Supplemental Materials
Additive Heredity Model for the Analysis of Mixture-of-Mixtures Experiments

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In the mixture-of-mixtures (MoM) experiments, the mixture components are called the major components and can be made up of sub-components. The sub-components within the major components are called the minor components. Assume that there are q major components, and let c_k be the proportion of the kth major component. Then,

$$\sum_{k=1}^{q} c_k = 1, 0 \leq c_k \leq 1, \quad k = 1, \ldots, q.$$

Moreover, each major component is composed of m_k minor components, whose proportions with respect to c_k are x_{kj}, such that,

$$\sum_{l=1}^{m_k} x_{kl} = 1, 0 \leq x_{kl} \leq 1, \quad l = 1, \ldots, m_k.$$

S1. Lemma 1

Lemma 1 *Any major-minor model can be written in the form of additive models.*

Proof: In the major-minor model, we denote g_1 as a function to capture the relationship between the response y and the major components. The coefficients in g_1 are functions of minor components.

Without loss of generality, consider the second-order Scheffé model on the major components for g_1:

$$g_1(c_1, ..., c_q) = \sum_{k=1}^{q} \alpha_k c_k + \sum_{1 \leq k < j \leq q} \alpha_{kj} c_k c_j + \epsilon.$$

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For the coefficient α_k, we consider the second-order Scheffé model on the corresponding minor components, that is,

$$\alpha_k(x_{k,1}, ..., x_{k,m_k}) = \sum_{l=1}^{m_k} \eta_l^{(k)} x_{kl} + \sum_{1 \le l < l' \le m_k} \eta_{ll'}^{(k)} x_{kl} x_{kl'},$$
$$\alpha_{kj} = \alpha_k \alpha_j,$$

where $\eta_l^{(k)}$ and $\eta_{l,l'}^{(k)}$ are the coefficients of the minor components x_{kl} and $x_{kl}x_{kl'}$, respectively. Thus, the major-minor model is given by:

$$\begin{aligned}
g_1(c_1, ..., c_q) &= \sum_{k=1}^{q} (\sum_{l=1}^{m_k} \eta_l^{(k)} x_{kl} + \sum_{1 \le l < l' \le m_k} \eta_{ll'}^{(k)} x_{kl} x_{kl'}) c_k \\
&+ \sum_{1 \le k < j \le q} \Big(\sum_{l=1}^{m_k} \eta_l^{(k)} x_{kl} + \sum_{1 \le l < l' \le m_k} \eta_{ll'}^{(k)} x_{kl} x_{kl'} \Big) \Big(\sum_{l=1}^{m_j} \eta_l^{(j)} x_{jl} + \sum_{1 \le l < l' \le m_j} \eta_{ll'}^{(j)} x_{jl} x_{jl'} \Big) c_k c_j + \epsilon \\
&= \sum_{k=1}^{q} \sum_{l=1}^{m_k} \eta_l^{(k)} x_{kl} c_k + \sum_{k=1}^{q} \sum_{1 \le l < l' \le m_k} \eta_{ll'}^{(k)} x_{kl} x_{kl'} c_k \\
&+ \sum_{1 \le k < j \le q} \Bigg[(\sum_{l=1}^{m_k} \eta_l^{(k)} x_{kl})(\sum_{l=1}^{m_j} \eta_l^{(j)} x_{jl}) + (\sum_{l=1}^{m_k} \eta_l^{(k)} x_{kl})(\sum_{1 \le l < l' \le m_j} \eta_{ll'}^{(j)} x_{jl} x_{jl'}) \\
&+ (\sum_{1 \le l < l' \le m_k} \eta_{ll'}^{(k)} x_{kl} x_{kl'})(\sum_{l=1}^{m_j} \eta_l^{(j)} x_{jl}) + (\sum_{1 \le l < l' \le m_k} \eta_{ll'}^{(k)} x_{kl} x_{kl'})(\sum_{1 \le l < l' \le m_j} \eta_{ll'}^{(j)} x_{jl} x_{jl'}) \Bigg] c_k c_j + \epsilon \\
&= \sum_{k=1}^{q} \sum_{j=1}^{m_k} \eta_l^{(k)} x_{kl} c_k + \sum_{k=1}^{q} \sum_{1 \le l < l' \le m_k} \eta_{ll'}^{(k)} x_{kl} x_{kl'} c_k \\
&+ \sum_{1 \le k < j \le q} \Big(\sum_{l=1}^{m_k} \sum_{l'=1}^{m_j} \eta_l^{(k)} \eta_{l'}^{(j)} x_{kl} x_{jl'} + \sum_{l=1}^{m_k} \sum_{1 \le l* < l*' \le m_j} \eta_l^{(k)} \eta_{l*l*'}^{(j)} x_{kl} x_{jl*} x_{jl*'} \\
&+ \sum_{l=1}^{m_j} \sum_{1 \le l* < l*' \le m_k} \eta_l^{(j)} \eta_{l*l*'}^{(k)} x_{jl} x_{kl*} x_{kl*'} + \sum_{1 \le l < l' \le m_k} \sum_{1 \le l* < l*' \le m_j} \eta_{ll'}^{(k)} \eta_{l*l*'}^{(j)} x_{kl} x_{kl'} x_{jl*} x_{jl*'} \Big) c_k c_j + \epsilon,
\end{aligned}$$

which is in the form of additive models. ■

S2. Algorithm of Generating Maximin Distance Designs for Major Components

Algorithm 2 is to generate the maximin distance design for major components in MoM experiments.

Algorithm 2 The maximin distance design for major components

Input: lower and upper bounds on the major components

2: Partition the design space into small elements with predefined precision

Combine the Simplex-centroid design points and additional random sampled points from the partition pool as the initial design points

4: Calculate the minimum distance, d_{old}, of all pairs in the initial design

for 1:T **do**

6: Sample one point out of the initial design as the old point

Sample one point out of the partition pool to form the new design by replacing the old point in the last design

8: Calculate the minimum distance, d_{new}, of all pairs in the new design

if $d_{new} > d_{old}$ **then** update d_{old} with d_{new}

10: **else** do not form the new design with the new point in line 7

end if

12: **end for**

Output: the maximin distance design

S3. More Details in Simulation

This section presents the details of simulation case (b), where there are three major components, c_1, c_2 and c_3, and the minor components nested under each major components are x_{11}, x_{12}, x_{13}, and x_{21}, x_{22}. Note that the major component c_3 has a single component.

There are five underlying models to be considered for generating the data:

$$\begin{aligned}
I:\ y =& 10c_1 + 30c_2 + 20c_3 + 18c_1c_2 + \epsilon,\\
II:\ y =& 15c_1x_{11} + 12.5c_1x_{12} + 15c_1x_{13} + 22.5c_2x_{21} + 20c_2x_{22} + \epsilon,\\
III:\ y =& 10c_1 + 30c_2 + 20c_3 + 15c_1^hx_{11} + 27.5c_2^hx_{21} + \epsilon,\ \text{where } h = 0.5,\\
IV:\ y =& 10c_1 + 30c_2 + 20c_3 + 25c_2x_{11} + 22.5c_3x_{21} + \epsilon,\\
V:\ y =& 10c_1 + 30c_2 + 20c_3 + 7c_2c_3 + 13.75c_1^2x_{11}x_{12} + \epsilon,
\end{aligned}$$

where the major and minor components are independent of ϵ, $\epsilon \sim N(0, \sigma^2)$ and σ^2 is chosen such that the signal-to-noise (SN) ratio is three.

Same as case (a), the compared method includes the multiple-Scheffé model

$$y = (\alpha_1 c_1 + \alpha_2 c_2 + \alpha_3 c_3) \times (\beta_{11} x_{11} + \beta_{12} x_{12} + \beta_{13} x_{13}) \times (\beta_{21} x_{21} + \beta_{22} x_{22}) + \epsilon,$$

The major-only linear Scheffé model and the major-only quadratic Scheffé model are expressed respectively as

$$y = \gamma_1 c_1 + \gamma_2 c_2 + \gamma_3 c_3 + \epsilon,$$

$$y = \gamma_1 c_1 + \gamma_2 c_2 + \gamma_3 c_3 + \gamma_4 c_1 c_2 + \gamma_5 c_1 c_3 + \gamma_6 c_2 c_3 + \epsilon.$$

The 1st-order major-minor model and the 2nd-order major-minor model are expressed respectively as

$$y = (\gamma_1 + \gamma_2 x_{11} + \gamma_3 x_{12}) c_1 + (\gamma_4 + \gamma_5 x_{21}) c_2 + \gamma_6 c_3 + \epsilon$$

$$\begin{aligned} y = {} & \gamma_1 c_1 + \gamma_2 c_2 + \gamma_3 c_3 + \gamma_4 x_{11} c_1 + \gamma_5 x_{12} c_1 + \gamma_6 x_{21} c_2 + \gamma_7 c_1 c_2 + \gamma_8 c_1 c_3 + \gamma_9 c_2 c_3 \\ & + \gamma_{10} x_{11} c_1 c_2 + \gamma_{11} x_{12} c_1 c_2 + \gamma_{12} x_{21} c_1 c_2 + \gamma_{13} x_{11} c_1 c_3 + \gamma_{14} x_{12} c_1 c_3 + \gamma_{15} x_{21} c_2 c_3 \\ & + \gamma_{16} x_{11} x_{21} c_1 c_2 + \gamma_{17} x_{12} x_{21} c_1 c_2 + \epsilon. \end{aligned}$$

Same as case (a), the metrics to evaluate the model performance are R^2, AICc, MSE, MSCV, MSCVnorm and model size.

For both the unconstrained and constrained major components, we consider two different designs: the I-optimal design and the maximin distance design. For the minor components x_{11}, x_{12}, x_{13}, we choose the three-component simplex-centroid design assuming seven design points. For the minor components x_{21}, x_{22}, we choose three design points: the two end points and the middle point in the domain, i.e., (1,0), (0.5,0.5), and (0,1). Same as case (a), we applied the idea of crossed design to combine the designs for the major and minor components.

Unconstrained MoM Experiments

Tables S1 and S2 show the simulation results in terms of R^2, MSE, MSCV, MSCVnorm, AICc, and model size among different models in the three-component simplex-centroid design and in the maximin distance design for the unconstrained MoM experiments based on 100 simulation replications. The proposed AHM generally outperform the other models in prediction regarding MSCV and MSCVnorm, and in fitting regrading AICc in all simulation models but IV. For the simulation model I, which only contains the major components, the AHM has comparable prediction performance with the MajorQuad model. For the simulation models II and III, the AHM has competitive prediction and fitting performance compared with the 1st_MM and the 2nd_MM. For the simulation model IV, the AHM as well as the 1st_MM, 2nd_MM, has similar prediction and fitting performance, but worse than the multiple Scheffé model. For the simulation model V, the prediction performance of AHM is best and close to that of the true model.

In terms of model fitting, the measure R^2, AICc, and MSE values in the tables indicate that the AHM has good fitting performance when it has competitive prediction performance.

The model size of the AHM varies across different settings because of the variable selection performed via the nonnegative garrote method. We also observe that the model size of the AHM is often larger than that of 1st_MM but smaller than that of 2nd_MM.

Table S1: Performance comparisons of models under the unconstrained MoM experiment using I-optimal design for major components from 100 simulation replications (means and standard errors (in parenthesis)).

	Model	R^2	MSE	MSCV	MSCVnorm	AICc	Size
I	1st_MM	0.970 (0.002)	15.06 (1.03)	15.76 (1.08)	0.31 (0.03)	407.0 (10.1)	6.0 (0.0)
	2nd_MM	0.977 (0.001)	12.78 (0.56)	14.66 (0.71)	0.29 (0.02)	397.7 (6.6)	17.0 (0.0)
	AHM	0.976 (0.001)	12.55 (0.40)	13.36 (0.40)	**0.26** (0.02)	**383.9** (4.6)	8.8 (1.5)
	MajorLinear	0.970 (0.002)	15.01 (0.97)	15.32 (0.98)	0.30 (0.02)	403.2 (9.5)	3.0 (0.0)
	MajorQuad	0.975 (0.001)	12.82 (0.26)	13.37 (0.28)	**0.26** (0.02)	**383.7** (3.0)	6.0 (0.0)
	MultipleScheffe	0.973 (0.002)	15.25 (1.21)	17.77 (1.52)	0.35 (0.04)	424.9 (11.7)	18.0 (0.0)
	trueModel	0.974 (0.001)	12.84 (0.20)	13.19 (0.21)	0.26 (0.02)	381.5 (2.3)	4.0 (0.0)
II	1st_MM	0.974 (0.001)	29.23 (0.82)	30.50 (0.87)	**0.26** (0.02)	**504.8** (4.3)	6.0 (0.0)
	2nd_MM	0.976 (0.001)	29.31 (1.13)	33.70 (1.71)	0.29 (0.03)	519.7 (5.9)	17.0 (0.0)
	AHM	0.975 (0.001)	28.70 (1.02)	30.50 (1.05)	**0.26** (0.02)	**504.8** (5.0)	8.3 (1.4)
	MajorLinear	0.963 (0.003)	40.28 (2.91)	41.22 (3.00)	0.36 (0.03)	548.1 (10.8)	3.0 (0.0)
	MajorQuad	0.963 (0.003)	40.59 (2.94)	42.40 (3.09)	0.37 (0.03)	552.7 (10.8)	6.0 (0.0)
	MultipleScheffe	0.976 (0.001)	29.21 (1.48)	33.94 (1.99)	0.29 (0.03)	520.6 (7.6)	18.0 (0.0)
	trueModel	0.974 (0.001)	29.23 (0.82)	30.50 (0.87)	0.26 (0.02)	504.8 (4.3)	6.0 (0.0)
III	1st_MM	0.918 (0.005)	157.02 (8.93)	164.26 (9.50)	0.31 (0.02)	751.7 (8.4)	6.0 (0.0)
	2nd_MM	0.935 (0.004)	135.62 (5.84)	155.85 (8.16)	0.29 (0.02)	744.9 (6.4)	17.0 (0.0)
	AHM	0.931 (0.004)	133.94 (4.26)	142.27 (4.49)	**0.26** (0.02)	**731.8** (4.6)	8.6 (1.8)
	MajorLinear	0.810 (0.013)	356.17 (25.58)	363.71 (26.25)	0.68 (0.04)	868.6 (10.5)	3.0 (0.0)
	MajorQuad	0.819 (0.013)	347.45 (25.06)	362.38 (26.14)	0.67 (0.04)	868.3 (10.5)	6.0 (0.0)
	MultipleScheffe	0.925 (0.006)	157.32 (10.54)	184.58 (14.03)	0.34 (0.03)	768.0 (9.9)	18.0 (0.0)
	trueModel	0.929 (0.003)	135.09 (2.21)	140.00 (2.44)	0.26 (0.02)	728.7 (2.4)	5.0 (0.0)
IV	1st_MM	0.844 (0.012)	240.46 (18.25)	251.44 (19.23)	0.65 (0.04)	814.2 (11.2)	6.0 (0.0)
	2nd_MM	0.865 (0.011)	225.36 (18.37)	246.82 (20.29)	0.64 (0.05)	819.2 (12.0)	17.0 (0.0)
	AHM	0.848 (0.012)	234.72 (17.38)	246.85 (18.07)	0.64 (0.04)	810.9 (10.8)	6.2 (1.2)
	MajorLinear	0.837 (0.012)	245.17 (18.80)	251.57 (19.29)	0.65 (0.04)	813.6 (11.3)	3.0 (0.0)
	MajorQuad	0.839 (0.012)	248.40 (19.06)	259.91 (19.97)	0.67 (0.04)	819.0 (11.3)	6.0 (0.0)
	MultipleScheffe	0.942 (0.004)	97.27 (4.13)	112.27 (5.90)	**0.29** (0.02)	**697.5** (6.3)	18.0 (0.0)
	trueModel	0.936 (0.003)	97.38 (1.71)	100.86 (1.88)	0.26 (0.02)	680.6 (2.6)	5.0 (0.0)
V	1st_MM	0.970 (0.002)	15.37 (1.04)	16.26 (1.16)	0.36 (0.03)	410.0 (10.0)	6.0 (0.0)
	2nd_MM	0.972 (0.002)	15.19 (1.20)	17.68 (1.56)	0.39 (0.04)	422.8 (11.8)	17.0 (0.0)
	AHM	0.978 (0.001)	11.29 (0.44)	12.08 (0.47)	**0.27** (0.02)	**370.3** (5.4)	10.4 (1.3)
	MajorLinear	0.968 (0.002)	15.91 (1.09)	16.32 (1.14)	0.36 (0.03)	411.6 (10.3)	3.0 (0.0)
	MajorQuad	0.969 (0.002)	15.60 (1.13)	16.31 (1.19)	0.36 (0.03)	412.1 (10.8)	6.0 (0.0)
	MultipleScheffe	0.972 (0.002)	15.73 (1.18)	18.68 (1.65)	0.41 (0.04)	429.5 (11.1)	18.0 (0.0)
	trueModel	0.977 (0.001)	11.40 (0.21)	11.83 (0.24)	0.26 (0.02)	365.3 (2.7)	5.0 (0.0)

Table S2: Performance comparisons of models under the unconstrained MoM experiment using the maximin distance design for major components from 100 simulation replications (means and standard errors (in parenthesis)).

	Model	R^2	MSE	MSCV	MSCVnorm	AICc	Size
I	1st_MM	0.973 (0.004)	13.69 (1.87)	14.24 (1.95)	0.30 (0.03)	446.4 (26.1)	6.0 (0.0)
	2nd_MM	0.978 (0.003)	11.94 (1.55)	13.46 (1.76)	0.28 (0.02)	437.7 (24.6)	17.0 (0.0)
	AHM	0.977 (0.003)	11.71 (1.50)	12.33 (1.56)	**0.26** (0.02)	**423.3** (24.2)	8.6 (1.8)
	MajorLinear	0.972 (0.004)	13.66 (1.84)	13.91 (1.87)	0.29 (0.02)	442.7 (25.7)	3.0 (0.0)
	MajorQuad	0.976 (0.003)	11.91 (1.47)	12.36 (1.53)	**0.26** (0.02)	**423.4** (23.4)	6.0 (0.0)
	MultipleScheffe	0.975 (0.004)	13.85 (1.93)	15.79 (2.20)	0.33 (0.03)	463.8 (26.3)	18.0 (0.0)
	trueModel	0.976 (0.003)	11.92 (1.47)	12.21 (1.51)	0.26 (0.02)	421.1 (23.6)	4.0 (0.0)
II	1st_MM	0.975 (0.003)	27.11 (3.60)	28.15 (3.73)	**0.26** (0.02)	**561.2** (26.2)	6.0 (0.0)
	2nd_MM	0.977 (0.003)	27.01 (3.69)	30.45 (4.20)	0.28 (0.02)	574.5 (26.9)	17.0 (0.0)
	AHM	0.976 (0.003)	26.53 (3.56)	28.06 (3.77)	**0.26** (0.02)	**560.4** (26.1)	8.4 (1.4)
	MajorLinear	0.965 (0.004)	37.71 (5.38)	38.46 (5.49)	0.36 (0.03)	613.0 (27.3)	3.0 (0.0)
	MajorQuad	0.966 (0.004)	37.88 (5.44)	39.35 (5.66)	0.37 (0.03)	617.1 (27.4)	6.0 (0.0)
	MultipleScheffe	0.977 (0.003)	27.10 (3.76)	30.81 (4.36)	0.29 (0.03)	576.5 (27.2)	18.0 (0.0)
	trueModel	0.975 (0.003)	27.11 (3.60)	28.15 (3.73)	0.26 (0.02)	561.2 (26.2)	6.0 (0.0)
III	1st_MM	0.924 (0.006)	148.32 (14.74)	154.20 (15.52)	0.31 (0.02)	847.6 (17.6)	6.0 (0.0)
	2nd_MM	0.939 (0.004)	128.91 (10.46)	145.23 (13.05)	0.29 (0.02)	838.4 (14.2)	17.0 (0.0)
	AHM	0.938 (0.005)	124.45 (10.13)	131.67 (10.78)	**0.26** (0.02)	**821.9** (14.3)	8.9 (1.6)
	MajorLinear	0.821 (0.014)	345.08 (33.99)	351.35 (34.58)	0.69 (0.04)	986.1 (17.2)	3.0 (0.0)
	MajorQuad	0.827 (0.013)	338.32 (32.65)	350.73 (33.68)	0.69 (0.04)	986.2 (16.9)	6.0 (0.0)
	MultipleScheffe	0.931 (0.007)	146.60 (15.74)	168.36 (19.05)	0.33 (0.03)	861.0 (19.1)	18.0 (0.0)
	trueModel	0.935 (0.004)	126.01 (9.51)	129.90 (9.88)	0.26 (0.02)	819.5 (13.4)	5.0 (0.0)
IV	1st_MM	0.848 (0.015)	229.44 (26.08)	238.20 (26.93)	0.64 (0.05)	920.6 (20.0)	6.0 (0.0)
	2nd_MM	0.874 (0.015)	204.81 (28.03)	222.52 (29.59)	0.60 (0.06)	915.1 (24.6)	17.0 (0.0)
	AHM	0.868 (0.016)	202.33 (29.02)	214.51 (30.81)	0.58 (0.06)	901.2 (26.5)	8.0 (1.4)
	MajorLinear	0.840 (0.015)	237.16 (24.39)	242.41 (24.92)	0.66 (0.05)	923.1 (17.7)	3.0 (0.0)
	MajorQuad	0.841 (0.015)	239.85 (24.82)	249.70 (25.79)	0.68 (0.05)	928.3 (17.8)	6.0 (0.0)
	MultipleScheffe	0.943 (0.005)	92.13 (7.58)	104.60 (9.28)	**0.28** (0.02)	**783.4** (14.4)	18.0 (0.0)
	trueModel	0.938 (0.005)	92.22 (6.55)	95.04 (6.71)	0.26 (0.02)	767.1 (12.5)	5.0 (0.0)
V	1st_MM	0.971 (0.004)	14.38 (1.86)	15.10 (1.97)	0.36 (0.03)	454.9 (23.8)	6.0 (0.0)
	2nd_MM	0.974 (0.004)	14.10 (1.88)	16.08 (2.23)	0.38 (0.04)	465.6 (24.6)	17.0 (0.0)
	AHM	0.979 (0.002)	10.59 (1.14)	11.27 (1.25)	**0.27** (0.02)	**409.4** (19.8)	10.5 (1.2)
	MajorLinear	0.970 (0.004)	14.77 (1.88)	15.09 (1.93)	0.36 (0.03)	456.0 (23.8)	3.0 (0.0)
	MajorQuad	0.971 (0.004)	14.40 (1.84)	14.99 (1.93)	0.35 (0.03)	455.1 (24.1)	6.0 (0.0)
	MultipleScheffe	0.973 (0.004)	14.68 (1.98)	16.91 (2.35)	0.40 (0.04)	473.8 (24.6)	18.0 (0.0)
	trueModel	0.979 (0.002)	10.68 (1.10)	11.03 (1.15)	0.26 (0.02)	404.3 (19.0)	5.0 (0.0)

Constrained MoM Experiments

We consider simulations where lower and upper bounds are placed on the major components. Specifically, we assume that the major and minor components satisfy the following constraints:

$$c_1 + c_2 + c_3 = 1, \quad 0.2 \leq c_1 \leq 0.45,$$
$$0.4 \leq c_2 \leq 0.6, \quad 0.1 \leq c_3 \leq 0.25,$$
$$x_{11} + x_{12} + x_{13} = 1, \quad x_{21} + x_{22} = 1.$$

The comparison results from using the I-optimal design and the maximin distance design for the major components are reported in Table S3 and Table S4, respectively. From both tables we can learn that the AHM has competitive prediction performance among all models. We also note that the 1st_MM, the 2nd_MM, and the multiple Scheffé model have relatively good prediction performance in simulation models I, II, III, and IV. Note that V favors the AHM.

It is worth noting that in IV, the AHM has comparable prediction performance as the true model, which is different from the results for the unconstrained MoM experiments. This observation is likely due to the difference between the two scenarios in terms of the constraints of the design space. The more highly constrained design space, the less negative effects of model misspecification on the model's prediction performance. The AHM has similar R^2, AICc and MSE values as the 1st_MM and the 2nd_MM in all simulation models but V. The model size of the AHM is larger than that of the 1st_MM but smaller than that of the 2nd_MM.

Table S3: Performance comparisons of models under the constrained MoM experiment using I-optimal design for major components from 100 simulation replications (means and standard errors (in parenthesis)).

	Model	R^2	MSE	MSCV	MSCVnorm	AICc	Size
I	1st_MM	0.999 (0.000)	0.48 (0.01)	0.49 (0.01)	**0.26** (0.02)	-116.3 (4.0)	6.0 (0.0)
	2nd_MM	0.999 (0.000)	0.47 (0.02)	0.52 (0.02)	0.28 (0.02)	-104.8 (5.7)	17.0 (0.0)
	AHM	0.999 (0.000)	0.47 (0.01)	0.49 (0.01)	**0.26** (0.02)	-117.3 (4.8)	8.3 (1.7)
	MajorLinear	0.999 (0.000)	0.48 (0.01)	0.48 (0.01)	**0.26** (0.02)	**-119.5** (3.3)	3.0 (0.0)
	MajorQuad	0.999 (0.000)	0.47 (0.01)	0.49 (0.01)	**0.26** (0.02)	-118.3 (2.7)	6.0 (0.0)
	MultipleScheffe	0.999 (0.000)	0.47 (0.02)	0.53 (0.02)	0.29 (0.02)	-101.3 (6.7)	18.0 (0.0)
	trueModel	0.999 (0.000)	0.47 (0.01)	0.48 (0.01)	0.26 (0.02)	-120.7 (2.2)	4.0 (0.0)
II	1st_MM	0.997 (0.000)	4.54 (0.08)	4.70 (0.08)	**0.26** (0.02)	**262.6** (2.9)	6.0 (0.0)
	2nd_MM	0.997 (0.000)	4.54 (0.14)	5.06 (0.18)	0.28 (0.02)	276.9 (5.4)	17.0 (0.0)
	AHM	0.997 (0.000)	4.50 (0.12)	4.74 (0.14)	**0.26** (0.02)	265.2 (4.9)	9.3 (1.1)
	MajorLinear	0.988 (0.001)	15.51 (1.02)	15.79 (1.04)	0.87 (0.03)	465.4 (11.2)	3.0 (0.0)
	MajorQuad	0.988 (0.001)	15.72 (1.04)	16.30 (1.08)	0.90 (0.03)	471.1 (11.3)	6.0 (0.0)
	MultipleScheffe	0.997 (0.000)	4.54 (0.15)	5.12 (0.21)	0.28 (0.02)	278.3 (5.5)	18.0 (0.0)
	trueModel	0.997 (0.000)	4.54 (0.08)	4.70 (0.08)	0.26 (0.02)	262.6 (2.9)	6.0 (0.0)
III	1st_MM	0.963 (0.002)	100.73 (2.90)	104.59 (2.96)	0.27 (0.02)	783.4 (4.9)	6.0 (0.0)
	2nd_MM	0.966 (0.002)	98.74 (3.32)	110.52 (3.91)	0.28 (0.02)	794.1 (5.7)	17.0 (0.0)
	AHM	0.964 (0.002)	98.12 (2.50)	102.63 (2.83)	**0.26** (0.02)	**782.2** (4.2)	8.7 (1.4)
	MajorLinear	0.851 (0.008)	394.24 (24.60)	401.47 (25.00)	1.01 (0.01)	1009.0 (10.5)	3.0 (0.0)
	MajorQuad	0.852 (0.008)	399.84 (25.03)	414.67 (25.90)	1.05 (0.01)	1014.8 (10.6)	6.0 (0.0)
	MultipleScheffe	0.966 (0.002)	98.70 (3.49)	111.76 (4.70)	0.28 (0.02)	795.5 (6.0)	18.0 (0.0)
	trueModel	0.963 (0.001)	98.61 (1.62)	101.71 (1.61)	0.26 (0.02)	778.7 (2.8)	5.0 (0.0)
IV	1st_MM	0.968 (0.002)	43.47 (2.75)	45.30 (2.92)	0.36 (0.03)	641.9 (10.7)	6.0 (0.0)
	2nd_MM	0.977 (0.001)	32.96 (1.43)	36.84 (1.68)	**0.29** (0.02)	**609.7** (7.4)	17.0 (0.0)
	AHM	0.975 (0.001)	34.81 (1.56)	36.47 (1.72)	**0.29** (0.02)	**609.0** (7.8)	9.5 (1.4)
	MajorLinear	0.909 (0.006)	120.75 (8.42)	122.97 (8.57)	0.96 (0.02)	810.2 (11.7)	3.0 (0.0)
	MajorQuad	0.909 (0.006)	122.40 (8.64)	126.95 (8.96)	0.99 (0.02)	815.8 (11.8)	6.0 (0.0)
	MultipleScheffe	0.978 (0.001)	32.27 (1.26)	36.47 (1.62)	**0.29** (0.02)	**607.6** (6.7)	18.0 (0.0)
	trueModel	0.976 (0.001)	32.24 (0.71)	33.24 (0.74)	0.26 (0.02)	590.9 (3.8)	5.0 (0.0)
V	1st_MM	0.998 (0.000)	1.09 (0.08)	1.13 (0.09)	0.37 (0.03)	22.7 (12.9)	6.0 (0.0)
	2nd_MM	0.998 (0.000)	1.11 (0.09)	1.25 (0.10)	0.40 (0.03)	40.1 (13.2)	17.0 (0.0)
	AHM	0.999 (0.000)	0.76 (0.02)	0.80 (0.02)	**0.26** (0.02)	**-32.1** (4.7)	9.9 (1.6)
	MajorLinear	0.998 (0.000)	1.14 (0.09)	1.16 (0.09)	0.38 (0.03)	26.0 (13.5)	3.0 (0.0)
	MajorQuad	0.998 (0.000)	1.14 (0.09)	1.18 (0.10)	0.38 (0.03)	30.2 (13.6)	6.0 (0.0)
	MultipleScheffe	0.998 (0.000)	1.12 (0.09)	1.26 (0.10)	0.41 (0.03)	42.0 (13.4)	18.0 (0.0)
	trueModel	0.999 (0.000)	0.77 (0.01)	0.79 (0.01)	0.26 (0.02)	-37.1 (2.4)	5.0 (0.0)

Table S4: Performance comparisons of models under the constrained MoM experiment using the maximin distance design for major components from 100 simulation replications (means and standard errors (in parenthesis)).

	Model	R^2	MSE	MSCV	MSCVnorm	AICc	Size
I	1st_MM	0.999 (0.000)	0.44 (0.04)	0.46 (0.05)	**0.26** (0.02)	-129.7 (17.0)	6.0 (0.0)
	2nd_MM	0.999 (0.000)	0.44 (0.05)	0.49 (0.05)	0.28 (0.02)	-117.2 (17.5)	17.0 (0.0)
	AHM	0.999 (0.000)	0.43 (0.04)	0.45 (0.04)	**0.26** (0.02)	-130.0 (17.0)	8.5 (1.6)
	MajorLinear	0.999 (0.000)	0.44 (0.04)	0.45 (0.04)	**0.26** (0.02)	**-132.9** (17.0)	3.0 (0.0)
	MajorQuad	0.999 (0.000)	0.44 (0.04)	0.45 (0.04)	**0.26** (0.02)	-131.0 (16.8)	6.0 (0.0)
	MultipleScheffe	0.999 (0.000)	0.44 (0.05)	0.50 (0.05)	0.29 (0.02)	-112.8 (18.2)	18.6 (0.5)
	trueModel	0.999 (0.000)	0.44 (0.04)	0.45 (0.04)	0.26 (0.02)	-133.7 (16.9)	4.0 (0.0)
II	1st_MM	0.997 (0.000)	4.43 (0.15)	4.60 (0.15)	**0.26** (0.02)	**258.7** (5.6)	6.0 (0.0)
	2nd_MM	0.997 (0.000)	4.42 (0.22)	4.93 (0.25)	0.28 (0.02)	272.3 (8.5)	17.0 (0.0)
	AHM	0.997 (0.000)	4.40 (0.17)	4.64 (0.19)	**0.26** (0.02)	261.8 (6.6)	9.5 (1.2)
	MajorLinear	0.988 (0.001)	15.11 (1.09)	15.39 (1.12)	0.87 (0.03)	461.0 (12.2)	3.0 (0.0)
	MajorQuad	0.988 (0.001)	15.31 (1.11)	15.88 (1.15)	0.89 (0.03)	466.6 (12.2)	6.0 (0.0)
	MultipleScheffe	0.997 (0.000)	4.43 (0.22)	5.03 (0.27)	0.28 (0.02)	274.8 (8.5)	18.6 (0.5)
	trueModel	0.997 (0.000)	4.43 (0.15)	4.60 (0.15)	0.26 (0.02)	258.7 (5.6)	6.0 (0.0)
III	1st_MM	0.963 (0.002)	99.16 (3.01)	102.87 (3.20)	**0.26** (0.02)	**780.8** (5.1)	6.0 (0.0)
	2nd_MM	0.966 (0.002)	97.15 (3.65)	108.37 (4.33)	0.28 (0.02)	791.4 (6.3)	17.0 (0.0)
	AHM	0.964 (0.002)	96.90 (2.80)	101.33 (2.80)	**0.26** (0.02)	**780.3** (4.6)	8.9 (1.5)
	MajorLinear	0.851 (0.011)	392.16 (28.65)	399.35 (29.12)	1.01 (0.01)	1008.0 (12.4)	3.0 (0.0)
	MajorQuad	0.851 (0.011)	397.70 (29.23)	412.49 (30.25)	1.05 (0.01)	1013.7 (12.5)	6.0 (0.0)
	MultipleScheffe	0.966 (0.002)	97.11 (3.59)	110.02 (4.47)	0.28 (0.02)	793.6 (6.3)	18.6 (0.5)
	trueModel	0.963 (0.001)	97.52 (1.87)	100.49 (1.95)	0.26 (0.02)	776.9 (3.2)	5.0 (0.0)
IV	1st_MM	0.968 (0.003)	42.11 (3.58)	43.85 (3.76)	0.35 (0.03)	636.4 (14.3)	6.0 (0.0)
	2nd_MM	0.978 (0.001)	32.08 (1.47)	35.84 (1.76)	**0.28** (0.02)	**605.2** (7.8)	17.0 (0.0)
	AHM	0.975 (0.001)	34.37 (2.05)	36.08 (2.07)	0.29 (0.02)	607.0 (10.0)	9.7 (1.3)
	MajorLinear	0.907 (0.007)	121.09 (9.39)	123.33 (9.56)	0.97 (0.02)	810.5 (13.1)	3.0 (0.0)
	MajorQuad	0.908 (0.007)	122.72 (9.54)	127.30 (9.90)	1.00 (0.02)	816.1 (13.2)	6.0 (0.0)
	MultipleScheffe	0.978 (0.001)	31.57 (1.40)	35.80 (1.82)	**0.28** (0.03)	**604.7** (7.6)	18.6 (0.5)
	trueModel	0.976 (0.001)	31.62 (0.79)	32.60 (0.81)	0.26 (0.02)	587.6 (4.3)	5.0 (0.0)
V	1st_MM	0.998 (0.000)	1.02 (0.09)	1.06 (0.10)	0.38 (0.03)	11.7 (15.3)	6.0 (0.0)
	2nd_MM	0.998 (0.000)	1.04 (0.10)	1.16 (0.11)	0.42 (0.04)	28.2 (16.7)	17.0 (0.0)
	AHM	0.999 (0.000)	0.69 (0.05)	0.73 (0.06)	**0.26** (0.02)	**-48.1** (13.2)	10.2 (1.3)
	MajorLinear	0.998 (0.000)	1.08 (0.10)	1.10 (0.10)	0.39 (0.03)	16.7 (15.6)	3.0 (0.0)
	MajorQuad	0.998 (0.000)	1.08 (0.10)	1.12 (0.10)	0.40 (0.03)	21.1 (15.7)	6.0 (0.0)
	MultipleScheffe	0.998 (0.000)	1.05 (0.10)	1.19 (0.12)	0.42 (0.04)	31.7 (17.0)	18.6 (0.5)
	trueModel	0.999 (0.000)	0.70 (0.05)	0.72 (0.05)	0.26 (0.02)	-53.8 (12.5)	5.0 (0.0)