Selection of Designs in Ordinal Regression Models under Linear Predictor Misspecification

Ishapathik Das

Abstract—The purpose of this article is to find a method of comparing designs for ordinal regression models using quantile dispersion graphs in the presence of linear predictor misspecification. The true relationship between response variable and the corresponding control variables are usually unknown. Experimenter assumes certain form of the linear predictor of the ordinal regression models. The assumed form of the linear predictor may not be correct always. Thus, the maximum likelihood estimates (MLE) of the unknown parameters of the model may be biased due to misspecification of the linear predictor. In this article, the uncertainty in the linear predictor is represented by an unknown function. An algorithm is provided to estimate the unknown function at the design points where observations are available. The unknown function is estimated at all points in the design region using multivariate parametric kriging. The comparison of the designs are based on a scalar valued function of the mean squared error of prediction (MSEP) matrix, which incorporates both variance and bias of the prediction caused by the misspecification in the linear predictor. The designs are compared using quantile dispersion graphs approach. The graphs also visually depict the robustness of the designs on the changes in the parameter values. Numerical examples are presented to illustrate the proposed methodology.

Keywords—Model misspecification, multivariate kriging, multivariate logistic link, ordinal response models, quantile dispersion graphs.

I. INTRODUCTION

THIS article presents a method of selecting robust designs for ordinal response models under model misspecification. Several authors discussed about the model misspecification and its effect on design selection for linear and generalized linear models (with a single response) till date; however, there is a lack in works for the situation where the responses are ordinal. In case of generalized linear models (GLMs), model misspecification may occur when the assumptions regarding the form of the linear predictor and/or the link function is wrong. For addressing the uncertainty in the linear predictor, we assume an unknown function and an iterative method is provided for estimating the unknown function at the design points of the model. Then, the multivariate kriging method is used to estimate the function at all points of the design region using the estimates at design points as a training data sets. The designs are compared using the quantile dispersion graphs approach on the basis of a scalar valued function of the mean squared error of prediction. These graphs allow design comparison over the entire experimental region. Also they provide assessment of the designs’ sensitivity to changes in the parameter values.

Some of the references for selecting optimal designs in multivariate GLMs are [1]–[3]. Reference [1] provides optimal designs for bivariate logistic models while [3] discussed designs for multinomial responses. However, neither of these papers investigate the effect of model misspecification on design selection for ordinal responses or multivariate GLMs.

Here, we provide a method of comparing designs in ordinal response models using QDGs under model misspecification. The comparison criterion is the mean squared error of prediction (MSEP) of the designs which takes into account the variance and the bias in the parameter estimates due to model misspecification. The QDGs technique allows a comparison of the designs on the entire experimental designs and not just at a single point like A, D or G optimal designs. QDGs also allow one to study the robustness of the designs to parameter changes.

The rest of the article is organised as follows: Section II discusses the multivariate generalized models and ordinal regression models. In Section III, the problem of model misspecification in ordinal response models and the expression for the MSEP under misspecification are given. The comparison criterion and the QDGs approach is explained in Section IV. In Section V, numerical examples illustrating the proposed methodology are discussed followed by concluding remarks in Section VI.

II. MULTIVARIATE GENERALIZED LINEAR MODELS

In multivariate GLMs (generalized linear models), we assume that $y_1, y_2, \ldots, y_n$ are independent $q$ dimensional response variables such that each $y_i$ belongs to an exponential family, which has the form

$$s(y_i|\theta_i, \phi) = \exp\left\{\frac{y_i\theta_i - b(\theta_i)}{\phi} + c(y_i, \phi, \omega_i)\right\},$$

where $b(.)$ and $c(.)$ are known function and $\phi$ is dispersion parameter possibly unknown. Here, mean response $\mu_i = \mu(\theta_i) = E(y_i|\theta_i) = [\mu_{i1}, \mu_{i2}, \ldots, \mu_{iq}]^T$ and linear predictor $\eta_i = [\eta_{i1}, \eta_{i2}, \ldots, \eta_{iq}]^T$ are $q$ dimensional vectors. The mean response $\mu_i$ is related to the linear predictor $\eta_i = Z_i \beta$ by link function $g$ as

$$\eta_i = g(\mu_i),$$

where

$$Z_i = \begin{bmatrix} f_1(x_i) & O_{1 \times p_2} & \cdots & O_{1 \times p_q} \\ O_{1 \times p_1} & f_2(x_i) & \cdots & O_{1 \times p_q} \\ \vdots & \vdots & \ddots & \vdots \\ O_{1 \times p_1} & O_{1 \times p_2} & \cdots & f_q(x_i) \end{bmatrix},$$

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\( \mathbf{f}(x) \) is known vector function of \( x \), \( \mathbf{O}_{1 \times p_j} \) is matrix of order \( 1 \times p_j \) with all elements zero, \( \beta = [\beta_1, \beta_2, \ldots, \beta_q]^T \) is \( p \times 1 \) vector of unknown parameters such that each \( \beta_j = [\beta_{j1}, \beta_{j2}, \ldots, \beta_{jp_j}]^T \) is \( p_j \times 1 \) vector of unknown parameters for jth response with \( p = \sum_{j=1}^{q} p_j \). For simplicity we denote \( \beta = [\beta_1, \beta_2, \ldots, \beta_q]^T \) such that first \( p_1 \) elements of \( \beta \) come from \( \beta_1 \), next \( p_2 \) elements of \( \beta \) come from \( \beta_2 \) and so on. It is usually assumed that inverse of \( g \) exists and it is denoted as \( h \). For natural link function we have \( \theta_i = \eta_i \). In general, we can relate \( \theta_i \) to linear predictor \( \eta_i \) using \( \mu_i = \mu(\theta_i) \) by function \( u \) which is defined as

\[
\theta_i = u(\eta_i) = u(Z_i, \beta) = \mu^{-1}(h(Z_i, \beta)) [4, \text{pp. 347}] \tag{4}
\]

For example, if \( y_1, y_2, \ldots, y_n \) are independent random variables such that each \( y_i \) is multinomial distributed having \( (q + 1) \) categories with parameter \( (\pi_i, n_i) \) with the density given by

\[
P(y_i = (y_{i1}, y_{i2}, \ldots, y_{iq})) = \frac{n_i!}{y_{i1}! y_{i2}! \cdots y_{iq}!} \prod_{j=1}^{q} \pi_{ij}^{y_{ij}} \prod_{j=q+1}^{q} (1 - \pi_{ij})^{n_i - y_{ij}} \tag{5}
\]

Then the density of \( y_i = y_{i1}/n_i \) has the form

\[
s(y_{i1}/n_i, \phi, \omega) = \exp\left\{ \frac{\{y_{i1}/n_i - b(\theta_i)\}}{\phi} + c(y_{i1}/n_i, \phi, \omega) \right\}, \tag{6}
\]

where \( \theta_i = \left( \frac{1}{n_i} \pi_{i1}, \frac{1}{n_i} \pi_{i2}, \ldots, \frac{1}{n_i} \pi_{iq} \right)^T, b(\theta_i) = \log(\frac{1}{n_i} \pi_{i1} - \frac{1}{n_i} \pi_{i2} - \cdots - \frac{1}{n_i} \pi_{iq}), c(y_{i1}/n_i, \phi, \omega) = \log(\frac{1}{n_i} \pi_{i1} - \frac{1}{n_i} \pi_{i2} - \cdots - \frac{1}{n_i} \pi_{iq}) \). Here \( \mu_i = E(y_{i1}/n_i) = \pi_{i1} \) and \( \phi = 1 \).

The logistic link function is given by

\[
\eta_i = g(\pi_i) = \theta_i.
\]

Then, \( \theta_i = \eta_i \) and hence \( u \) is identity function.

A. Ordinal Response Models

Suppose \( y_1, y_2, \ldots, y_n \) are independent \( q \) dimensional ordinal responses so that each \( y_i \) is multinomial distributed having \( (q + 1) \) ordered categories with parameter \( (\pi_i, n_i) \). The simple cumulative model [5, pp. 243] for ordinal responses is given by

\[
\tau_{ij} = \sum_{r=1}^{j} \pi_{ir} = P(y_i \leq j) = F(\theta_{0j} + x_i^T \theta) \tag{7}
\]

for \( j = 1, 2, \ldots, q \),

where \( F^{-1} \) is link function, \( \theta_{01}, \theta_{02}, \ldots, \theta_{0q}, \theta \) are parameters and \( x_i \) is design vector. The general form of the multivariate GLMs for the categorical responses is given by \( \mathbf{g}(\mathbf{\mu}_i) = \mathbf{g}(\pi_i) = \mathbf{Z}_i \beta \) or \( \mathbf{\mu}_i = \pi_i = h(Z_i, \beta) \) [5, pp. 261]. The equivalent form for the ordinal responses is given by

\[
\mu_i = \pi_i = \begin{pmatrix} \pi_{i1} \\ \pi_{i2} \\ \vdots \\ \pi_{iq} \end{pmatrix} = h \left( \begin{pmatrix} 1 & \cdots & 0 & x_i^T \end{pmatrix} \begin{pmatrix} \theta_{01} \\ \vdots \\ \theta_{0q} \end{pmatrix} \right) \tag{8}
\]

which is given by

\[
h_j(\eta_{j1}, \ldots, \eta_{jq}) = F(\eta_j) - F(\eta_{j-1}), \tag{9}
\]

From (7), and (8), we should have

\[
\mu_{ij} = \pi_{ij} = h(Z_i, \beta), \tag{10}
\]

However, the correct form the linear predictor may be different. Suppose, the correct form of the linear predictor is

\[
\eta_{T}(x) = x(\beta) + f(x) \tag{11}
\]

Then, the estimated mean response using the correct form of linear predictor is

\[
\mu_{T}(x) = \pi_T(x) = h(\eta_{T}(x)) = h(x(\beta) + f(x)), \tag{12}
\]

Reference [6] provides an approximate bias and variance of \( \beta \) for univariate generalized linear models when the linear predictor is misspecified. We generalize it for ordinal response models.

Let \( \mu = [\mu_1, \mu_2, \ldots, \mu_n]^T \) and \( \mu_T = [\mu_{T1}, \mu_{T2}, \ldots, \mu_{Tn}]^T \) with \( \mu_i = h(Z_i, \beta_i) \) and \( \mu_{Ti} = h(Z_i, \beta + f(x_i)) \), where \( \beta_i \) is the model parameter vector. Let us denote \( \mathbf{W}_i(\beta) = \mathbf{D}_i(\beta) \Sigma^{-1}_i \mathbf{D}_i^T(\beta) \) and \( \mathbf{W}_{Ti}(\beta) = \mathbf{D}_i(\beta) \Sigma^{-1}_i \Sigma^{-1}_T \mathbf{D}_i^T(\beta) \), where \( \mathbf{D}_i(\beta) = \frac{\delta h(\eta_i)}{\delta \theta} \) is the derivative of \( h(\eta) \) evaluated at \( \eta_i = Z_i \beta, \Sigma_i \) and \( \Sigma_T \) are the variance of \( y_i \) under assumed model and true model respectively. Finally, let \( \mathbf{P} \) be the \( n_q \times n_q \) diagonal matrix having diagonal element \( \frac{1}{n_i} \), \( \mathbf{D} = \text{diag}(\mathbf{D}_i(\beta_i)), \Sigma = \text{diag}(\Sigma_i), \mathbf{W} = \text{diag}(\mathbf{W}_i(\beta_i)), \mathbf{W}_T = \text{diag}(\mathbf{W}_{Ti}(\beta)) \), and \( \mathbf{X} = [\mathbf{Z}_1^T, \mathbf{Z}_2^T, \ldots, \mathbf{Z}_n^T]^T \). Then
the approximate bias and variance of $\hat{\beta}$ are given by
\begin{align}
\text{Bias}(\hat{\beta}) &= \mathbf{H}_n^{-1}\mathbf{b}, \\
\text{Var}(\hat{\beta}) &= \frac{1}{n}\mathbf{H}_n^{-1}\mathbf{H}_n\mathbf{H}_n^{-1},
\end{align}
where $\mathbf{b} = X^T\mathbf{P}\mathbf{D}\Sigma^{-1}(\mu_T - \mu)$, $\mathbf{H}_n = X^T\mathbf{P}\mathbf{W}_T\mathbf{X}$ and $\mathbf{H}_n = X^T\mathbf{P}\mathbf{W}_X - \mathbf{R}$ with
\begin{equation}
\mathbf{R} = \frac{1}{n}\sum_{i=1}^{n}\sum_{r=1}^{q}Z_i^T\mathbf{U}_r(\beta_0)Z_i(\gamma_r - \mu_r(\beta_0)),
\end{equation}
where $\mathbf{U}_r(\beta_0) = \frac{\partial^2 u_r(Z_i\beta_0)}{\partial \eta^2}$.

Now, using the above expressions of bias and variance of $\hat{\beta}$, the mean squared error (MSE) of $\hat{\mu}(\mathbf{x})$ is given by
\begin{equation}
\text{MSE}(\hat{\mu}(\mathbf{x})) = \left[\frac{\partial \hat{\mu}(\mathbf{x})}{\partial \eta(x)}\right]_{\eta_T}Z(\mathbf{x})\text{Var}(\hat{\beta}) \times Z_i^T(\mathbf{x}) \left[\frac{\partial \hat{\mu}(\mathbf{x})}{\partial \eta(x)}\right]^T_{\eta_T} + \left[\frac{\partial \hat{\mu}(\mathbf{x})}{\partial \eta(x)}\right]_{\eta_T}Z(\mathbf{x})\text{Bias}(\hat{\beta}) - \mathbf{f}(\mathbf{x}) \right] \times [Z(\mathbf{x})\text{Bias}(\hat{\beta}) - \mathbf{f}(\mathbf{x})]^T \left[\frac{\partial \hat{\mu}(\mathbf{x})}{\partial \eta(x)}\right]^T_{\eta_T}.
\end{equation}

The derivation of the above expressions for $\text{Bias}(\hat{\beta})$, $\text{Var}(\hat{\beta})$ and $\text{MSE}(\hat{\mu}(\mathbf{x}))$ are given in Appendix A and B.

IV. COMPARISON CRITERIA FOR DESIGNS

Here, we want to compare designs in ordinal regression models under linear predictor misspecification. The MLEs of the unknown parameters are biased due to model misspecification. So, we compare designs on the basis of MSE of the estimated mean response as it takes into account both the variance and bias of the parameter estimates. In the univariate response case MSEP is a scalar. So, in univariate case, if MSEP of a design $D_1$ is smaller than that of design $D_2$, then we say that design $D_1$ has better prediction capabilities than design $D_2$. However, for multivariate case, MSEP is a matrix. So, we have to consider a scalar valued function of MSEP matrix for such comparison. Several scalar valued functions of a matrix such as determinant, largest eigen value, etc exist in literature. For our numerical example, we consider the largest eigen value of MSEP, denoted as EMSEP, for comparing the designs.

From (15), it is observed that, MSEP at a point $\mathbf{x}$ depends on unknown parameter vector $\beta$, and unknown function $\mathbf{f}$. Hence, EMSEP is a function of $\beta$, $\mathbf{f}$, and $\mathbf{x}$. For, evaluating EMSEP at a point $\mathbf{x}$, we need to have values of $\beta$, and $\mathbf{f}(\mathbf{x})$. We use the MLE $\hat{\beta}$ of $\beta$ for evaluating EMSEP at $\mathbf{x}$. In the next section, we describe an algorithm for estimating $\mathbf{f}(\mathbf{x})$.

A. Algorithm for Estimating $\mathbf{f}$

We first generalize the estimation technique of [7] for the multinomial response model case. This method can be used if an initial data set is available.

Let $\mathbf{d}(\mathbf{x})$ be the difference between the estimated and the true response at a design point $\mathbf{x}$.
\begin{equation}
\mathbf{d}(\mathbf{x}) = \pi_T(\mathbf{x}) - \pi(\mathbf{x}) = \mathbf{h}[\eta(\mathbf{x}) + \mathbf{f}(\mathbf{x})] - \mathbf{h}[\eta(\mathbf{x})].
\end{equation}

Using first order Taylor series expansion around $\eta(\mathbf{x})$, we have
\begin{equation}
\mathbf{d}(\mathbf{x}) = \int_{\eta(\mathbf{x})}^{\eta(\mathbf{x}) + \mathbf{f}(\mathbf{x})} \frac{\partial \mathbf{h}(\eta)}{\partial \eta} \mathbf{d}(\mathbf{x}).
\end{equation}

Thus, the estimate of $\mathbf{f}$ is given by,
\begin{equation}
\hat{\mathbf{f}}(\mathbf{x}) = \left[\frac{\partial \mathbf{h}(\eta)}{\partial \eta}\right]_{\eta(\mathbf{x})}^{-1} \mathbf{d}(\mathbf{x}),
\end{equation}
where $\mathbf{d}(\mathbf{x}) = \mathbf{y}(\mathbf{x}) - \pi(\mathbf{x}) = \mathbf{y}(\mathbf{x}) - \mathbf{h}[\mathbf{Z}(\mathbf{x})\hat{\beta}]$, and $\hat{\beta}$ is the MLEs of $\beta$ using assumed form of linear predictor $\eta(\mathbf{x}) = \mathbf{Z}(\mathbf{x})\beta$.

By estimating $\mathbf{f}$ by the above method, we expect to have better fit using true form of linear predictor over assumed form of linear predictor. That means the deviance using true form of linear predictor should be less than that of the fitted model using assumed form of linear predictor. However, it is observed that, as $\mathbf{f}$ is estimated using first order Taylor series approximation, the deviance is increased or not decreased significantly using true form of linear predictor for some data sets. So, when the approximation is not close enough then we don’t get desired results. Here, we propose an algorithm which ensure that we will get better fit using true form of linear predictor over assumed form of linear predictor of the model. In this algorithm, the function $\mathbf{f}(\mathbf{x})$ is estimated using an iterative method. Let us denote for $l \geq 1$, $\eta^{(l)}(\mathbf{x})$, $\mathbf{d}^{(l)}(\mathbf{x})$, and $\eta^{(l)}(\mathbf{x})$ for the estimates of $\eta(\mathbf{x})$, $\mathbf{d}(\mathbf{x})$, and $\mathbf{f}(\mathbf{x})$ respectively at $l$th iteration. Also, let $\text{Dev}(l)$ be the deviance of the fitted model using $\eta^{(l)}(\mathbf{x})$. For $l = 1$, $\eta^{(1)}(\mathbf{x}) = \mathbf{Z}(\mathbf{x})\beta$, where $\beta$ is the MLEs of $\beta$ using assumed form of linear predictor $\eta(\mathbf{x}) = \mathbf{Z}(\mathbf{x})\beta$, $\mathbf{d}^{(1)}(\mathbf{x}) = \mathbf{y}(\mathbf{x}) - \mathbf{h}[\eta^{(1)}(\mathbf{x})]$, and $\mathbf{f}^{(1)}(\mathbf{x}) = \left[\frac{\partial \mathbf{h}(\eta)}{\partial \eta}\right]_{\eta^{(1)}(\mathbf{x})}^{-1} \mathbf{d}^{(1)}(\mathbf{x})$. Now for $l \geq 1$, the algorithm goes as follows
\begin{equation}
\eta^{(l+1)}(\mathbf{x}) = \eta^{(l)}(\mathbf{x}) + r\mathbf{f}^{(l)}(\mathbf{x}),
\end{equation}
\begin{equation}
\mathbf{d}^{(l+1)}(\mathbf{x}) = \mathbf{y}(\mathbf{x}) - \mathbf{h}[\eta^{(l+1)}(\mathbf{x})],
\end{equation}
and
\begin{equation}
\mathbf{f}^{(l+1)}(\mathbf{x}) = \left[\frac{\partial \mathbf{h}(\eta)}{\partial \eta}\right]_{\eta^{(l+1)}(\mathbf{x})}^{-1} \mathbf{d}^{(l+1)}(\mathbf{x}).
\end{equation}

The above iteration is continued till $\text{Dev}(l)$ is close to zero, i.e., $\text{Dev}(l) < \epsilon$ for some chosen $\epsilon > 0$. Here, $r \in (0, 1]$ is a correction factor suitably chosen so that the iteration is converged. In several example, it is observed that smaller values of $r$ ensure the convergence of the algorithm. However, it increases the number of iteration. So, we have to choose $r$ suitably so that, the iteration is converged as well as it reduces the computation time.

Note the above described method can be used to estimate $\mathbf{f}$ only at the design points. However, we need to compute EMSEP at any point in the region $\mathcal{R}$, thus an estimate of $\mathbf{f}$ at any point in the design region is necessary. Using multivariate kriging ([8], [9]) details in Appendix C, we estimate $\mathbf{f}$ at any point in the design region. The estimates of $\mathbf{f}$ at the design points obtained by the above algorithm act as a training data...
set for kriging.

B. Quantile Dispersion Graphs for Comparing Designs

As we mentioned in Section IV, it is observed that the EMSEP values are functions of $f(x)$, $\beta$ and $x$. So, we may denote the EMSEP values corresponding to design $D$ as a function $t_D[x, \beta, f(x)]$. By using the method described in Section IV-A, we can get the estimates $\hat{f}(x)$ of $f(x)$, and the dependence on $f$ can be removed by using the estimates $\hat{f}(x)$. Here, it is assumed that $\beta$ lies in the parameter space $C$. If an initial data set is available, we use the $100(1-\alpha)\%$ confidence region of $\beta$ (10),

$$C = \{\gamma : (\beta - \gamma)'[\text{Var}(\beta)]^{-1}(\beta - \gamma) \leq \chi^2_{1, p}\}. \quad (20)$$

as the parameter space $C$. To compare over the entire experimental region $R$, we partition $R$ into several concentric regions $R_C$ by reducing its boundary by a shrinkage factor $\nu$. The values of $\nu$ are so chosen that the concentric regions cover the entire region $R$. For a design $D$ and a fixed $\beta \in C$, the quantiles of $\mathcal{T}_D(x, \beta)$ are computed for $x \in R_C$. The $p$th quantile of design $D$ is denoted by $Q_D(p, \beta, \nu)$. To address the dependency on $\beta$, a subset of values of $\beta$ is selected from $C$ and denoted by $C$. $Q_D(p, \beta, \nu)$ values are then found for $\beta \in C$. For a fixed $p$ and $\nu$ the minimum and maximum quantiles,

$$Q_D^{\min}(p, \nu) = \min_{\beta \in C} \{Q_D(p, \beta, \nu)\}, \quad (p \in [0, 1]),$$

$$Q_D^{\max}(p, \nu) = \max_{\beta \in C} \{Q_D(p, \beta, \nu)\}, \quad (p \in [0, 1]),$$

are computed over the values of $\beta$ in $C$. By plotting $Q_D^{\min}(p, \nu)$ and $Q_D^{\max}(p, \nu)$ against the probabilities $p \in [0, 1]$, we get the quantile dispersion graphs (QDGs) for design $D$ over the region $R_C$. Small and close values of $Q_D^{\min}(p, \nu)$ and $Q_D^{\max}(p, \nu)$ are desirable. Small values of the minimum and maximum quantiles indicate that the design $D$ has good prediction capability in the presence of linear predictor misspecification. While, close values of $Q_D^{\min}(p, \nu)$ and $Q_D^{\max}(p, \nu)$ imply that the design is robust to changes in the parameter values $\beta$.

V. EXAMPLES

The examples are based on simulated data where $q = 3$ (four categories) and there are two covariates $x_1$ and $x_2$. For generating the data set, the true linear predictor is

$$\eta_{1}(x) = -4.2 + 2.5x_1 - 3.7x_2 + f_{T,1}(x),$$

$$\eta_{2}(x) = -3.1 + 2.5x_1 - 3.7x_2 + f_{T,2}(x),$$

$$\eta_{3}(x) = -1.5 + 2.5x_1 - 3.7x_2 + f_{T,3}(x),$$

where the function $f_T = [f_{T,1}, f_{T,2}, f_{T,3}]'$ is defined by

$$f_{T,1}(x) = -[5\pi \sin(2\pi x_1) \cos(x_2)],$$

$$f_{T,2}(x) = [\pi \sin(2\pi x_1) \cos(x_2)],$$

$$f_{T,3}(x) = 6[\pi \sin(2\pi x_1) \cos(x_2)],$$

and the true link function is the multivariate logistic link function. The responses are taken at the design points of design $D_1$, a $5 \times 7$ factorial design and there are $n_1 = 6$ experimental units at each run. Designs and the corresponding responses are given in Table I.

Suppose the experimenter assumed the following model,

$$\eta_{1}(x) = \theta_{01} + \theta_{11}x_1 + \theta_{22}x_2,$$

$$\eta_{2}(x) = \theta_{02} + \theta_{12}x_1 + \theta_{22}x_2,$$

$$\eta_{3}(x) = \theta_{03} + \theta_{13}x_1 + \theta_{22}x_2$$

and the multivariate logistic link function. The parameter estimates are shown in Table II. The resultant deviance is $77.1884$ with $30$ degrees of freedom ($p$ value $< 0.0001$), indicating a lack of fit. A possible cause of the large deviance may be due to a misspecified linear predictor. Suppose we misspecified the linear function by a function $f$ which is unknown, then the true $\eta$ can be written as,

$$\eta_{1}(x) = \theta_{01} + \theta_{11}x_1 + \theta_{22}x_2 + f_{1}(x),$$

$$\eta_{2}(x) = \theta_{02} + \theta_{12}x_1 + \theta_{22}x_2 + f_{2}(x),$$

$$\eta_{3}(x) = \theta_{03} + \theta_{13}x_1 + \theta_{22}x_2 + f_{3}(x),$$

where $f(x) = [f_{1}(x), f_{2}(x), f_{3}(x)]'$.

Our interest here is to study the effect of the misspecification in the linear predictor on design selection. Suppose we compare the performance of design $D_1$ under misspecification with two other designs $D_2$ (uniform shell design) and $D_3$ (central composite design). Using QDGs we will study the effect of model misspecification on the prediction capabilities of the three designs and choose the one which is most robust under the current misspecification. The design points of $D_2$ and $D_3$ are listed in Table I, note they have the same number of experimental runs as the original design $D_1$. The prediction capabilities of the three designs are compared on the basis of their EMSEP values. Note that EMSEP depends on the unknown function $f(x)$, the parameter vector $\beta$ and the design points $x$.

To compare the designs on the entire experimental region, $R$ is divided into several concentric regions, $R_C$, given by

$$R_C = \{x : \text{lb}_i \leq x_i \leq \text{ub}_1, \text{lb}_2 \leq x_2 \leq \text{ub}_2\},$$

$$0.5 \leq \nu \leq 1,$$

with $\text{lb}_i = a_i + (1-\nu)(b_i - a_i)$ and $\text{ub}_i = b_i - (1-\nu)(b_i - a_i)$. Here, $a_i$ and $b_i$ are the upper and lower bounds of $x_i$ for $i = 1, 2$. For this example we choose $a_1 = -1$, $a_2 = -1$, $b_1 = 1$ and $b_2 = 1$. From the boundary of each region $R_C$, $1000$ points are selected.

For estimation of $f(x)$ at the selected points in $R$ we proceed in the following way. First we use the method described in Section IV-A to compute $\hat{f}(x)$ at the design points of $D_1$. Then, using $\hat{f}(x)$ at the design points as a training data, multivariate kriging is applied to find $f(x)$ at all points in the experimental region $R$, where, $R = \{x : -1 \leq x_1 \leq 1, -1 \leq x_2 \leq 1\}$.

For kriging, we fit the intercept only model with unknown parameter vector $\varpi_0$,

$$f(x) = \varpi_0 + \Pi(x),$$

where $\Pi(x)$ is a stationary Gaussian process with zero mean, unknown variance and correlation function. The form of the correlation function is assumed to be the generalized
TABLE I

DESIGNS $D_1$ (5 × 7 FACTORIAL), $D_2$ (UNIFORM SHELL DESIGN) AND $D_3$ (CENTRAL COMPOSITE DESIGN) AND THE RESPONSES FOR THE EXAMPLE: THERE ARE $n_1 = 6$ EXPERIMENTAL UNITS AT EACH RUN

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<th>$D_3$</th>
<th>Responses</th>
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Fig. 1 Quantile dispersion graphs for designs $D_1$, $D_2$, and $D_3$. p > 0.5. Hence, away from the center of the region, designs $D_1$ and $D_2$ have better prediction capabilities than the design $D_3$ under the misspecification of the linear predictor. However, the maximum quantiles of designs $D_1$ and $D_2$ are close to each other implying that designs $D_1$ and $D_2$ has comparable prediction capabilities near the boundary of the region. As we move towards the center of the region, the maximum quantiles of designs $D_2$ and $D_3$ move close to each other, while the maximum quantiles of the design $D_1$ are smaller than those of designs $D_2$ and $D_3$. Hence, near the center of the experimental region, designs $D_2$ and $D_3$ have comparable performances and the design $D_1$ has better prediction capabilities than designs $D_2$ and $D_3$. Another point to note is that the differences between $Q_{D_{1 \text{min}}}^{p}$ and $Q_{D_{2 \text{max}}}^{p}$ values of design $D_1$ are smaller than those of designs $D_2$ and $D_3$, implying that design $D_1$ is more robust to the changes in the regression parameter vector $\beta$ as compared to $D_2$ and $D_3$ throughout the experimental region.

VI. CONCLUDING REMARKS

In this article, we use the QDGs approach to compare designs for ordinal response models when the form of the linear predictor is uncertain. The QDGs approach compares the designs over the entire experimental region not just at a
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where we use an unknown function point like a single value criterion, such as D efficiency. We change as points are selected from various locations in the linear predictor. Multivariate parametric kriging is used to link \( \mu \) and \( U \).

\[ U = \sum_{i=1}^{n} \left[ Z_i \Sigma^{-1} \{ y_i - \mu \} \right] \]

and

\[ V_{\text{ar}}(\hat{\beta}_0) = \frac{1}{n \sigma^2} \left[ \sum_{i=1}^{n} Z_i^T D_i (\beta_0) \Sigma_i^{-1} \{ y_i - \mu \} \right] \]

By central limit theorem for independent not identical distributed random variables we get \( \frac{d \hat{\beta}_0}{d \beta} \) has a multivariate normal distribution with mean \( \sqrt{n} \epsilon \) and variance \( X^T P \epsilon X \).

Now, expanding \( \frac{d \hat{\beta}_0}{d \beta} \) around \( \beta_0 \), we get

\[ \frac{d \beta}{d \beta} = \frac{d \hat{\beta}_0}{d \beta} + \frac{p}{2} \sum_{k=1}^{p} \left( \beta_k - \beta_{0,k} \right) \frac{d^2 \beta}{d \beta_k^2} \]

Here, \( \beta_j \) and \( \beta_{0,j} \) are denoted for the \( j \)th term of the vector \( \beta \) and \( \beta_0 \), respectively and \( \beta \) is the point lying on the line segment joining by \( \beta \) and \( \beta_0 \). Now, putting \( \beta \) (MLE of \( \beta \)) in (33) and using \( \frac{d \hat{\beta}_0}{d \beta} = 0 \) we get,

\[ \begin{align*}
E \left[ \frac{1}{\sqrt{n}} \frac{d \hat{\beta}_0}{d \beta} \right] &= \frac{1}{\sqrt{n}} E \left[ \sum_{i=1}^{n} Z_i^T D_i (\beta_0) \Sigma_i^{-1} \{ y_i - \mu \} \right] \\
&= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} Z_i^T D_i (\beta_0) \Sigma_i^{-1} (\mu - \mu) \\
&= \sqrt{n} \sum_{i=1}^{n} Z_i^T D_i (\beta_0) \Sigma_i^{-1} (\mu - \mu) \\
&= \sqrt{n} \sum_{i=1}^{n} \left[ Z_i^T \phi \Sigma_i^{-1} (\mu - \mu) \right] = \sqrt{n} \left[ \phi \Sigma^{-1} (\mu - \mu) \right]
\end{align*} \]

Now, \( \frac{d^2 \beta}{d \beta^2} \) is bounded when the distribution of response variables follow multinomial distribution. Also, by consistency of \( \beta \), we have \( \beta - \beta_0 \rightarrow 0 \) as \( n \rightarrow \infty \). Hence, \( \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\hat{\beta}_i - \beta_0) \rightarrow \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \epsilon_i \rightarrow 0 \).
\( \beta_{0,1} \) \( \frac{d^3 \hat{\beta}_{0,1}}{d \beta_1^2 d \beta_3^2 d \beta_5^2} \to 0 \) as \( n \to \infty \). So,

\[
\left[ \frac{1}{n} \frac{d^3 \hat{\beta}_{0,1}}{d \beta_1^2 d \beta_3^2 d \beta_5^2} + \frac{1}{2n} \sum_{i=1}^{n} \left( \hat{\beta}_i - \beta_{0,1} \right) \frac{d^3 \hat{\beta}_{0,1}}{d \beta_1^2 d \beta_3^2 d \beta_5^2} \right] \\
= \frac{1}{n} \frac{d^3 \hat{\beta}_{0,1}}{d \beta_1^2 d \beta_3^2 d \beta_5^2} - H_{jk}
\]

(35)

Where \( H_{jk} \) is the element of the matrix \( H_n = \frac{1}{n} \frac{d^3 \hat{\beta}_{0,1}}{d \beta_1^2 d \beta_3^2 d \beta_5^2} \).

This gives the limit distribution of \( \frac{1}{\sqrt{n}} (\beta - \beta_0) \) as the solution of

\[
\sum_{k=1}^{n} H_{jk} \sqrt{n} (\hat{\beta}_k - \beta_{0,k}) = \frac{1}{\sqrt{n}} \frac{d \eta}{d \beta_j}
\]

(36)

This follows asymptotically multivariate normal distribution with mean \( \sqrt{n} \beta \) and variance \( X^T PWX - \mathbf{R} \) (by (32)).

**APPENDIX B**

**DERIVATION OF FORMULA 15**

The mean squared error of \( \hat{\beta}(x) \) is given by

\[
MSE(\hat{\beta}(x)) = Var(\hat{\beta}(x)) + Bias(\hat{\beta}(x))(Bias(\hat{\beta}(x))^T
\]

(37)

Since \( \hat{\beta}(x) = h(\hat{\eta}(x)) \), expanding \( \hat{\beta}(x) = h(\hat{\eta}(x)) \) around \( \eta_T(x) \) and approximating up to first order derivative of the Taylor series, we have,

\[
\hat{\beta}(x) = h(\hat{\eta}(x)) = h(\hat{\eta}_T(x)) + \frac{d h(\hat{\eta}(x))}{d \hat{\eta}(x)} (\hat{\eta}(x) - \eta_T(x))
\]

(38)

Now, taking expectation on both sides of (38), we get

\[
E(\hat{\beta}(x)) = \hat{\beta}(x) + \frac{d h(\hat{\eta}(x))}{d \hat{\eta}(x)} E(\hat{\eta}(x) - \eta_T(x))
\]

(39)

From (38), we get

\[
Var(\hat{\beta}(x)) = Var(h(\hat{\eta}(x)) + \frac{d h(\hat{\eta}(x))}{d \hat{\eta}(x)} \eta_T(x))
\]

(40)

Now,

\[
Bias(\hat{\beta}(x)) = E[\hat{\beta}(x)] - \beta(x)
\]

(41)

**PARAMETRICAL EMPIRICAL KRIGING FOR MULTIPLE OUTPUTS**

Let us consider the regression model where for \( x \in S \subset R^d \), we have multiple outputs \( T_1(x), T_2(x), \ldots, T_m(x) \) and the model is given by (9) (page 102, equation (4.2.1))

\[
T_i(x) = \Lambda_i(x) \delta_i + G_i(x)
\]

(43)

where for each \( i = 1, 2, \ldots, m \), the \( G_i(x) \) has multivariate normal distribution having mean zero, unknown variance and unknown correlation function. Here, \( \Lambda_i(x) \) is a \( p_i \times 1 \) known vector function and \( \delta_i \) is a \( p_i \times 1 \) vector of unknown parameters. For simplicity, let us denote \( \delta = \delta_1, \delta_2, \ldots, \delta_m \) as the \( p \times 1 \) unknown parameter with \( p = \sum_{i=1}^{m} p_i \). For the above model, we assume that the covariance between \( G_i(x_1) \) and \( G_i(x_2) \) depends only on \( x_1 - x_2 \) and it is given by \( Cov(G_i(x_1), G_i(x_2)) = \sigma_i^2 \rho_i(x_1 - x_2) \), where \( \rho_i(x_1 - x_2) \) is the correlation between \( G_i(x_1) \) and \( G_i(x_2) \). Also, we assume joint covariance structure of the \{\( G_i(x) \)\} given by \( Cov(G_i(x_1), G_j(x_2)) = \sigma_{ij} \rho_i(x_1 - x_2) \), where \( \rho_{ij}(x_1 - x_2) \) is the cross correlation function of \( Z_i(x) \) and \( Z_j(x) \) for \( i \neq j \).

Reference [9] discusses various types of correlation functions for \( \rho_i(x) \) and \( \rho_{ij}(x) \). In our numerical example we use the Generalized exponential correlation function for \( \rho_i(x) \) and \( \rho_{ij}(x) \) given below.

Suppose we need to find \( \rho_i(x_1 - x_2) \) and \( \rho_{ij}(x_1 - x_2) \), where \( x_1 \) and \( x_2 \) are two realization of \( x \) and let \( e = x_1 - x_2 \in \mathbb{R}^d \). Then \( \rho(e) \) and \( \rho_{ij}(e) \) have the form \( \zeta(\Theta(e)) \), where \( \zeta(e) \) is given by

\[
\zeta(e) = \prod_{k=1}^{d} \exp(-\Theta_k |e_k| ^{\Theta_{k+1}}), 0 < \Theta_{d+1} \leq 2.
\]

Suppose, we want to predict \( \hat{Y}_1(x_0) \) at new design point \( x_0 \).

Then the estimate of \( \hat{Y}_1(x_0) \), \( \hat{Y}_1(x_0) \) is given by [9, pp. 107,
equation (4.2.12)]

\[ \hat{\mathbf{Y}}_N(x_0) = \mathbf{\Lambda}'_0 \hat{\delta} + \mathbf{r}_0' \mathbf{\Sigma}^{-1} (\mathbf{Y}^N - \mathbf{F}\hat{\delta}), \tag{44} \]

where \( \hat{\delta} \) is the generalized least square estimate of \( \delta \) using \( N = \sum_{i=1}^{m} n_i \) observations \( \mathbf{Y}^N = [(\mathbf{Y}^N_1)']', (\mathbf{Y}^N_2)']', \ldots, (\mathbf{Y}^N_m)']' \) with \( n_i \) observations for the \( i \)th design points \( x_1', x_2', \ldots, x_{n_i}' \). Here

\[ F = \begin{pmatrix} \mathbf{A}_1'(x_0) & \mathbf{O}_{1 \times (p-m)} \\ \mathbf{F}_1 & \mathbf{O}_{n_1 \times p_1} \\ \vdots & \vdots \\ \mathbf{O}_{n \times p_1} & \mathbf{F}_m \end{pmatrix}, \tag{45} \]

\[ \mathbf{\Sigma} = \begin{pmatrix} \mathbf{R}_1 & \tau_1 \mathbf{R}_{12} & \ldots & \tau_m \mathbf{R}_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ \tau_m \mathbf{R}_{1m} & \tau_m \mathbf{R}_{2m} & \ldots & \tau_m \mathbf{R}_{m} \end{pmatrix}, \tag{46} \]

\[ \mathbf{\Lambda}'_0 = [\mathbf{A}_1'(x_0), \mathbf{O}_{1 \times (p-m)}], \text{ and } \mathbf{r}_0' = [\mathbf{r}_1', \tau_2 \mathbf{r}_2', \ldots, \tau_m \mathbf{r}_m'], \]

where

- \( \tau_i = \sigma_i / \sigma_1, \quad 2 \leq i \leq m, \)
- \( \mathbf{A}_1(x_0) \) is the vector of regressor at the design point \( x_0 \) for \( \mathbf{Y}_1(x) \),
- \( \mathbf{F}_i = (\mathbf{A}_1'(x)) \) is the \( n_i \times p_1 \) matrix of regressor for \( i \)th response,
- \( \mathbf{R}_i \) is the matrix of order \( n_i \times n_i \) for the correlations between the elements of \( \mathbf{Y}_i \),
- \( \mathbf{r}_{ij} \) is the \( n_i \times 1 \) vector of correlations between \( \mathbf{Y}_1(x_0) \) and \( \mathbf{Y}_i \), and
- \( \mathbf{R}_{ij} \) is the matrix of order \( n_i \times n_j \) for the correlations between \( \mathbf{Y}_i \) and \( \mathbf{Y}_j \).

The unknown parameter vector \( \Theta \) for the correlation function is estimated using maximum likelihood estimation.

REFERENCES