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SUPPLEMENT TO "MAXIMIN AND MAXIMIN-EFFICIENT EVENT-RELATED FMRI DESIGNS UNDER A NONLINEAR MODEL"

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1. Near-invariance property. Let d be a design in the restricted design class Ξ_0 that involves two stimulus types ($Q = 2$) and has a length $L = rQ$ for a positive integer r. We show that, under a simplified model, the Φ_A-value yielded by d is nearly invariant to permutations of the components of $\boldsymbol{\theta}$. With the notation as in (2.1) in the main article, the model that we consider here can be written as:

$$\boldsymbol{y} = \boldsymbol{X}_1\boldsymbol{h}(\boldsymbol{p})\theta_1 + \boldsymbol{X}_2\boldsymbol{h}(\boldsymbol{p})\theta_2 + \boldsymbol{e};\ \boldsymbol{e} \sim (\boldsymbol{0}, \boldsymbol{I}).$$

In contrast to (2.1), this simplified model does not include a nuisance term and that the error terms are uncorrelated. For the design d in Ξ_0, the matrices $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ can approximately have the following form:

$$\boldsymbol{X}_1 = \begin{bmatrix} \boldsymbol{A} \\ \boldsymbol{B} \end{bmatrix};\ \boldsymbol{X}_2 = \begin{bmatrix} \boldsymbol{B} \\ \boldsymbol{A} \end{bmatrix}.$$

The $\boldsymbol{L}_d(\boldsymbol{\theta}, \boldsymbol{p})$ for the information matrix $\boldsymbol{M}(d; \boldsymbol{\theta}, \boldsymbol{p})$ is approximately:

$$\boldsymbol{L}_d(\boldsymbol{\theta}, \boldsymbol{p}) = [\boldsymbol{L}_1, \boldsymbol{L}_6],\ \boldsymbol{L}_i = \begin{bmatrix} \boldsymbol{A}(\partial\boldsymbol{h}(\boldsymbol{p})/\partial p_i)\theta_1 + \boldsymbol{B}(\partial\boldsymbol{h}(\boldsymbol{p})/\partial p_i)\theta_2 \\ \boldsymbol{B}(\partial\boldsymbol{h}(\boldsymbol{p})/\partial p_i)\theta_1 + \boldsymbol{A}(\partial\boldsymbol{h}(\boldsymbol{p})/\partial p_i)\theta_2 \end{bmatrix},\ i = 1, 6.$$

After exchanging the values of θ_1 and θ_2, we have

$$\boldsymbol{L}_d(\boldsymbol{\theta}^N, \boldsymbol{p}) = \boldsymbol{G}\boldsymbol{L}_d(\boldsymbol{\theta}, \boldsymbol{p}),\ \text{where } \boldsymbol{G} = \begin{bmatrix} \boldsymbol{O} & \boldsymbol{I} \\ \boldsymbol{I} & \boldsymbol{O} \end{bmatrix},$$

$\boldsymbol{O}$ is a matrix of zeros, $\boldsymbol{I}$ is an identity matrix and $\boldsymbol{\theta}^N = (\theta_2, \theta_1)'$. We thus have:

$$\begin{aligned} \boldsymbol{M}(d; \boldsymbol{\theta}^N, \boldsymbol{p}) &= \boldsymbol{E}_d(\boldsymbol{p})'[\boldsymbol{I} - w\{\boldsymbol{L}_d(\boldsymbol{\theta}^N, \boldsymbol{p})\}]\boldsymbol{E}_d(\boldsymbol{p}) \\ &= \boldsymbol{E}_d(\boldsymbol{p})'[\boldsymbol{I} - \boldsymbol{G}w\{\boldsymbol{L}_d(\boldsymbol{\theta}, \boldsymbol{p})\}\boldsymbol{G}']\boldsymbol{E}_d(\boldsymbol{p}) \\ &= [\boldsymbol{G}'\boldsymbol{E}_d(\boldsymbol{p})]'[\boldsymbol{I} - w\{\boldsymbol{L}_d(\boldsymbol{\theta}, \boldsymbol{p})\}]\boldsymbol{G}'\boldsymbol{E}_d(\boldsymbol{p}). \end{aligned}$$

In addition,

$$\boldsymbol{G}'\boldsymbol{E}_d(\boldsymbol{p}) = [\boldsymbol{G}\boldsymbol{X}_1\boldsymbol{h}(\boldsymbol{p}), \boldsymbol{G}\boldsymbol{X}_2\boldsymbol{h}(\boldsymbol{p})] \\ = [\boldsymbol{X}_2\boldsymbol{h}(\boldsymbol{p}), \boldsymbol{X}_1\boldsymbol{h}(\boldsymbol{p})] = \boldsymbol{E}_d(\boldsymbol{p}) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Consequently,

$$\Phi_A(\boldsymbol{M}(d; \boldsymbol{\theta}^N, \boldsymbol{p})) = \Phi_A(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \boldsymbol{M}(d; \boldsymbol{\theta}, \boldsymbol{p}) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}) = \Phi_A(\boldsymbol{M}(d; \boldsymbol{\theta}, \boldsymbol{p})).$$

2. A search algorithm. Here, we describe a genetic algorithm for searching for an ER-fMRI design.

Step 1. Generate N (an even number) initial designs, including block, m-sequence(-based), and random designs, and mixed designs with partial block design and partial m-sequence(-based) or random design. Obtain the fitness (value of the objectives function) of each initial design.

Step 2. With probability proportional to fitness, select with replacement $N/2$ pairs of designs to generate $N/2$ pairs of offsprings via crossover and mutation. Specifically, the crossover operator exchanges the corresponding subsequences of the paired designs. The mutation operator perturbs a randomly selected portion α_m of elements of all offspring designs. Obtain the fitness of the resulting designs.

Step 3. Add to the population another $\alpha_i N$ (an integer) immigrants drawn from random and block designs, and their combinations. Obtain their fitness.

Step 4. Combine the N designs in the current generation, the N offspring designs and $\alpha_i N$ immigrants. According to their fitness, keep the best N designs to form the next generation, and discard the others.

Step 5. Repeat steps 2 through 4 until a stopping rule is met; e.g., no significant improvement. Keep track of the best design over generations.

When implementing the algorithm, we follow Kao, Mandal, Lazar, and Stufken (2009) to set $N = 20$, $\alpha_m = 1\%$ and $\alpha_i = 20\%$. The search is terminated if there is no significant improvement in the objective function. Specifically, the improvement is checked every 100 generations and is compared to that of the first 100 generations. We stop the search if the relative improvement is no more than 10^{-7}. In our experience, this stopping rule works well. See Kao (2009) for details.

References.

Kao, M. H. (2009), "Multi-Objective Optimal Experimental Designs for ER-fMRI Using Matlab," *Journal of Statistical Software*, 30, 1–13.

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