Appendix A: Parametric Variance Estimation

In this appendix, the details of parametric variance estimation will be discussed. Recall that in parametric dual modeling, the data used for variance estimation is the squared, EWLS means model residuals and in DMRR, the data used is the squared, MMRR residuals. Although the variance data is different in the two dual modeling procedures, the procedure itself can be generalized to specific situations by introducing some general notation. In Appendix A.1 we will define this general notation and in Appendix A.2 the parametric variance estimation procedure will be discussed in detail.

Appendix A.1: Notation and Results

The following is a list of notation and results that will be useful in deriving the parametric variance estimate in Appendix A.2:

1. Parametric variance estimation involves the weighted least squares analysis of the "generalized linear model" (GLM):

$$\mathbf{e}^{2\,(\text{method})} = \exp\{\mathbf{Z}\boldsymbol{\theta}\} + \boldsymbol{\eta} \qquad \text{(A.1.1)}$$

where the superscript "method" may be replaced by the "method" in which the means model is estimated (For example, "method" = "ewls" if the method used is estimated weighted least squares and "method" = "mmrr" if the method used is DMRR.).

2. The estimated parametric variance function is given by

$$\hat{\boldsymbol{\sigma}}^{2\,(\text{glm})} = \exp\left\{\mathbf{Z}\hat{\boldsymbol{\theta}}^{(\text{glm})}\right\} \qquad \text{(A.1.2)}$$

where the superscript "glm" refers to the weighted least squares analysis of the GLM given in A.1.1.

3. We define the *n*x*n* matrix $\mathbf{V}_e$ as :

$$\mathbf{V}_e = \text{diag}\left\langle 2\exp\left\{2\mathbf{z}_1'\boldsymbol{\theta}^{(\text{glm})}\right\}, \cdots, 2\exp\left\{2\mathbf{z}_n'\boldsymbol{\theta}^{(\text{glm})}\right\}\right\rangle \qquad \text{(A.1.3)}$$

where the elements of $\mathbf{V}_e$ are the variances of the squared, means model residuals implied by the GLM given in A.1.1.

4. The *n*x*n* matrix Δ is defined as follows:

$$\Delta = \operatorname{diag}\left\langle \left[\left. \frac{\partial \exp\left(\mathbf{z}_i'\hat{\boldsymbol{\theta}}^{(glm)}\right)}{\partial\left(\mathbf{z}_i'\hat{\boldsymbol{\theta}}^{(glm)}\right)} \right|_{\hat{\boldsymbol{\theta}}^{(glm)} = \boldsymbol{\theta}^{(glm)}} \right] \right\rangle \qquad \text{(A.1.4)}$$

where $\boldsymbol{\theta}^{(glm)} = E\left[\hat{\boldsymbol{\theta}}^{(glm)}\right]$, obtained by regressing $E\left[\mathbf{e}^{2\,(method)}\right]$ vs. $\mathbf{Z}$ through the function $\exp\left\{\mathbf{Z}\boldsymbol{\theta}\right\}$. It is important to note that the value of $\boldsymbol{\theta}^{(glm)}$ depends on the type of squared residuals used to model the variance.

5. The scalar δ_o can be defined for any point z_o, as

$$\delta_o = \left. \frac{\partial \exp\left(\mathbf{z}_o'\hat{\boldsymbol{\theta}}^{(glm)}\right)}{\partial\left(\mathbf{z}_o'\hat{\boldsymbol{\theta}}^{(glm)}\right)} \right|_{\hat{\boldsymbol{\theta}}^{(glm)} = \boldsymbol{\theta}^{(glm)}} . \qquad \text{(A.1.5)}$$

6. From a Taylor series expansion of $\exp\left\{\mathbf{Z}\hat{\boldsymbol{\theta}}^{(glm)}\right\}$ about $\boldsymbol{\theta}^{(glm)}$ and retaining only the linear terms, the parametric variance estimate is approximated by

$$\exp\left\{\mathbf{Z}\hat{\boldsymbol{\theta}}^{(glm)}\right\} \approx \exp\left\{\mathbf{Z}\boldsymbol{\theta}^{(glm)}\right\} + \boldsymbol{\Delta}\ \mathbf{Z}\left(\hat{\boldsymbol{\theta}}^{(glm)} - \boldsymbol{\theta}^{(glm)}\right). \qquad \text{(A.1.6)}$$

7. Using the Gauss-Newton algorithm (discussed in Appendix A.2) we have

$$\hat{\boldsymbol{\theta}}^{(glm)} - \boldsymbol{\theta}^{(glm)} \approx \left(\mathbf{Z}'\boldsymbol{\Delta}\,\mathbf{V}_e^{-1}\boldsymbol{\Delta}\,\mathbf{Z}\right)^{-1}\mathbf{Z}'\boldsymbol{\Delta}\,\mathbf{V}_e^{-1}\left(\mathbf{e}^{2(method)} - \exp\left\{\mathbf{Z}\boldsymbol{\theta}^{(glm)}\right\}\right) \qquad \text{(A.1.7)}$$

and defining

$$\mathbf{H}^{(glm)} = \boldsymbol{\Delta}\,\mathbf{Z}\ \left(\mathbf{Z}'\boldsymbol{\Delta}\,\mathbf{V}_e^{-1}\boldsymbol{\Delta}\,\mathbf{Z}\right)^{-1}\mathbf{Z}'\boldsymbol{\Delta}\,\mathbf{V}_e^{-1}, \qquad \text{(A.1.8)}$$

we can write

$$\boldsymbol{\Delta}\,\mathbf{Z}\left(\hat{\boldsymbol{\theta}}^{(glm)} - \boldsymbol{\theta}^{(glm)}\right) \approx \mathbf{H}^{(glm)}\left(\mathbf{e}^{2\,(method)} - \exp\left\{\mathbf{Z}\boldsymbol{\theta}^{(glm)}\right\}\right). \qquad \text{(A.1.9)}$$

8. Combining the A.1.5 and A.1.8, we have that the parametric variance estimate can be approximated by

$$\exp\left\{\mathbf{Z}\hat{\boldsymbol{\theta}}^{(\mathrm{glm})}\right\} \approx \exp\left\{\mathbf{Z}\boldsymbol{\theta}^{(\mathrm{glm})}\right\} + \mathbf{H}^{(\mathrm{glm})}\left(\mathbf{e}^{2\ (\mathrm{method})} - \exp\left\{\mathbf{Z}\boldsymbol{\theta}^{(\mathrm{glm})}\right\}\right) \qquad (\mathrm{A.1.10})$$

Appendix A.2: Obtaining $\exp\left\{\mathbf{Z}\hat{\boldsymbol{\theta}}^{(\mathbf{glm})}\right\}$

The parametric variance estimate, $\exp\left\{\mathbf{Z}\hat{\boldsymbol{\theta}}^{(\mathrm{glm})}\right\}$, is obtained by first estimating the parameter $\boldsymbol{\theta}$ in the model

$$\mathbf{e}^{2\ (\mathrm{method})} = \exp\{\mathbf{Z}\boldsymbol{\theta}\} + \boldsymbol{\eta}. \qquad (\mathrm{A.2.1})$$

Parameter estimation is accomplished via weighted least squares, which can be expressed in matrix notation as

$$\min_{\boldsymbol{\theta}^*} \left(\mathbf{e}^{2\ (\mathrm{method})} - \exp\left\{\mathbf{Z}\boldsymbol{\theta}^*\right\}\right)' \mathbf{V}_{\mathrm{e}}^{-1} \left(\mathbf{e}^{2\ (\mathrm{method})} - \exp\left\{\mathbf{Z}\boldsymbol{\theta}^*\right\}\right) \qquad (\mathrm{A.2.2})$$

where $\boldsymbol{\theta}^*$ is a qx1 vector of variance model parameters and $\theta_i \in \Re\ (i = 1, \cdots, q)$. Since the minimization expressed in A.2.2 is nonlinear in $\boldsymbol{\theta}^*$, it is necessary to use numerical techniques such as the Gauss-Newton algorithm to obtain a solution. Essentially, the Gauss-Newton procedure is iterative and requires a set of starting values. Applied to parametric variance estimation, the Gauss-Newton procedure is given as follows.

1. Obtain initial estimates of the parameters. Usually the initial estimates are obtained by regressing $ln\left(\mathbf{e}^{2\ (\mathrm{method})}\right)$ vs $\mathbf{Z}$ using ordinary least squares. Thus, the initial solution to A.2.1 is given as:

$$\hat{\boldsymbol{\theta}}^* = \hat{\boldsymbol{\theta}}_0^{(\mathrm{glm})} = \left(\mathbf{Z}'\mathbf{Z}\right)^{-1}\mathbf{Z}'\left[ln\left(\mathbf{e}^{2\ (\mathrm{method})}\right)\right]. \qquad (\mathrm{A.2.3})$$

2. In the attempt to find the value of $\boldsymbol{\theta}^*$ that minimizes A.2.2, use Taylor Series to expand $\exp\left\{\mathbf{Z}\boldsymbol{\theta}^*\right\}$ about $\hat{\boldsymbol{\theta}}^* = \hat{\boldsymbol{\theta}}_0^{(\mathrm{glm})}$ and retain only the linear terms:

$$\exp\left\{\mathbf{Z}\boldsymbol{\theta}^*\right\} \approx \exp\left\{\mathbf{Z}\hat{\boldsymbol{\theta}}_0^{(\mathrm{glm})}\right\} + \left(\boldsymbol{\theta}^* - \hat{\boldsymbol{\theta}}_0^{(\mathrm{glm})}\right)\left[\left(\frac{\partial \exp\left\{\mathbf{Z}\boldsymbol{\theta}^*\right\}}{\partial \boldsymbol{\theta}^*}\right)\Bigg|_{\boldsymbol{\theta}^* = \hat{\boldsymbol{\theta}}_o^{(\mathrm{glm})}}\right] \tag{A.2.4}$$

Notice from the chain rule we have that

$$\left[\left(\frac{\partial \exp\left\{\mathbf{Z}\boldsymbol{\theta}^*\right\}}{\partial \boldsymbol{\theta}^*}\right)\Bigg|_{\boldsymbol{\theta}^* = \hat{\boldsymbol{\theta}}_o^{(\mathrm{glm})}}\right] = \boldsymbol{\Delta}\,\mathbf{Z} \tag{A.2.5}$$

where $\boldsymbol{\Delta}$ and $\mathbf{Z}$ are given as follows:

$$\boldsymbol{\Delta} = \left[\left(\frac{\partial \exp\left\{\mathbf{Z}\boldsymbol{\theta}^*\right\}}{\partial\left(\mathbf{Z}\boldsymbol{\theta}^*\right)}\right)\Bigg|_{\boldsymbol{\theta}^* = \hat{\boldsymbol{\theta}}_o^{(\mathrm{glm})}}\right], \tag{A.2.6}$$

$$\mathbf{Z} = \left[\left(\frac{\partial\left(\mathbf{Z}\boldsymbol{\theta}^*\right)}{\partial \boldsymbol{\theta}^*}\right)\Bigg|_{\boldsymbol{\theta}^* = \hat{\boldsymbol{\theta}}_o^{(\mathrm{glm})}}\right]. \tag{A.2.7}$$

3. Substitute the Taylor Series expansion of $\exp\left\{\mathbf{Z}\boldsymbol{\theta}^*\right\}$ into expression (A.2.2) and compute the solution by differentiating with respect to $\hat{\boldsymbol{\theta}}^*$ and setting equal to zero. The solution is given by:

$$\hat{\boldsymbol{\theta}}_1^{(\mathrm{glm})} \approx \hat{\boldsymbol{\theta}}_0^{(\mathrm{glm})} + \left(\mathbf{Z}'\boldsymbol{\Delta}\,\mathbf{V}_e^{-1}\boldsymbol{\Delta}\,\mathbf{Z}\right)^{-1}\mathbf{Z}'\boldsymbol{\Delta}\,\mathbf{V}_e^{-1}\left(\mathbf{e}^{2(\mathrm{method})} - \exp\left\{\mathbf{Z}\hat{\boldsymbol{\theta}}_0^{(\mathrm{glm})}\right\}\right). \tag{A.2.8}$$

4. If $\hat{\boldsymbol{\theta}}_1^{(\mathrm{glm})} \approx \hat{\boldsymbol{\theta}}_0^{(\mathrm{glm})}$, then stop. Otherwise, replace $\hat{\boldsymbol{\theta}}_0^{(\mathrm{glm})}$ with $\hat{\boldsymbol{\theta}}_1^{(\mathrm{glm})}$ and return to step 2. At convergence set $\hat{\boldsymbol{\theta}}^{(\mathrm{glm})} = \hat{\boldsymbol{\theta}}_1^{(\mathrm{glm})}$.

The parametric variance estimate is then given as

$$\hat{\boldsymbol{\sigma}}^{2(\mathrm{glm})} = \exp\left\{\mathbf{Z}\hat{\boldsymbol{\theta}}^{(\mathrm{glm})}\right\} \tag{A.2.9}$$

where $\hat{\theta}^{(glm)}$ is found by the Gauss-Newton algorithm mentioned above.