50

Number of training samples Number of predictor variables Population coefficient of determination 15 and 40 0.5 and 0.9

Position of relevant components $\triangleright 1, 2 \triangleright 1, 3 \triangleright 2, 3 \text{ and } \triangleright 1, 2, 3$

Decay factor of eigenvalues of X 0.5 and 0.9

Table 1: Parameters used for simulating calibration sets

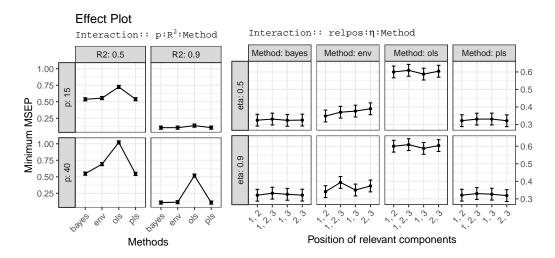
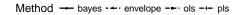


Figure 1: Third order interaction effects



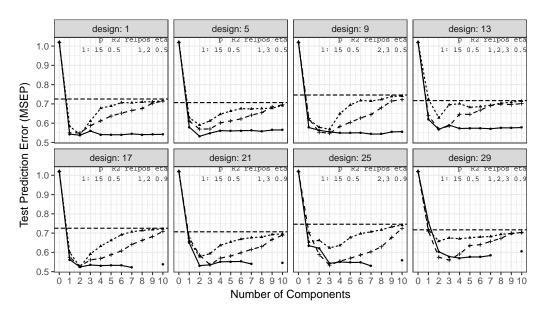


Figure 2: Average Prediction Error for designs with 15 predictor variables where Coefficient of determination is 0.5



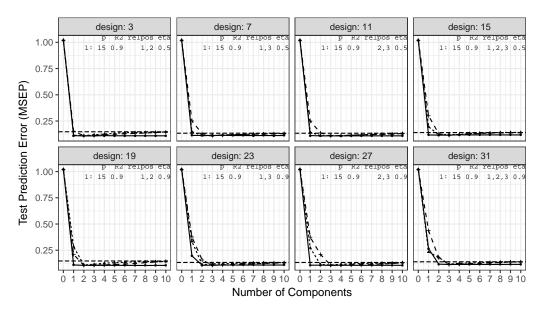
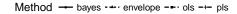


Figure 3: Average Prediction Error for designs with 15 predictor variables where Coefficient of determination is 0.9



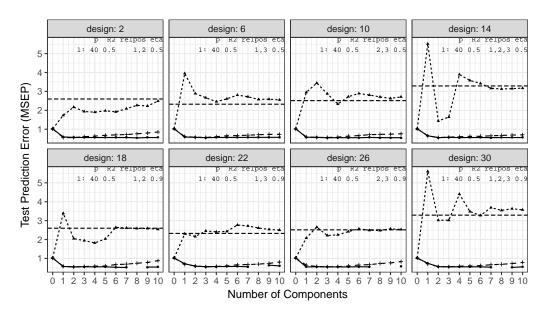


Figure 4: Average Prediction Error for designs with 40 predictor variables where Coefficient of determination is 0.5



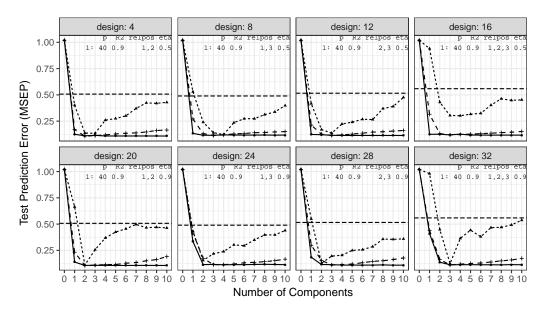


Figure 5: Average Prediction Error for designs with 40 predictor variables where Coefficient of determination is 0.9

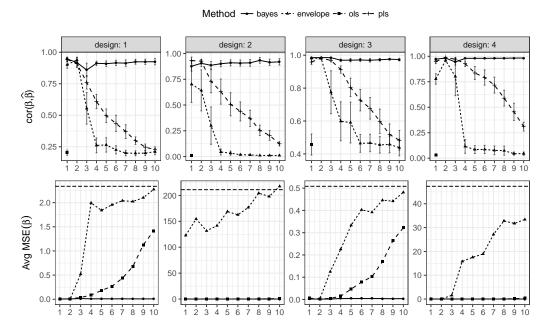


Figure 6: Correlation between true and estimated beta coefficient and Beta Estimation Error