

## **Appendix G:**

### **Bayesian Equivalence Theory for the $k$ -regressor Case**

This Appendix contains the steps for deriving the Bayesian equivalence theory function for the two regressor no interaction model. The notation used in this Appendix is defined in Sections 5.1-5.1 of Chapter 5.

To ensure concavity, the log determinant is used rather than the determinant for the Bayesian D-optimality criterion,  $f$ , is defined in expression (1).

$$\phi = \int R(\boldsymbol{\delta}, \boldsymbol{\beta}) \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta} = \log \int \det \mathbf{I}(\mathbf{x}, \boldsymbol{\beta}) \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta}. \quad (1)$$

With  $f$  defined, the Frechet derivative is given by

$$F_{\phi}[\mathbf{M}(\boldsymbol{\eta}^*, \boldsymbol{\beta}), \mathbf{J}(\mathbf{x}, \boldsymbol{\beta})] = \lim_{\boldsymbol{\varepsilon} \rightarrow 0^+} \frac{1}{\boldsymbol{\varepsilon}} \left[ \log \frac{\int \det \{(1 - \boldsymbol{\varepsilon}) \mathbf{M}(\boldsymbol{\eta}^*, \boldsymbol{\beta}) + \boldsymbol{\varepsilon} \mathbf{J}(\mathbf{x}, \boldsymbol{\beta})\} \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta}}{\int \det \mathbf{M}(\boldsymbol{\eta}^*, \boldsymbol{\beta}) \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta}} \right]. \quad (2)$$

where  $\mathbf{M}(\boldsymbol{\eta}, \boldsymbol{\beta}) = \begin{bmatrix} \sum \lambda_i & \sum \lambda_i \mathbf{x}_{1i} & \sum \lambda_i \mathbf{x}_{2i} \\ \sum \lambda_i \mathbf{x}_{1i} & \sum \lambda_i \mathbf{x}_{1i}^2 & \sum \lambda_i \mathbf{x}_{1i} \mathbf{x}_{2i} \\ \sum \lambda_i \mathbf{x}_{2i} & \sum \lambda_i \mathbf{x}_{1i} \mathbf{x}_{2i} & \sum \lambda_i \mathbf{x}_{2i}^2 \end{bmatrix} = \begin{bmatrix} a & d & f \\ d & b & g \\ f & g & c \end{bmatrix}$  and

$$\mathbf{J}(\mathbf{x}, \boldsymbol{\beta}) = \begin{bmatrix} \lambda_j & \lambda_j \mathbf{x}_{1j} & \lambda_j \mathbf{x}_{2j} \\ \lambda_j \mathbf{x}_{1j} & \lambda_j \mathbf{x}_{1j}^2 & \lambda_j \mathbf{x}_{1j} \mathbf{x}_{2j} \\ \lambda_j \mathbf{x}_{2j} & \lambda_j \mathbf{x}_{1j} \mathbf{x}_{2j} & \lambda_j \mathbf{x}_{2j}^2 \end{bmatrix}. \quad \text{The numerator of this argument of the log in (3) can be}$$

expressed as

$$\int \det \mathbf{M}(\mathbf{x}, \boldsymbol{\beta}) \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta} + \boldsymbol{\varepsilon} \int Q_1 \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta} + \boldsymbol{\varepsilon}^2 \int Q_2 \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta} + \boldsymbol{\varepsilon}^3 \int Q_3 \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta} \quad (4)$$

Taking the limit of (4) yields the indeterminant form of  $\frac{0}{0}$  so L'Hopitals Rule is employed to find the limit which yields

$$F_{\phi}[\mathbf{M}(\boldsymbol{\eta}^*, \boldsymbol{\beta}), \mathbf{J}(\mathbf{x}, \boldsymbol{\beta})] = \frac{\int Q_1 \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta}}{\int \det \mathbf{M}(\boldsymbol{\eta}^*, \boldsymbol{\beta}) \boldsymbol{\pi}(\boldsymbol{\beta}) d\boldsymbol{\beta}} \quad (5)$$

where

$$Q_1 = \lambda_j \left( acx_{1j}^2 - fx_{1j}^2 + abx_{2j}^2 - dx_{2j}^2 - 2agx_{1j}x_{2j} + 2dfx_{1j}x_{2j} + 2fgx_{1j} - 2dcx_{1j} + 2d\xi \right) + (3cd^2 + 3bf^2 - 3abc - 6dfg) \quad (6)$$

To demonstrate the use of Bayesian equivalence theory, the optimality of the design in Table 10.2.1 in Chapter 10 was verified. Recall that  $\beta_1 \sim U(-4, -2)$  and  $\beta_2 \sim U(-3, -1)$  so this is the Bayesian D-optimal design based on the ratios of (4,3). It is listed in tabular form below.

Table 1. Bayesian D-optimal Design where  $\beta_1 \sim U(-4, -2)$  and  $\beta_2 \sim U(-3, -1)$ .

<i>i</i>	<i>p<sub>i</sub></i>	<i>x<sub>1i</sub></i>	<i>x<sub>2i</sub></i>	<i>Contour</i>
<b>1</b>	0.3	IEC <sub>100</sub>	IEC <sub>100</sub>	MEC <sub>100</sub>
<b>2</b>	0.3	IEC <sub>100</sub>	IEC <sub>8.55</sub>	MEC <sub>8.55</sub>
<b>3</b>	0.3	IEC <sub>11.44</sub>	IEC <sub>100</sub>	MEC <sub>11.44</sub>

Monte Carlo integration was used to simulate the value of the Frechet derivative in (5) for this particular design. That function is graphed in Figure 1.

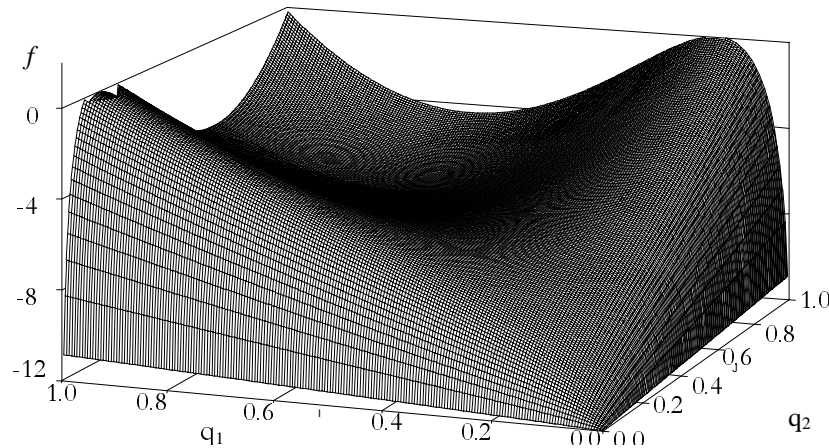


Figure 1 Bayesian equivalence function for the D-optimal design where  $\beta_1 \sim U(-4, -2)$  and  $\beta_2 \sim U(-3, -1)$ .

Thus, the optimality of this design is verified since this function is less than zero in the design space and equal to zero at the design points. Note that this same procedure can be used to verify the optimality of Bayesian designs in the k-regressor model.