Appendices

A Proofs

Proof of Theorem 1

Lemma 1. *Let $h : \mathbb{R}^p \to \mathbb{R}_+$ be a strictly convex function, and let $g : \mathbb{R}_+ \to \mathbb{R}_+$ be a convex and strictly increasing function. Then the composition $g \circ h : \mathbb{R}^p \to \mathbb{R}_+$ is strictly convex.*

Proof. (Lemma 1) This is easy to show using first principles. Let $\alpha \in (0, 1)$ and let $\mathbf{z} \neq \mathbf{z}'$ be two points in $\mathbb{R}^p$. By strict convexity, we have:

$$h(\alpha\mathbf{z} + (1 - \alpha)\mathbf{z}') < \alpha h(\mathbf{z}) + (1 - \alpha)h(\mathbf{z}').$$

Moreover, since g is strictly increasing and convex, it follows that:

$$(g \circ h)(\alpha\mathbf{z} + (1 - \alpha)\mathbf{z}') < g(\alpha h(\mathbf{z}) + (1 - \alpha)h(\mathbf{z}')) \leq \alpha(g \circ h)(\mathbf{z}) + (1 - \alpha)(g \circ h)(\mathbf{z}'),$$

which proves the strict convexity of $g \circ h$. $\square$

Proof. (Theorem 1) Let $g(x) = x^{q/2}$ and $h(\mathbf{z}) = \|\mathbf{z} - \mathbf{z}_i\|_2^2$. It is easy to verify that h is strictly convex, and g is convex and strictly increasing on $\mathbb{R}_+$. By Lemma 1, it follows that $(g \circ f)(\mathbf{x}) = \|\mathbf{z} - \mathbf{z}_i\|_2^q$ is strictly convex. Hence, for any $\alpha \in (0, 1)$ and $\mathbf{z}, \mathbf{z}' \in \mathbb{R}^p, \mathbf{z} \neq \mathbf{z}'$, we have:

$$\begin{aligned}
D_q(\alpha\mathbf{z} + (1 - \alpha)\mathbf{z}'; \mathcal{Z}) &= \frac{1}{mq}\sum_{i=1}^{n} \| \{(\alpha\mathbf{z} + (1 - \alpha)\mathbf{z}') - \mathbf{z}_i\} \|_2^q \\
&< \frac{1}{mq}\sum_{i=1}^{n} \{\alpha\|\mathbf{z} - \mathbf{z}_i\|_2^q + (1 - \alpha)\|\mathbf{z}' - \mathbf{z}_i\|_2^q\} \\
&= \alpha D_q(\mathbf{z}; \mathcal{Z}) + (1 - \alpha)D_q(\mathbf{z}'; \mathcal{Z}),
\end{aligned}$$

so the objective $D_q(\mathbf{z}; \mathcal{Z})$ is strictly convex in $\mathbf{z}$.

Using this fact, we show that (5) has a unique minimizer. Note that the objective $D_q(\mathbf{z}; \mathcal{Z})$ is continuous and coercive on the closed set $\mathbb{R}^p$, where the latter term implies that for all sequences $\{\mathbf{z}_k\}_{k=1}^{\infty}$ satisfying $\|\mathbf{z}_k\|_2 \to \infty$, $\lim_{k\to\infty} D_q(\mathbf{z}_k; \mathcal{Z}) = \infty$. It follows from Proposition A.8 in Bertsekas (1999) and the strict convexity of $D_q(\mathbf{z};\mathcal{Z})$ that there exists exactly one one global minimum of (5), so $C_q(\mathcal{Z})$ is uniquely defined.

To prove that the unique minimizer $C_q(\mathcal{Z})$ is contained in conv($\mathcal{Z}$), note that by first-order optimality conditions, $C_q(\mathcal{Z})$ must satisfy:

$$\nabla D_q(C_q(\mathcal{Z});\mathcal{Z}) = \frac{1}{n}\sum_{i=1}^{m}\left\{\|C_q(\mathcal{Z})-\mathbf{z}_i\|_2^{q-2}(C_q(\mathcal{Z})-\mathbf{z}_i)\right\} = \mathbf{0}$$

$$\Leftrightarrow C_q(\mathcal{Z}) = \sum_{i=1}^{m}\left\{\frac{\|C_q(\mathcal{Z})-\mathbf{z}_i\|_2^{q-2}}{\sum_{j=1}^{n}\|C_q(\mathcal{Z})-\mathbf{z}_j\|_2^{q-2}}\,\mathbf{z}_i\right\} \equiv \sum_{i=1}^{m}\alpha_i\mathbf{z}_i.$$

Since the weights $\{\alpha_i\}_{i=1}^m$ satisfy $\alpha_i \geq 0$ and $\sum_{i=1}^m \alpha_i = 1$, it follows by definition that $C_q(\mathcal{Z}) \in \text{conv}(\mathcal{Z})$, which is as desired.

□

Proof of Theorem 2

Lemma 2. *Let $\mathcal{Z} = \{\mathbf{z}_i\}_{i=1}^m$ be a set of points in $\mathbb{R}^p$. Then there exists some point $\mathbf{z}_j \in \mathcal{Z}$ such that $D_q(\mathbf{z}_j;\mathcal{Z}) \geq D_q(\mathbf{z};\mathcal{Z})$ for all $\mathbf{z} \in$ conv($\mathcal{Z}$).*

Proof. (Lemma 2) Since conv($\mathcal{Z}$) is a compact set, the set of maximizers in:

$$\mathcal{M} = \text{argmax}_{\mathbf{z}\in\text{conv}(\mathcal{Z})} D_q(\mathbf{z};\mathcal{Z})$$

is non-empty, so an equivalent claim is that $\mathbf{z}_j \in \mathcal{M}$ for some $j = 1,\cdots,m$. Suppose, for contradiction, that $\mathbf{z}_j \notin \mathcal{M}$ for all $j = 1,\cdots,m$, and let $\mathbf{z}' = \sum_{i=1}^m \alpha_j\mathbf{z}_j \notin \mathcal{Z}$ be a maximizer in $\mathcal{M}$, with $\alpha_j \geq 0$ and $\sum_{j=1}^m \alpha_j = 1$. Then, by convexity, we have:

$$D_q(\mathbf{z}';\mathcal{Z}) = \frac{1}{mq}\sum_{i=1}^{m}\left\|\sum_{j=1}^{m}\alpha_j(\mathbf{z}_j-\mathbf{z}_i)\right\|_2^q \leq \frac{1}{mq}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_j\|\mathbf{z}_j-\mathbf{z}_i\|_2^q = \frac{1}{mq}\sum_{j=1}^{m}\alpha_j\left(\sum_{i=1}^{m}\|\mathbf{z}_j-\mathbf{z}_i\|_2^q\right)$$
$$= \sum_{j=1}^{m}\alpha_j D_q(\mathbf{z}_j;\mathcal{Z}),$$

which implies that $D_q(\mathbf{z}';\mathcal{Z}) \leq D_q(\mathbf{z}_j;\mathcal{Z})$ for at least one $j = 1,\cdots,m$. Since $\mathbf{z}' \in \mathcal{M}$, this implies that $\mathbf{z}_j \in \mathcal{M}$, which is a contradiction. The lemma therefore holds. □

Proof. (Theorem 2) Since $D_q(\mathbf{z};\mathcal{Z})$ is twice-differentiable, it is β-smooth on conv($\mathcal{Z}$) if and only if:

$$\nabla^2 D_q(\mathbf{z};\mathcal{Z}) \preceq \beta\mathbf{I} \quad \text{for all } \mathbf{z} \in \text{conv}(\mathcal{Z}). \tag{A.1}$$

Letting $\lambda_{max}\{\mathbf{A}\}$ denote the largest eigenvalue of $\mathbf{A}$, it follows that:

$$\begin{aligned}
\lambda_{max}\{\nabla^2 D_q(\mathbf{z};\mathcal{Z})\} &= \lambda_{max}\left\{\frac{q-2}{m}\sum_{i=1}^m \left\{\|\mathbf{z}-\mathbf{z}_i\|_2^{q-4}(\mathbf{z}-\mathbf{z}_i)(\mathbf{z}-\mathbf{z}_i)^T\right\} + \frac{1}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-2}\mathbf{I}\right\} \\
&\leq \frac{q-2}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-4}\lambda_{max}\left\{(\mathbf{z}-\mathbf{z}_i)(\mathbf{z}-\mathbf{z}_i)^T\right\} + \frac{1}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-2}\lambda_{max}\{\mathbf{I}\} \\
&= \frac{q-2}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-4}\cdot\|\mathbf{z}-\mathbf{z}_i\|_2^2 + \frac{1}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-2} \\
&= \frac{q-1}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-2} \leq \frac{q-1}{m}\max_{j=1,\cdots,m}\sum_{i=1}^m \|\mathbf{z}_j-\mathbf{z}_i\|_2^{q-2} = \bar{\beta},
\end{aligned}$$

where the last inequality holds by Lemma 2. Hence, $\nabla^2 D_q(\mathbf{z};\mathcal{Z}) \preceq \bar{\beta}\mathbf{I}$ for all $\mathbf{z} \in \text{conv}(\mathcal{Z})$, so $D_q(\mathbf{z};\mathcal{Z})$ is $\bar{\beta}$-smooth on conv($\mathcal{Z}$) by (A.1).

Likewise, since $D_q(\mathbf{z};\mathcal{Z})$ is twice-differentiable, it is μ-strongly convex on conv($\mathcal{Z}$) if and only if:

$$\mu\mathbf{I} \preceq \nabla^2 D_q(\mathbf{z};\mathcal{Z}) \quad \text{for all } \mathbf{z} \in \text{conv}(\mathcal{Z}). \tag{A.2}$$

Letting $\lambda_{min}\{\mathbf{A}\}$ denote the smallest eigenvalue of $\mathbf{A}$, we have:

$$\begin{aligned}
\lambda_{min}\{\nabla^2 D_q(\mathbf{z};\mathcal{Z})\} &= \lambda_{min}\left\{\frac{q-2}{m}\sum_{i=1}^m \left\{\|\mathbf{z}-\mathbf{z}_i\|_2^{q-4}(\mathbf{z}-\mathbf{z}_i)(\mathbf{z}-\mathbf{z}_i)^T\right\} + \frac{1}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-2}\mathbf{I}\right\} \\
&\geq \frac{q-2}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-4}\lambda_{min}\left\{(\mathbf{z}-\mathbf{z}_i)(\mathbf{z}-\mathbf{z}_i)^T\right\} + \frac{1}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-2}\lambda_{min}\{\mathbf{I}\} \\
&\geq \frac{q-2}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-4}\cdot 0 + \frac{1}{m}\sum_{i=1}^m \|\mathbf{z}-\mathbf{z}_i\|_2^{q-2} \geq \frac{1}{m}\sum_{i=1}^m \|C_{q-2}(\mathcal{Z})-\mathbf{z}_i\|_2^{q-2} = \bar{\mu},
\end{aligned}$$

where the last inequality holds by definition of $C_{q-2}(\mathcal{Z})$. Hence by (A.2), $D_q(\mathbf{z};\mathcal{Z})$ is $\bar{\mu}$-strongly convex. □

Proof of Corollary 1

Consider a β-smooth and μ-strongly convex function h with unique minimizer $\mathbf{u}^*$. It can be shown (Nesterov, 2007) that an iteration upper bound of $t = O\left(\sqrt{\frac{\beta}{\mu}}\log\frac{1}{\epsilon_{in}}\right)$ guarantees an ϵ_{in}-accuracy in objective, i.e. $|h(\mathbf{u}^{[t]}) - h(\mathbf{u}^*)| < \epsilon_{in}$. Combining this iteration bound with the result in Theorem 2, and using the fact that each update requires $O(mp)$ work, we get the desired result.

Proof of Theorem 3

The three parts of this theorem are individually easy to verify. For finite termination, we showed in Section 3.1 that the objective in (7) strictly decreases after each loop iteration of Algorithm 1. Moreover, there are exactly N^n possible assignments of the sample $\{\mathbf{y}_j\}_{j=1}^N$ to the design points $\{\mathbf{m}_i\}_{i=1}^n$. Suppose, for contradiction, that Algorithm 1 does not terminate after N^n iterations. Then there exists at least two iterations which begin with the same assignment of $\{\mathbf{y}_j\}_{j=1}^N$. This, in turn, generates the same design $\{\mathbf{m}_i\}_{i=1}^n$ at the end of both iterations, which presents a contradiction to the strictly decreasing objective values induced by each loop iteration of Algorithm 1. The first claim therefore holds.

Next, regarding running time, consider the two updates in a single loop iteration of Algorithm 1. The first update assigns each sample point in $\{\mathbf{y}_j\}$ to its closest design point, which requires $O(Nnp)$ work. The second update computes, for each design point, the C_q-center of samples assigned to it. Let $\mathcal{Z} = \{\mathbf{z}_j\}_{j=1}^{m_i}$ be the m_i points assigned to the i-th design point. From Corollary 1, the computation of its C_q-center requires $O(m_i p\sqrt{(q-1)\kappa_{q-2}(\mathcal{Z})\log(1/\epsilon_{in})})$ work. Letting $\tilde{\mathbf{z}} = \text{argmax}_{j=1,\cdots,m_i} D_q(\mathbf{z}_j;\mathcal{Z})$, it follows that for any $q \geq 2$:

$$\kappa_q(\mathcal{Z}) = \frac{D_q(\tilde{\mathbf{z}};\mathcal{Z})}{D_q(C_q(\mathcal{Z});\mathcal{Z})} \leq \frac{\sum_{i=1}^{m_i}\|\mathbf{z}_i - C_q(\mathcal{Z})\|_2^q + m_i\|\tilde{\mathbf{z}} - C_q(\mathcal{Z})\|_2^q}{\sum_{i=1}^{m_i}\|\mathbf{z}_i - C_q(\mathcal{Z})\|_2^q}$$
$$\leq 1 + \frac{m_i\|\tilde{\mathbf{z}} - C_q(\mathcal{Z})\|_2^q}{\sum_{i=1}^{m_i}\|\mathbf{z}_i - C_q(\mathcal{Z})\|_2^q} \leq m_i + 1.$$

Hence, updating C_q-centers for all n design points require a total work of:

$$\begin{aligned}\sum_{i=1}^n O(m_i p\sqrt{(q-1)\kappa_{q-2}(\mathcal{Z})\log(1/\epsilon_{in})}) &\leq O\left(\left\{\sum_{i=1}^n m_i^{3/2}\right\} p\sqrt{q-1}\log\frac{1}{\epsilon_{in}}\right)\\ &\leq O\left(\left\{\sum_{i=1}^n m_i\right\}^{3/2} p\sqrt{q-1}\log\frac{1}{\epsilon_{in}}\right)\\ &= O\left(N^{3/2}p\sqrt{q-1}\log\frac{1}{\epsilon_{in}}\right).\end{aligned}$$

Finally, since $n \leq N^{1/2}$, the running time of the second step dominates the first, which completes the argument.

Finally, assume that the C_q-center updates in (5) are exact. By the termination conditions of Algorithm 1, the converged design is optimal given fixed assignments, and the converged assignment variables are optimal given a fixed design. Hence, the converged design (as well as its corresponding assignment) are locally optimal for (7).

Proof of Proposition 1

This can be shown by a simple application of the triangle inequality. Let $\mathcal{D} = \{\mathbf{m}_i\}_{i=1}^n$ be the design at the current iteration, and without loss of generality, suppose the first design point $\mathbf{m}_1$ is to be updated. Also, let $\{d_i\}_{i=1}^n$ be the minimax distances for each design point (defined in (15)), with $d^* = \max_i d_i$ being the overall minimax distance of $\mathcal{D}$.

Let $\tilde{\mathbf{m}}_1$ be the optimal design point in (16), and note that, by optimization constraints, $\|\tilde{\mathbf{m}}_1 - \mathbf{m}_1\| \leq d^* - d_1$. Denoting $\tilde{d}^*$ as the overall minimax distance of the new design $\tilde{\mathcal{D}} = \{\tilde{\mathbf{m}}_1, \mathbf{m}_2, \cdots, \mathbf{m}_n\}$, the claim is that $\tilde{d}^* \leq d^*$. To prove this, let $\mathbf{x}$ be the point in $\mathcal{X}$ achieving the minimax distance $\tilde{d}^*$, and consider the following three cases:

- If $Q(\mathbf{x}, \tilde{\mathcal{D}})$, the closest design point to $\mathbf{x}$ in $\tilde{\mathcal{D}}$, equals $\tilde{\mathbf{m}}_1$, then:

$$\tilde{d}^* = \|\mathbf{x} - \tilde{\mathbf{m}}_1\| \leq \|\mathbf{x} - \mathbf{m}_1\| + \|\mathbf{m}_1 - \tilde{\mathbf{m}}_1\| \leq d_1 + (d^* - d_1) = d^*.$$

- If $Q(\mathbf{x}, \tilde{\mathcal{D}}) = \mathbf{m}_i$ for some $i = 2, \cdots, n$, and $Q(\mathbf{x}, \mathcal{D}) = \mathbf{m}_1$, then:

$$\tilde{d}^* = \|\mathbf{x} - \mathbf{m}_i\| \leq \|\mathbf{x} - \tilde{\mathbf{m}}_1\| \leq \|\mathbf{x} - \mathbf{m}_1\| + \|\mathbf{m}_1 - \tilde{\mathbf{m}}_1\| \leq d_1 + (d^* - d_1) = d^*.$$

- If $Q(\mathbf{x}, \tilde{\mathcal{D}}) = \mathbf{m}_i$ for some $i = 2, \cdots, n$, and $Q(\mathbf{x}, \mathcal{D}) = \mathbf{m}_j$ for some $j = 1, \cdots, n$, then it must be the case that $i = j$, since the only change from $\mathcal{D}$ to $\tilde{\mathcal{D}}$ is the first design point. Hence:

$$\tilde{d}^* = \|\mathbf{x} - \mathbf{m}_i\| \leq d_i \leq d^*.$$

This proves the proposition.

B Minimax designs on $[0, 1]^p$

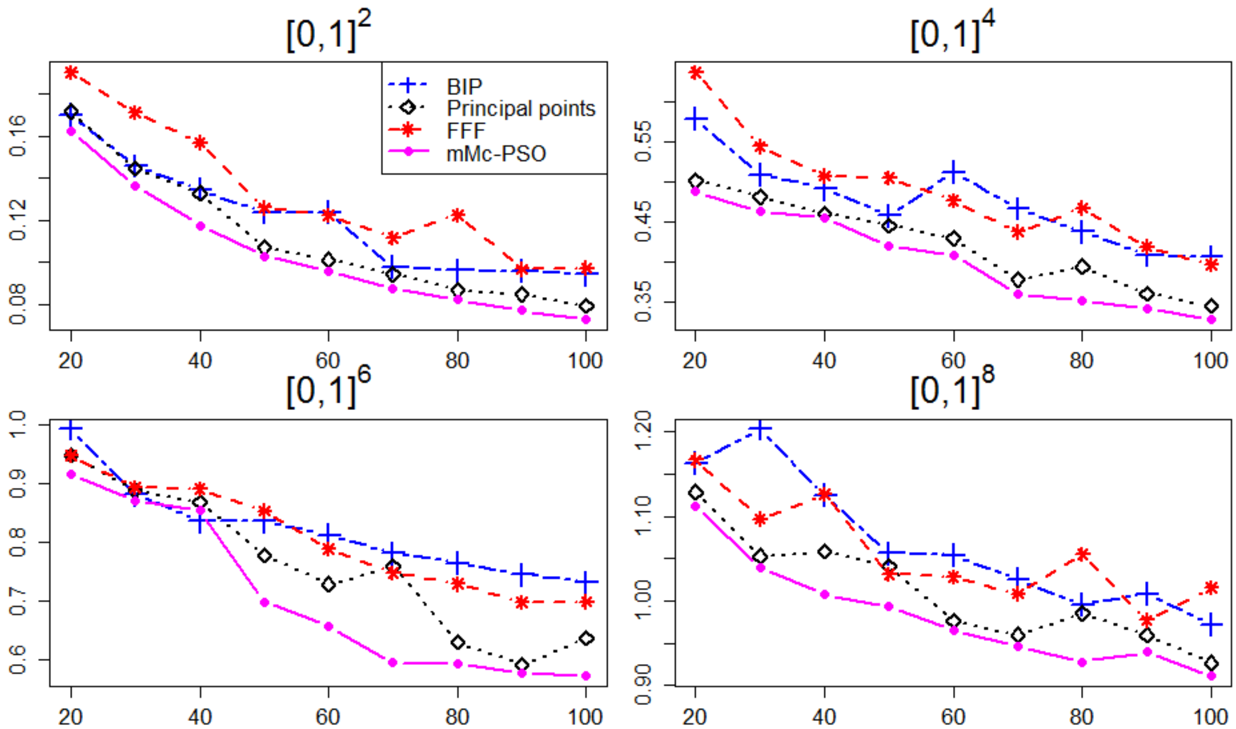

Figure B.1: Minimax criterion on $[0, 1]^p$ for $p = 2, 4, 6$ and 8.

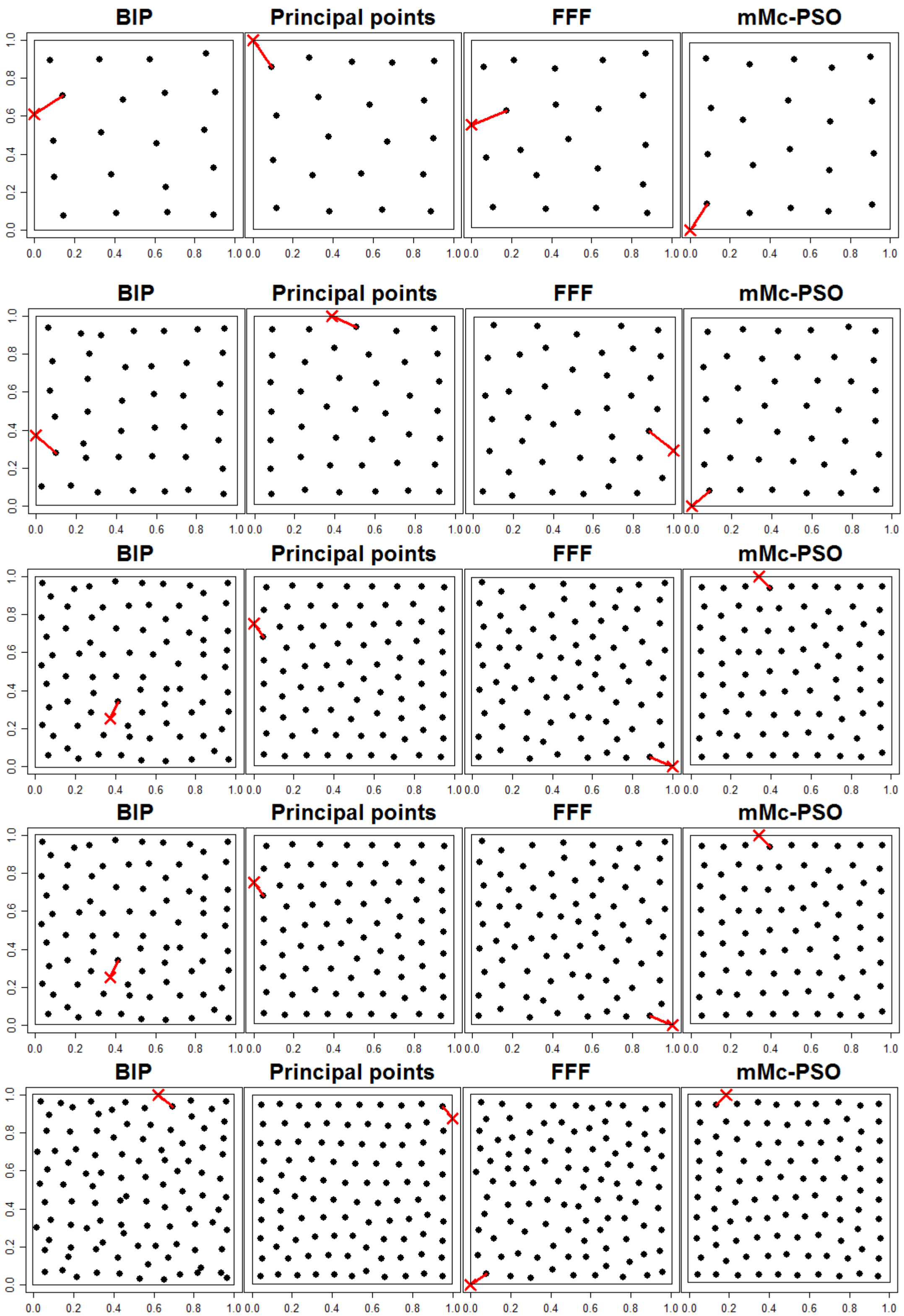

Figure B.2: 20-, 40-, 60-, 80- and 100-point designs on the unit hypercube $[0,1]^2$.

C Minimax designs on A_p and B_p

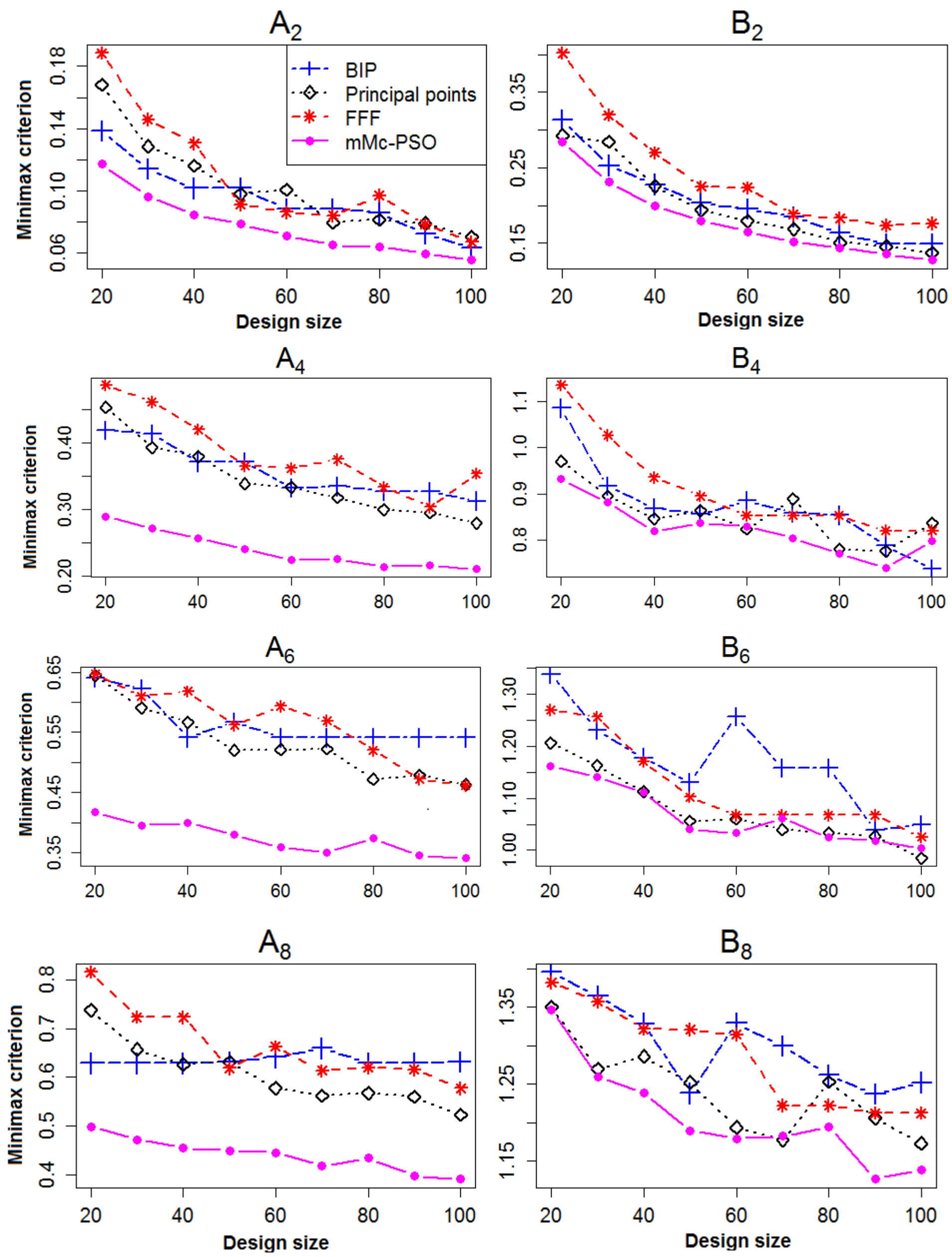

Figure C.1: Minimax criterion on A_p and B_p for $p = 2, 4, 6$ and 8.

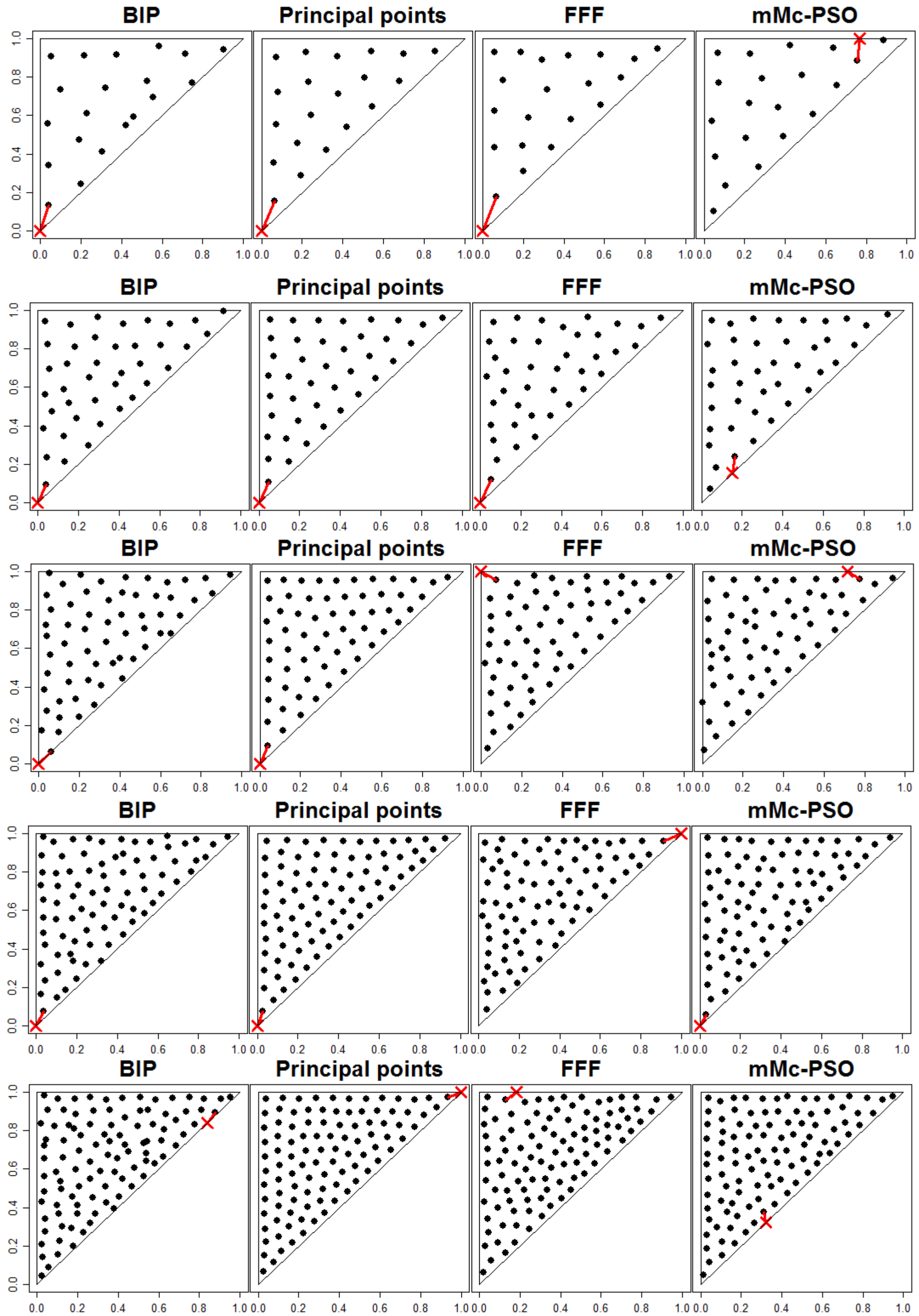

Figure C.2: 20-, 40-, 60-, 80- and 100-point designs on the unit simplex A_2.

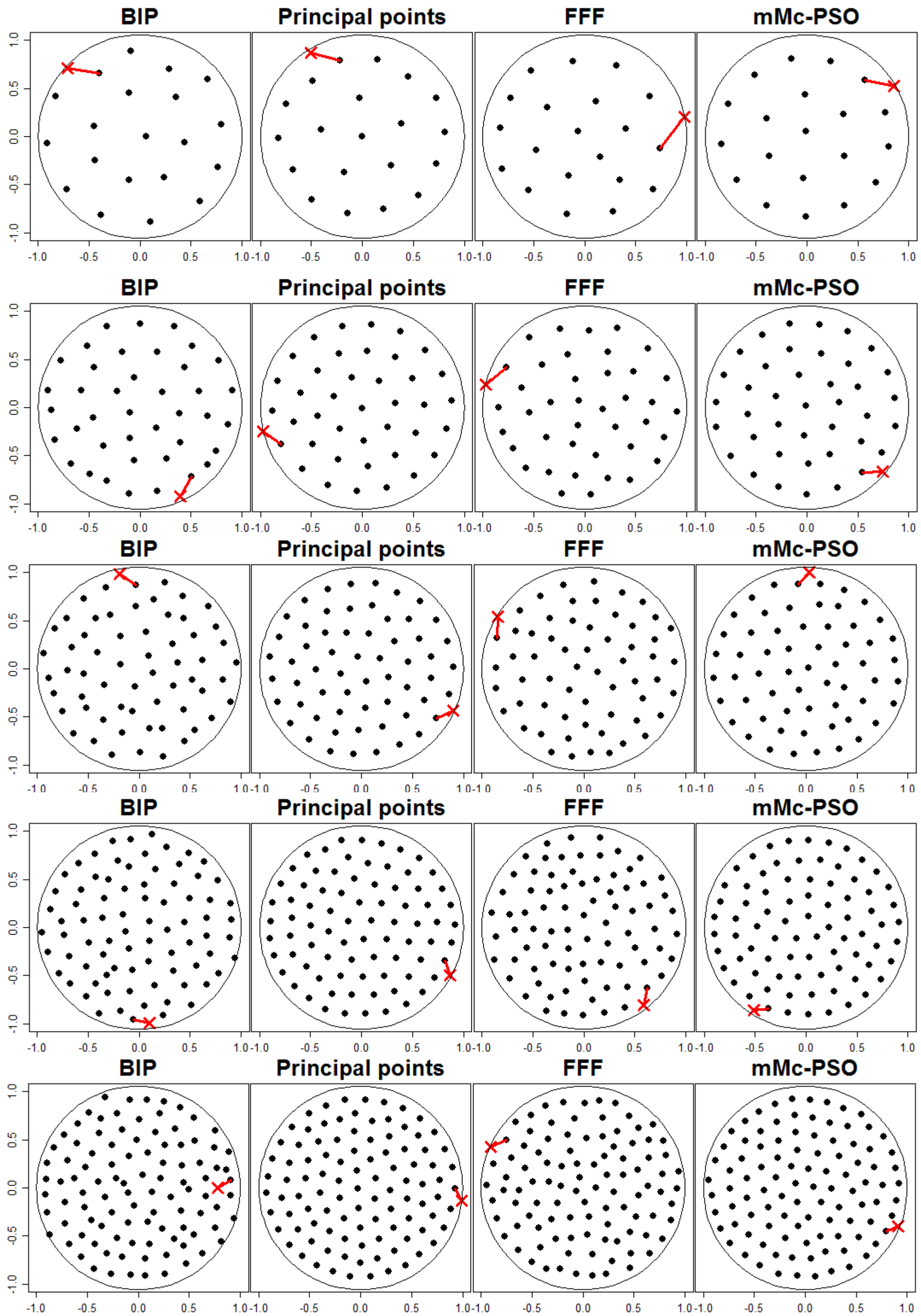

Figure C.3: 20-, 40-, 60-, 80- and 100-point designs on the unit ball B_2.

D Minimax designs on Georgia

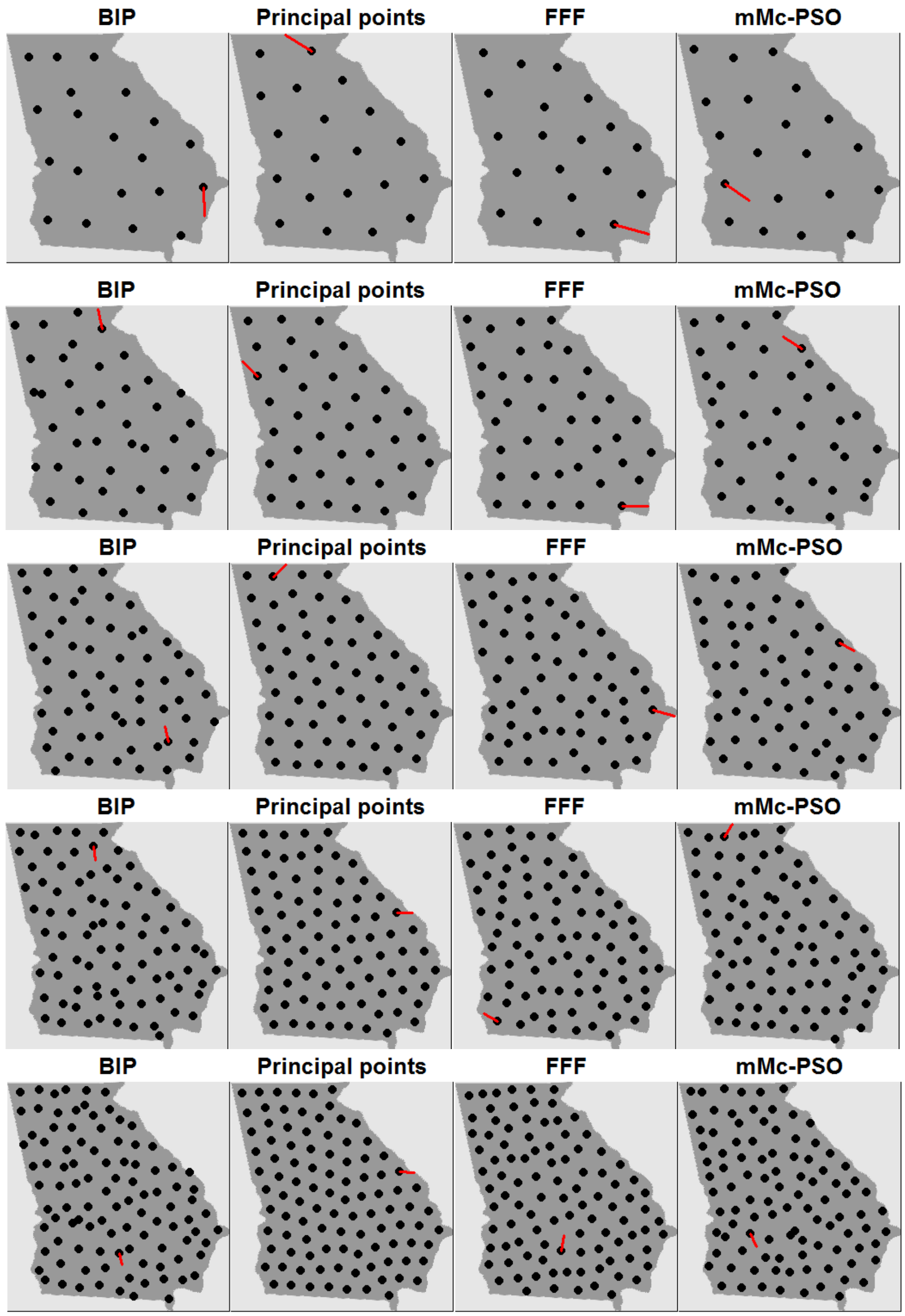

Figure D.1: 20-, 40-, 60-, 80- and 100-point designs on Georgia.