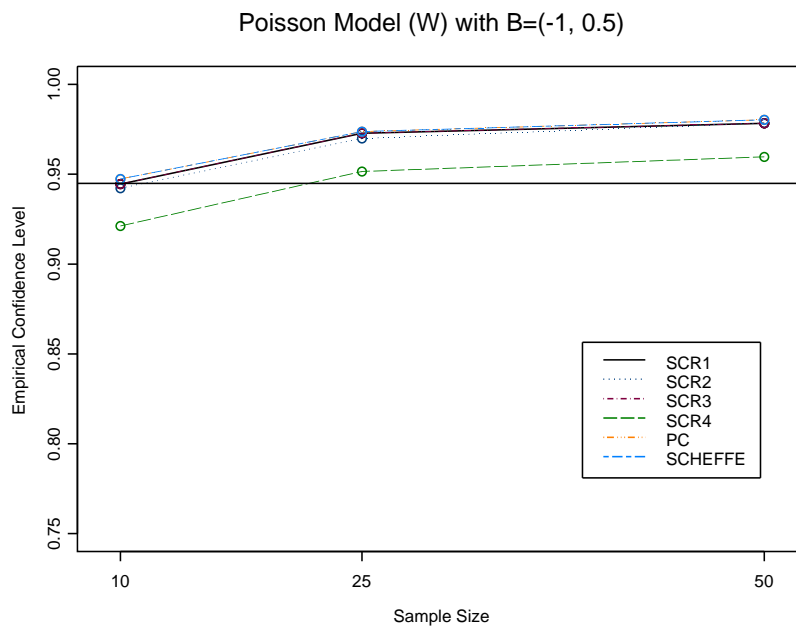


Figure A.9: MLE Intervals Poisson-Wide Range $B=1$

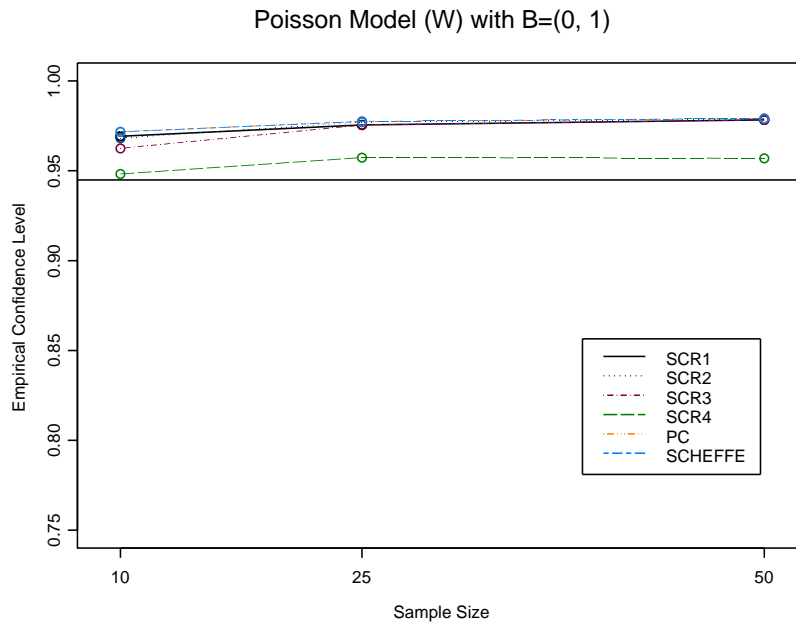


Figure A.10: MLE Intervals Poisson-Wide Range $B=2$

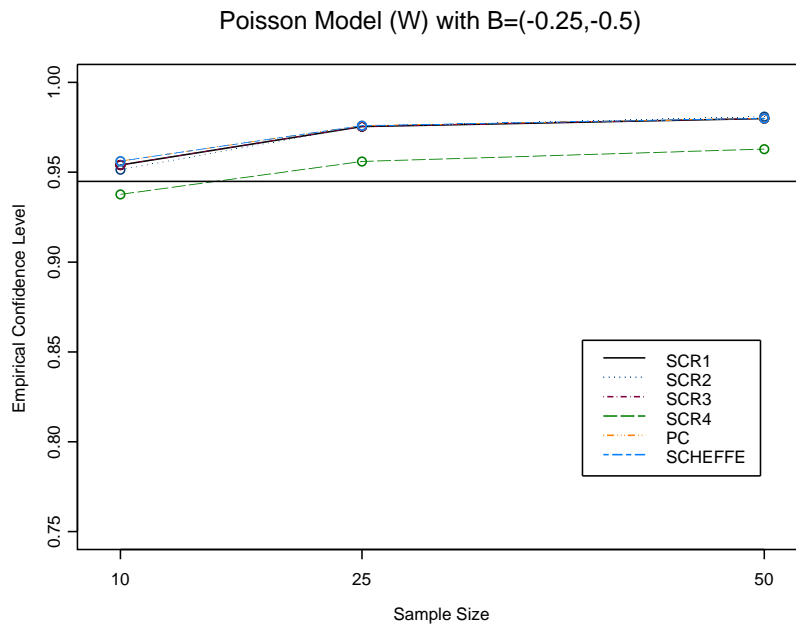


Figure A.11: MLE Intervals Poisson-Wide Range $B=3$

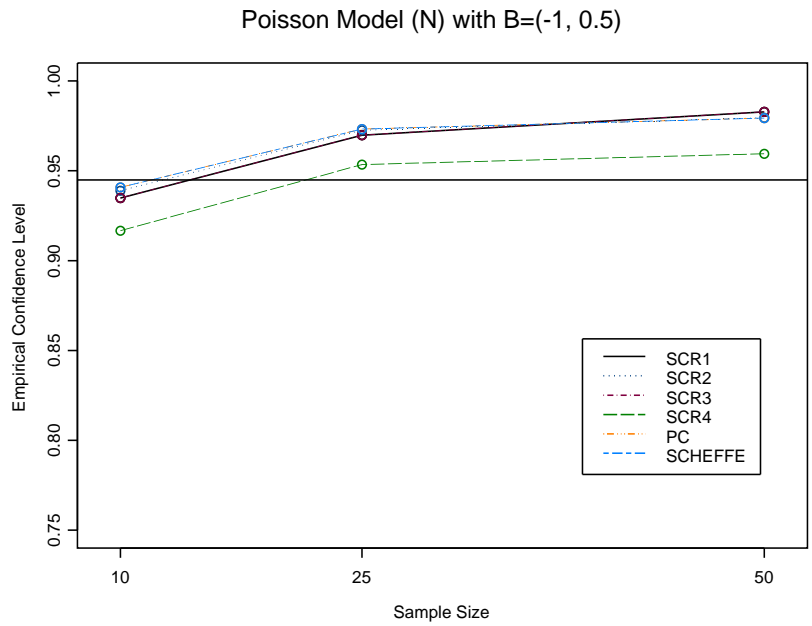


Figure A.12: MLE Intervals Poisson-Narrow Range $B=1$

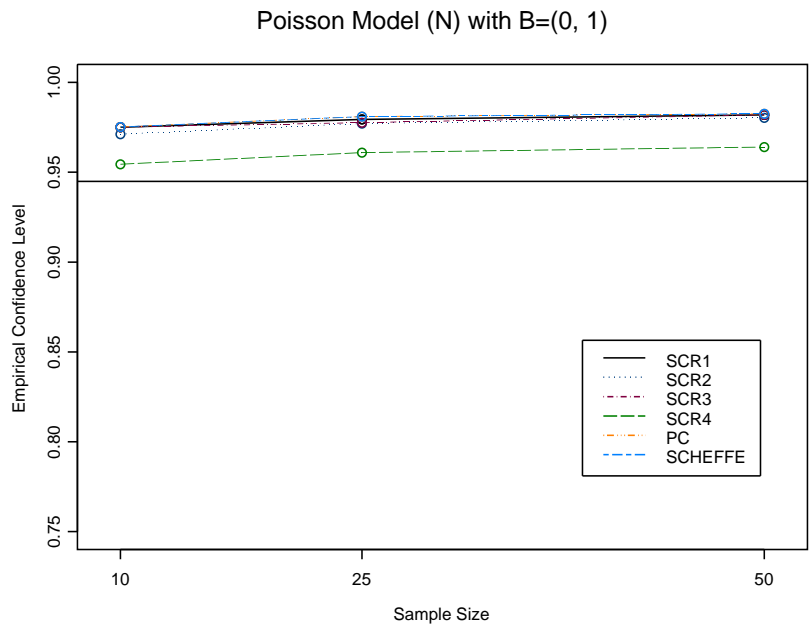


Figure A.13: MLE Intervals Poisson-Narrow Range $B=2$

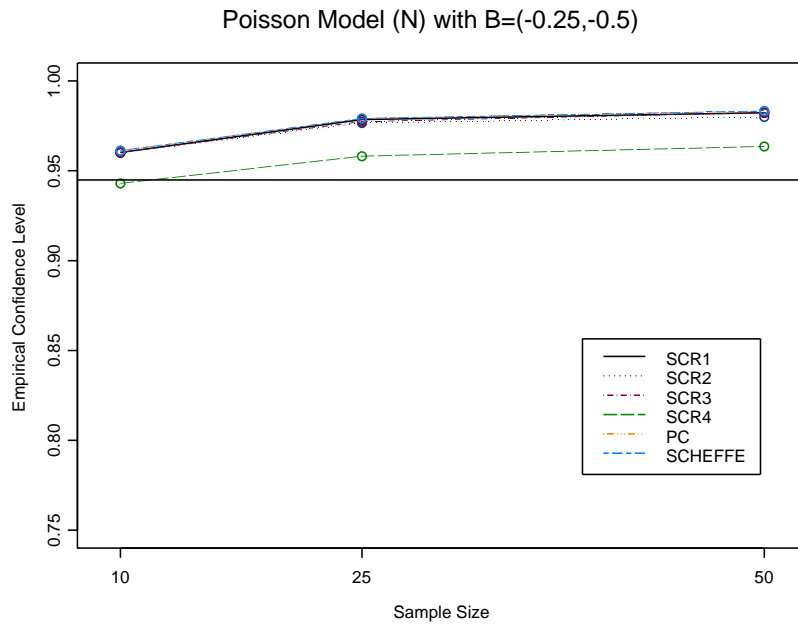


Figure A.14: MLE Intervals Poisson-Narrow Range $B=3$

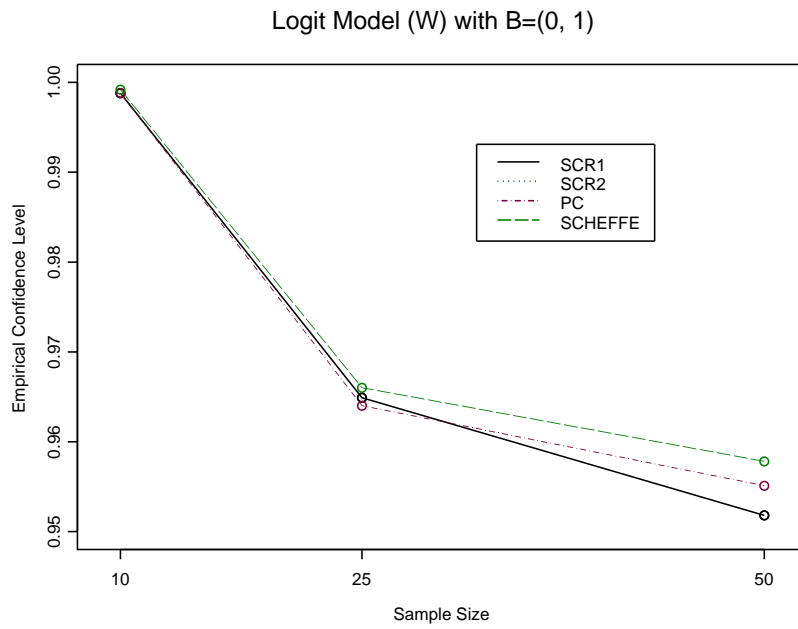


Figure A.15: pMLE Intervals Logit-Wide Range $B=2$

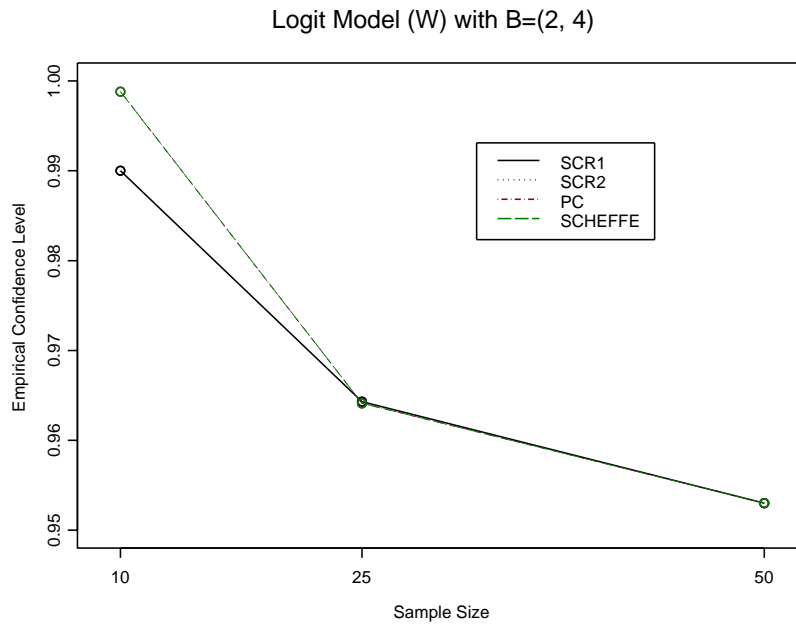


Figure A.16: pMLE Intervals Logit-Wide Range B=3

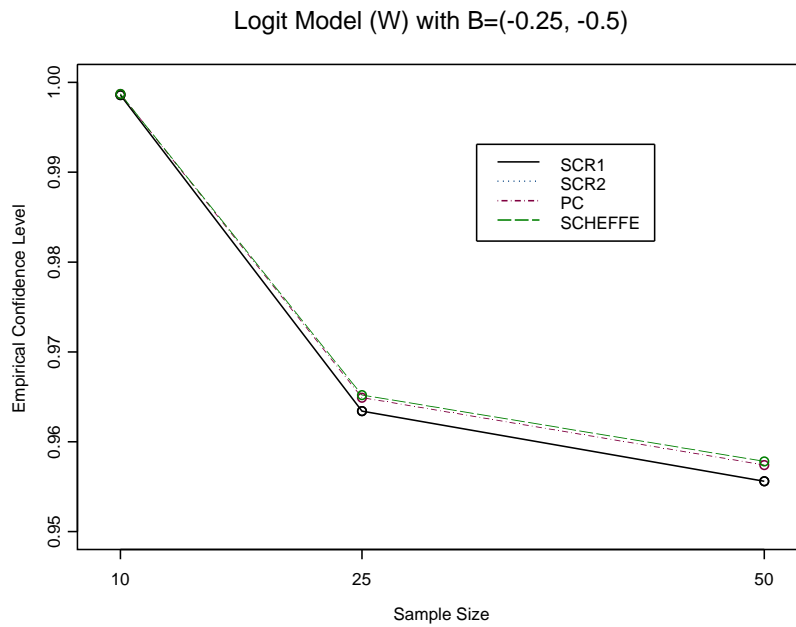


Figure A.17: pMLE Intervals Logit-Wide Range B=4

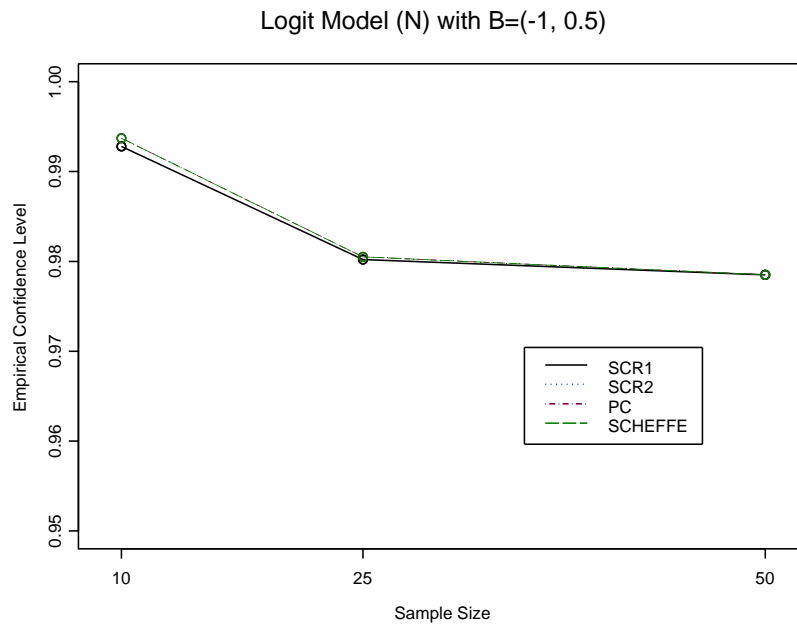


Figure A.18: pMLE Intervals Logit-Narrow Range $B=1$

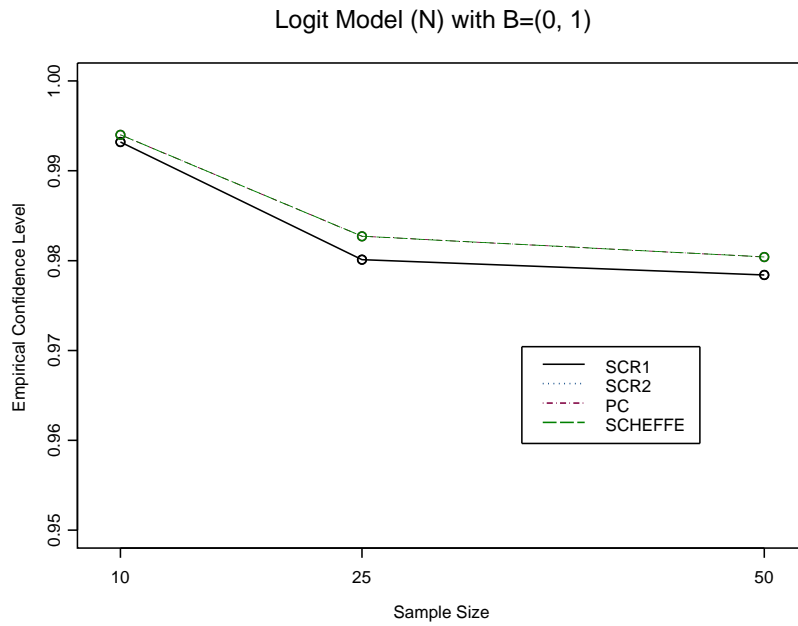


Figure A.19: pMLE Intervals Logit-Narrow Range B=2

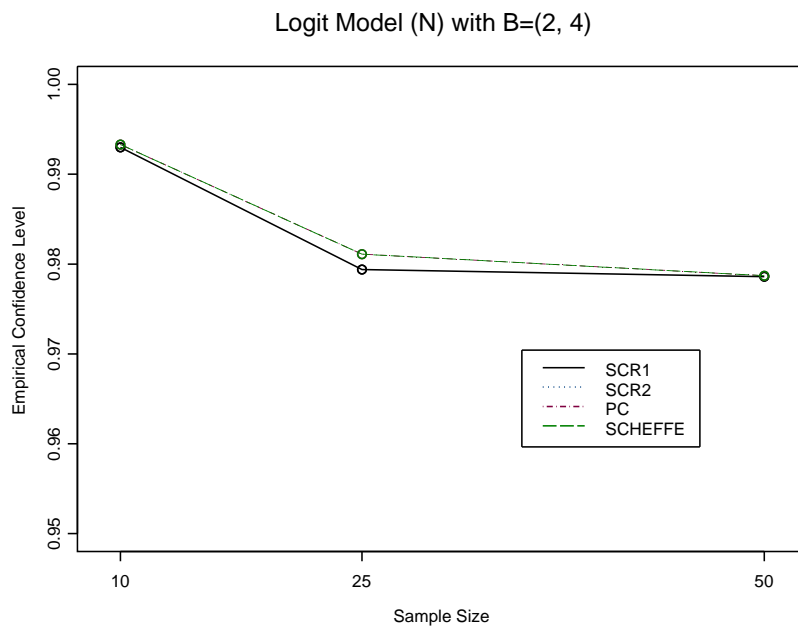


Figure A.20: pMLE Intervals Logit-Narrow Range B=3

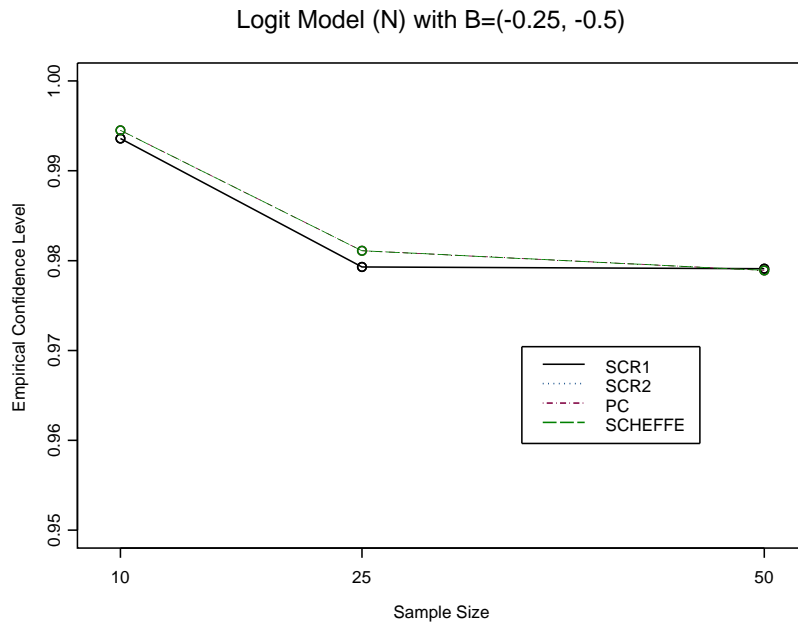


Figure A.21: pMLE Intervals Logit-Narrow Range $B=4$

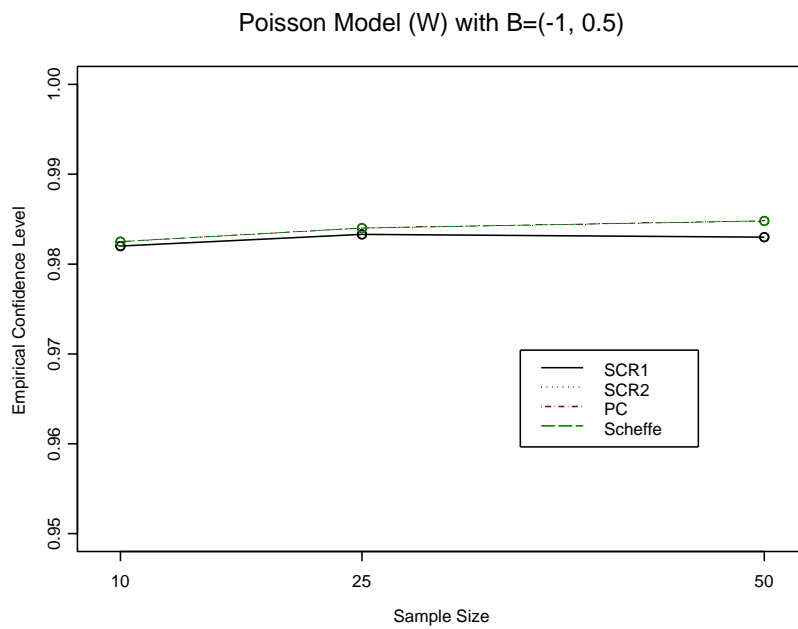


Figure A.22: pMLE Intervals Poisson-Wide Range $B=1$

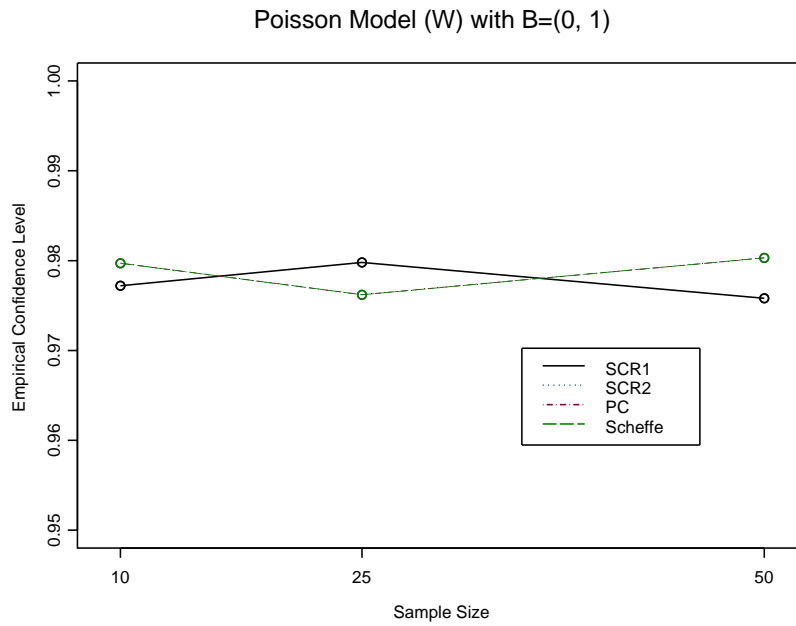


Figure A.23: pMLE Intervals Poisson-Wide Range $B=2$

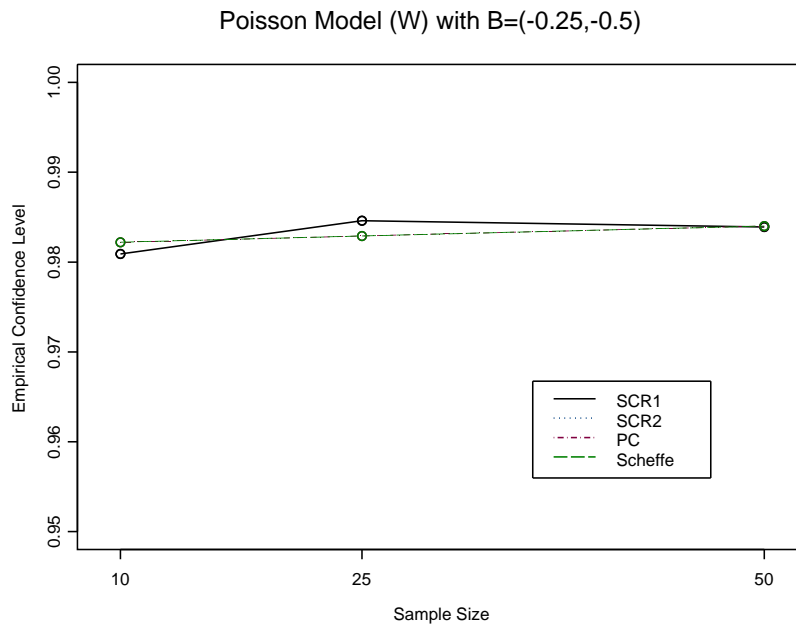


Figure A.24: pMLE Intervals Poisson-Wide Range $B=3$

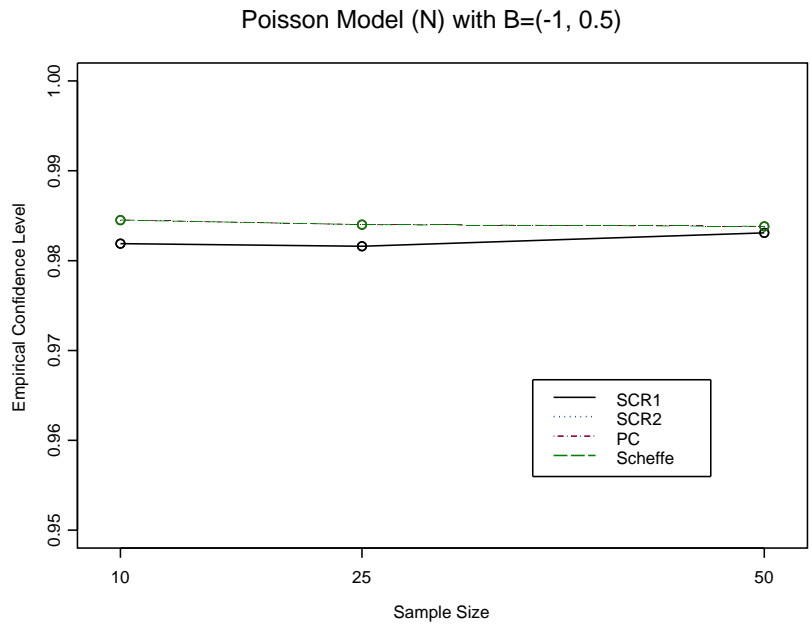


Figure A.25: pMLE Intervals Poisson-Narrow Range $B=1$

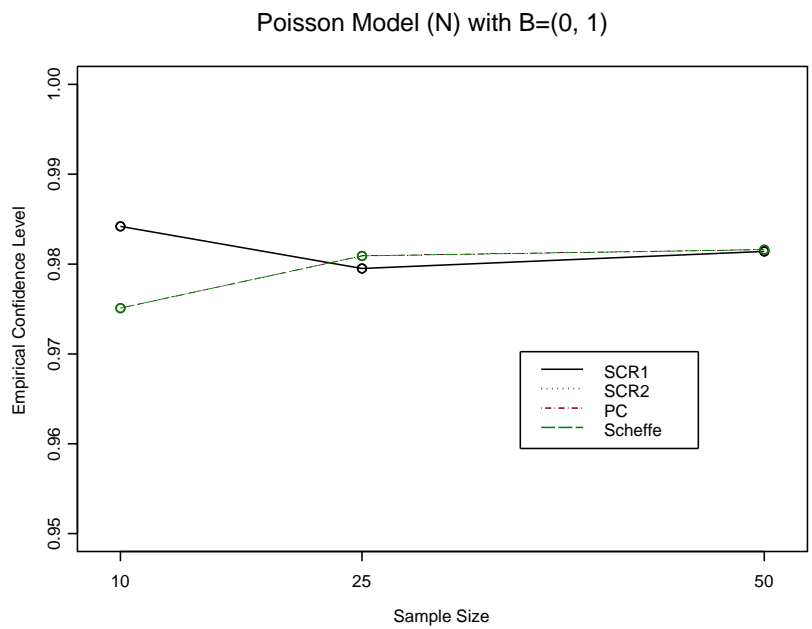


Figure A.26: pMLE Intervals Poisson-Narrow Range $B=2$

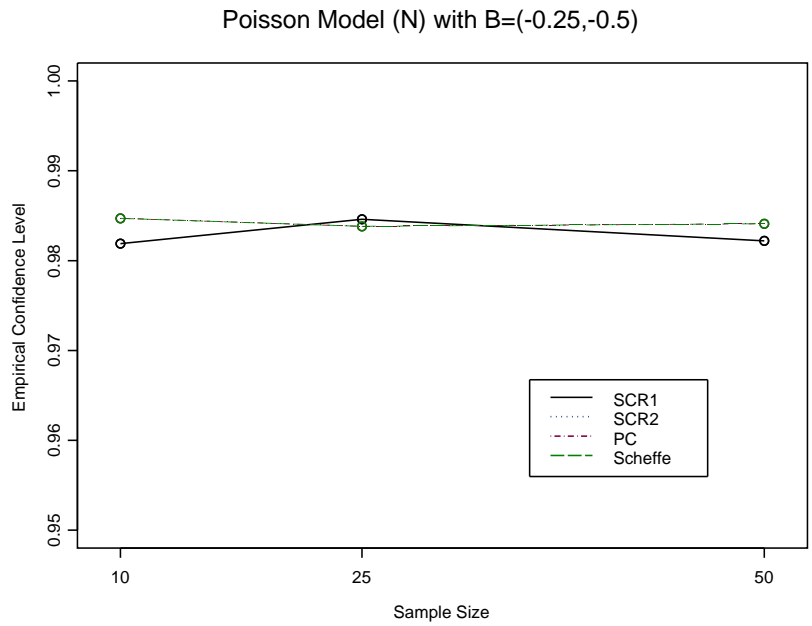


Figure A.27: pMLE Intervals Poisson-Narrow Range $B=3$

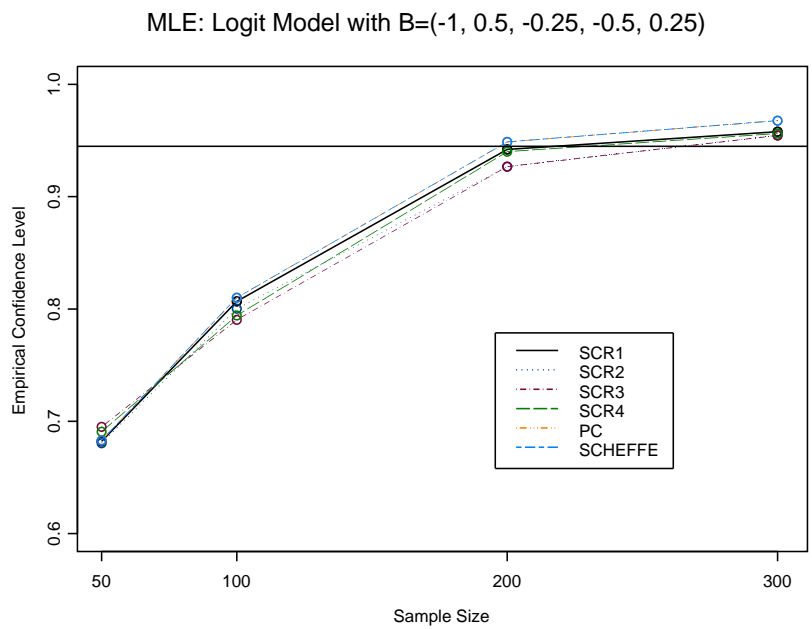


Figure A.28: MLE Intervals for the Parameters - Logit

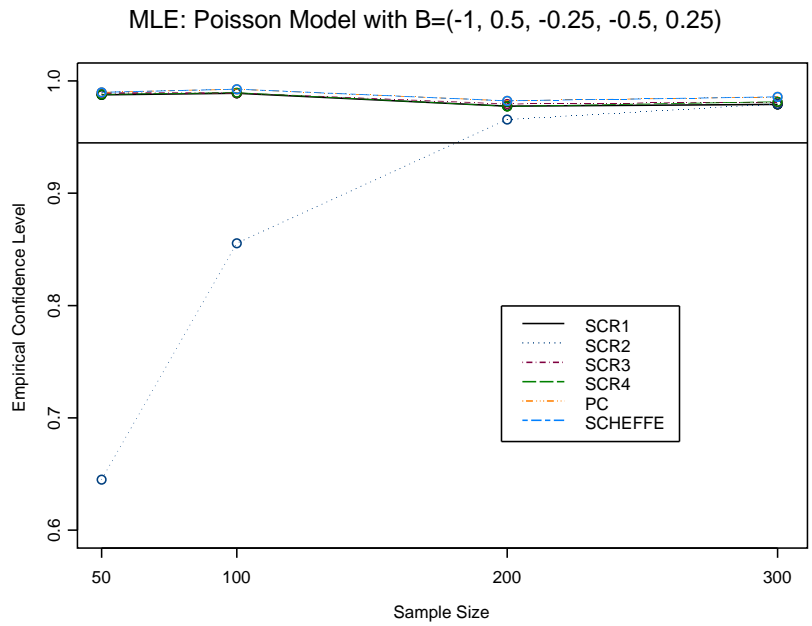


Figure A.29: MLE Intervals for the Parameters - Poisson

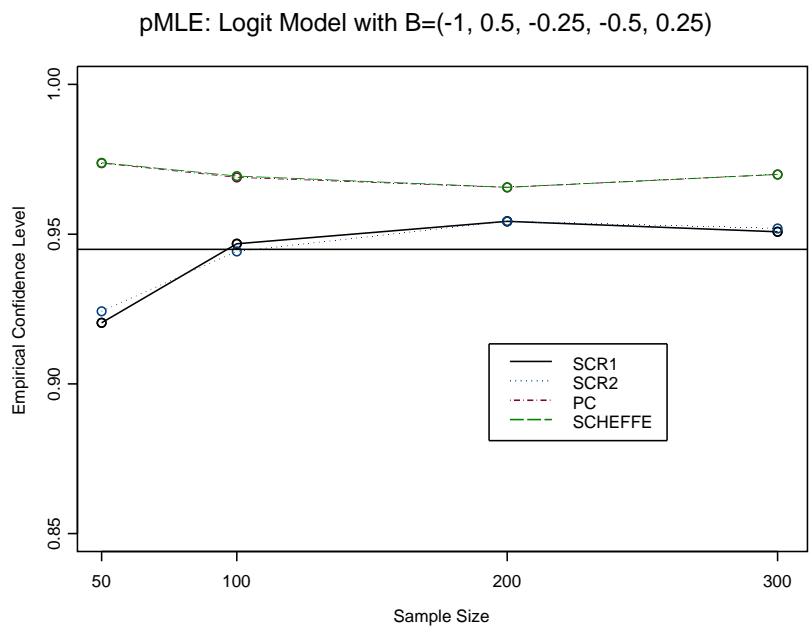


Figure A.30: pMLE Intervals for the Parameters - Logit

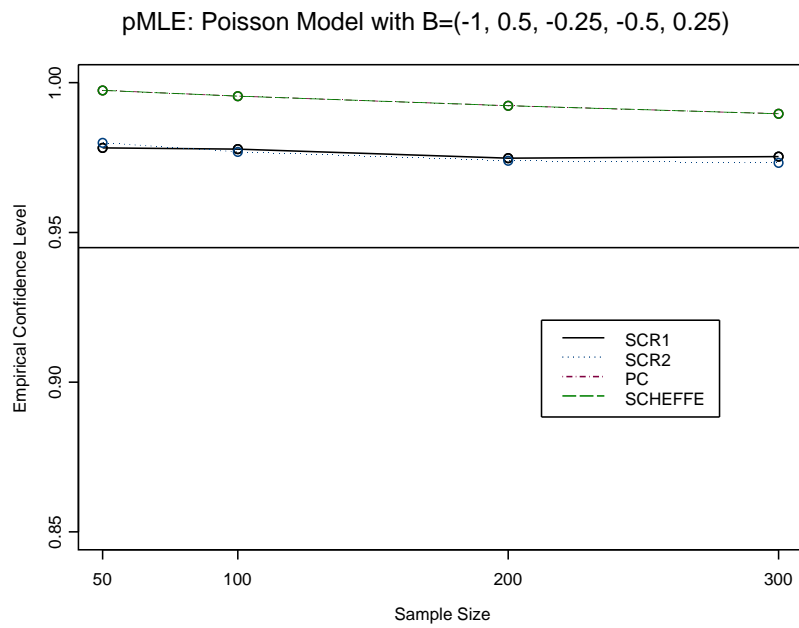


Figure A.31: pMLE Intervals for the Parameters - Poisson

APPENDIX B

Moments of Binomial and Poisson Random Variables

The moments of the binomial and poisson random variables are utilized in the SCR methodology. The following lays out the derivation of these as used in the coding for calculating the various SCR critical values. Both derivations calculate the generalized linear model moment, $b(\theta)$ based on the exponential class form $exp\{y\theta - b(\theta) + a(y)\}$ as in [13].

B.1 The Binomial Random Variable

If $Y \sim \text{BIN}(n, \pi)$, then the likelihood is given by,

$$\binom{n}{\pi} \pi^{\sum y} (1 - \pi)^{n - \sum y} = exp\left\{\sum y(\log \pi - \log(1 - \pi)) + n \log(1 - \pi) + \log \binom{n}{\pi}\right\}$$

. Thus, $b(\pi) = -n \log(1 - \pi)$ where $\pi = \frac{e^\eta}{1 + e^\eta}$ for $\eta = \theta$ given that the logit or log is a canonical link. Then, if we reparameterize $b(\pi)$ in terms of θ , then $b(\theta) = n \log(1 + e^\theta)$. Then the moments of the binomial random variable are given by the derivatives of $b(\theta)$. The first moment is:

$$\mu_\theta = b'(\theta) = \frac{ne^\theta}{1 + e^\theta} = \frac{n \frac{\pi}{1 - \pi}}{1 + \frac{\pi}{1 - \pi}} = n\pi.$$

The second moment is

$$\sigma_\theta^2 = b''(\theta) = \frac{ne^\theta}{(1 + e^\theta)^2}.$$

The third moment is

$$b^3(\theta) = \frac{ne^\theta(1 - e^\theta)}{(1 + e^\theta)^3}$$

and the fourth moment is

$$b^4(\theta) = ne^\theta(1 - e^\theta) \frac{-3e^\theta}{(1 + e^\theta)^4} + \frac{e^\theta - 2e^\theta}{(1 + e^\theta)^3} = \frac{e^\theta - 4e^{2\theta} + e^{3\theta}}{(1 + e^\theta)^4}.$$

B.2 The Poisson Random Variable

When $Y \sim \text{POI}(\mu)$, then the likelihood is given by,

$$\frac{e^{n\mu} \mu^{\sum y}}{y!} = \exp\{-\log(y!) + \sum y \log \mu - \mu\}.$$

Thus, $b(\mu) = \mu$ and given that $\theta = \log \mu$, then $b(\theta) = e^\theta$. Then the derivatives are all given by

$$b'(\theta) = b''(\theta) = b^3(\theta) = b^4(\theta) = e^\theta.$$

APPENDIX C

Restricted-Scheffé Methodology

The following algorithm is adapted from both Casella and Strawderman (1980) and Piegorsch and Casella (1988) for any GLM. Suppose we have interest in constrained regions of the form $R_{\mathbf{x}_i} = \{a_{11} \leq x_1 \leq a_{12}, a_{21} \leq x_2 \leq a_{22}, \dots, a_{k1} \leq x_k \leq a_{k2}\}$ where the a_{mi} ($m = 1, \dots, K$ and $i = 1, 2$) are specified. Generally, this algorithm finds a set of vertices that are of the form $\Omega_{\mathbf{x}_i} = \{\mathbf{x} : \sum_{m=1}^r x_m^2 \geq q^2 \sum_{m=r+1}^{K+1} z_m^2\}$ that contain the true set of vertices for the estimation space of interest. This subset, $\Omega_{\mathbf{x}_i}^R$, is the $\Omega_{\mathbf{x}_i}$ that most closely matches $R_{\mathbf{x}_i}$ and on which we will base the critical point for the Scheffé-based intervals. The algorithm, closely following the one outlined by Piegorsch and Casella [7], is as follows:

- 1) Find the 2^k vertices of the hyper-rectangle defined by $R_{\mathbf{x}_i}$. These are denoted $v_j = \{v_{mj}\}_{m=1}^k$ where each $v_{mj} = (a_{ml}, a_{m'l})$ for $j = 1, \dots, 2^k$, $m = 1, \dots, k$, $m' = 1, \dots, k$, and $l = 1, \dots, K$. Note that when estimating the mean response all $v_{0j} = 1$ while estimating the vector of the regression coefficients all $v_{0j} = 0$.
- 2) Compute the diagonalized vertices, $\boldsymbol{\psi}_j = \mathbf{D}^{-1/2} \mathbf{U}' \mathbf{v}_j = \{\psi_{Mj}\}_{M=1}^{k+1}$ where $j = 1, \dots, 2^k$ ranges the dimension of the k -dimensional real set, \mathbb{R}^k . The M^{th} element of this vector can be written as $\psi_{Mj} = \lambda_M^{-1/2} \sum_{L=1}^{K+1} u_{LM} v_{L-1,j}$ where λ_M is the M^{th} diagonal of the eigenvalue matrix \mathbf{D} , u_{LM} is in the L^{th} and M^{th} row and column of the eigenvector matrix \mathbf{U} , and $M = 1, \dots, k$. At this step, we have the diagonalized vertices that need to be matched as closely as possible to vertices of sets of the form of $\Omega_{\mathbf{z}_i}$.

- 3) In order to find the set of vertices that are the closest match to R_z , compute the minimum and maximum among the diagonalized vertices $z_M^{max} = \max|\psi_{Mj}|$ and

$$z_M^{min} = \begin{cases} 0 & \text{if } \min_j\{\psi_{Mj}\} < 0 < \max_j\{\psi_{Mj}\} \\ \min_j\{|\psi_{Mj}|\} & \text{otherwise} \end{cases}$$

This summarizes the vertices by recovering the maximum and minimum.

- 4) Calculate the following quantity,

$$Q_r^2 = \sum_{M=1}^r (z_M^{min})^2 / \sum_{M=r+1}^{k+1} (z_M^{max})^2$$

for each $r = 1, \dots, k$. These values are informative about R_{x_i} . For example, if $Q_r^2 = 0$, the set Ω_{x_i} does not contain the image of R_{x_i} . Whenever, $Q_r^2 > 0$, the set Ω_{x_i} does contains the image of R_{x_i} and $Q_r^2 \geq d^2$ for any $r = 1, \dots, k$. Thus, this step finds the sets which contain the R_z set so now all that needs to be done is to pick out the set most resembling R_z .

- 5) Now each d_r^2 is estimated. If $Q_r^2 = 0$, then $d_r^2 = \chi_{k+1, \alpha}^2$ which is the typical value using the Scheffé bounds. This reflects that fact that if a region of R_{x_i} is not restricted then the typical Scheffé bounds are the most appropriate. Whenever $Q_r^2 > 0$, then Q_r^2 is the largest d^2 that allows Ω_{z_i} to contain R_z . In this case, let $B^2 = (1 + Q_r^2)^{-1}$. This may be considered a measure of the size of the constraint region. Then the value of d_r^2 can be given by a table [6] or found by computer. Specifically, this value is found by finding the solution to the following equality:

$$P(E_{r,s}(b, d^2) + P(E_{s,r}(a, d^2) = P(a\chi_r + b\chi_s)^2 \leq d^2) - P(\chi_p^2 \leq d^2)$$

where $E_{r,s}(b, d^2)$ and $E_{s,r}(a, d^2)$ are as defined previously. This is a very tedious calculation and requires a computer to provide a solution.

- 6) Finally, let $d_S^2 = \min_r \{d_r^2\}$. This is the value that bounds the GLM when applied to the formula. Alternatively, one may choose, in step 5) the small of all Q_r^2

which also yields the smallest d^2 .

$$\mathbf{x}'\hat{\boldsymbol{\beta}} \pm |d_S|(\mathbf{x}'\mathbf{F}^{-1}\mathbf{x})^{1/2} \quad \forall \mathbf{x} \in R_{\mathbf{x}_i}$$

When the domain of interest for the predictor variable is continuous this algorithm may be followed explicitly for any set of restrictions given by R_x . However, when estimating linear combinations of the parameters, a slight change must be made. Now the limits on the domain are not given by R_x but are rectangular regions defined by the c_i 's. For example, when considering the simultaneous estimation of the vector of parameters $(\beta_1, \dots, \beta_k)$, our contrast matrix is a sequence of 0's and 1's as described in chapter 3. Since we are trying to estimate the actual β_i 's ($i=1, \dots, k$) instead of $\mathbf{X}'\boldsymbol{\beta}$, we need to capture the rectangular region defined by all the 0's and 1's. The easiest way to do this is to shift that rectangular region. For example, in two dimensions, we are trying to capture a rectangular region with the vertices (0,0), (1,0), (0,1), and (1,1). Simply shift this rectangle to have the vertices (1,1), (1,2), (2,1), and (2,2) so that the quadric form $\Omega_{\mathbf{x}_i}$ contains the rectangle. This concept may be extended to higher dimensions so that a hyper-rectangle is defined in k dimensions and the calculation of the quantity Q_r^2 is given by (C).

APPENDIX D

SCR Methodology

The SCR1 solution utilized the "tube" formula proposed recently by Naiman [10]. Assume there are d points in n -dimensional Euclidean space of interest. If these points are connected they form a curve. Tube formulas compute the volume of a tube of radius r about this curve. Tube-based intervals utilize the following solution for d , the critical value, when $k = 1$ (k =dimension)

$$\alpha \approx \frac{\kappa_0}{\pi} \exp(-d^2/2) + \delta * (1 - \Phi(d))$$

where κ_0 is the volume of the region defined by the points and δ is the Euler-Poincare characteristic of the region.

Then for $k > 1$

$$\begin{aligned} \alpha \approx & \frac{\kappa_0 \delta(\frac{k+1}{2})}{\pi^{\frac{k+1}{2}}} (1 - F_{k+1,\nu}(\frac{d^2}{k+1})) \\ & + \frac{\zeta_0 \delta(\frac{k}{2})}{2\pi^{\frac{k+1}{2}}} (1 - F_{k,\nu}(\frac{d^2}{k})) \\ & + \frac{(\kappa_2 + \zeta_1 + m_0) \delta(\frac{k-1}{2})}{2\pi^{\frac{k+1}{2}}} \\ & (1 - F_{k-1,\nu}(\frac{d^2}{k-1})) \end{aligned}$$

where κ_0 is the volume of the region defined by the points, ζ_0 is the surface area of this region, κ_2 is the curvature of the region, ζ_1 is the curvature of the boundary of this region, and m_0 is the rotation angle. The naive or SCR1 solution directly utilizes these formulas.

The SCR3 solution utilized the bias correction of the Gaussian random field,

$W_n(\mathbf{x})$, via the equality

$$|W_n(\mathbf{x})| = |\mathbf{W}(\mathbf{x})| - \mathbf{p}_2(\mathbf{x}, \mathbf{W}_n(\mathbf{x})). \quad (\text{D.1})$$

The biasing constant is given by

$$\begin{aligned} p_2(x, z) &= -z \left\{ \frac{1}{2} [\kappa_2(\mathbf{x}) - \mathbf{1} + \kappa_1^2(\mathbf{x})] \right. \\ &\quad \left. + \frac{1}{24} [\kappa_4(\mathbf{x}) + 4\kappa_1(\mathbf{x})\kappa_3(\mathbf{x})] (z^2 - \mathbf{3}) \right. \\ &\quad \left. + \frac{1}{72} \kappa_3^2(\mathbf{x}) (z^4 - 10z^2 + \mathbf{15}) \right\} = \mathbf{O}\left(\frac{\mathbf{1}}{\mathbf{n}}\right) \end{aligned}$$

The moments of $W_n(\mathbf{x})$ are given by the following,

$$\begin{aligned} \kappa_1(\mathbf{x}) &= E[W_n(\mathbf{x})] = \mu'_n(\mathbf{x}) \\ \kappa_2(\mathbf{x}) &= E[W_n(\mathbf{x}) - \mathbf{E}[\mathbf{W}_n(\mathbf{x})]]^2 \\ &= 1 + \frac{1}{2}C_1 - \frac{1}{2}C_2 - 3C_3 + \frac{1}{2}C_4 \\ &\quad + C_6 - \frac{1}{2}C_7 + \frac{7}{4}C_8 \\ \kappa_3(\mathbf{x}) &= E[W_n(\mathbf{x}) - \mathbf{E}[\mathbf{W}_n(\mathbf{x})]]^3 \\ \kappa_4(\mathbf{x}) &= E[W_n(\mathbf{x}) - \mathbf{E}[\mathbf{W}_n(\mathbf{x})]]^4 - \mathbf{3}\kappa_2^2(\mathbf{x}) \\ &= -9C_3 = 3C_6 + 6C_8 + 3C_9. \end{aligned}$$

The C_i 's ($i = 1, \dots, 9$) utilized in the above calculations are given in the following equations. Note that the quantities, b^j 's, are based on the distribution of the response variable and the estimated parameters. Thus, they depend on whether the usual MLE estimators or alternative pMLE estimators are used. See Appendix B for the description of the b^j 's.

$$C_1 = \frac{1}{n^3} \sum_i \sum_j b_i^{(3)} b_j^{(3)} \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_i \rangle \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_j \rangle \langle \mathbf{u}_i, \mathbf{u}_j \rangle^2 \quad (\text{D.2})$$

$$C_2 = \frac{1}{n^2} \sum_i b_i^{(4)} b_j^{(3)} \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_i \rangle^2 \langle \mathbf{u}_i, \mathbf{u}_j \rangle \quad (\text{D.3})$$

$$C_3 = \frac{1}{n^3} \sum_i \sum_j b_i^{(3)} b_j^{(3)} \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_i \rangle^2 \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_j \rangle^2 \langle \mathbf{u}_i, \mathbf{u}_j \rangle \quad (\text{D.4})$$

$$C_4 = \frac{1}{n^3} \sum_i \sum_j b_i^{(3)} b_j^{(3)} \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_i \rangle^2 \langle \mathbf{u}_j, \mathbf{u}_j \rangle \langle \mathbf{u}_i, \mathbf{u}_j \rangle \quad (\text{D.5})$$

$$C_5 = C_1 \quad (\text{D.6})$$

$$C_6 = \frac{1}{n^2} \sum_i b_i^{(4)} \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_i \rangle^4 \quad (\text{D.7})$$

$$C_7 = \frac{1}{n^3} \sum_i \sum_j b_i^{(3)} b_j^{(3)} \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_i \rangle \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_j \rangle^3 \langle \mathbf{u}_i, \mathbf{u}_i \rangle \quad (\text{D.8})$$

$$C_8 = \frac{1}{n^3} \sum_i \sum_j b_i^{(3)} b_j^{(3)} \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_i \rangle^3 \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_j \rangle^3 \quad (\text{D.9})$$

$$C_9 = \frac{1}{n^2} \sum_i [b_i^{(2)}]^2 \langle \mathbf{s}(\mathbf{x}), \mathbf{u}_i \rangle^4. \quad (\text{D.10})$$

APPENDIX E

Fortran Code: Piegorsch-Casella PMLE for the Mean Response

```
USE MSIMSL
INTEGER PINT, REPS
DOUBLE PRECISION P, R
PARAMETER(PINT=2, REPS=5000, LDA=PINT, LDEVEC=PINT, LDAINV=PINT)
DOUBLE PRECISION RANGEX(2), VER(PINT, 2**(PINT-1)),
DVER(PINT, 2**(PINT-1)), ZMAX(2**(PINT-1)), ZMIN(2**(PINT-1))
DOUBLE PRECISION S, A2, B2, Q2, C, Dp, Z(2), ECL(REPS),
ECL2(REPS), N, MEANECL, MEANECL2, LEFT, RIGHT, MUTEMP
DOUBLE PRECISION BETAP(2), XMAT(:, :), LINEAR(:), LINEARP, U(:),
MU(:), MUHAT(:), FACT
REAL MEANTEMP
INTEGER PTEMP(:), DONE, ITER, Y2(:)
ALLOCATABLE XMAT, LINEAR, U, MU, MUHAT, PTEMP, Y2
INTEGER L, RT, ISEED, STEP, NINT, CONF, CONF2, ITER2
DOUBLE PRECISION ERS
DOUBLE PRECISION CHIP
DOUBLE PRECISION BETAF(PINT), DELTAF(PINT), LOGLIK, LOGLIKOLD,
DET1, DET2, FISH(PINT, PINT)
DOUBLE PRECISION USTAR(PINT), LOGLIK1, LOGLIK2, FACU(PINT, PINT),
MX, BIAS(PINT), MEANBIAS(PINT)
COMMON S, R, P, A2, B2, C
```

```

INTEGER IRULE,K,I,J,RINT,IPVT(PINT)
DOUBLE PRECISION LOW(2),UP(2),ERRABS,ERREL,TEMP,COVLIN,TEMP2(2),XSUM
DOUBLE PRECISION ERSRESULT1,ERSRESULT2,ERSTEMP,CHIPTEMP,FX,FX1,CO,C1,C2
DOUBLE PRECISION ERREST,CHIPRESULT1
DOUBLE PRECISION CHIPRESULT2
EXTERNAL ERS, CHIP
PARAMETER(Delta=1.0D-3,Epsilon=1.0D-6,Max=1000,Small=1.0D-6)
DOUBLE PRECISION EPS,MUL(2)
PARAMETER (EPS=1.0D-2, ICEN=0, IFIX=0, IFRQ=0, ILT=0, INIT=0,INTCEP=1)
DOUBLE PRECISION CASE(:,,:), COEF(:,,:),COV(:,,:),H2(:,,:)
DOUBLE PRECISION H3(:,,:),HAT(:,,:),WGT(:,,:)
DOUBLE PRECISION X(:,,:), RESULTS(7),INTER,VTEMP(PINT,PINT),X2(:,,:)
DOUBLE PRECISION F(PINT,PINT),D(LDA),UMAT(LDEVEC,PINT),
D2(PINT,PINT),D3(PINT,PINT)
ALLOCATABLE CASE,COEF,COV,X,X2,H2,H3,HAT,WGT

OPEN (UNIT=8, FILE='C:/Results/pc results/Dferror.txt')
OPEN (UNIT=9, FILE='C:/Results/pc results/RESULTS.txt')
OPEN (UNIT=10, FILE='C:/Results/pc results/RELERR.txt')
OPEN (UNIT=11, FILE='C:/Results/pc results/ECL.txt')
OPEN (UNIT=12, FILE='C:/Results/pc results/DATA.txt')

! DEFINE R, S, AND P AND INTEGER VERSIONS FOR LATER
P=2.0D0
R=1.0D0
S=P-R
RINT=INT(R)

```

```

ISEED=34271
CALL RNSET(ISEED)
C10=P*DFIN(9.5D-1,P,1.0D6)
! LOOP FOR MODEL TYPE 1=LOGIT, 2=POISSON, 3=PROBIT
DO 2 B=1,2
  IF (B.EQ.1) THEN
    MODEL=3
  ELSEIF (B.EQ.2) THEN
    MODEL=0
  ELSEIF (B.EQ.3) THEN
    MODEL=4
  ENDIF
! LOOP FOR BETA PARAMETERS 1=(-1,.5), 2=(0,1), 3=(2,4),
4=(-.25,-.5)
DO 3 H=1,4
  IF (H.EQ.1) THEN
    BETAP(1)=-1.0D0
    BETAP(2)=5.0D-1
  ELSEIF (H.EQ.2) THEN
    BETAP(1)=0.0D0
    BETAP(2)=1.0D0
  ELSEIF (H.EQ.3) THEN
    BETAP(1)=2.0D0
    BETAP(2)=4.0D0
  ELSEIF (H.EQ.4) THEN
    BETAP(1)=-2.5D-1
    BETAP(2)=-5.0D-1

```



```

ENDIF
! LOOP FOR N (N=10,25,50,100,200)
DO 4 W=1,3
IF (W.EQ.1) THEN
N=1.0D1
ELSEIF (W.EQ.2) THEN
N=2.5D1
ELSEIF (W.EQ.3) THEN
N=5.0D1
ELSEIF (W.EQ.4) THEN
N=1.0D2
ELSEIF (W.EQ.5) THEN
N=2.0D2
ENDIF
NINT=INT(N)
LDCASE=NINT
LDCOEF=PINT
LDCOV=PINT
LDX=NINT
NCOL=PINT+1
NOBS=NINT
ALLOCATE (Y2(NINT),CASE(LDCASE,5),COEF(LDCOEF,4),
COV(LDCOV,4),X(LDX,NCOL))
ALLOCATE (XMAT(NINT,2),LINEAR(NINT),PTEMP(NINT),
U(NINT),MU(NINT),MUHAT(NINT))
ALLOCATE (X2(LDX,NCOL),H2(PINT,NINT),H3(NINT,PINT),
HAT(NINT,NINT),WGT(NINT,NINT))

```

```

! LOOP FOR RESTRICTED DOMAIN TYPES 1=UNRESTRICTED, 2=WIDE,
3=NARROW

DO 5 G=2,3
  IF (G.EQ.1) THEN
    MUL(1)=1.0D-4
    MUL(2)=1.0D0-1.0D-4
  ELSEIF (G.EQ.2) THEN
    MUL(1)=1.0D-1
    MUL(2)=9.0D-1
  ELSEIF (G.EQ.3) THEN
    MUL(1)=2.5D-1
    MUL(2)=7.5D-1
  ENDIF

  IF (MODEL.EQ.3) THEN
    RANGEX=(DLOG(MUL/(1-MUL))-BETAP(1))/BETAP(2)
  ELSEIF (MODEL.EQ.0) THEN
    RANGEX(2)=0.0D0
    RANGEX(1)=1.0D0
  ELSEIF (MODEL.EQ.4) THEN
    K=1
    DO WHILE (K.LE.2)
      RANGEX(K)=(DNORDF(MUL(K))-BETAP(1))/BETAP(2)
      K=K+1
    ENDDO
  ENDIF

! LOOP FOR DOMAIN TYPES 1=EQUALLY SPACED, 2=ONE CLUSTER
DO 6 E=1,1

```

```

ECL=0.0D0
ECL2=0.0D0
MEANBIAS=0.0D0
DO 7 A=1,REPS
BETAF=0.0D0
IF (E.EQ.1) THEN
IF ((MODEL.EQ.3).OR.(MODEL.EQ.4)) THEN
K=1
EQSPACE:DO WHILE (K.LT.N)
INTER=(RANGEX(2)-RANGEX(1))/(N-1)
X(K,1)=RANGEX(1)+INTER*(K-1)+1.0D-8
X(K+1,1)=RANGEX(1)+INTER*K+1.0D-8
K=K+1
ENDDO EQSPACE
ELSEIF (MODEL.EQ.0) THEN
IF (G.EQ.2) THEN
CALL DRNUN(NINT,X(:,1))
ELSEIF (G.EQ.3) THEN
CALL DRNUN(NINT,U)
X(:,1)=5.0D-1*U
ENDIF
ENDIF
ELSEIF (E.EQ.2) THEN
NCLUS=NINT*0.2
! GENERATE N-NUM CLUSTER EQUALLY SPACED PTS
CALL DRNUN(NINT-NCLUS,U(1:NINT-NCLUS))
MUHAT(1:NINT-NCLUS)=MUL(1)+U(1:NINT-NCLUS)*

```

```

(MUL(2)-MUL(1))
!   GENEATE A POINT IN THE RANGE TO CLUSTER PTS ABOUT
    UTEMP=DRNUNF()
    MUTEMP=MUL(1)+UTEMP*(MUL(2)-MUL(1))
    CALL DRNUN(NCLUS,U(1:NCLUS))
!   CLUSTER ABOUT POINT WITH WIDTH=0.2
    MUHAT(NINT-NCLUS+1:NINT)=(MUTEMP-1.0D-1)+
    U(1:NCLUS)*2.0D-1
!   FIX IF CLUSTERED POINTS FALL OUTSIDE RANGE OF X
    DO 8 Y=1,NCLUS
    IF ((MUHAT(NINT-NCLUS+Y).LT.MUL(1))) THEN
    MUHAT(NINT-NCLUS+Y)=MUL(1)
    ELSEIF (MUHAT(NINT-NCLUS+Y).GT.MUL(2)) THEN
    MUHAT(NINT-NCLUS+Y)=MUL(2)
    ENDIF
    8 CONTINUE
    IF (MODEL.EQ.3) THEN
    X(:,1)=(DLOG(MUHAT/(1.0D0-MUHAT)+Small)-
    BETAP(1))/BETAP(2)
    ELSEIF (MODEL.EQ.0) THEN
    X(:,1)=(DLOG(MUHAT+Small)-BETAP(1))/BETAP(2)
    ELSEIF (MODEL.EQ.4) THEN
    K=1
    DO WHILE (K.LE.2)
    RANGEX(K)=(DNORDF(MUL(K))-BETAP(1))
    /BETAP(2)
    K=K+1

```

```

ENDDO

ENDIF

ENDIF

XMAT(:,1)=1.0D0

XMAT(:,2)=X(:,1)

!NOTE: TEMP VALUE FOR LINEAR - LATER WILL BE
      USING EST BETAS!!!

      LINEAR=MATMUL(XMAT,BETAP)

!   SIMULATE Y NOW !   SIMULATE UNIFORM(0,1) RV'S

      CALL DRNUN(NINT,U)

!   SIMULATE RESPONSE Y

      DO 10 I=1,NINT
      IF (MODEL.EQ.3) THEN
      MU(I)=DEXP(LINEAR(I))/(1+DEXP(LINEAR(I)))
      ELSEIF (MODEL.EQ.0) THEN
      MU(I)=DEXP(LINEAR(I))
      ELSEIF (MODEL.EQ.4) THEN
      MU(I)=DNORDF(LINEAR(I))
      ENDIF

!   THE 3RD COLUMN OF X IS Y

      IF ((MODEL.EQ.3).OR.(MODEL.EQ.4)) THEN
      IF (U(I).LT.MU(I)) THEN
      X(I,3)=1.0D0
      ELSE
      X(I,3)=0.0D0
      ENDIF
      ELSE

```

```

RANGEX(1)=DMIN1(X(I,1),RANGEX(1))
RANGEX(2)=DMAX1(X(I,1),RANGEX(2))
MEANTEMP=REAL(MU(I))
CALL RNPOI(NINT,MEANTEMP,PTEMP)
X(I,3)=DBLE(PTEMP(I))
ENDIF
10 CONTINUE
!PMLE CALCULATIONS START HERE
IF (MODEL.EQ.3) THEN
X(:,2)=1.0D0
ELSEIF (MODEL.EQ.0) THEN
X(:,2)=MU
ENDIF
WGT=0.0D0
LOGLIK1=0.0D0
LOGLIK2=0.0D0
MUSUM1=0.0D0
MUSUM2=0.0D0
XSUM=SUM(X(:,3))/N
Y2=INT(X(:,3))
IF (MODEL.EQ.3) THEN
BETAF(1)=DLOG((XSUM)/((1.0D0-XSUM+Small))+Small)
ELSEIF (MODEL.EQ.0) THEN
BETAF(1)=DLOG(XSUM+Small)
ENDIF
BETAF(2)=0.0D0
LINEAR=MATMUL(XMAT,BETAF)

```

```

DO 55 I=1,NINT
IF (MODEL.EQ.3) THEN
MUHAT(I)=DEXP(LINEAR(I))/(1+DEXP(LINEAR(I)))
WGT(I,I)=DSQRT(MUHAT(I)*(1.0DO-MUHAT(I)))
IF (X(I,3).EQ.1.0DO) THEN
LOGLIK1=LOGLIK1+(DLOG(MUHAT(I)+Small))
ELSE
LOGLIK2=LOGLIK2+(DLOG(1-MUHAT(I)+Small))
ENDIF
ELSEIF (MODEL.EQ.0) THEN
MUHAT(I)=DEXP(LINEAR(I))
WGT(I,I)=DSQRT(MUHAT(I))
IF (Y2(I).GT.169) THEN
Y2(I)=169
ENDIF
FACT=DFAC(Y2(I))
LOGLIK1=LOGLIK1-MUHAT(I)+X(I,3)*
DLOG(MUHAT(I)+Small)-DLOG(FACT)
LOGLIK2=0.0DO
ELSEIF (MODEL.EQ.4) THEN
MUHAT(I)=DNORDF(LINEAR(I))
WGT(I,I)=DSQRT(MUHAT(I)*(1.0DO-MUHAT(I)))
ENDIF
55 CONTINUE
LOGLIK=LOGLIK1+LOGLIK2
IPRINT=0
TEMP3=0

```

```

H2=MATMUL (TRANSPOSE (XMAT) ,WGT)
FISH=MATMUL (H2,TRANSPOSE (H2))
CALL DLFTSF (PINT,FISH , LDA, FACU, LDA, IPVT)
! Compute the determinant
CALL DLFDSF (PINT, FACU, LDA, IPVT, DET1, DET2)
LOGLIK=LOGLIK+5.0D-1*(DET1*1.0D1**DET2)
ITER=0
LOGLIKOLD=0.0D0
ITER=0
DO WHILE (ITER.LT.25)
ITER=ITER+1
H2=MATMUL (TRANSPOSE (XMAT) ,WGT)
FISH=MATMUL (H2,TRANSPOSE (H2))
CALL DLINRG (PINT,FISH,LDA,F,LDAINV)
H3=MATMUL (TRANSPOSE (H2) ,F)
HAT=MATMUL (H3,H2)
DO 66 0=1,NINT
IF (MODEL.EQ.3) THEN
X2(0,3)=X(0,3)-MUHAT(0)+HAT(0,0)*
(5.0D-1-MUHAT(0))
ELSEIF (MODEL.EQ.0) THEN
X2(0,3)=X(0,3)-MUHAT(0)+HAT(0,0)/2.0D0
ENDIF
66 CONTINUE
USTAR=MATMUL (TRANSPOSE (XMAT) ,X2(: ,3))
DELTAF=MATMUL (F,USTAR)
MX=DMAX1 (DABS (DELTAF (1)) ,DABS (DELTAF (2))) /10

```



```

IF (MX.GT.1.0D0) THEN
DELTAf=DELTAf/MX
ENDIF
BETAf=BETAf+DELTAf
LINEAR=MATMUL(XMAT,BETAf)
LOGLIKOLD=LOGLIK
! DO HALF-STEPS
  DONE=0
  ITER2=0
  DO WHILE (DONE.EQ.0)
    ITER2=ITER2+1
    IF (MODEL.EQ.3) THEN
      DO 65 I=1,NINT
        MUHAT(I)=1.0D0/(1.0D0+DEXP(-LINEAR(I)))
        IF (X(I,3).EQ.1.0D0) THEN
          LOGLIK1=LOGLIK1+(DLOG(MUHAT(I)+Small))
        ELSE
          LOGLIK2=LOGLIK2+(DLOG(1-MUHAT(I)+Small))
        ENDIF
      65 CONTINUE
    ELSEIF (MODEL.EQ.0) THEN
      !FACT=DFAC(Y2(I))
      DO 67 I=1,NINT
        MUHAT(I)=DEXP(LINEAR(I))
        LOGLIK1=LOGLIK1-MUHAT(I)+X(I,3)*
          DLOG(MUHAT(I)+Small)-DLOG(FACT)
        LOGLIK2=0.0D0

```

```

67 CONTINUE
ENDIF
LOGLIK=LOGLIK1+LOGLIK2
H2=MATMUL(TRANSPPOSE(XMAT),WGT)
FISH=MATMUL(H2,XMAT)
CALL DLFTSF (PINT,FISH , LDA, FACU, LDA, IPVT)
!
!                                     Compute the determinant
CALL DLFDSF (PINT, FACU, LDA, IPVT, DET1, DET2)
LOGLIK=LOGLIK+5.0D-1*(DET1*1.0D1**DET2)
IF ((LOGLIK.GT.LOGLIKOLD).OR.(ITER2.EQ.5)) THEN
DONE=1
!ITER=30
ELSE
BETAF=BETAF-DELTA*2.0D0**(-I)
ENDIF
ENDDO
IF (SUM(DABS(DELTA)).LT.1.0D-4) THEN
ITER=250
ENDIF
ENDDO
LINEAR=MATMUL(XMAT,BETAF)
BIAS=BETAF-BETAP
!ENDDO
! RETRIVE VERTICES FROM RECTANGULAR RESTRICTIONS ON X
VER(1,:) = 1.0D0
L=1
DO 11 I=2,PINT

```

```

STEP=2**(PINT-I)
DO 12 J=1,L,2*STEP
VER(I,J:STEP+J-1)=RANGEX(1)
VER(I,STEP+J:2*STEP+J-1)=RANGEX(2)
12 CONTINUE
L=L+STEP
!   CALCULATE Q2 FROM P.867-868 OF CS !   FIRST CALCULATE
DIAGONALIZED VERTICES
CALL DEVCSF (PINT, FISH, LDA, D, UMAT, LDEVEC)
DO 16 K=1,PINT
DO 17 L=1,PINT
IF (K.EQ.L) THEN
D2(K,L)=D(K)**5.0D-1
ELSE
D2(K,L)=0.0D0
ENDIF
17 CONTINUE
16 CONTINUE
CALL DLINRG(PINT,D2,LDA,D3,LDAINV)
VTEMP=MATMUL(D3,TRANSPPOSE(UMAT))
DVER=MATMUL(VTEMP,VER)
IF (PINT.EQ.2) THEN
ZMAX(2)=DVER(2,2)
ZMIN(1)=DVER(2,1)
IF ((ZMAX(2).GT.0.0D0).AND.(ZMIN(1).LT.0.0D0))
THEN
ZMIN(1)=0.0D0

```

```

ELSE
ZMIN(1)=DMIN1(DABS(DVER(1,1)),
DABS(DVER(1,2)),DABS(DVER(2,1)),
DABS(DVER(2,2)))
ENDIF

ZMAX(2)=DMAX1(DABS(DVER(1,1)),
DABS(DVER(1,2)),DABS(DVER(2,1)),
DABS(DVER(2,2)))

ELSE
DO 13 K=1,(2**(PINT-1)-1)
Z(I-1)=DVER(I-1,K)
Z(I)=DVER(I,K)
ZMAX(K)=(DMAX1(Z(I-1),Z(I)))
TEMP=(DMIN1(Z(I-1),Z(I)))
IF ((TEMP.LT.0.0D0).AND.
(ZMAX(K).GT.0.0D0)) THEN
ZMIN(K)=0.0D0
ELSE
ZMIN(K)=DABS(TEMP)
ENDIF
ZMAX(K)=DMAX1(DABS(ZMAX(K)),
DABS(Z(I)))
13 CONTINUE
ENDIF
11 CONTINUE
RT=1
Q2=0.0D0

```

```

DO WHILE (RT.LT.(2**(PINT-1)))
Q2TEMP=SUM(ZMIN(1:RT)**2.0D0)/
SUM(ZMAX(RT+1:2**(PINT-1))**2.0D0)
IF (Q2TEMP.EQ.0.0D0) THEN
RT=RT+1
Q2=Q2TEMP
RT=2**(PINT-1)
ENDIF
ENDDO
B2=(1.0D0+Q2)**(-1.0D0)
A2=1-B2
! STARTING VALUES FOR THE SECANT METHOD
C0=1.96D0**2.0D0
C1=C10
! DEFINE UPPER AND LOWER LIMITS FOR ERS INTEGRAL
LOW(1)=C0
LOW(2)=C1
! BE CAREFUL WHEN B2=0
IF (B2.GT.1.0D-6) THEN
UP(1)=(C0)/(B2)
UP(2)=(C1)/(B2)
ELSE
UP(1)=9.99D9
UP(2)=9.99D9
END IF
C=DSQRT(C0)
ERRABS=1.0d-6

```

```

ERREL=1.0d-6
IRULE=2
! Call 1st ERS integral
IF (B2.EQ.0.0D0) THEN
CALL DQDAGI(ERS,LOW(1),1,ERRABS,ERREL,
ERSRESULT1,ERREST)
ELSE IF (B2.EQ.1.0D0) THEN
ERSRESULT1=0.0D0
ELSE
CALL DQDAG(ERS,LOW(1),UP(1),ERRABS,ERREL,
IRULE,ERSRESULT1,ERREST)
END IF
! Call 2nd ERS integral
C=DSQRT(C1)
IF (B2.EQ.0.0D0) THEN
CALL DQDAGI(ERS,LOW(2),1,ERRABS,ERREL,
ERSRESULT2,ERREST)
ELSE IF (B2.EQ.1.0D0) THEN
ERSRESULT2=0.0D0
ELSE
CALL DQDAG(ERS,LOW(2),UP(2),ERRABS,ERREL,
IRULE,ERSRESULT2,ERREST)
END IF
! SET LIMITS FOR CHIP INTEGRAL
LOW(1)=0.0D0
LOW(2)=0.0D0
UP(1)=C0

```

```

UP(2)=C1
! Call the 1st chi square (p) integral
CALL DQDAG(CHIP,LOW(1),UP(1),ERRABS,ERREL,
IRULE,CHIPRESULT1,ERREST)
! Call the 2nd chi square (p) integral
CALL DQDAG(CHIP,LOW(2),UP(2),ERRABS,ERREL,
IRULE,CHIPRESULT2,ERREST)
! COMPUTE FIRST TWO VALUES OF THE FUNCTION F - SHOULD HAVE 0.95
BETWEEN THESE
FX=ERSRESULT1+CHIPRESULT1
FX1=ERSRESULT2+CHIPRESULT2
! K COUNTS HOW MANY ITERATIONS
K=0
AbsErr=1.0d0
! BEGIN LOOP TO OPTIMIZE F FOR C2 UNTIL ABSERR < EPS
SECANTLOOP: DO WHILE ((K.LT.Max).AND.
(AbsErr.GT.Epsilon))
! CALCULATES NEW ITERATION OF C
Df=(FX1-FX)/(C1-C0)
IF (Df.EQ.0) THEN
WRITE (8,*) Df
ELSE
! CALCULATES NEW ITERATION OF C
Dp=(FX1-9.5D-1)/Df
C2=(C1-Dp)**1.0D0
ENDIF
! CALCULATE NEW FX FOR C2

```

```

LOW(1)=C2
IF (B2.NE.0.0D0) THEN
UP(1)=(C2)/(B2)
ENDIF
ERRABS=1.0d-6
ERREL=1.0d-6
IRULE=2
! Call ERS integral
C=DSQRT(C2)
IF (B2.EQ.0.0D0) THEN
CALL DQDAGI(ERS,LOW(1),1,ERRABS,
ERREL,ERSTEMP,ERREST)
ELSEIF (B2.EQ.1.0D0) THEN
ERSTEMP=0.0D0
ELSE
CALL DQDAG(ERS,LOW(1),UP(1),ERRABS,
ERREL,IRULE,ERSTEMP,ERREST)
ENDIF
LOW(1)=0.0D0
UP(1)=C2
! Call the chi square (p) integral
CALL DQDAG(CHIP,LOW(1),UP(1),ERRABS,
ERREL,IRULE,CHIPTEMP,ERREST)
! CALCULATES THE NEW F VALUE (SOMEWHERE BETWEEN FX AND FX1)
TEMP=ERSTEMP+CHIPTEMP
! CALCULATE THE ERRORS
AbsErr=DABS(TEMP-9.5D-1)

```



```

RelErr=DABS(Dp)/(DABS(C2)+Small)
! RECORDS SMALL RELERR
IF (RelErr.GT.Delta) THEN
  WRITE(10,*) K,RelErr
ENDIF
! IF TEMP < 0.95 THEN OVERESTIMATED C2
IF (TEMP.LT.9.5D-1) THEN
  C0=C2
  FX=TEMP
ELSE
! IF TEMP >= 0.95 THEN C2 UNDERESTIMATED
  C1=C2
  FX1=TEMP
ENDIF
K=K+1
ENDDO SECANTLOOP
CONF=0
CONF2=0
DO 60 I=1,NINT
LINEARP=DDOT(PINT,XMAT(I,:),1,BETAP,1)
TEMP2=MATMUL(XMAT(I,:),F)
COVLIN=DDOT(PINT,TEMP2,1,XMAT(I,:),1)
      +F(2,2)*XMAT(I,2)**2.0D0
! RECORD WHEN BOUNDS ARE ESTIMATED CORRECTLY
LEFT=(LINEAR(I)-LINEARP)**2.0D0
RIGHT=C2*((COVLIN))
IF (LEFT.LE.RIGHT) THEN

```

```

CONF=CONF+1

ENDIF

LEFT=(LINEAR(I)-LINEARP)**2.0D0

RIGHT=C10*((COVLIN))

IF (LEFT.LE.RIGHT) THEN

    CONF2=CONF2+1

ENDIF

60 CONTINUE

ECL(A)=DBLE(CONF)/N

ECL2(A)=DBLE(CONF2)/N

MEANECL=SUM(ECL)/REPS

MEANECL2=SUM(ECL2)/REPS

MEANBIAS=(MEANBIAS+BIAS)/REPS

RESULTS(1)=MODEL

RESULTS(2)=H

RESULTS(3)=NINT

RESULTS(4)=G

RESULTS(5)=E

RESULTS(6)=MEANECL

RESULTS(7)=MEANECL2

7 CONTINUE

WRITE(11,*) MEANECL,MEANECL2,MEANBIAS

WRITE(9,*) RESULTS

6 CONTINUE

5 CONTINUE

DEALLOCATE (Y2,CASE,COEF,COV,X)

```

```
DEALLOCATE (XMAT,LINEAR,U,MU,MUHAT,PTEMP)
```

```
DEALLOCATE (X2,H2,H3,HAT,WGT)
```

```
4 CONTINUE
```

```
3 CONTINUE
```

```
2 CONTINUE
```

```
STOP
```

```
END
```

```
! Now start defining the functions ! used in the above main  
program ! Define the ERS function
```

```
DOUBLE PRECISION FUNCTION ERS(T)
```

```
DOUBLE PRECISION PART1, PART2, PART3, DFD, DFN
```

```
COMMON S,R,P,A2,B2,C
```

```
DOUBLE PRECISION T,S,R,P,A2,B2,C, TEMP, TEMP2, TEMP3, TEMP4,TEMP5,TEMP6
```

```
DOUBLE PRECISION DGAMMA, DFDF
```

```
!
```

```
DFD=S
```

```
DFN=R
```

```
TEMP4=C*(T-C**2.0D0)**5.0D-1
```

```
TEMP5=DSQRT(A2)*DSQRT(B2)*T
```

```
TEMP6=A2*T-C**2.0D0
```

```
PART1=DFDF*((S/R)*((TEMP4-TEMP5)/TEMP6)**2.d0,DFN,DFD)
```

```
PART2=T**((P/2.d0)-1.d0)
```

```
TEMP=P/2.0D0
```

```
TEMP2=2.0D0**TEMP
```

```
TEMP3=DGAMMA(TEMP)*TEMP2
```

```
PART3=DEXP(-T/2.d0)/TEMP3
```

```
ERS=PART1*(PART2*PART3)
```

```
RETURN
```

```
END
```

```
! Define the chi-square function
```

```
DOUBLE PRECISION FUNCTION CHIP(T)
```

```
DOUBLE PRECISION PART1, PART2, PART3
```

```
COMMON S,R,P,A2,B2,C
```

```
DOUBLE PRECISION T,S,R,P
```

```
DOUBLE PRECISION DGAMMA
```

```
PART1=T**((P/2.d0)-1.d0)
```

```
PART2=DEXP(-T/2.d0)
```

```
PART3=DGAMMA(P/2.d0)*2.d0**(P/2.d0)
```

```
CHIP=(PART1*PART2)/(PART3)
```

```
RETURN
```

```
END
```

APPENDIX F

Fortran Code: SCR PMLE for the Mean Response

```
USE MSIMSL
INTEGER N,P,M,INCX,LDA,LDR,LDAINV,VER,REPS
DOUBLE PRECISION Small
PARAMETER(N=100,P=2,M=41,REPS=5000,LDA=P,LDR=P,LDFAC=P,
LDAINV=P,Small=1.0D-6)
REAL MEANTEMP
DOUBLE PRECISION B2(N),B3(N),B4(N),B(P,P),A(P,P)
DOUBLE PRECISION AINV(P,P),LO(N),HI(N)
DOUBLE PRECISION SU(N,N),S(P,N),UI(P,N),U(N,N),K1,UITEMP(P)
DOUBLE PRECISION CRIT,C(9),KAP(5,N),KAQ(5,N),MAX_P2(N)
DOUBLE PRECISION BT(P,P),TEMP2(P),TEMP3,TEMP4,BTINV(P,P)
DOUBLE PRECISION P2,Q2,F,P3,N2,XMAT(N,P),INFO(P,P)
DOUBLE PRECISION UCRIT(N),K0,CRITLO,CRITHI,FX,FX1,ALPHA,MAX,ABSERR
DOUBLE PRECISION DF,DP,TEMPFX,LINEAR(N),LINEARP(N),VAR(N),MU(N),K3,TOL
DOUBLE PRECISION XLO,XHI,YLO,YHI,PI,X1,X2,Y1,Y2,XT,YT,CRITHIO
DOUBLE PRECISION FIRST(P),SECOND(P),DIF(P),NORMDIF,T(P,M),INTER,RESULTS(6)
DOUBLE PRECISION SUM1,SUM2,MEAN1,MEAN2,NORMC,UNIF(N),RANGEX(2),
ECL(REPS),MEANECL
EXTERNAL P2,Q2,F
INTEGER I,J,K,V,IRANK,CONF,PTEMP(N)
LOGICAL PIVOT
```

```

DOUBLE PRECISION H2(P,N),H3(N,P),HAT(N,N)
INTEGER ITER,ITER2,YF(N)
DOUBLE PRECISION X(N,P),XF(N,P),WGT(N,N)
DOUBLE PRECISION BETAP(P),MUL(2),MUHAT(N),UTEMP,MUTEMP,FACT
DOUBLE PRECISION BETAF(P),LOGLIK1,LOGLIK2,MUSUM1,MUSUM2,XSUM
DOUBLE PRECISION FISH(P,P),USTAR(P),DELTAF(P),FCOV(P,P)
DOUBLE PRECISION MX,LOGLIK,LOGLIKOLD,LEFT,RIGHT
INTEGER COUNT,NCLUS

COMMON KAP,KAQ,P3,N2,C,C2
OPEN (UNIT=9, FILE='C:/Results/RESULTS_SCR100_bothmean.txt')
OPEN (UNIT=10, FILE='C:/Results/ECL100_bothmean.txt')

MAX=500
EPSILON=1.0D-6
ALPHA=5.0D-2
PI=3.1415926535897932D0
P3=DBLE(P)
N2=DBLE(N)
K0=0.0D0
RINT=INT(R)
CALL RNSET(34271)
COUNT=0
! THIS IS SCHEFFE SOLUTION
CRITHIO=(P3*DFIN(9.5D-1,P3,1.0D6))
! LOOP FOR MODEL TYPE 1=LOGIT, 2=POISSON, 3=PROBIT
DO 2 Z=1,2

```

```

      IF (Z.EQ.1) THEN
          MODEL=3
      ELSEIF (Z.EQ.2) THEN
          MODEL=0
      ELSEIF (Z.EQ.3) THEN
          MODEL=4
      ENDIF

!   LOOP FOR BETA PARAMETERS 1=(-1,.5), 2=(0,1), 3=(2,4),
4=(-.25,-.5)

      DO 3 H=1,4
          IF (H.EQ.1) THEN
              BETAP(1)=-1.0D0
              BETAP(2)=5.0D-1
          ELSEIF (H.EQ.2) THEN
              BETAP(1)=0.0D0
              BETAP(2)=1.0D0
          ELSEIF (H.EQ.3) THEN
              BETAP(1)=2.0D0
              BETAP(2)=4.0D0
          ELSEIF (H.EQ.4) THEN
              BETAP(1)=-2.5D-1
              BETAP(2)=-5.0D-1
          ENDIF
      ENDIF

!   LOOP FOR RESTRICTED DOMAIN TYPES 1=UNRESTRICTED, 2=WIDE,
3=NARROW

      DO 5 G=2,3
          IF (G.EQ.1) THEN

```

```

      MUL(1)=1.0D-8
      MUL(2)=1.0D0-1.0D-8
    ELSEIF (G.EQ.2) THEN
      MUL(1)=1.0D-1
      MUL(2)=9.0D-1
    ELSEIF (G.EQ.3) THEN
      MUL(1)=2.5D-1
      MUL(2)=7.5D-1
    ENDIF

    IF (MODEL.EQ.3) THEN
      RANGEX=(DLOG(MUL/(1-MUL))
      -BETAP(1))/BETAP(2)
    ELSEIF (MODEL.EQ.0) THEN
      RANGEX(2)=0.0D0
      RANGEX(1)=1.0D0
    ELSEIF (MODEL.EQ.4) THEN
      K=1
      DO WHILE (K.LE.2)
        RANGEX(K)=(DNORDF(MUL(K))
        -BETAP(1))/BETAP(2)
        K=K+1
      ENDDO
    ENDIF

```

```

!   LOOP FOR DOMAIN TYPES 1=EQUALLY SPACED, 2=ONE CLUSTER

```

```

      DO 6 D=1,1
      ECL=0.0D0

```



```

DO 7 R=1,4
      VER=R
!   COUNTS EACH COMBINATION OF SIMULATION SPECS (THERE ARE
3*4*2*3=72 COMBINATIONS)
DO 8 L=1,REPS
      DONE=0
      CONF=0
      DO WHILE (DONE.EQ.0)
      CALL RNSET(0)
      IF (D.EQ.1) THEN
!   GENERATE EQUALLY SPACED X'S
      IF ((MODEL.EQ.3).OR.(MODEL.EQ.4)) THEN
      K=1
EQSPACE:DO WHILE (K.LT.N)
      INTER=(RANGEX(2)-RANGEX(1))/(N-1)
      X(K,1)=RANGEX(1)+INTER*(K-1)+1.0D-8
      X(K+1,1)=RANGEX(1)+INTER*K+1.0D-8
      K=K+1
      ENDDO EQSPACE
      ELSEIF (MODEL.EQ.0) THEN
      IF (G.EQ.2) THEN
      CALL DRNUN(N,X(:,1))
      ELSEIF (G.EQ.3) THEN
      CALL DRNUN(N,UNIF)
      X(:,1)=5.0D-1*UNIF
      ENDIF
      ENDIF

```

```

ELSEIF (D.EQ.2) THEN
    NCLUS=N*2.0D-1
    ! GENERATE N-NUM CLUSTER EQUALLY SPACED PTS
    CALL DRNUN(N-NCLUS,UNIF(1:N-NCLUS))
    MUHAT(1:N-NCLUS)=MUL(1)+UNIF(1:N-NCLUS)
    *(MUL(2)-MUL(1))
    ! GENEATE A POINT IN THE RANGE TO CLUSTER PTS ABOUT
    UTEMP=DRNUNF()
    MUTEMP=MUL(1)+UTEMP*(MUL(2)-MUL(1))
    CALL DRNUN(NCLUS,UNIF(1:NCLUS))
    ! CLUSTER ABOUT POINT WITH WIDTH=0.2
    MUHAT(N-NCLUS+1:N)=(MUTEMP-1.0D-1)+
    UNIF(1:NCLUS)*
        2.0D-1
        ! FIX IF CLUSTERED POINTS FALL OUTSIDE RANGE OF X
DO 9 J=1,NCLUS
    IF ((MUHAT(N-NCLUS+J).LT.MUL(1))) THEN
        MUHAT(N-NCLUS+J)=MUL(1)
    ELSEIF (MUHAT(N-NCLUS+J).GT.MUL(2)) THEN
        MUHAT(N-NCLUS+J)=MUL(2)
    ENDIF
9 CONTINUE
IF (MODEL.EQ.3) THEN
    X(:,1)=(DLOG(MUHAT/(1.0D0-MUHAT)+Small)-
        BETAP(1))/BETAP(2)
ELSEIF (MODEL.EQ.0) THEN
    X(:,1)=(DLOG(MUHAT+Small)-BETAP(1))/BETAP(2)

```

```

ELSEIF (MODEL.EQ.4) THEN
    K=1
    DO WHILE (K.LE.N)
        X(K,1)=(DNORDF(MUL(K))-BETAP(1))/BETAP(2)
        K=K+1
    ENDDO
ENDIF
ENDIF
XMAT(:,1)=1.0DO
XMAT(:,2)=X(:,1)
LINEARP=MATMUL(XMAT,BETAP)
!   SIMULATE Y NOW
!   SIMULATE UNIFORM(0,1) RV'S
        CALL DRNUN(N,UNIF)
!   SIMULATE RESPONSE Y
    DO 10 I=1,N
    IF (MODEL.EQ.3) THEN
        MU(I)=DEXP(LINEARP(I))/
            (1+DEXP(LINEARP(I)))
    ELSEIF (MODEL.EQ.0) THEN
        MU(I)=DEXP(LINEARP(I))
    ELSEIF (MODEL.EQ.4) THEN
        MU(K)=DNORDF(LINEARP(I))
    ENDIF
    IF ((MODEL.EQ.3).OR.(MODEL.EQ.4)) THEN
        IF (UNIF(I).LT.MU(I)) THEN
            X(I,3)=1.0DO

```

```

        ELSE
            X(I,3)=0.0D0
        ENDIF
ELSE
    RANGEX(1)=DMIN1(X(I,1),RANGEX(1))
    RANGEX(2)=DMAX1(X(I,1),RANGEX(2))
!
    IF (UNIF(I).LT.MU(I)) THEN
        MEANTEMP=REAL(MU(I))
        CALL RNPOI(N,MEANTEMP,PTEMP)
        X(I,3)=DBLE(PTEMP(I))
    ENDIF
10 CONTINUE

!PMLE CALCULATIONS START HERE
    IF (MODEL.EQ.3) THEN
        X(:,2)=1.0D0
    ELSEIF (MODEL.EQ.0) THEN
        X(:,2)=MU
    ENDIF
    WGT=0.0D0
    LOGLIK1=0.0D0
    LOGLIK2=0.0D0
    MUSUM1=0.0D0
    MUSUM2=0.0D0
    XSUM=SUM(X(:,3))/N
    YF=INT(X(:,3))
    IF (MODEL.EQ.3) THEN

```

```

      BETAF(1)=DLOG((XSUM)/
      ((1.0D0-XSUM+Small))+Small)
ELSEIF (MODEL.EQ.0) THEN
      BETAF(1)=DLOG(XSUM+Small)
ENDIF
BETAF(2)=0.0D0
LINEAR=MATMUL(XMAT,BETAF)
DO 55 I=1,N
      IF (MODEL.EQ.3) THEN
          MUHAT(I)=DEXP(LINEAR(I))/
          (1+DEXP(LINEAR(I)))
          IF (MUHAT(I).LT.1.0D-5) THEN
              MUHAT(I)=1.0D-5
          ENDIF
          WGT(I,I)=DSQRT(MUHAT(I)*
          (1.0D0-MUHAT(I)))
          IF (X(I,3).EQ.1.0D0) THEN
              LOGLIK1=LOGLIK1+(DLOG
              (MUHAT(I)+Small))
          ELSE
              LOGLIK2=LOGLIK2+
              (DLOG(1-MUHAT(I)+Small))
          ENDIF
      ELSEIF (MODEL.EQ.0) THEN
          MUHAT(I)=DEXP(LINEAR(I))
          WGT(I,I)=DSQRT(MUHAT(I))
          IF (YF(I).GT.169) THEN

```

```

      YF(I)=169
ENDIF
      FACT=DFAC(YF(I))
      LOGLIK1=LOGLIK1-MUHAT(I)+X(I,3)*
      DLOG(MUHAT(I)+Small)-DLOG(FACT)
      LOGLIK2=0.0D0
      ELSEIF (MODEL.EQ.4) THEN
      MUHAT(I)=DNORDF(LINEAR(I))
      WGT(I,I)=DSQRT(MUHAT(I)*
      (1.0D0-MUHAT(I)))
ENDIF
55 CONTINUE
      LOGLIK=LOGLIK1+LOGLIK2
      IPRINT=0
      TEMP3=0
      ITER=0
      LOGLIKOLD=0.0D0
      ITER=0
      DO WHILE (ITER.LT.25)
          ITER=ITER+1
          H2=MATMUL(TRANSPPOSE(XMAT),WGT)
          FISH=MATMUL(H2,TRANSPPOSE(H2))
          CALL DLINRG(P,FISH,LDA,FCOV,LDAINV)
          H3=MATMUL(TRANSPPOSE(2),FCOV)
          HAT=MATMUL(H3,H2)
          DO 66 0=1,N
              IF (MODEL.EQ.3) THEN

```

```

        XF(0,3)=X(0,3)-MUHAT(0)+HAT(0,0)*(5.0D-1-MUHAT(0))
ELSEIF (MODEL.EQ.0) THEN
        XF(0,3)=X(0,3)-MUHAT(0)+HAT(0,0)/2.0D0
ENDIF
66 CONTINUE
USTAR=MATMUL(TRANPOSE(XMAT),XF(:,3))
DELTA F=MATMUL(FCOV,USTAR)
MX=DMAX1(DABS(DELTA F(1)),DABS(DELTA F(2)))/10
IF (MX.GT.1.0D0) THEN
        DELTA F=DELTA F/MX
ENDIF
BETA F=BETA F+DELTA F
LINEAR=MATMUL(XMAT,BETA F)
LOGLIKOLD=LOGLIK
! DO HALF-STEPS
DONE=0
ITER2=0
DO WHILE (DONE.EQ.0)
        ITER2=ITER2+1
        IF (MODEL.EQ.3) THEN
                DO 65 I=1,N
                        MUHAT(I)=1.0D0/(1.0D0+
                                DEXP(-LINEAR(I)))
                        IF (X(I,3).EQ.1.0D0) THEN
                                LOGLIK1=LOGLIK1+
                                        (DLOG(MUHAT(I)+Small))
                        ELSE

```

```

        LOGLIK2=LOGLIK2+
        (DLOG(1-MUHAT(I)+Small))
    ENDIF
65 CONTINUE
ELSEIF (MODEL.EQ.0) THEN
    !FACT=DFAC(Y2(I))
    DO 67 I=1,N
        MUHAT(I)=DEXP(LINEAR(I))
        LOGLIK1=LOGLIK1-MUHAT(I)+
        X(I,3)*DLOG(MUHAT(I)+Small)-
        DLOG(FACT)
        LOGLIK2=0.0D0
    67 CONTINUE
    ENDIF
    LOGLIK=LOGLIK1+LOGLIK2
    IF ((LOGLIK.GT.LOGLIKOLD).OR.
        (ITER2.EQ.5)) THEN
        DONE=1
        !ITER=30
    ELSE
        BETAF=BETAF-DELTA*2.0D0**(-I)
    ENDIF
ENDDO
IF (SUM(DABS(DELTA)).LT.1.0D-4) THEN
    ITER=250
ENDIF
ENDDO

```



```

        LINEAR=MATMUL(XMAT,BETAF)
        CALL DLINRG(P,FCOV,LDA,INFO,LDAINV)
!   COMPUTE SCALED INFO P.433
        A=INFO/N2
!   COMPUTE A INVERSE
        CALL DLINRG(P,A,LDA,AINV,LDAINV)
        IF (IERCD().EQ.0) THEN
            DONE=1
        ENDIF
        ENDIF
        ENDDO
        TOL=100*DMACH(4)

        PIVOT=.FALSE.
!   COMPUTE CHOLESKY DECOMP OF INFORMATION SCALED !   THIS SOLUTION
GIVES B'B=A
        CALL DCHFAC(P,A,LDA,TOL,IRANK,B,LDR)
        BT=TRANSPOSE(B)
!   COMPUTES BT_INV
        CALL DLINRG(P,BT,LDA,BTINV,LDAINV)

!   START CALCULATION OF S(X) FOR ALL V=1,N !   NOTE THAT THERE IS A
UNIQUE S(X) FOR EACH UNIQUE X !   CALCULATE S(X) FROM P.435 CALL IT
S !   COMPUTE UI FROM P.437
        IF ((MODEL.EQ.3).OR.(MODEL.EQ.4)) THEN
            B2=N2*(DEXP(LINEAR))/((1.0D0+

```

```

        DEXP(LINEAR)**2.0D0)
        B3=N2*(DEXP(LINEAR)*(1.0D0-DEXP(LINEAR)))/
            (1.0D0+DEXP(LINEAR))**3.0D0
        B4=N2*((DEXP(LINEAR)-4.0D0*
            DEXP(2.0D0*LINEAR)+DEXP(3.0D0*LINEAR)))/
            ((1.0D0+DEXP(LINEAR))**4.0D0)
        ELSEIF (MODEL.EQ.0) THEN
            B2=DEXP(LINEAR)
            B3=B2
            B4=B2
        ENDIF
        DO 13 V=1,N
!   MUST DIVIDE UI BY N GIVEN HOW DATA IS ENTERED FOR CTGLM
SUBROUTINE!!!!!!
            TEMP2=MATMUL(BTINV,XMAT(V,:))
            CALL DVCAL (P,1/N2,TEMP2,1,UI(:,V),1)
            TEMP2=MATMUL(AINV,XMAT(V,:))
            TEMP3=DDOT(P,XMAT(V,:), 1, TEMP2, 1)
            TEMP4=1/DSQRT(TEMP3)
!   THIS MULTIPLIES A SCALAR (TEMP4) BY VECTOR (UI) TO GET S(X) FOR I
            CALL DVCAL (P, TEMP4, UI(:,V), 1, S(:,V), 1)
        13 CONTINUE

        DO 30 I=1,N
            DO 31 J=1,N
                U(I,J)=DDOT(P,UI(:,I),1,UI(:,J),1)
!   DOT PRODUCT OF S(X) AND UI

```

```

          SU(I,J)=DDOT(P,S(:,I),1,UI(:,J),1)
31 CONTINUE
30 CONTINUE

      DO 14 V=1,N
!   NOTE THAT VAR(X'BLINEAR)=X*VAR(BETA)*X' !   FORMULA FROM AGRESTI
P. 172

          TEMP2=MATMUL(XMAT(V,:),FCOV)
          VAR(V)=DDOT(P,TEMP2,1,XMAT(V,:),1)
!   SET K1 AND K3 TO 0 (SO IT DOESN'T BUILD ON PAST VALUES)
          K1=0.0D0
          K3=0.0D0
!   INITIALIZE C VECTOR
          C=0.0D0
          DO 20 I=1,N
!   C CALCS P.437
          C(2)=C(2)+(B4(I)*(SU(V,I)**2.0D0)
            *U(I,I))
          C(6)=C(6)+(B4(I)*(SU(V,I)**4.0D0))
          C(9)=C(9)+((B2(I)**2.0D0)*SU(V,I)**4.0D0)
!   SEE P 436
          K1=K1+(B3(I)*((SU(V,I)**3.0D0)-
            SU(V,I)*U(I,I)))
          K3=K3+(B3(I)*(SU(V,I)**3.0D0))
          DO 32 J=1,N
          C(1)=C(1)+(B3(I)*B3(J)*SU(V,I)*
            SU(V,J)*U(I,J)**2.0D0)

```

```

C(3)=C(3)+(B3(I)*B3(J)*(SU(V,I)
**2.0D0)*(SU(V,J)**2.0D0)*U(I,J))
C(4)=C(4)+(B3(I)*B3(J)*U(I,J)*
(SU(V,I)**2.0D0)*U(I,J)*U(J,J))
C(7)=C(7)+(B3(I)*B3(J)*SU(V,I)*
(SU(V,J)**3.0D0)*U(I,I))
C(8)=C(8)+(B3(I)*B3(J)*(SU(V,I)
**3.0D0)*(SU(V,J)**3.0D0))
32 CONTINUE
20 CONTINUE
C(1)=C(1)/(N2**3.0D0)
C(2)=C(2)/(N2**2.0D0)
C(3)=C(3)/(N2**3.0D0)
C(4)=C(4)/(N2**3.0D0)
C(5)=C(1)
C(6)=C(6)/(N2**2.0D0)
C(7)=C(7)/(N2**3.0D0)
C(8)=C(8)/(N2**3.0D0)
C(9)=C(9)/(N2**2.0D0)
K1=K1/(2.0D0*(N2**1.5D0))
K3=K3/(N2**1.5D0)
!   CONSTANTS USED IN P(X,Z) COMPUTATION P.437
KAP(1,V)=K1
TEMP3=C(1)-C(2)+C(4)-C(7)
KAP(2,V)=1.0D0+5.0D-1*TEMP3-3.0D0*C(3)
+C(6)+1.75D0*C(8)
KAP(3,V)=K3

```

```
KAP(4,V)=-9.0D0*C(3)+3.0D0*C(6)+6.0D0*  
C(8)+3.0D0*C(9)
```

```
!   CONSTANTS USED IN Q(X,U) COMPUTATIONS P.438
```

```
KAQ(2,V)=C(3)-1.5D0*C(8)-C(5)-C(4)+  
5.0D-1*C(7)+C(6)-C(2)
```

```
KAQ(3,V)=KAP(3,V)
```

```
KAQ(4,V)=-3.0D0*C(3)-6.0D0*C(4)-6.0D0*  
C(5)+3.0D0*C(6)+3.0D0*C(7)-3.0D0*C(8)+3.0D0*C(9)
```

```
14 CONTINUE
```

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!! !
```

```
THIS SECTION NOW STARTS NAIMAN CRITICAL VALUE CALCS !   CREATE  
MATRIX T THAT CONTAINS DOMAIN PARTITIONED LIKE ON P.441
```

```
T(1,:) = 1.0D0  
DO 50 I=2,P  
K=1  
GETT:DO WHILE ((K.LE.M).AND.(I.GT.1))  
INTER=(RANGEX(2)-RANGEX(1))/(M-1)  
T(I,K)=RANGEX(1)+INTER*(K-1)  
T(I,K+1)=RANGEX(1)+INTER*K  
K=K+1  
ENDDO GETT  
50 CONTINUE  
K0=0.0D0  
DO 40 K=1,(M-1)
```

```
!   APPROXIMATE THE MANIFOLD VOLUME (K0) LIKE ON P.441 !   COMPUTE  
S(T(K))
```

```
UITEMP=MATMUL(BTINV,T(:,K))
```

```

!      CALL DLINRG(P,A,LDA,AINV,LDAINV)
          TEMP2=MATMUL(AINV,T(:,K))
          TEMP3=DDOT(P,T(:,K), 1, TEMP2, 1)
          TEMP4=1/DSQRT(TEMP3)
          CALL DVCAL (P, TEMP4, UITEMP, 1, SECOND, 1)
!      COMPUTE S(T(K+1))
          UITEMP=MATMUL(BTINV,T(:,K+1))
!      CALL DLINRG(P,A,LDA,AINV,LDAINV)
          TEMP2=MATMUL(AINV,T(:,K+1))
          TEMP3=DDOT(P,T(:,K+1), 1, TEMP2, 1)
          TEMP4=1/DSQRT(TEMP3)
          CALL DVCAL (P, TEMP4, UITEMP, 1, FIRST, 1)
!      COMPUTE DIFFERENCE OF S(T(K))-S(T(K+1))
          DIF=FIRST-SECOND
          INCX=1
!      GET THE NORM OF THE DIFF
          NORMDIF=DNRM2(P,DIF,INCX)
!      ADD TO PREVIOUS NORMS TO APPROXIMATE KO
          KO=KO+NORMDIF
40  CONTINUE

!      CONTINUE CALC CRIT HERE !   GET S(A) TO SEE IF S(A)=S(B) FOR
INTERVAL [A,B] !   T(:,1) CONTAINS POINT A
          CRITHI=CRITHIO
          CRITLO=1.96D0**2.0D0
          UITEMP=MATMUL(BTINV,T(:,1))
          TEMP2=MATMUL(AINV,T(:,1))

```

```

        TEMP3=DDOT(P,T(:,1), 1, TEMP2, 1)
        TEMP4=1/DSQRT(TEMP3)
        CALL DVCAL (P, TEMP4, UITEMP, 1, FIRST, 1)
!   GET S(B) !   T(:,M) CONTAINS POINT B
        UITEMP=MATMUL(BTINV,T(:,M))
        TEMP2=MATMUL(AINV,T(:,M))
        TEMP3=DDOT(P,T(:,M), 1, TEMP2, 1)
        TEMP4=1/DSQRT(TEMP3)
        CALL DVCAL (P, TEMP4, UITEMP, 1, SECOND, 1)
!   COMPUTE DIFFERENCE OF S(A)-S(B) AND THEN TAKE NORM !   IF NORM=0
THEN S(A)=S(B)
        DIF=FIRST-SECOND
        INCX=1
        NORMDIF=DNRM2(P,DIF,INCX)
        IF (NORMDIF.EQ.0) THEN
            E=0.0D0
        ELSE
            E=1.0D0
        ENDIF
!   STARTING VALUES FOR SECANT METHOD !   SEE P.438 FOR FORMULA FOR
FX

        NORMC=1-DNORDF(CRITLO)
        FX=K0/(PI)*DEXP(-(CRITLO**2.0D0)/2.0D0)+
        2.0D0*E*NORMC-ALPHA
        NORMC=1-DNORDF(CRITHI)
        FX1=K0/(PI)*DEXP(-(CRITHI**2.0D0)/2.0D0)+

```

```

      2.0D0*E*NORMC-ALPHA

K=1

ABSERR=1.0D0

SECANT: DO WHILE ((K.LT.MAX).AND.
      (ABSERR.GT.EPSILON))

      DF=(FX1-FX)/(CRITHI-CRITLO+Small)

      DP=(FX1)/(DF+Small)

      CRIT=CRITHI-DP

      NORMC=1-DNORDF(CRIT)

      TEMPFX=K0/(PI)*DEXP(-(CRIT**2.0D0)/2.0D0)+
      2.0D0*E*NORMC-ALPHA

ABSERR=DABS(TEMPFX)

      IF (TEMPFX.LT.0) THEN

          CRITHI=CRIT

          FX1=TEMPFX

          ELSE

          CRITLO=CRIT

          FX=TEMPFX

          ENDIF

      K=K+1

      ENDDO SECANT

      IF (CRIT.GT.CRITHIO) THEN

          CRIT=CRITHIO

      ENDIF

      SUM1=0.0D0

      SUM2=0.0D0

      MEAN1=0.0D0

```



```

        MEAN2=0.0D0

        DO 60 V=1,N

!    CALCULATE CI FOR ETA=X'BETA THEN TRANSFORM TO GET CI ON MEAN
RESP !    CONSTRUCT CI'S HERE (RECALL 4 SCB CI'S)

        IF (VER.EQ.1) THEN

!    BASIC SCR (N IS NUMBER OF POINTS IN X TO MAKE PREDICTIONS
FOR-NEVER MIND FOR NOW!)

        LO(V)=LINEAR(V)-DSQRT(CRIT)*DSQRT(VAR(V))
        HI(V)=LINEAR(V)+DSQRT(CRIT)*DSQRT(VAR(V))
        LEFT=(LINEAR(V)-LINEARP(V))*2.0D0
        RIGHT=(CRIT**2.0D0)*VAR(V)

! IF ((LINEARP(V).GE.LO(V)).AND.(LINEARP(V).
        LE.HI(V))) THEN

        IF (LEFT.LE.RIGHT) THEN

            CONF=CONF+1

        ENDIF

!    CENTERED SCR SEE P.637 OF SUN(2001)

        ELSEIF (VER.EQ.2) THEN

        LO(V)=LINEAR(V)-KAP(1,V)*DSQRT(VAR(V))-
            (CRIT)*DSQRT(VAR(V))*DSQRT(KAP(2,V))
        HI(V)=LINEAR(V)-KAP(1,V)*DSQRT(VAR(V))+
            (CRIT)*DSQRT(VAR(V))*DSQRT(KAP(2,V))
        SUM1=SUM1+KAP(1,V)
        SUM2=SUM2+KAP(2,V)

        IF ((LINEARP(V).GE.LO(V)).AND.(LINEARP(V)
            .LE.HI(V))) THEN

            CONF=CONF+1

```

```

ENDIF
ELSEIF (VER.EQ.3) THEN
!   CORRECTED 2 SCR
      !U=SOLVE Q2 FOR U: |u|+q2=c
      XLO=1.0D-2
      XHI=2.0D0*CRIT
      YLO=Q2(XLO)-CRIT
      YHI=Q2(XHI)-CRIT
      X1=XLO
      X2=XHI
      Y1=YLO
      Y2=YHI
      ABSERR=1.0D0
      COUNT=1
      SECANTLOOP: DO WHILE ((ABSERR.GT.EPSILON)
        .AND.(COUNT.LT.25))
        XT = X2 - ((X2-X1)*Y2)/(Y2-Y1+Small)
        YT = Q2(XT) - CRIT
        IF (YT*YLO>0) THEN
          XLO = XT
        YLO = YT
        ELSE
          XHI = XT
        YHI = YT
        ENDIF
      X1=XLO
      X2=XHI

```

```

Y1=YLO
Y2=YHI
ABSERR=DABS(YT)
COUNT=COUNT+1
ENDDO SECANTLOOP
UCRIT(V)=Q2(XT)
LO(V)=LINEAR(V)-UCRIT(V)*DSQRT(VAR(V))
HI(V)=LINEAR(V)+UCRIT(V)*DSQRT(VAR(V))
SUM1=SUM1+UCRIT(V)
IF ((LINEAR(V).GE.LO(V)).AND.
(LINEAR(V).LE.HI(V))) THEN
CONF=CONF+1
ENDIF
ELSEIF (VER.EQ.4) THEN
! CORRECTED SCR ! GET MAX OF P2 BY SECANT METHOD
XLO=1.0D-2
XHI=2.0D0*CRIT
YLO=P2(XLO)
YHI=P2(XHI)
X1=XLO
X2=XHI
Y1=YLO
Y2=YHI
ABSERR=1.0D0
K=1
SECANTLOOP2: DO WHILE ((K.LT.MAX).AND.
(ABSERR.GT.EPSILON))

```

```

XT = X2 - ((X2-X1)*Y2)/(Y2-Y1+Small)
  YT = P2(XT)
  IF (YT*YLO>0) THEN
    XLO = XT
  XLO = YT
  ELSE
    XHI = XT
    YHI = YT
  ENDIF
  X1=XLO
  X2=XHI
  Y1=YLO
  Y2=YHI
  ABSERR=DABS(YT)
  K=K+1
  ENDDO SECANTLOOP2
  MAX_P2(V) = DABS(P2(XT))
  UCRIT(V)=CRIT-MAX_P2(V)
!  NOW USE SECANT METHOD AGAIN TO FIND CRIT FOR EQ.41 P. 440
  CRITLO=1.96D0
!  THIS IS SCHEFFE SOLUTION
  CRITHI=CRITHIO
  NORMC=1-DNORDF(CRITLO-MAX_P2(V))
  FX=K0/(2.0D0*PI)*DEXP(-((CRITLO-MAX_P2(V))
    **2.0D0)/2.0D0)+E*NORMC-ALPHA
  NORMC=1-DNORDF(CRITHI-MAX_P2(V))
  FX1=K0/(2.0D0*PI)*DEXP(-((CRITHI-MAX_P2(V))

```

```

                **2.0D0)/2.0D0)+E*NORMC-ALPHA
K=1
ABSERR=1.0D0
SECANT2: DO WHILE ((K.LT.MAX).AND.
                (ABSERR.GT.EPSILON))
DF=(FX1-FX)/(CRITHI-CRITLO+Small)
DP=(FX1)/(DF+Small)
!NOTE: THIS IS AUCRIT REALLY
CRIT=CRITHI-DP
NORMC=1-DNORDF(CRIT-MAX_P2(V))
TEMPFX=K0/(2.0D0*PI)*DEXP(-((CRIT-
MAX_P2(V))**2.0D0)/2.0D0)+E*NORMC-ALPHA
                ABSERR=DABS(TEMPFX)
IF (TEMPFX.LT.0) THEN
CRITHI=CRIT
FX1=TEMPFX
ELSE
CRITLO=CRIT
FX=TEMPFX
ENDIF
K=K+1
ENDDO SECANT2
LO(V)=LINEAR(V)-UCRIT(V)*DSQRT(VAR(V))
HI(V)=LINEAR(V)+UCRIT(V)*DSQRT(VAR(V))
SUM2=SUM2+MAX_P2(V)
IF ((LINEAR(V).GE.LO(V)).AND.
(LINEAR(V).LE.HI(V))) THEN

```

```
      CONF=CONF+1
    ENDIF
  ENDIF
60 CONTINUE
    ECL(L)=CONF/N2
  8 CONTINUE
MEANECL=SUM(ECL)/DBLE(REPS)
  RESULTS(1)=MODEL
  RESULTS(2)=H
  RESULTS(3)=G
  RESULTS(4)=N
  RESULTS(5)=MEANECL
  RESULTS(6)=VER
WRITE(9,*) RESULTS
  WRITE(10,*) MEANECL
  7 CONTINUE
  6 CONTINUE
  5 CONTINUE
  3 CONTINUE
  2 CONTINUE
END
```

```

DOUBLE PRECISION FUNCTION P2(U)
DOUBLE PRECISION U,KAP(5),KAQ(5),C(9),C2,N2,P3,
PART1,PART2,PART3
COMMON KAP,KAQ,P3,N2,C,C2
PART1=KAP(2)-1.0D0+KAP(1)**2.0D0
PART2=(KAP(4)+4.0D0*KAP(1)*KAP(3))*(U**2.0D0-3.0D0)
PART3=KAP(3)*(U**4.0D0-1.0D1*U**2.0D0+1.5D1)
P2=U*(3.6D1*PART1+3.0D0*PART2+PART3)/7.2D1
RETURN
END

```

```

DOUBLE PRECISION FUNCTION Q2(U)
DOUBLE PRECISION U,KAQ(5),KAP(5),P3,N2,C2,C(9),
PART1,PART2
COMMON KAP,KAQ,P3,N2,C,C2
PART1=U*U-3.0D0
PART2=(U*U-1.0D1)*U*U+1.5D1
Q2=-U*(3.6D1*KAQ(2) + 3.0D0*KAQ(4)*PART1 + KAP(3)
**2.0D0*PART2)/7.2D1
RETURN
END

```

APPENDIX G

Fortran Code: Piegorsch-Casella PMLE for the Parameters

```
USE MSIMSL
INTEGER PINT,REPS,KINT,LDA,LDEVEC,LDAINV
DOUBLE PRECISION P,R
PARAMETER(PINT=5,NINT=300,REPS=5000, KINT=PINT-1,
LDA=PINT, LDEVEC=PINT,LDAINV=PINT)
DOUBLE PRECISION RANGEX(2),RX(2),VER(2**(PINT-1),PINT),
DVER(PINT,2**(PINT-1)),ZMAX(PINT),ZMIN(PINT)
DOUBLE PRECISION S,A2, B2 ,Q2,C, Dp,Z(2),ECL(REPS),
ECL2(REPS),N,MEANECL,MEANECL2,LEFT,RIGHT
DOUBLE PRECISION BETAP(PINT),XMAT(NINT,PINT),CMAT(KINT,PINT),
LINEAR(NINT),LINEARP(NINT),MU(NINT)
DOUBLE PRECISION VTEMP(PINT,PINT),LINEARCP(KINT),
LINEARC(KINT),UNIF(NINT)
DOUBLE PRECISION RESULTS(6),D(PINT),D2(PINT,PINT),D3(PINT,PINT),
F(PINT,PINT),UMAT(PINT,PINT)
REAL MEANTEMP,PS
INTEGER PTEMP(KINT),DONE,TEMPX(NINT)
INTEGER L,ISEED,NINT,CONF,CONF2
DOUBLE PRECISION ERS
DOUBLE PRECISION CHIP
COMMON S, R, P, A2, B2, C
```



```

INTEGER IRULE,K,I,J,RINT
DOUBLE PRECISION LOW(2),UP(2),ERRABS,ERREL,TEMP,COVLIN,TEMP2(PINT)
DOUBLE PRECISION ERSRESULT1,ERSRESULT2,ERSTEMP,CHIPTEMP,FX,FX1,CO,C1,C2
DOUBLE PRECISION ERREST,CHIPRESULT1,ZMAXTEMP,CRIT
DOUBLE PRECISION CHIPRESULT2
EXTERNAL ERS,CHIP
PARAMETER(Delta=1.0D-3,Epsilon=1.0D-6,Max=1000,Small=1.0D-10)
INTEGER IPVT(PINT),COUNT2
DOUBLE PRECISION H2(PINT,NINT),H3(NINT,PINT),HAT(NINT,NINT)
INTEGER COUNT,ITER,ITER2,YF(NINT),ICODE
DOUBLE PRECISION X(NINT,PINT+1),X2(NINT,PINT+1),WGT(NINT,NINT)
DOUBLE PRECISION MUHAT(NINT),FACT
DOUBLE PRECISION BETAF(PINT),LOGLIK1,LOGLIK2,MUSUM1,MUSUM2,XSUM
DOUBLE PRECISION FISH(PINT,PINT),FACU(PINT,PINT),DET1,DET2,
USTAR(PINT),DELTA(PINT)
DOUBLE PRECISION MX,LOGLIK,LOGLIKOLD,C10

OPEN (UNIT=8, FILE='C:/Results/CMAT RESULTS/DferrorPMLE300.txt')
OPEN (UNIT=9, FILE='C:/Results/CMAT RESULTS/RESULTS_PCPMLE300.txt')
OPEN (UNIT=10, FILE='C:/Results/CMAT RESULTS/RELERR.txt')
OPEN (UNIT=11, FILE='C:/Results/CMAT RESULTS/ECL_PCPMLE300.txt')
OPEN (UNIT=12, FILE='C:/Results/CMAT RESULTS/DATA.txt')

```

```

!   DEFINE R, S, AND P AND INTEGER VERSIONS FOR LATER
P=DBLE(PINT)
R=DBLE(KINT)
N=DBLE(NINT)
S=P-R
RINT=INT(R)
ISEED=3427
CALL RNSET(ISEED)
C10=P*DFIN(9.5D-1,P,1.0D6)

!   LOOP FOR MODEL TYPE 1=LOGIT, 2=POISSON, 3=PROBIT
      DO 2 B=1,2
          IF (B.EQ.1) THEN
              MODEL=3
          ELSEIF (B.EQ.2) THEN
              MODEL=0
          ELSEIF (B.EQ.3) THEN
              MODEL=4
          ENDIF

!   LOOP FOR BETA PARAMETERS 1=(-1,.5), 2=(0,1), 3=(2,4),
4=(-.25,-.5)
      DO 3 H=1,2
          IF (H.EQ.1) THEN
              BETAP(1)=-1.0D0
              BETAP(2)=5.0D-1
              BETAP(3)=-2.5D-1

```

```

        BETAP(4)=-5.0D-1
        BETAP(5)=2.5D-1
ELSEIF (H.EQ.2) THEN
        BETAP(1)=1.0D0
        BETAP(2)=2.0D0
        BETAP(3)=4.0D0
        BETAP(4)=2.0D0
        BETAP(5)=4.0D0
ELSEIF (H.EQ.3) THEN
        BETAP(1)=-1.0D0
        BETAP(2)=2.0D0
        BETAP(3)=4.0D0
        BETAP(4)=2.0D0
        BETAP(5)=4.0D0
ENDIF

! LOOP FOR DOMAIN TYPES 1=EQUALLY SPACED, 2=ONE CLUSTER
DO 6 E=1,1
DO 7 A=1,REPS
        DONE=0
        CONF=0
        CONF2=0
        88 CONTINUE
! GENERATE X'S - THESE ARE BINOMIAL RV'S
        DONE=1
        RANGEX(1)=DRNUNF()
        RANGEX(2)=DRNUNF()
        X=0.0D0

```

```

XMAT=0.0DO
PS=5.0D-1
CALL RNBIN (NINT, KINT, PS, TEMPX)
DO 33 Q=1,NINT
    IF (TEMPX(Q).EQ.0) THEN
        X(Q,1)=1.0DO
        XMAT(Q,2)=1.0DO
    ELSEIF (TEMPX(Q).EQ.1) THEN
        X(Q,2)=1.0DO
        XMAT(Q,3)=1.0DO
    ELSEIF (TEMPX(Q).EQ.2) THEN
        X(Q,3)=1.0DO
        XMAT(Q,4)=1.0DO
    ELSEIF (TEMPX(Q).EQ.3) THEN
        X(Q,4)=1.0DO
        XMAT(Q,5)=1.0DO
    ENDIF
33 CONTINUE
DO 34 Q=2,PINT
    IF (SUM(XMAT(:,Q)).EQ.0) THEN
        GOTO 88
    ENDIF
34 CONTINUE

    XMAT(:,1)=1.0DO
! CRATE C MATRIX
DO 11 K=1,PINT-1

```

```

DO 12 W=1,KINT
  IF (W.EQ.K) THEN
    CMAT(W,K+1)=1.0DO
  ELSE
    CMAT(W,K+1)=0.0DO
  ENDIF
12 CONTINUE
11 CONTINUE
CMAT(:,1)=0.0DO
LINEARP=MATMUL(XMAT,BETAP)
LINEARCP=MATMUL(CMAT,BETAP)
! SIMULATE Y NOW
! SIMULATE UNIFORM (0,1) RV'S
CALL DRNUN(NINT,UNIF)
! SIMULATE RESPONSE Y
DO 10 I=1,NINT
  IF (MODEL.EQ.3) THEN
    MU(I)=DEXP(LINEARP(I))/
    (1+DEXP(LINEARP(I)))
  ELSEIF (MODEL.EQ.0) THEN
    MU(I)=DEXP(LINEARP(I))
  ELSEIF (MODEL.EQ.4) THEN
    MU(I)=DNORDF(LINEARP(I))
  ENDIF
  IF ((MODEL.EQ.3).OR.(MODEL.EQ.4)) THEN
    IF (UNIF(I).LT.MU(I)) THEN
      X(I,PINT+1)=1.0DO
    
```

```

ELSE
  X(I,PINT+1)=0.0D0
ENDIF
ELSE
  RANGEX(1)=DMIN1(X(I,1),RANGEX(1))
  RANGEX(2)=DMAX1(X(I,1),RANGEX(2))
  !IF (UNIF(I).LT.MU(I)) THEN
  MEANTEMP=REAL(MU(I))
  CALL RNPOI(NINT,MEANTEMP,PTEMP)
  X(I,PINT+1)=DBLE(PTEMP(I))

  ENDIF
  10 CONTINUE

```

```

!PMLE CALCULATIONS START HERE

```

```

IF (MODEL.EQ.3) THEN
  X(:,PINT)=1.0D0
ELSEIF (MODEL.EQ.0) THEN
  X(:,PINT)=MU
  ENDIF
  WGT=0.0D0
  LOGLIK1=0.0D0
  LOGLIK2=0.0D0
  MUSUM1=0.0D0
  MUSUM2=0.0D0
  XSUM=SUM(X(:,PINT+1))/N
  YF=INT(X(:,PINT+1))

```

```

BETAF=0.0D0
IF (MODEL.EQ.3) THEN
BETAF(1)=DLOG((XSUM)/((1.0D0-XSUM+Small))+Small)
ELSEIF (MODEL.EQ.0) THEN
BETAF(1)=DLOG(XSUM+Small)
ENDIF
BETAF(2)=0.0D0
LINEAR=MATMUL(XMAT,BETAF)
DO 55 I=1,NINT
IF (MODEL.EQ.3) THEN
MUHAT(I)=DEXP(LINEAR(I))/(1+DEXP(LINEAR(I)))
IF (MUHAT(I).LT.1.0D-4) THEN
MUHAT(I)=1.0D-4
ENDIF
WGT(I,I)=DSQRT(MUHAT(I)*(1.0D0-MUHAT(I)))
IF (X(I,PINT+1).EQ.1.0D0) THEN
LOGLIK1=LOGLIK1+(DLOG(MUHAT(I)+Small))
ELSE
LOGLIK2=LOGLIK2+(DLOG(1-MUHAT(I)+Small))
ENDIF
ELSEIF (MODEL.EQ.0) THEN
MUHAT(I)=DEXP(LINEAR(I))
WGT(I,I)=DSQRT(MUHAT(I))
IF (YF(I).GT.169) THEN
YF(I)=169
ENDIF
FACT=DFAC(YF(I))

```

```

LOGLIK1=LOGLIK1-MUHAT(I)+X(I,PINT+1)*
DLOG(MUHAT(I)+Small)-DLOG(FACT)
LOGLIK2=0.0D0
ELSEIF (MODEL.EQ.4) THEN
MUHAT(I)=DNORDF(LINEAR(I))
WGT(I,I)=DSQRT(MUHAT(I)*(1.0D0-MUHAT(I)))
ENDIF
55 CONTINUE

LOGLIK=LOGLIK1+LOGLIK2
TEMP3=0
H2=MATMUL(TRANSPPOSE(XMAT),WGT)
FISH=MATMUL(H2,TRANSPPOSE(H2))
CALL ERSET(0,0,0)
CALL DLFTSF (PINT,FISH , LDA, FACU, LDA, IPVT)
!                                     Compute the determinant

CALL DLFDSF (PINT, FACU, LDA, IPVT, DET1, DET2)

LOGLIK=LOGLIK+5.0D-1*(DET1*1.0D1**DET2)
ITER=0
LOGLIKOLD=0.0D0
ITER=0
DO WHILE (ITER.LT.25)
ITER=ITER+1
H2=MATMUL(TRANSPPOSE(XMAT),WGT)
FISH=MATMUL(H2,TRANSPPOSE(H2))

```



```

CALL ERSET(0,0,0)
CALL DLINRG(PINT,FISH,LDA,F,LDAINV)
ICODE=IERCD()
IF ((ICODE.EQ.1).OR.(ICODE.EQ.2)) THEN
COUNT2=COUNT2+1
WRITE(8,*) ICODE,L,H,R,COUNT2
GOTO 88
ENDIF

H3=MATMUL(TRANSPPOSE(H2),F)
HAT=MATMUL(H3,H2)
LINEAR=MATMUL(XMAT,BETAF)
DO 66 O=1,NINT
IF (MODEL.EQ.3) THEN
MUHAT(O)=1.0D0/(1.0D0+DEXP(-LINEAR(O)))
X2(O,PINT+1)=X(O,PINT+1)-MUHAT(O)+HAT(O,O)*(5.0D-1-MUHAT(O))
ELSEIF (MODEL.EQ.0) THEN
MUHAT(O)=DEXP(LINEAR(O))
X2(O,PINT+1)=X(O,PINT+1)-MUHAT(O)+HAT(O,O)/2.0D0
ENDIF
66 CONTINUE
USTAR=MATMUL(TRANSPPOSE(XMAT),X2(:,PINT+1))
DELTAF=MATMUL(F,USTAR)
MX=DMAX1(DABS(DELTAF(1)),DABS(DELTAF(2)))/10
IF (MX.GT.1.0D0) THEN
DELTAF=DELTAF/MX
ENDIF

```

```

BETAF=BETAF+DELTAF
LOGLIKOLD=LOGLIK
! DO HALF-STEPS
DONE=0
ITER2=0
LINEAR=MATMUL(XMAT,BETAF)
DO WHILE (DONE.EQ.0)
ITER2=ITER2+1
IF (MODEL.EQ.3) THEN
DO 65 I=1,NINT
MUHAT(I)=1.0D0/(1.0D0+DEXP(-LINEAR(I)))
IF (X(I,3).EQ.1.0D0) THEN
LOGLIK1=LOGLIK1+(DLOG(MUHAT(I)+Small))
ELSE
LOGLIK2=LOGLIK2+(DLOG(1-MUHAT(I)+Small))
ENDIF
65 CONTINUE
ELSEIF (MODEL.EQ.0) THEN

DO 67 I=1,NINT
MUHAT(I)=DEXP(LINEAR(I))
LOGLIK1=LOGLIK1-MUHAT(I)+
X(I,PINT+1)*DLOG(MUHAT(I)+Small)-
DLOG(FACT)
LOGLIK2=0.0D0
67 CONTINUE

ENDIF

```

```

LOGLIK=LOGLIK1+LOGLIK2
H2=MATMUL(TRANPOSE(XMAT),WGT)
FISH=MATMUL(H2,XMAT)
CALL DLFTSF (PINT,FISH , LDA, FACU,LDA, IPVT)
!                                     Compute the determinant

CALL DLFDSF (PINT, FACU, LDA, IPVT,DET1, DET2)
LOGLIK=LOGLIK+5.0D-1*(DET1*1.0D1**DET2)
IF ((LOGLIK.GT.LOGLIKOLD).OR.
(ITER2.EQ.5)) THEN
DONE=1
ELSE
BETAF=BETAF-DELTA*2.0D0**(-I)
ENDIF
ENDDO
IF (SUM(DABS(DELTA)).LT.1.0D-2) THEN
ITER=2.5D5
ENDIF
ENDDO
LINEAR=MATMUL(XMAT,BETAF)
LINEARC=MATMUL(CMAT,BETAF)

IF (DONE.EQ.1) THEN
CALL DLINRG(PINT,FISH,LDA,F,LDAINV)
ENDIF

```

```

IF (IERCD().NE.0) THEN
  DONE=1
ENDIF

!   CALCULATE Q2 FROM P.867-868 OF CS !   FIRST CALCULATE
DIAGONALIZED VERTICES

CALL DEVCSF (PINT, F, LDA, D, UMAT, LDEVEC)

DO 16 K=1,PINT
DO 17 L=1,PINT
IF (K.EQ.L) THEN
D2(K,L)=D(K)
ELSE
D2(K,L)=0.0D0
ENDIF

17 CONTINUE
16 CONTINUE

RX(1)=1.0D0
RX(2)=2.0D0
COUNT=1
DO 98 I=1,2
DO 97 J=1,2
DO 96 K=1,2
DO 95 L=1,2
VER(COUNT,2)=RX(I)
VER(COUNT,3)=RX(J)
VER(COUNT,4)=RX(K)

```

```

VER(COUNT,5)=RX(L)
COUNT=COUNT+1
95 CONTINUE
96 CONTINUE
97 CONTINUE
98 CONTINUE

CALL DLINRG(PINT,D2**5.0-1,LDA,D3,LDAINV)
VTEMP=MATMUL(D3,TRANSPPOSE(UMAT))
DVER=MATMUL(VTEMP,TRANSPPOSE(VER))

DO 25 K=1,PINT
ZMAXTEMP=-1.0D10
DO 13 I=1,2**KINT-1
Z(1)=DVER(K,I)
Z(2)=DVER(K,I+1)
ZMAXTEMP=(DMAX1(Z(1),Z(2),ZMAXTEMP))
TEMP=(DMIN1(Z(1),Z(2),ZMAXTEMP))
IF ((TEMP.LT.0.0D0).AND.(ZMAXTEMP.GT.0.0D0)) THEN
ZMIN(K)=0.0D0
ELSE
ZMIN(K)=DMIN1(DABS(Z(1)),DABS(Z(2)),DABS(ZMAXTEMP))
ENDIF
ZMAX(K)=DMAX1(DABS(Z(1)),DABS(Z(2)),DABS(ZMAXTEMP))
13 CONTINUE
25 CONTINUE
CRIT=1.0D10

```

```
DO 26 K=1,KINT
```

```
Q2=SUM((ZMIN(1:K)+1.0D0)**2.0D0)/SUM((ZMAX(K+1:PINT)-5.0D-1)**2.0D0)
```

```
B2=(1.0D0+Q2)**(-1.0D0)
```

```
A2=1-B2
```

```
! STARTING VALUES FOR THE SECANT METHOD
```

```
C0=1.96D0**2.0D0
```

```
C1=C10
```

```
! DEFINE UPPER AND LOWER LIMITS FOR ERS INTEGRAL
```

```
LOW(1)=C0
```

```
LOW(2)=C1
```

```
! BE CAREFUL WHEN B2=0
```

```
IF (B2.GT.1.0D-6) THEN
```

```
UP(1)=(C0)/(B2)
```

```
UP(2)=(C1)/(B2)
```

```
ELSE
```

```
UP(1)=9.99D9
```

```
UP(2)=9.99D10
```

```
END IF
```

```
C=DSQRT(C0)
```

```
ERRABS=1.0d-6
```

```
ERREL=1.0d-6
```

```
IRULE=2
```

```
! Call 1st ERS integral
```

```
IF (B2.EQ.0.0D0) THEN
```

```
CALL DQDAGI(ERS,LOW(1),1,ERRABS,ERREL,ERSRESULT1,ERREST)
```

```

ELSE IF (B2.EQ.1.0D0) THEN
ERSRESULT1=0.0D0

ELSE

CALL DQDAG(ERS,LOW(1),UP(1)+Small,ERRABS,ERREL,IRULE,ERSRESULT1,ERREST)

END IF

! Call 2nd ERS integral
C=DSQRT(C1)

IF (B2.EQ.0.0D0) THEN

CALL DQDAGI(ERS,LOW(2),1,
ERRABS,ERREL,ERSRESULT2,ERREST)

ELSE IF (B2.EQ.1.0D0) THEN

ERSRESULT2=0.0D0

ELSE

CALL DQDAG(ERS,LOW(2),UP(2)+Small,ERRABS,ERREL,IRULE,ERSRESULT2,ERREST)

END IF

! SET LIMITS FOR CHIP INTEGRAL

LOW(1)=0.0D0

LOW(2)=0.0D0

UP(1)=C0

UP(2)=C1

! Call the 1st chi square (p) integral

CALL DQDAG(CHIP,LOW(1),UP(1),ERRABS,
ERREL,IRULE,CHIPRESULT1,ERREST)

! Call the 2nd chi square (p) integral

CALL DQDAG(CHIP,LOW(2),UP(2),ERRABS,
ERREL,IRULE,CHIPRESULT2,ERREST)

! COMPUTE FIRST TWO VALUES OF THE FUNCTION F - SHOULD HAVE 0.95

```

```

BETWEEN THESE

FX=ERSRESULT1+CHIPRESULT1

FX1=ERSRESULT2+CHIPRESULT2

!   K COUNTS HOW MANY ITERATIONS

L=0

AbsErr=1.0d0

!   BEGIN LOOP TO OPTIMIZE F FOR C2 UNTIL ABSERR < EPS
SECANTLOOP: DO WHILE ((L.LT.Max).AND.(AbsErr.GT.Epsilon))

!   CALCULATES NEW ITERATION OF C
Df=(FX1-FX)/(C1-C0)
IF (Df.EQ.0) THEN
WRITE (8,*) Df
ELSE
!   CALCULATES NEW ITERATION OF C
Dp=(FX1-9.5D-1)/Df
C2=(C1-Dp)**1.0D0
ENDIF

!   CALCULATE NEW FX FOR C2
LOW(1)=C2
IF (B2.NE.0.0D0) THEN
UP(1)=(C2)/(B2)
ENDIF

ERRABS=1.0d-6
ERREL=1.0d-6
IRULE=2

!   Call ERS integral

```



```

C=DSQRT(C2)
IF (B2.EQ.0.0D0) THEN
CALL DQDAGI(ERS,LOW(1),1,ERRABS,
ERREL,ERSTEMP,ERREST)
ELSEIF (B2.EQ.1.0D0) THEN
ERSTEMP=0.0D0
ELSE
CALL DQDAG(ERS,LOW(1),UP(1),ERRABS,ERREL,IRULE,ERSTEMP,ERREST)
ENDIF
LOW(1)=0.0D0
UP(1)=C2
! Call the chi square (p) integral
CALL DQDAG(CHIP,LOW(1),UP(1),ERRABS,ERREL,IRULE,CHIPTEMP,ERREST)
! CALCULATES THE NEW F VALUE (SOMEWHERE BETWEEN FX AND FX1)
TEMP=ERSTEMP+CHIPTEMP
! CALCULATE THE ERRORS
AbsErr=DABS(TEMP-9.5D-1)
RelErr=DABS(Dp)/(DABS(C2)+Small)
! RECORDS SMALL RELERR
IF (RelErr.GT.Delta) THEN
WRITE(10,*) L,RelErr
ENDIF
! IF TEMP < 0.95 THEN OVERESTIMATED C2
IF (TEMP.LT.9.5D-1) THEN
C0=C2
FX=TEMP
ELSE

```

```

!   IF TEMP >= 0.95 THEN C2 UNDERESTIMATED
C1=C2
FX1=TEMP
ENDIF
L=L+1

ENDDO SECANTLOOP
26 CONTINUE
CONF=0
CONF2=0
DO 60 I=1,KINT
TEMP2=MATMUL(CMAT(I,:),F)
COVLIN=DDOT(PINT,TEMP2,1,CMAT(I,:),1)
!   RECORD WHEN BOUNDS ARE ESTIMATED CORRECTLY
LEFT=(LINEARC(I)-LINEARCP(I))**2.0D0
RIGHT=CRIT*COVLIN
IF (LEFT.LE.RIGHT) THEN
CONF=CONF+1
ENDIF
LEFT=(LINEARC(I)-LINEARCP(I))**2.0D0
RIGHT=C10*COVLIN
IF (LEFT.LE.RIGHT) THEN
CONF2=CONF2+1
ENDIF
60 CONTINUE
K=DBLE(KINT)
ECL(A)=DBLE(CONF)/K

```

```

ECL2(A)=DBLE(CONF2)/K
MEANECL=SUM(ECL)/REPS
MEANECL2=SUM(ECL2)/REPS
RESULTS(1)=MODEL
RESULTS(2)=H
RESULTS(3)=NINT
RESULTS(4)=E
RESULTS(5)=MEANECL
RESULTS(6)=MEANECL2
7 CONTINUE
WRITE(11,*) MEANECL,MEANECL2
WRITE(9,*) C2,RESULTS
6 CONTINUE
5 CONTINUE
4 CONTINUE
3 CONTINUE
2 CONTINUE

```

```

STOP

```

```

END

```

```

! Now start defining the functions ! used in the above main
program ! Define the ERS function

```

```

DOUBLE PRECISION FUNCTION ERS(T)

```

```

DOUBLE PRECISION PART1, PART2, PART3, DFD, DFN

```

```

COMMON S,R,P,A2,B2,C

```

```

DOUBLE PRECISION T,S,R,P,A2,B2,C, TEMP, TEMP2, TEMP3, TEMP4,TEMP5,TEMP6

```

```

DOUBLE PRECISION DGAMMA, DFDF
!
DFD=S
DFN=R
TEMP4=C*(T-C**2.0D0)**5.0D-1
TEMP5=DSQRT(A2)*DSQRT(B2)*T
TEMP6=A2*T-C**2.0D0
PART1=DFDF((S/R)*((TEMP4-TEMP5)/TEMP6)**2.d0,DFN,DFD)
PART2=T**((P/2.d0)-1.d0)
TEMP=P/2.0D0
TEMP2=2.0D0**TEMP
TEMP3=DGAMMA(TEMP)*TEMP2
PART3=DEXP(-T/2.d0)/TEMP3
ERS=PART1*(PART2*PART3)

RETURN
END

```

```

! Define the chi-square function
DOUBLE PRECISION FUNCTION CHIP(T)
DOUBLE PRECISION PART1, PART2, PART3
COMMON S,R,P,A2,B2,C
DOUBLE PRECISION T,S,R,P
DOUBLE PRECISION DGAMMA

```

```
PART1=T**((P/2.d0)-1.d0)
PART2=DEXP(-T/2.d0)
PART3=DGAMMA(P/2.d0)*2.d0**(P/2.d0)
CHIP=(PART1*PART2)/(PART3)
RETURN
END
```

APPENDIX H

Fortran Code: SCR PMLE for the Parameters

```
USE MSIMSL

INTEGER N,P,M,INCX,LDA,LDR,LDAINV,VER,REPS,NCOMP,MAXK

DOUBLE PRECISION Small

PARAMETER(N=200,P=5,REPS=5000,NCOMP=P-1,M=NCOMP*(NCOMP+1)-1,
Small=1.0D-10,MAXK=100,LDA=P,LDR=P,LDFAC=P,LDAINV=P)

REAL MEANTEMP,PS

DOUBLE PRECISION B2(NCOMP),B3(NCOMP),B4(NCOMP),B(NCOMP,NCOMP),
A(NCOMP,NCOMP)

DOUBLE PRECISION AINV(NCOMP,NCOMP),LO(NCOMP),HI(NCOMP),
CMAT(NCOMP,P),XMAT(N,P)

DOUBLE PRECISION SU(NCOMP,NCOMP),S(P,NCOMP),UI(P,NCOMP),
U(NCOMP,NCOMP),K1,UITEMP(NCOMP)

DOUBLE PRECISION CRIT,C(9),KAP(5,NCOMP),KAQ(5,NCOMP),MAX_P2(NCOMP)

DOUBLE PRECISION BT(NCOMP,NCOMP),TEMP2(NCOMP),TEMP3,TEMP4,
TEMP5(NCOMP)

DOUBLE PRECISION TEMP6(NCOMP),K2VEC(NCOMP),BTINV(NCOMP,NCOMP)

DOUBLE PRECISION P2,Q2,F,P3,N2

DOUBLE PRECISION UCRIT(NCOMP),K0,CRITLO,CRITHI,FX,FX1,ALPHA,
MAX,ABSERR,KSI2VEC(NCOMP)

DOUBLE PRECISION KSI,UIT(NCOMP,M**(NCOMP-2)),ST(NCOMP,M**(NCOMP-2)),
K2(10),K2MEAN
```

```

DOUBLE PRECISION STEMP1(NCOMP),STEMP2(NCOMP),STEMP3(NCOMP),KSI2,
KSI2MEAN
DOUBLE PRECISION DF,DP,TEMPFX,LINEAR(N),LINEARP(N),VAR(NCOMP),K3,TOL,C10
DOUBLE PRECISION XLO,XHI,YLO,YHI,PI,X1,X2,Y1,Y2,XT,YT,LINEARC(NCOMP),
TEMPT(NCOMP,M**NCOMP)
DOUBLE PRECISION FIRST(NCOMP),SECOND(NCOMP),DIF(NCOMP),NORMDIF,T(NCOMP,
M**NCOMP),INTER,RESULTS(6)
DOUBLE PRECISION SUM1,SUM2,MEAN1,MEAN2,UNIF(N),RANGEX(2),ECL(REPS),MEANECL
DOUBLE PRECISION PART1,PART2,PART3,PART4,PART5,PART6,GRAD(NCOMP,M**NCOMP),MO
DOUBLE PRECISION CROSS(2,3),CROSSDOT,NORM1,NORM2,COSTH,THETA
DOUBLE PRECISION GRADIENT1(NCOMP),GRADIENT2(NCOMP),LINEARCP(NCOMP)
EXTERNAL P2,Q2,F
INTEGER I,J,K,IRANK,CONF,PTEMP(NCOMP),IPVT(P),COUNT2,LOOP
DOUBLE PRECISION H2(P,N),H3(N,P),HAT(N,N)
DOUBLE PRECISION MU(N),V
INTEGER COUNT,TEMPX(N),ITER,ITER2,YF(N),ICODE
DOUBLE PRECISION COV2(NCOMP,NCOMP),X(N,P+1),XF(N,P+1),WGT(N,N)
DOUBLE PRECISION BETAP(P),MUHAT(N),FACT
DOUBLE PRECISION BETAF(P),LOGLIK1,LOGLIK2,MUSUM1,MUSUM2,XSUM
DOUBLE PRECISION FISH(P,P),FACU(P,P),DET1,DET2,USTAR(P),DELTAF(P),FCOV(P,P)
DOUBLE PRECISION MX,LOGLIK,LOGLIKOLD,GG,HH

COMMON KAP,KAQ,P3,N2,C,C2,LOOP

OPEN (UNIT=8, FILE='C:/Results/ERRORS.txt')
OPEN (UNIT=9, FILE='C:/Results/RESULTS.txt')

```

```

OPEN (UNIT=10, FILE='C:/Results/ECL.txt')

MAX=500

EPSILON=1.0D-6

ALPHA=5.0D-2

PI=3.1415926535897932D0

P3=DBLE(P)

N2=DBLE(N)

K0=0.0D0

RINT=INT(R)

CALL RNSET(34271)

COUNT=0

! THIS IS SCHEFFE SOLUTION

C10=(P3*DFIN(9.5D-1,P3,1.0D6))

! LOOP FOR MODEL TYPE 1=LOGIT, 2=POISSON, 3=PROBIT
DO 2 Z=1,2
    IF (Z.EQ.1) THEN
        MODEL=3
    ELSEIF (Z.EQ.2) THEN
        MODEL=0
    ELSEIF (Z.EQ.3) THEN
        MODEL=4
    ENDIF
! LOOP FOR BETA PARAMETERS
DO 3 H=1,2

```



```
IF (H.EQ.1) THEN
    BETAP(1)=-1.0D0
    BETAP(2)=5.0D-1
    BETAP(3)=-2.5D-1
    BETAP(4)=-5.0D-1
    BETAP(5)=2.5D-1
```

```
ELSEIF (H.EQ.2) THEN
    BETAP(1)=1.0D0
    BETAP(2)=2.0D0
    BETAP(3)=4.0D0
    BETAP(4)=2.0D0
    BETAP(5)=4.0D0
```

```
ELSEIF (H.EQ.3) THEN
    BETAP(1)=-1.0D0
    BETAP(2)=2.0D0
    BETAP(3)=4.0D0
    BETAP(4)=2.0D0
    BETAP(5)=4.0D0
```

```
ENDIF
```

```
! LOOP FOR RESTRICTED DOMAIN TYPES 1=UNRESTRICTED, 2=WIDE,
3=NARROW
```

```
! LOOP FOR DOMAIN TYPES 1=EQUALLY SPACED, 2=ONE CLUSTER
```

```
DO 7 R=1,4
    VER=R
    COUNT2=0
```

```

!   COUNTS EACH COMBINATION OF SIMULATION SPECS

      DO 8 L=1,REPS

          DONE=0

          CONF=0

      88 CONTINUE

! !   GENERATE X'S

      DONE=1

      RANGEX(1)=DRNUNF()

      RANGEX(2)=DRNUNF()

      X=0.0D0

      XMAT=0.0D0

      PS=5.0D-1

      CALL RNBIN (N, NCOMP, PS, TEMPX)

      DO 33 Q=1,N

          IF (TEMPX(Q).EQ.0) THEN

              X(Q,1)=1.0D0

              XMAT(Q,2)=1.0D0

          ELSEIF (TEMPX(Q).EQ.1) THEN

              X(Q,2)=1.0D0

              XMAT(Q,3)=1.0D0

          ELSEIF (TEMPX(Q).EQ.2) THEN

              X(Q,3)=1.0D0

              XMAT(Q,4)=1.0D0

          ELSEIF (TEMPX(Q).EQ.3) THEN

              X(Q,4)=1.0D0

              XMAT(Q,5)=1.0D0

```

```

        ENDIF
33 CONTINUE
DO 34 Q=2,P
    IF (SUM(XMAT(:,Q)).EQ.0) THEN
        GOTO 88
    ENDIF
34 CONTINUE

XMAT(:,1)=1.0D0

! CREATE C MATRIX

DO 11 K=1,P-1
    DO 12 W=1,NCOMP
        IF (W.EQ.K) THEN
            CMAT(W,K+1)=1.0D0
        ELSE
            CMAT(W,K+1)=0.0D0
        ENDIF
    12 CONTINUE
11 CONTINUE
CMAT(:,1)=0.0D0
LINEARP=MATMUL(XMAT,BETAP)
LINEARCP=MATMUL(CMAT,BETAP)

! SIMULATE Y NOW
! SIMULATE UNIFORM(0,1) RV'S
CALL DRNUN(N,UNIF)
! SIMULATE RESPONSE Y
DO 10 I=1,N

```

```

IF (MODEL.EQ.3) THEN
    MU(I)=DEXP(LINEARP(I))/(1+DEXP(LINEARP(I)))
ELSEIF (MODEL.EQ.0) THEN
    MU(I)=DEXP(LINEARP(I))
ELSEIF (MODEL.EQ.4) THEN
    MU(I)=DNORDF(LINEARP(I))
ENDIF
IF ((MODEL.EQ.3).OR.(MODEL.EQ.4)) THEN
    IF (UNIF(I).LT.MU(I)) THEN
        X(I,P+1)=1.0D0
    ELSE
        X(I,P+1)=0.0D0
    ENDIF
ELSE
    RANGEX(1)=DMIN1(X(I,1),RANGEX(1))
    RANGEX(2)=DMAX1(X(I,1),RANGEX(2))
    MEANTEMP=REAL(MU(I))
    CALL RNPOI(N,MEANTEMP,PTEMP)
    X(I,P+1)=DBLE(PTEMP(I))
ENDIF
10 CONTINUE

```

!PMLE CALCULATIONS START HERE

```

IF (MODEL.EQ.3) THEN
X(:,P)=1.0D0
ELSEIF (MODEL.EQ.0) THEN
X(:,P)=MU

```

```

ENDIF
WGT=0.0D0
LOGLIK1=0.0D0
LOGLIK2=0.0D0
MUSUM1=0.0D0
MUSUM2=0.0D0
XSUM=SUM(X(:,P+1))/N
YF=INT(X(:,P+1))
BETAF=0.0D0
IF (MODEL.EQ.3) THEN
BETAF(1)=DLOG((XSUM)/((1.0D0-XSUM+Small))+Small)
ELSEIF (MODEL.EQ.0) THEN
BETAF(1)=DLOG(XSUM+Small)
ENDIF
BETAF(2)=0.0D0
LINEAR=MATMUL(XMAT,BETAF)
DO 55 I=1,N
IF (MODEL.EQ.3) THEN
MUHAT(I)=DEXP(LINEAR(I))/
(1+DEXP(LINEAR(I)))
WGT(I,I)=DSQRT(MUHAT(I)*(1.0D0-MUHAT(I)))
IF (X(I,3).EQ.1.0D0) THEN
LOGLIK1=LOGLIK1+(DLOG(MUHAT(I)+Small))
ELSE
LOGLIK2=LOGLIK2+(DLOG(1-MUHAT(I)+Small))
ENDIF

```

```

ELSEIF (MODEL.EQ.0) THEN
MUHAT(I)=DEXP(LINEAR(I))
WGT(I,I)=DSQRT(MUHAT(I))
IF (YF(I).GT.169) THEN
YF(I)=169
ENDIF
FACT=DFAC(YF(I))
LOGLIK1=LOGLIK1-MUHAT(I)+X(I,P+1)*
DLOG(MUHAT(I)+Small)-DLOG(FACT)
LOGLIK2=0.0D0
ELSEIF (MODEL.EQ.4) THEN
MUHAT(I)=DNORDF(LINEAR(I))
WGT(I,I)=DSQRT(MUHAT(I)*(1.0D0-MUHAT(I)))
ENDIF
55 CONTINUE

LOGLIK=LOGLIK1+LOGLIK2
TEMP3=0
H2=MATMUL(TRANPOSE(XMAT),WGT)
FISH=MATMUL(H2,TRANPOSE(H2))
CALL ERSET(0,0,0)
CALL DLFTSF (P,FISH , LDA, FACU, LDA, IPVT)
!           Compute the determinant

CALL DLFDSF (P, FACU, LDA, IPVT, DET1, DET2)

LOGLIK=LOGLIK+5.0D-1*(DET1*1.0D1**DET2)

```

```

ITER=0
LOGLIKOLD=0.0D0
ITER=0
DO WHILE (ITER.LT.25)
ITER=ITER+1
H2=MATMUL (TRANSPOSE (XMAT) ,WGT)
FISH=MATMUL (H2, TRANSPOSE (H2))
CALL DLINRG (P, FISH, LDA, FCOV, LDAINV)
ICODE=IERCD()
IF ((ICODE.EQ.1).OR.(ICODE.EQ.2)) THEN
COUNT2=COUNT2+1
WRITE(8,*) ICODE,L,H,R,COUNT2
GOTO 88
ENDIF
H3=MATMUL (TRANSPOSE (H2) ,FCOV)
HAT=MATMUL (H3,H2)
LINEAR=MATMUL (XMAT,BETAF)
DO 66 O=1,N
IF (MODEL.EQ.3) THEN
MUHAT(O)=1.0D0/(1.0D0+DEXP(-LINEAR(O)))
XF(O,P+1)=X(O,P+1)-MUHAT(O)+HAT(O,O)*(5.0D-1+(1.0D0-MUHAT(O)))
ELSEIF (MODEL.EQ.0) THEN
MUHAT(O)=DEXP(LINEAR(O))
XF(O,P+1)=X(O,P+1)-MUHAT(O)+HAT(O,O)*5.0D-1
ENDIF
66 CONTINUE
USTAR=MATMUL (TRANSPOSE (XMAT) ,XF(:,P+1))

```

```

DELTA F=MATMUL (FCOV, USTAR)
MX=D MAX1 (DABS (DELTA F (1)), DABS (DELTA F (2))) /10.0D0
IF (MX.GT.1.0D0) THEN
DELTA F=DELTA F/MX
ENDIF
BETA F=BETA F+DELTA F
LOGLIKOLD=LOGLIK
! DO HALF- STEPS
DONE=0
ITER2=0
LINEAR=MATMUL (XMAT, BETA F)
DO WHILE (DONE.EQ.0)
ITER2=ITER2+1
IF (MODEL.EQ.3) THEN
DO 65 I=1, N
MUHAT (I)=1.0D0/(1.0D0+DEXP (-LINEAR (I)))

WGT (I, I)=DSQRT (MUHAT (I)*(1.0D0-MUHAT (I)))
IF (X (I, P+1).EQ.1.0D0) THEN
LOGLIK1=LOGLIK1+(DLOG (MUHAT (I)+Small))
ELSE
LOGLIK2=LOGLIK2+(DLOG (1-MUHAT (I)+Small))
ENDIF
65 CONTINUE
ELSEIF (MODEL.EQ.0) THEN
DO 67 I=1, N
MUHAT (I)=DEXP (LINEAR (I))

```



```

WGT(I,I)=DSQRT(MUHAT(I))
LOGLIK1=LOGLIK1-MUHAT(I)+X(I,P+1)*
DLOG(MUHAT(I)+Small)-DLOG(FACT)
LOGLIK2=0.0D0
67 CONTINUE
ENDIF
LOGLIK=LOGLIK1+LOGLIK2
H2=MATMUL(TRANPOSE(XMAT),WGT)
FISH=MATMUL(H2,XMAT)
CALL DLFTSF (P,FISH , LDA, FACU, LDA, IPVT)
!           Compute the determinant

CALL DLFDSF (P, FACU, LDA, IPVT, DET1, DET2)
LOGLIK=LOGLIK+5.0D-1*(DET1*1.0D1**DET2)
IF ((LOGLIK.GT.LOGLIKOLD).OR.(ITER2.EQ.5)) THEN
DONE=1
ELSE
BETAF=BETAF-DELTA*2.0D0**(-I)
ENDIF
ENDDO
IF (SUM(DABS(DELTA)).LT.1.0D-2) THEN
ITER=2.5D5
ENDIF
ENDDO
LINEAR=MATMUL(XMAT,BETAF)

```

```

CALL DLINRG(P,FISH,P,FCOV,P)
!   THIS IS COV MAT OF BETAS (COV2)
COV2=FCOV(2:P,2:P)
!   COMPUTE INFORMATION MATRIX P.432 !   FIRST COMPUTE
LINEAR=X'BETAHAT
LINEARC=MATMUL(CMAT,BETAF)

!   COMPUTE SCALED INFO P.433

!   COMPUTE A INVERSE

AINV=COV2*N2
CALL DLINRG(NCOMP,AINV,NCOMP,A,NCOMP)

!   COMPUTE CHOLESKY DECOMP OF INFORMATION SCALED !   THIS SOLUTION
GIVES B'B=A
TOL=100*DMACH(4)
CALL DCHFAC(NCOMP,A,NCOMP,TOL,IRANK,B,NCOMP)
BT=TRANSPOSE(B)
!   COMPUTES BT_INV
CALL DLINRG(NCOMP,BT,NCOMP,BTINV,NCOMP)

!   START CALCULATION OF S(X) FOR ALL V=1,N !   NOTE THAT THERE IS A
UNIQUE S(X) FOR EACH UNIQUE X !   CALCULATE S(X) FROM P.435 CALL IT
S !   COMPUTE UI FROM P.437

```

```

IF ((MODEL.EQ.3).OR.(MODEL.EQ.4)) THEN
B2=N2*(DEXP(LINEARC))/(1.0D0+DEXP(LINEARC)**2.0D0)
B3=N2*(DEXP(LINEARC)*(1.0D0-DEXP(LINEARC)))/
(1.0D0+DEXP(LINEARC)**3.0D0)
B4=N2*((DEXP(LINEARC)-4.0D0*DEXP(2.0D0*LINEARC)
+DEXP(3.0D0*LINEARC)))/(1.0D0+DEXP(LINEARC)**4.0D0)
ELSEIF (MODEL.EQ.0) THEN
B2=DEXP(LINEARC)
B3=B2
B4=B2
ENDIF

DO 13 V=1,NCOMP

! MUST DIVIDE UI BY N GIVEN HOW DATA IS ENTERED FOR CALCULATION OF
BETAS!!!!
TEMP2=MATMUL(BTINV,CMAT(V,2:P))
CALL DVCAL (P,1/N2,TEMP2,1,UI(:,V),1)
TEMP2=MATMUL(AINV,CMAT(V,2:P))
TEMP3=DDOT(P,CMAT(V,2:P), 1, TEMP2, 1)
IF (TEMP3.LT.1.0D-5) THEN
TEMP3=1.0D-5
ENDIF
TEMP4=1/DSQRT(TEMP3)
! THIS MULTIPLIES A SCALAR (TEMP4) BY VECTOR (UI) TO GET S(X) FOR
I
CALL DVCAL (P, TEMP4, UI(:,V), 1, S(:,V), 1)

```

13 CONTINUE

DO 30 I=1, NCOMP

DO 31 J=1, NCOMP

U(I, J)=DDOT(P, UI(:, I), 1, UI(:, J), 1)

! DOT PRODUCT OF S(X) AND UI

SU(I, J)=DDOT(P, S(:, I), 1, UI(:, J), 1)

31 CONTINUE

30 CONTINUE

DO 14 V=1, NCOMP

! NOTE THAT VAR(X'BLINEAR)=X*VAR(BETA)*X' ! FORMULA FROM AGRESTI

P. 172

VAR(V)=FCOV(V, V)

! SET K1 AND K3 TO 0 (SO IT DOESN'T BUILD ON PAST VALUES)

K1=0.0D0

K3=0.0D0

! INITIALIZE C VECTOR

C=0.0D0

DO 20 I=1, NCOMP

! C CALCS P. 437

C(2)=C(2)+(B4(I)*(SU(V, I)**2.0D0)*U(I, I))

C(6)=C(6)+(B4(I)*(SU(V, I)**4.0D0))

C(9)=C(9)+((B2(I)**2.0D0)*SU(V, I)**4.0D0)

! SEE P 436

K1=K1+(B3(I)*((SU(V, I)**3.0D0)-SU(V, I)*U(I, I)))

```

K3=K3+(B3(I)*(SU(V,I)**3.0D0))
DO 32 J=1,N
C(1)=C(1)+(B3(I)*B3(J)*SU(V,I)*SU(V,J)*
U(I,J)**2.0D0)
C(3)=C(3)+(B3(I)*B3(J)*(SU(V,I)**2.0D0)*
(SU(V,J)**2.0D0)*U(I,J))
C(4)=C(4)+(B3(I)*B3(J)*U(I,J)*(SU(V,I)**2.0D0)
*U(I,J)*U(J,J))
C(7)=C(7)+(B3(I)*B3(J)*SU(V,I)*(SU(V,J)
**3.0D0)*U(I,I))
C(8)=C(8)+(B3(I)*B3(J)*(SU(V,I)**3.0D0)*
(SU(V,J)**3.0D0))
32 CONTINUE
20 CONTINUE

```

! FINISH CALCULATION OF C CONSTANTS FOR EDGEWORTH EXPANSIONS

```

C(1)=C(1)/(N2**3.0D0)
C(2)=C(2)/(N2**2.0D0)
C(3)=C(3)/(N2**3.0D0)
C(4)=C(4)/(N2**3.0D0)
C(5)=C(1)
C(6)=C(6)/(N2**2.0D0)
C(7)=C(7)/(N2**3.0D0)
C(8)=C(8)/(N2**3.0D0)
C(9)=C(9)/(N2**2.0D0)
K1=K1/(2.0D0*(N2**1.5D0))

```



```
DO 51 J=1,M
DO 53 K=1,M
DO 54 Q=1,M
DO 56 O=1,M
TEMPT(1,COUNT)=INTER*(J-1)
TEMPT(2,COUNT)=INTER*(K-1)
TEMPT(3,COUNT)=INTER*(Q-1)
TEMPT(4,COUNT)=INTER*(O-1)
COUNT=COUNT+1
56 CONTINUE
54 CONTINUE
53 CONTINUE
51 CONTINUE
ENDIF
```

```
COUNT=0
DO 50 I=1,M**NCOMP
SUMCOL=(SUM(TEMPT(:,I)))
IF (SUMCOL.EQ.1) THEN
COUNT=COUNT+1
T(:,COUNT)=TEMPT(:,I)
ENDIF
SUMCOL=0.0D0
50 CONTINUE
KO=0.0D0
KSI=0.0D0
```

```

DO 40 K=1, (COUNT-1)
!   APPROXIMATE THE MANIFOLD VOLUME (KO) LIKE ON P.441 !   COMPUTE
S(T(K))
UITEMP=MATMUL(BTINV,T(:,K))
TEMP2=MATMUL(AINV,T(:,K))
TEMP3=DDOT(NCOMP,T(:,K), 1, TEMP2, 1)
IF (TEMP3.LT.1.0D-5) THEN
TEMP3=1.0D-5
ENDIF
TEMP4=1/DSQRT(TEMP3)
CALL DVCAL (NCOMP, TEMP4, UITEMP, 1, SECOND, 1)
!   COMPUTE S(T(K+1))
UITEMP=MATMUL(BTINV,T(:,K+1))
TEMP2=MATMUL(AINV,T(:,K+1))
TEMP3=DDOT(NCOMP,T(:,K+1), 1, TEMP2, 1)
IF (TEMP3.LT.1.0D-5) THEN
TEMP3=1.0D-5
ENDIF
TEMP4=1/DSQRT(TEMP3)
CALL DVCAL (NCOMP, TEMP4, UITEMP, 1, FIRST, 1)
!   COMPUTE DIFFERENCE OF S(T(K))-S(T(K+1))
DIF=FIRST-SECOND
INCX=1
!   GET THE NORM OF THE DIFF
NORMDIF=DNRM2(NCOMP,DIF,INCX)
!   ADD TO PREVIOUS NORMS TO APPROXIMATE KO
KO=KO+NORMDIF

```


40 CONTINUE

```
! APPROXIMATE THE MANIFOLD SURFACE AREA (KSI)
! TO DO THIS WE CALC VOLUME ON D-1 DIMENSIONS
DO 42 Q=1, NCOMP
DO 41 J=1, (COUNT-1)
TEMPT(:, J)=T(:, J)
TEMPT(:, J+1)=T(:, J+1)
TEMPT(Q, J)=0.0D0
TEMPT(Q, J+1)=0.0D0
UITEMP=MATMUL(BTINV, TEMPT(:, J))
! CALL DLINRG(P, A, LDA, AINV, LDAINV)
TEMP2=MATMUL(AINV, TEMPT(:, J))
TEMP3=DDOT(NCOMP, TEMPT(:, J), 1, TEMP2, 1)
IF (TEMP3.LT.1.0D-5) THEN
TEMP3=1.0D-5
ENDIF
TEMP4=1/DSQRT(TEMP3)
CALL DVCAL (NCOMP, TEMP4, UITEMP, 1, SECOND, 1)
! COMPUTE S(T(K+1))
UITEMP=MATMUL(BTINV, TEMPT(:, J+1))
! CALL DLINRG(P, A, LDA, AINV, LDAINV)
TEMP2=MATMUL(AINV, TEMPT(:, J+1))
TEMP3=DDOT(NCOMP, TEMPT(:, J+1), 1, TEMP2, 1)
IF (TEMP3.LT.1.0D-5) THEN
TEMP3=1.0D-5
ENDIF
```

```

TEMP4=1/DSQRT(TEMP3)
CALL DVCAL (NCOMP, TEMP4, UITEMP,1, FIRST, 1)
!   COMPUTE DIFFERENCE OF S(T(K))-S(T(K+1))
DIF=FIRST-SECOND
INCX=1
!   GET THE NORM OF THE DIFF
NORMDIF=DNRM2(NCOMP,DIF,INCX)
!   ADD TO PREVIOUS NORMS TO APPROXIMATE KO
KSI=KSI+NORMDIF
41 CONTINUE
42 CONTINUE

!   CALCULATE CURVATURE FOR (NCOMP) CHOOSE (NCOMP-3) 3 TUPLES AND
TAKE THE MEAN
DO 76 V=1,(COUNT-1)
!   MUST DIVIDE UI BY N GIVEN HOW DATA IS ENTERED FOR CTGLM
SUBROUTINE!!!!!!
DO 99 J=1,P-2
DO 98 K=J+1,P
DO 97 I=0,P-J
GG=J
HH=K
TEMPT(:,V)=T(:,V)
TEMPT(GG,V)=0.0D0
TEMPT(HH,V)=0.0D0
TEMPT(:,V+1)=T(:,V+1)
TEMPT(GG+I,V+1)=0.0D0

```

```

TEMPT(HH+I,V+1)=0.0D0
TEMP2=MATMUL(BTINV,TEMPT(:,V))
CALL DVCAL (NCOMP,1/N2,TEMP2,1,UIT(:,V),1)
TEMP2=MATMUL(AINV,TEMPT(:,V))
TEMP3=DDOT(NCOMP,TEMPT(:,V),1,TEMP2,1)
IF (TEMP3.LT.1.0D-5) THEN
TEMP3=1.0D-5
ENDIF
TEMP4=1/DSQRT(TEMP3)
! THIS MULTIPLIES A SCALAR (TEMP4) BY VECTOR (UI) TO GET S(X) FOR
I
CALL DVCAL (NCOMP,TEMP4,UIT(:,V),1,ST(:,V),1)
TEMP2=MATMUL(BTINV,TEMPT(:,V+1))
CALL DVCAL (NCOMP,1/N2,TEMP2,1,UIT(:,V+1),1)
TEMP2=MATMUL(AINV,TEMPT(:,V+1))
TEMP3=DDOT(NCOMP,TEMPT(:,V+1),1,TEMP2,1)
IF (TEMP3.LT.1.0D-5) THEN
TEMP3=1.0D-5
ENDIF
TEMP4=1/DSQRT(TEMP3)
! HIS MULTIPLIES A SCALAR (TEMP4) BY VECTOR (UI) TO GET S(X) FOR
I
CALL DVCAL (NCOMP,TEMP4,UIT(:,V+1),1,ST(:,V+1),1)
CALL DVCAL(NCOMP,2.0D0,ST(:,V),1,TEMP5,1)
TEMP6=ST(:,V+1)-TEMP5+ST(:,V-1)
CALL DVCAL(NCOMP,INTER**2.0D0,TEMP6,1,K2VEC,1)
K2(V)=DNRM2(NCOMP,K2VEC,INCX)

```

97 CONTINUE

98 CONTINUE

99 CONTINUE

76 CONTINUE

K2MEAN=SUM(K2)

! CALCULATE CURVATURE FOR (NCOMP) CHOOSE(NCOMP-3) 3 TUPLES AND TAKE THE MEAN

IF (P.EQ.5) THEN

DO 47 I=2,P

DO 49 J=2,P

DO 46 K=2,P

DO 48 V=1,(COUNT-1)

STEMP1=ST(:,V+1)

STEMP1(I)=0.0D0

STEMP2=ST(:,V)

STEMP2(J)=0.0D0

STEMP3=ST(:,V-1)

STEMP3(K)=0.0D0

CALL DVCAL(NCOMP,2.0D0,STEMP2,1,TEMP5,1)

TEMP6=STEMP1-TEMP5+STEMP3

CALL DVCAL(NCOMP,INTER**2.0D0,TEMP6,1,KSI2VEC,1)

KSI2=KSI2+DNRM2(NCOMP,KSI2VEC,INCX)

48 CONTINUE

46 CONTINUE

49 CONTINUE

47 CONTINUE

ENDIF

```

KSI2MEAN=KSI2/4.0D0

!   CALC ROTATION ANGLE HERE !   ASSUMES ANGLE BETWEEN ALL POSSIBLE
TWO SIDES MEETING
MO=0.0D0
INTER=1.0D0/(DBLE(P)-1.0D0)
DO 81 J=1,NCOMP-1
DO 82 K=1,2
DO 80 V=1,100,99
IF (K.EQ.1) THEN
TEMP(:,V)=T(:,V)-INTER
TEMP(J,V)=0.0D0
ELSE
TEMP(:,V)=T(:,V)-INTER
TEMP(J+1,V)=0.0D0
ENDIF
TEMP2=MATMUL(BTINV,TEMP(:,V))
CALL DVCAL (NCOMP,1/N2,TEMP2,1,UIT(:,V),1)
TEMP2=MATMUL(AINV,TEMP(:,V))
TEMP3=DDOT(NCOMP,TEMP(:,V), 1, TEMP2, 1)
IF (TEMP3.LT.1.0D-5) THEN
TEMP3=1.0D-5
ENDIF
TEMP4=1/DSQRT(TEMP3)
!   THIS MULTIPLIES A SCALAR (TEMP4) BY VECTOR (UI) TO GET S(X) FOR
I
CALL DVCAL (NCOMP, TEMP4, UIT(:,V), 1, ST(:,V), 1)

```

```

IF (K.EQ.1) THEN
TEMP(:,V+1)=T(:,V+1)+INTER
TEMP(J,V+1)=0.0D0
ELSE
TEMP(:,V+1)=T(:,V+1)+INTER
TEMP(J+1,V+1)=0.0D0
ENDIF

TEMP2=MATMUL(BTINV,TEMP(:,V+1))
CALL DVCAL (NCOMP,1/N2,TEMP2,1,UIT(:,V+1),1)
TEMP2=MATMUL(AINV,TEMP(:,V+1))
TEMP3=DDOT(NCOMP,TEMP(:,V+1), 1, TEMP2, 1)
IF (TEMP3.LT.1.0D-5) THEN
TEMP3=1.0D-5
ENDIF
TEMP4=1/DSQRT(TEMP3)
! THIS MULTIPLIES A SCALAR (TEMP4) BY VECTOR (UI) TO GET S(X) FOR
I
CALL DVCAL (NCOMP, TEMP4, UIT(:,V+1), 1, ST(:,V+1), 1)

GRAD(:,V)=ST(:,V+1)-ST(:,V)

IF (V.EQ.1) THEN
CALL DVCAL(NCOMP,INTER,GRAD(:,V),1,GRADIENT1,1)
ELSE
CALL DVCAL(NCOMP,INTER,GRAD(:,V),1,GRADIENT2,1)

```

ENDIF

80 CONTINUE

! NOW CHOOSE THREE POINTS WITHIN EACH SURFACE DEFINED BY THE
GRADIENT SO THAT ! WE CAN COMPUTE THE NORMAL VECTORS FOR EACH
SURFACE ! THEN THE CROSS PRODUCT OF (B-A)X(C-A) GIVES ME THE
NORMAL VECTOR (COMPUTE A NORMAL ! VECTOR FOR EACH SURFACE) THEN
USE COS(THETA) TO GET THETA

! COMPUTE NORMAL VECTORWS TO EACH SURFACE
GRAD1 AND GRAD2

! NOW CALCULATE THE ROTATION ANGLE BETWEEN EACH OF THE 4 CHOOSE 2
=6 FACES\

IF (J.EQ.1) THEN

CROSS(K,1)=GRADIENT1(4)*GRADIENT2(3)-
GRADIENT1(3)*GRADIENT2(4)

CROSS(K,2)=GRADIENT1(4)*GRADIENT2(2)-
GRADIENT1(2)*GRADIENT2(4)

CROSS(K,3)=GRADIENT1(3)*GRADIENT2(2)-
GRADIENT1(2)*GRADIENT2(3)

ELSEIF (J.EQ.2) THEN

CROSS(K,1)=GRADIENT1(4)*GRADIENT2(3)-
GRADIENT1(3)*GRADIENT2(4)

CROSS(K,2)=GRADIENT1(4)*GRADIENT2(1)-
GRADIENT1(1)*GRADIENT2(4)

```

CROSS(K,3)=GRADIENT1(3)*GRADIENT2(1)-
GRADIENT1(1)*GRADIENT2(3)
ELSEIF (J.EQ.3) THEN
CROSS(K,1)=GRADIENT1(4)*GRADIENT2(2)-
GRADIENT1(2)*GRADIENT2(4)
CROSS(K,2)=GRADIENT1(4)*GRADIENT2(1)-
GRADIENT1(1)*GRADIENT2(4)
CROSS(K,3)=GRADIENT1(2)*GRADIENT2(1)-
GRADIENT1(1)*GRADIENT2(2)
ELSEIF (J.EQ.4) THEN
CROSS(K,1)=GRADIENT1(3)*GRADIENT2(2)-
GRADIENT1(2)*GRADIENT2(3)
CROSS(K,2)=GRADIENT1(3)*GRADIENT2(1)-
GRADIENT1(1)*GRADIENT2(3)
CROSS(K,3)=GRADIENT1(2)*GRADIENT2(1)-
GRADIENT1(1)*GRADIENT2(2)
ENDIF
82 CONTINUE
CROSSDOT=DDOT(3,CROSS(1,:),1,CROSS(2,:),1)
NORM1=DNRM2(3,CROSS(1,:),INCX)
NORM2=DNRM2(3,CROSS(2,:),INCX)
COSTH=CROSSDOT/(NORM1*NORM2+Small)
THETA=DACOS(COSTH)
MO=MO+THETA
81 CONTINUE

```


! NOW GET CONSTANT USING IDENTITY FROM SU(2000)

CRITLO=1.96D0

CRITHI=DSQRT(C10)

! STARTING VALUES FOR SECANT METHOD

PART1=(K0*DGAMMA((DBLE(NCOMP)+1.0D0)/2.0D0))/

(PI**((DBLE(NCOMP)+1.0D0)/2.0D0))

PART2=1.0D0-DFDF(CRITLO**2.0D0/(DBLE(NCOMP)

+1.0D0),DBLE(NCOMP+1),DBLE(N-P))

PART3=(KSI*DGAMMA(DBLE(NCOMP)/2.0D0))/

(2.0D0*PI**((DBLE(NCOMP)/2.0D0))

PART4=1.0D0-DFDF(CRITLO**2.0D0/

DBLE(NCOMP),DBLE(NCOMP),DBLE(N-P))

PART5=((K2MEAN+KSI2MEAN+M0)*DGAMMA(

(DBLE(NCOMP)-1.0D0)/2.0D0))/

(2.0D0*PI*PI**((DBLE(NCOMP)-1.0D0)/2.0D0))

PART6=1.0D0-DFDF(CRITLO**2.0D0/(DBLE

(NCOMP)-1.0D0),DBLE(NCOMP-1),DBLE(N-P))

FX=PART1*PART2+PART3*PART4+PART5*PART6-ALPHA

PART1=(K0*DGAMMA((DBLE(NCOMP)+1.0D0)/2.0D0))

/(PI**((DBLE(NCOMP)+1.0D0)/2.0D0))

PART2=1.0D0-DFDF(CRITHI**2.0D0/(DBLE(NCOMP)

+1.0D0),DBLE(NCOMP+1),DBLE(N-P))

PART3=(KSI*DGAMMA(DBLE(NCOMP)/2.0D0))/

(2.0D0*PI**((DBLE(NCOMP)/2.0D0))

```

PART4=1.0D0-DFDF(CRITHI**2.0D0/DBLE(NCOMP),
DBLE(NCOMP),DBLE(N-P))
PART5=((K2MEAN+KSI2MEAN+M0)*DGAMMA(
(DBLE(NCOMP)-1.0D0)/2.0D0))/(2.0D0*PI*PI**
((DBLE(NCOMP)-1.0D0)/2.0D0))
PART6=1.0D0-DFDF(CRITHI**2.0D0/(DBLE(NCOMP)
-1.0D0),DBLE(NCOMP-1),DBLE(N-P))
FX1=PART1*PART2+PART3*PART4+PART5*PART6-ALPHA

K=1
ABSERR=1.0D0
SECANT: DO WHILE ((K.LT.MAXK).AND.(ABSERR.GT.EPSILON))
DF=(FX1-FX)/(CRITHI-CRITLO+Small)

DP=(FX1)/(DF+Small)
CRIT=CRITHI-DP
PART1=(K0*DGAMMA((DBLE(NCOMP)+1.0D0)/2.0D0))
/(PI**((DBLE(NCOMP)+1.0D0)/2.0D0))
PART2=1.0D0-DFDF(CRIT**2.0D0/(DBLE(NCOMP)
+1.0D0),DBLE(NCOMP+1),DBLE(N-P))
PART3=(KSI*DGAMMA(DBLE(NCOMP)/2.0D0))/
(2.0D0*PI**((DBLE(NCOMP)/2.0D0))
PART4=1.0D0-DFDF(CRIT**2.0D0/DBLE(NCOMP),
DBLE(NCOMP),DBLE(N-P))
PART5=((K2MEAN+KSI2MEAN+M0)*DGAMMA((
DBLE(NCOMP)-1.0D0)/2.0D0))/(2.0D0*PI*PI**
((DBLE(NCOMP)-1.0D0)/2.0D0))

```

```

PART6=1.0D0-DFDF(CRIT**2.0D0/(DBLE(NCOMP)
-1.0D0),DBLE(NCOMP-1),DBLE(N-P))
TEMPFX=PART1*PART2+PART3*PART4+PART5*PART6-ALPHA
ABSERR=DABS(TEMPFX)
IF (TEMPFX.LT.0) THEN
CRITHI=CRIT
FX1=TEMPFX
ELSE
CRITLO=CRIT
FX=TEMPFX
ENDIF
K=K+1
ENDDO SECANT

```

```

SUM1=0.0D0
SUM2=0.0D0
MEAN1=0.0D0
MEAN2=0.0D0

```

```

DO 60 V=1, NCOMP

```

```

!   CALCULATE CI FOR ETA=X'BETA THEN TRANSFORM TO GET CI ON MEAN
RESP

```

```

!   CONSTRUCT CI'S HERE (RECALL 4 SCB CI'S)
IF (VER.EQ.1) THEN
!   BASIC SCR (N IS NUMBER OF POINTS IN X TO MAKE PREDICTIONS
FOR-NEVER MIND FOR NOW!)

LO(V)=LINEARC(V)-(CRIT)*DSQRT(VAR(V))
HI(V)=LINEARC(V)+(CRIT)*DSQRT(VAR(V))
IF ((LINEARCP(V).GE.LO(V)).AND.
(LINEARCP(V).LE.HI(V))) THEN
CONF=CONF+1
ENDIF

!   CENTERED SCR SEE P.637 OF SUN(2001)
ELSEIF (VER.EQ.2) THEN
IF (KAP(2,V).LT.1.0D-5) THEN
KAP(2,V)=1.0D-5
ENDIF

LO(V)=LINEARC(V)-KAP(1,V)*DSQRT(VAR(V))
-(CRIT)*DSQRT(VAR(V))*DSQRT(KAP(2,V))
HI(V)=LINEARC(V)-KAP(1,V)*DSQRT(VAR(V))
+(CRIT)*DSQRT(VAR(V))*DSQRT(KAP(2,V))
SUM1=SUM1+KAP(1,V)
SUM2=SUM2+KAP(2,V)
IF ((LINEARCP(V).GE.LO(V)).AND.
(LINEARCP(V).LE.HI(V))) THEN
CONF=CONF+1
ENDIF

```

```

ELSEIF (VER.EQ.3) THEN
!   CORRECTED 2 SCR

      !U=SOLVE Q2 FOR U: |u|+q2=c
      XLO=0.0D0
      XHI=1.4D0
      !LOOP=V
      YLO=Q2(XLO,V)
      YHI=Q2(XHI,V)
      X1=XLO
      X2=XHI
      Y1=YLO
      Y2=YHI
      ABSERR=1.0D0
      COUNT=1
      SECANTLOOP: DO WHILE ((ABSERR.GT.EPSILON)
      .AND.(COUNT.LT.250))
      XT = X2 - ((X2-X1)*Y2)/(Y2-Y1+Small)
      YT = Q2(XT,V) - CRIT
      IF (YT*YLO>0) THEN
      XLO = XT
      YLO = YT
      ELSE
      XHI = XT
      YHI = YT
      ENDIF
      X1=XLO
      X2=XHI

```

```

Y1=YLO
Y2=YHI
ABSERR=DABS(YT)
COUNT=COUNT+1
ENDDO SECANTLOOP
UCRIT(V)=Q2(XT,V)-CRIT
IF (DABS(UCRIT(V)).LT.1.0D-4) THEN
UCRIT(V)=1.0D-4
ENDIF
LO(V)=LINEARC(V)-(DABS(UCRIT(V)))*DSQRT(VAR(V))
HI(V)=LINEARC(V)+(DABS(UCRIT(V)))*DSQRT(VAR(V))
SUM1=SUM1+UCRIT(V)
IF ((LINEARCP(V).GE.LO(V)).AND.
(LINEARCP(V).LE.HI(V))) THEN
CONF=CONF+1
ENDIF
ELSEIF (VER.EQ.4) THEN
!   CORRECTED SCR !   GET MAX OF P2 BY SECANT METHOD
XLO=1.0D-2
XHI=2.0D0*CRIT
YLO=P2(XLO,V)
YHI=P2(XHI,V)
X1=XLO
X2=XHI
Y1=YLO
Y2=YHI
ABSERR=1.0D0

```

```

K=1
LOOP=V
SECANTLOOP2: DO WHILE ((K.LT.MAX) .
AND.(ABSERR.GT.EPSILON))
XT = X2 - ((X2-X1)*Y2)/(Y2-Y1+Small)
YT = P2(XT,V)
IF (YT*YLO>0) THEN
XLO = XT
YLO = YT
ELSE
XHI = XT
YHI = YT
ENDIF
X1=XLO
X2=XHI
Y1=YLO
Y2=YHI
ABSERR=DABS(YT)
K=K+1
ENDDO SECANTLOOP2
MAX_P2(V) = DABS(P2(XT,V))
UCRIT(V)=CRIT-MAX_P2(V)
!   NOW USE SECANT METHOD AGAIN TO FIND CRIT FOR EQ.41 P. 440
CRITLO=1.96D0
!   THIS IS SCHEFFE SOLUTION
CRITHI=DSQRT(C10)
!   STARTING VALUES FOR SECANT METHOD

```

```

PART1=(K0*DGAMMA((DBLE(NCOMP)+1.0D0)/2.0D0))/
(PI**((DBLE(NCOMP)+1.0D0)/2.0D0))
PART2=1.0D0-DFDF((CRITLO-MAX_P2(V))**2.0D0/
(DBLE(NCOMP)+1.0D0),DBLE(NCOMP+1),DBLE(N-P))
PART3=(KSI*DGAMMA(DBLE(NCOMP)/2.0D0))/
(2.0D0*PI**((DBLE(NCOMP)/2.0D0))
PART4=1.0D0-DFDF((CRITLO-MAX_P2(V))**2.0D0/
DBLE(NCOMP),DBLE(NCOMP),DBLE(N-P))
PART5=((K2MEAN+KSI2MEAN+M0)*DGAMMA(
(DBLE(NCOMP)-1.0D0)/2.0D0))/(2.0D0*PI*
PI**((DBLE(NCOMP)-1.0D0)/2.0D0))
PART6=1.0D0-DFDF((CRITLO-MAX_P2(V))**2.0D0/
(DBLE(NCOMP)-1.0D0),DBLE(NCOMP-1),DBLE(N-P))
FX=PART1*PART2+PART3*PART4+PART5*PART6-ALPHA
PART1=(K0*DGAMMA((DBLE(NCOMP)+1.0D0)/2.0D0))/
(PI**((DBLE(NCOMP)+1.0D0)/2.0D0))
PART2=1.0D0-DFDF((CRITHI-MAX_P2(V))**2.0D0/
(DBLE(NCOMP)+1.0D0),DBLE(NCOMP+1),DBLE(N-P))
PART3=(KSI*DGAMMA(DBLE(NCOMP)/2.0D0))/
(2.0D0*PI**((DBLE(NCOMP)/2.0D0))
PART4=1.0D0-DFDF((CRITHI-MAX_P2(V))**2.0D0/
DBLE(NCOMP),DBLE(NCOMP),DBLE(N-P))
PART5=((K2MEAN+KSI2MEAN+M0)*DGAMMA(
(DBLE(NCOMP)-1.0D0)/2.0D0))/(2.0D0*PI*
PI**((DBLE(NCOMP)-1.0D0)/2.0D0))
PART6=1.0D0-DFDF((CRITHI-MAX_P2(V))**2.0D0/
(DBLE(NCOMP)-1.0D0),DBLE(NCOMP-1),DBLE(N-P))

```


FX1=PART1*PART2+PART3*PART4+PART5*PART6-ALPHA

K=1

ABSERR=1.0D0

SECANT2: DO WHILE ((K.LT.MAXK).AND.(ABSERR.GT.EPSILON))

DF=(FX1-FX)/(CRITHI-CRITLO+Small)

DP=(FX1)/(DF+Small)

CRIT=CRITHI-DP

PART1=(K0*DGAMMA((DBLE(NCOMP)+1.0D0)/2.0D0))/(

PI**((DBLE(NCOMP)+1.0D0)/2.0D0))

PART2=1.0D0-DFDF((CRIT-MAX_P2(V))**2.0D0/

(DBLE(NCOMP)+1.0D0),DBLE(NCOMP+1),DBLE(N-P))

PART3=(KSI*DGAMMA(DBLE(NCOMP)/2.0D0))/

(2.0D0*PI**((DBLE(NCOMP)/2.0D0))

PART4=1.0D0-DFDF((CRIT-MAX_P2(V))**2.0D0/

DBLE(NCOMP),DBLE(NCOMP),DBLE(N-P))

PART5=((K2MEAN+KSI2MEAN+M0)*DGAMMA(

(DBLE(NCOMP)-1.0D0)/2.0D0))/(2.0D0*PI*

PI**((DBLE(NCOMP)-1.0D0)/2.0D0))

PART6=1.0D0-DFDF((CRIT-MAX_P2(V))**2.0D0/

(DBLE(NCOMP)-1.0D0),DBLE(NCOMP-1),DBLE(N-P))

TEMPFX=PART1*PART2+PART3*PART4+PART5*PART6-ALPHA

ABSERR=DABS(TEMPFX)

IF (TEMPFX.LT.0) THEN

CRITHI=CRIT

FX1=TEMPFX

ELSE

```

CRITLO=CRIT
FX=TEMPFX
ENDIF
K=K+1
ENDDO SECANT2
IF (CRIT.LT.1.0D-5) THEN
CRIT=1.0D-5
ENDIF

LO(V)=LINEARC(V)-(CRIT)*DSQRT(VAR(V))
HI(V)=LINEARC(V)+(CRIT)*DSQRT(VAR(V))
SUM2=SUM2+MAX_P2(V)
IF ((LINEARCP(V).GE.LO(V)).AND.(LINEARCP(V)
.LE.HI(V))) THEN
CONF=CONF+1
ENDIF
ENDIF

60 CONTINUE
ECL(L)=DBLE(CONF)/DBLE(NCOMP)
8 CONTINUE
MEANECL=SUM(ECL)/DBLE(REPS)
RESULTS(1)=MODEL
RESULTS(2)=H
RESULTS(4)=N
RESULTS(5)=MEANECL
RESULTS(6)=VER
WRITE(9,*) RESULTS

```

```

WRITE(10,*) MEANECL
CALL ERSET(0,2,2)
7 CONTINUE
3 CONTINUE
2 CONTINUE
END

```

```

DOUBLE PRECISION FUNCTION P2(U,V)
DOUBLE PRECISION U,KAP(5,4),KAQ(5,4),C(9),C2,N2,P3,
PART1,PART2,PART3,V
INTEGER LOOP
COMMON KAP,KAQ,P3,N2,C,C2,LOOP
PART1=KAP(2,V)-1.0D0+KAP(1,V)**2.0D0
PART2=(KAP(4,V)+4.0D0*KAP(1,V)*KAP(V,3))*(U**2.0D0-3.0D0)
PART3=KAP(3,V)*(U**4.0D0-1.0D1*U**2.0D0+1.5D1)
P2=U*(3.6D1*PART1+3.0D0*PART2+PART3)/7.2D1
RETURN
END

```

```

DOUBLE PRECISION FUNCTION Q2(U,V)
DOUBLE PRECISION U,KAQ(5,4),KAP(5,4),P3,N2,C2,C(9),

```

```
PART1,PART2,V
INTEGER LOOP
COMMON KAP,KAQ,P3,N2,C,C2,LOOP
PART1=U*U-3.0D0
PART2=(U*U-1.0D1)*U*U+1.5D1
Q2=-U*(3.6D1*KAQ(2,V) + 3.0D0*KAQ(4,V)*PART1 +
  KAP(3,V)**2.0D0*PART2)/7.2D1
RETURN
END
```

VITA

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Generalized Linear Models (GLM's) are utilized in a variety of statistical applications. Many times the estimated quantities from the models are of primary interest. These estimated quantities may include the mean response, odds ratio, relative risk, or attributable proportion. In these cases overall conclusions about these quantities may be desirable. Currently few sophisticated methods exist to simultaneously estimate these quantities from a GLM. I propose several methods of estimating these quantities simultaneously and compare them to the existing methods. Intervals for the expected response of the GLM and any set of linear combinations of the GLM are explored. Most existing methods emphasis the simultaneous estimation of the expected response; few consider estimation of the sets of regression parameters, and hence quantities such as the odds ratio or relative risk. Additionally, almost all intervals employ maximum likelihood estimators (MLEs) for the model parameters. MLEs are often biased estimators for GLMs, particularly at small sample sizes. Thus, another set of intervals is proposed that utilize an alternative estimator for the parameters, the penalized maximum likelihood estimator (pMLE). This estimator is very similar to the usual MLE, but it is shifted in order to account for the bias typically present in the MLE for GLMs. Various critical values of the simultaneous intervals are explored for both the MLE and pMLE based intervals. Emphasis is placed on scenarios where the sample size is small relative to the number of parameters being estimated. Simulation studies compare the various intervals and suggest general recommendations. The pMLE based intervals proposed exhibit superior performance, particularly at small and moderate sample sizes. While usual MLE based intervals typically do not attain the desired level of confidence at the small sample sizes, the pMLE based intervals do. Additionally, at moderate to large sample sizes the pMLE based intervals are, in many cases, less conservative than the usual MLE based intervals.

ADVISOR'S APPROVAL: _____