APPENDIX B. COMPUTATION OF Q AND R FOR TESTING FOR EQUALITY OF CONSTRAINED AND UNCONSTRAINED RESIDUALS

To show that $\boldsymbol{Q}$ and $\boldsymbol{R}$ must be computed using $\boldsymbol{\theta} \neq \tilde{\boldsymbol{\theta}}$ for the test of equality of constrained and unconstrained weighted residuals, we need to use results from the constrained regression. The constrained regression involves finding the minimum value of $S(\boldsymbol{\theta}), S(\tilde{\boldsymbol{\theta}})$, subject to the constraint $g(\gamma\boldsymbol{\theta}) = g(\gamma\boldsymbol{\theta}_*)$. This is accomplished using the Lagrange function given as equation E-7 in Cooley (2004, p. 145):

$$L(\boldsymbol{\theta}, \lambda) = S(\boldsymbol{\theta}) + 2\lambda\big(g(\gamma\boldsymbol{\theta}_*) - g(\gamma\boldsymbol{\theta})\big). \tag{B-1}$$

The method used is the same one used for equation 8. First, we substitute equations A-1 and A-2, appendix A, into equation B-1, take the derivatives of $L(\boldsymbol{\theta}, \lambda)$ with respect to $\boldsymbol{\theta}$ and λ, and set the results to zero to yield, for iteration r+1

$$\boldsymbol{\theta}_{r+1} - \boldsymbol{\theta}_r = \lambda_{r+1}\left(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r\right)^{-1}\boldsymbol{Dg}_r' + \left(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r\right)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}\big(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)\big) \tag{B-2}$$

and

$$g(\gamma\boldsymbol{\theta}_*) = g(\gamma\boldsymbol{\theta}_r) + \boldsymbol{D}g_r\left(\boldsymbol{\theta}_{r+1} - \boldsymbol{\theta}_r\right). \tag{B-3}$$

Second, we put equation B-2 into equation B-3 and solve for λ to obtain for iteration r+1

$$\lambda_{r+1} = \frac{g(\gamma\boldsymbol{\theta}_*) - g(\gamma\boldsymbol{\theta}_r) - \boldsymbol{D}g_r\left(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r\right)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}\big(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)\big)}{\boldsymbol{Q}_r'\boldsymbol{Q}_r}. \tag{B-4}$$

At convergence $\boldsymbol{\theta}_{r+1} \approx \boldsymbol{\theta}_r \approx \tilde{\boldsymbol{\theta}}$ so that equation B-4 can be substituted into equation B-2 to give

$$\begin{aligned}
&\left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\big(\boldsymbol{Y} - \boldsymbol{f}(\gamma\tilde{\boldsymbol{\theta}})\big) - \frac{\left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\tilde{g}'\boldsymbol{D}\tilde{g}\left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\big(\boldsymbol{Y} - \boldsymbol{f}(\gamma\tilde{\boldsymbol{\theta}})\big)}{\tilde{\boldsymbol{Q}}'\tilde{\boldsymbol{Q}}} \\
&= \left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}\left(\boldsymbol{I} - \frac{\boldsymbol{D}\tilde{g}'\boldsymbol{D}\tilde{g}\left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}}{\tilde{\boldsymbol{Q}}'\tilde{\boldsymbol{Q}}}\right)\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\big(\boldsymbol{Y} - \boldsymbol{f}(\gamma\tilde{\boldsymbol{\theta}})\big) \\
&= \boldsymbol{0},
\end{aligned} \tag{B-5}$$

where the tildes over variables indicate evaluation using $\tilde{\boldsymbol{\theta}}$. Cooley (2004, equation E-14) showed that equation B-5 can be written in the form

$$\left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}^{1/2}\left(\tilde{\boldsymbol{R}}-\frac{\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{Q}}'}{\tilde{\boldsymbol{Q}}'\tilde{\boldsymbol{Q}}}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)=\boldsymbol{0}. \tag{B-6}$$

Premultiplication of equation B-6 by $\boldsymbol{\omega}^{1/2}\boldsymbol{D}\tilde{\boldsymbol{f}}$ and use of the definition and properties of $\tilde{\boldsymbol{R}}$ lead to the result needed to complete the proof:

$$\left(\tilde{\boldsymbol{R}}-\frac{\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{Q}}'}{\tilde{\boldsymbol{Q}}'\tilde{\boldsymbol{Q}}}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)=\boldsymbol{0}. \tag{B-7}$$

To derive the equations needed to show that weighted residuals from the constrained regression, defined as $\left(\boldsymbol{I}-\boldsymbol{Q}\boldsymbol{Q}'/\boldsymbol{Q}'\boldsymbol{Q}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)$, equal standard weighted residuals $\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right)\right)$ when model intrinsic and model combined intrinsic types of nonlinearity are negligible, we substitute equation 6-17 of Cooley (2004) into the constrained weighted residuals to get

$$\begin{aligned}&\left(\boldsymbol{I}-\frac{\boldsymbol{Q}\boldsymbol{Q}'}{\boldsymbol{Q}'\boldsymbol{Q}}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)\\&=\left(\boldsymbol{I}-\boldsymbol{R}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\boldsymbol{\theta}_*\right)\right)+\left(\boldsymbol{I}-\boldsymbol{R}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{f}\left(\gamma\boldsymbol{\theta}_*\right)-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)+\left(\boldsymbol{R}-\frac{\boldsymbol{Q}\boldsymbol{Q}'}{\boldsymbol{Q}'\boldsymbol{Q}}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right).\end{aligned} \tag{B-8}$$

If model intrinsic nonlinearity is negligible, then from Cooley (2004, equations 6-2 and I-1 - I-5) the first term on the right side of equation B-8 is equal to the weighted residual vector and the second term is negligible. If model combined intrinsic nonlinearity is negligible, then from Cooley (2004, equation I-21) the last term is negligible. However, from equation B-7, if $\tilde{\boldsymbol{R}}$ and $\tilde{\boldsymbol{Q}}$ were used in place of $\boldsymbol{R}$ and $\boldsymbol{Q}$, then this term always would be zero.