

MAXIMIN DISTANCE DESIGNS FOR MIXED CONTINUOUS, ORDINAL, AND BINARY VARIABLES

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Supplementary Material

The supplementary material contains the proofs of the theorems in Section S1 and additional details on the implementation and specification of the numerical studies in Section S2.

S1 Proofs of theorems

Preliminary Notation and Omitted Proofs for Theorems 1-3

For a point $\mathbf{x} = (x_1, \dots, x_p) \in \mathbb{R}^p$ and a set $\mathcal{A} \subset \{1, \dots, p\}$. Let

$$\mathbf{x}_{\mathcal{A}} = \{(x_{k_1}, \dots, x_{k_h}) : k_i \text{ is the } i\text{-th smallest number in } \mathcal{A}, i = 1, \dots, m(\mathcal{A})\},$$

i.e., $\mathbf{x}_{\mathcal{A}}$ consists of the dimensions in $\mathcal{A}$ of the point $\mathbf{x}$. Theorems 1-3 can be proved in the same way as their counterparts in He (2019) and thus we omit the proofs.

Proof of Theorem 4

Proof. Let

$$\mathcal{B} = \prod_{k=1}^p \{0, \dots, s_k - 1\}, \quad \mathcal{I}_v = (\mathcal{L} \oplus v) \cap \mathcal{B},$$

and define

$$\Phi(\mathbf{a}) = (\mathcal{Y}_{1(a_1+1)}, \dots, \mathcal{Y}_{p(a_p+1)})$$

for $\mathbf{a} \in \mathcal{B}$. Write

$$\mathcal{D}_v = \mathcal{D}(\mathcal{L}, \mathbf{s}, \mathcal{Y}, v) = \{\Phi(\mathbf{a}) : \mathbf{a} \in \mathcal{I}_v\}.$$

The map Φ is injective because each $\mathcal{Y}_k$ contains s_k distinct levels. By assumption, the projection of $\mathcal{I}_u$ onto coordinate k is $\{0, \dots, s_k - 1\}$ for every k .

We first show that $\mathcal{I}_{\mathbf{0}_p}$ has the same coordinate projections. Since $\mathbf{0}_p \in \mathcal{I}_{\mathbf{0}_p}$, this is immediate when $s_k = 1$. For $s_k \geq 2$, choose $\mathbf{a}, \mathbf{b} \in \mathcal{I}_u$ with $a_k = 0$ and $b_k = 1$, and let $\mathbf{c} = (\mathbf{b} - \mathbf{a}) \bmod 2$, with the reduction taken coordinatewise. Because $\mathbf{b} - \mathbf{a} \in \mathcal{L}$ and $2\mathbb{Z}^p \subseteq \mathcal{L}$, we have $\mathbf{c} \in \mathcal{L}$. Moreover, $c_k = 1$, and $c_j = 0$ whenever $s_j = 1$. Hence $\mathbf{c} \in \mathcal{I}_{\mathbf{0}_p}$. For every even $\ell \in \{0, \dots, s_k - 1\}$, the vector $\ell \mathbf{e}_k$ belongs to $\mathcal{I}_{\mathbf{0}_p}$; for every odd ℓ in this range, the vector $\mathbf{c} + (\ell - 1)\mathbf{e}_k$ belongs to $\mathcal{I}_{\mathbf{0}_p}$. Thus, every prescribed index occurs in each coordinate of $\mathcal{I}_{\mathbf{0}_p}$. In particular, $\mathcal{D}_{\mathbf{0}_p}$ has at least two runs and the same coordinate level sets as $\mathcal{D}_u$.

Fix $v, v' \in \{\mathbf{0}_p, \mathbf{u}\}$, and choose distinct $\mathbf{a}, \mathbf{b} \in \mathcal{I}_v$ such that $\rho(\mathcal{D}_v) = \|\Phi(\mathbf{a}) - \Phi(\mathbf{b})\|_2$. If $|b_k - a_k| \geq 3$ for some k , subtracting $2\mathbf{e}_k$ from the endpoint with the larger k th coordinate

gives a distinct feasible pair with strictly smaller distance, contradicting minimality. The same argument applies if $|b_k - a_k| = 2$ and the two indices also differ in another coordinate. Consequently, either $|b_k - a_k| \leq 1$ for every k , or, after interchanging $\mathbf{a}$ and $\mathbf{b}$ if necessary, $\mathbf{b} = \mathbf{a} + 2\mathbf{e}_k$ for some k .

First, suppose that $|b_k - a_k| \leq 1$ for every k . Choose any $\mathbf{t} \in \mathcal{I}_{\mathbf{v}'}$ and construct $\mathbf{a}'$ and $\mathbf{b}'$ coordinatewise. If $a_k \neq b_k$, retain or exchange the two indices a_k and b_k so that $a'_k \equiv t_k \pmod{2}$. This is possible because the two indices are adjacent and therefore have opposite parity. If $a_k = b_k$, set $a'_k = b'_k = t_k$. Then $\mathbf{a}', \mathbf{b}' \in \mathcal{B}$ and $\mathbf{a}' - \mathbf{t} \in 2\mathbb{Z}^p \subseteq \mathcal{L}$, $\mathbf{b}' - \mathbf{a}' \equiv \mathbf{b} - \mathbf{a} \pmod{2}$. Since $\mathbf{b} - \mathbf{a} \in \mathcal{L}$, it follows that $\mathbf{b}' - \mathbf{a}' \in \mathcal{L}$. Thus, $\mathbf{a}'$ and $\mathbf{b}'$ are distinct elements of $\mathcal{I}_{\mathbf{v}'}$. The construction preserves every absolute coordinate difference after applying Φ , so $\|\Phi(\mathbf{a}') - \Phi(\mathbf{b}')\|_2 = \|\Phi(\mathbf{a}) - \Phi(\mathbf{b})\|_2$.

Next, suppose that $\mathbf{b} = \mathbf{a} + 2\mathbf{e}_k$. Because $\mathcal{I}_{\mathbf{v}'}$ contains every prescribed index in coordinate k , there exists $\mathbf{t} \in \mathcal{I}_{\mathbf{v}'}$ with $t_k = a_k$. Since $2\mathbf{e}_k \in \mathcal{L}$ and $a_k + 2 = b_k \leq s_k - 1$, we also have $\mathbf{t} + 2\mathbf{e}_k \in \mathcal{I}_{\mathbf{v}'}$. Therefore, $\|\Phi(\mathbf{t} + 2\mathbf{e}_k) - \Phi(\mathbf{t})\|_2 = \mathcal{Y}_{k(b_k+1)} - \mathcal{Y}_{k(a_k+1)} = \rho(\mathcal{D}_{\mathbf{v}})$.

In either case, $\mathcal{D}_{\mathbf{v}'}$ contains two distinct points whose distance equals $\rho(\mathcal{D}_{\mathbf{v}})$, and hence $\rho(\mathcal{D}_{\mathbf{v}'}) \leq \rho(\mathcal{D}_{\mathbf{v}})$. Applying this argument with $(\mathbf{v}, \mathbf{v}') = (\mathbf{u}, \mathbf{0}_p)$ and then with $(\mathbf{v}, \mathbf{v}') = (\mathbf{0}_p, \mathbf{u})$ proves the claimed equality. $\square$

Proof of Theorem 5

Proof. We use the product-space assumptions on $\mathcal{G}$ given in the definition of an ILDM and consider a feasible target run size n .

We first show that every admissible design has a counterpart with the same run size, no smaller separation distance, and at least two actual levels in every coordinate. Consider $\bar{\mathcal{D}} = \mathcal{D}(\bar{\mathcal{L}}, \bar{\mathbf{s}}, \bar{\mathcal{Y}}, \mathbf{0}_p)$. If every $\bar{s}_k \geq 2$, no modification is needed at this stage. Otherwise, relabel the coordinates so that $\bar{s}_k \geq 2$ for $k \leq h$ and $\bar{s}_k = 1$ for $k > h$, where $1 \leq h < p$ because $m(\bar{\mathcal{D}}) \geq 2$. Define

$$\mathcal{M} = \{\mathbf{z} \in \mathbb{Z}^h : (\mathbf{z}, \mathbf{0}_{p-h}) \in \bar{\mathcal{L}}\}, \quad \hat{\mathcal{L}} = \mathcal{M} \times \mathbb{Z}^{p-h}.$$

The set $\mathcal{M}$ is a lattice containing $2\mathbb{Z}^h$. Since each of the first h coordinates actually uses index 1, the projection of $\mathcal{M}$ onto each coordinate contains 1 and is therefore $\mathbb{Z}$. Thus, $\mathcal{M}$ and $\hat{\mathcal{L}}$ are standard ILs. Because the last $p - h$ index coordinates are fixed at zero,

$$\mathcal{D}(\hat{\mathcal{L}}, \bar{\mathbf{s}}, \bar{\mathcal{Y}}, \mathbf{0}_p) = \bar{\mathcal{D}}.$$

Let $\mathcal{M}_0 = \{\mathbf{z} \in \mathcal{M} : z_1 \text{ is even}\}$ and $\mathcal{M}_1 = \{\mathbf{z} \in \mathcal{M} : z_1 \text{ is odd}\}$. The first set is an index-two sublattice of $\mathcal{M}$, and the second is its complementary coset. Set

$$\tilde{\mathcal{L}} = (\mathcal{M}_0 \times \mathbb{E}^{p-h}) \cup (\mathcal{M}_1 \times (\mathbb{E}^{p-h} \oplus \mathbf{1}_{p-h})).$$

This is a lattice containing $2\mathbb{Z}^p$. Its first h coordinate projections are inherited from $\mathcal{M}$, and its remaining projections contain both parities, so it is a standard IL. Retain $\tilde{s}_k = \bar{s}_k$

and $\tilde{\mathcal{Y}}_k = \bar{\mathcal{Y}}_k$ for $k \leq h$, and set $\tilde{s}_k = 2$ and $\tilde{\mathcal{Y}}_k = \{0, w_k\}$ for $k > h$. Every old index $(\mathbf{a}, \mathbf{0}_{p-h})$ corresponds uniquely to the new index $(\mathbf{a}, \epsilon(\mathbf{a})\mathbf{1}_{p-h})$, where $\epsilon(\mathbf{a}) = a_1 \bmod 2$. This correspondence is a bijection between the two finite index sets. Both values of ϵ occur because the first coordinate actually uses indices 0 and 1. Thus, each added coordinate uses both levels. The first h coordinates are unchanged, and the previously constant coordinates cannot decrease any pairwise distance. Consequently,

$$m(\tilde{\mathcal{D}}) = m(\bar{\mathcal{D}}), \quad \rho(\tilde{\mathcal{D}}) \geq \rho(\bar{\mathcal{D}}), \quad \tilde{s}_k \geq 2 \quad (k = 1, \dots, p).$$

Next, replace the smallest and largest levels in each coordinate by 0 and w_k , respectively, leaving the interior levels unchanged. The new levels remain admissible and distinct. The index set and run size are unchanged, and no absolute difference between coordinate levels decreases. Hence every admissible design has a counterpart satisfying the stated span and endpoint conditions, with the same run size and no smaller separation distance.

We now prove the distance formula. For a standard IL $\mathcal{L}$ and $s_k \geq 2$ for every k , let

$$\mathcal{I} = \mathcal{L} \cap \prod_{k=1}^p \{0, \dots, s_k - 1\}, \quad \Phi(\mathbf{a}) = (\mathcal{Y}_{1(a_1+1)}, \dots, \mathcal{Y}_{p(a_p+1)}).$$

Then $\mathcal{D} = \{\Phi(\mathbf{a}) : \mathbf{a} \in \mathcal{I}\}$, and Φ is injective. Write

$$A = \min_{\mathbf{c} \in \mathcal{H} \setminus \{\mathbf{0}_p\}} \left\{ \sum_{k:c_k=1} d^*(\mathcal{Y}_k)^2 \right\}^{1/2}, \quad B = \min_{k=1, \dots, p} d^+(\mathcal{Y}_k).$$

For distinct $\mathbf{a}, \mathbf{b} \in \mathcal{I}$, the coordinatewise reduction $\mathbf{c} = (\mathbf{b} - \mathbf{a}) \bmod 2$ belongs to $\mathcal{H}$. If $\mathbf{c} \neq \mathbf{0}_p$, then

$$\|\Phi(\mathbf{b}) - \Phi(\mathbf{a})\|_2 \geq \left\{ \sum_{k:c_k=1} d^*(\mathcal{Y}_k)^2 \right\}^{1/2} \geq A.$$

Otherwise, some coordinate indices differ by at least two, giving

$$\|\Phi(\mathbf{b}) - \Phi(\mathbf{a})\|_2 \geq |\mathcal{Y}_{k(b_k+1)} - \mathcal{Y}_{k(a_k+1)}| \geq d^+(\mathcal{Y}_k) \geq B.$$

Thus, $\rho(\mathcal{D}) \geq \min\{A, B\}$.

For the reverse inequality, fix a nonzero $\mathbf{c} \in \mathcal{H}$. Whenever $c_k = 1$, choose i_k attaining $\mathcal{Y}_{k(i_k+1)} - \mathcal{Y}_{k(i_k)} = d^*(\mathcal{Y}_k)$. Of the consecutive indices $i_k - 1$ and i_k , assign the even index to a_k and the odd index to b_k . Set $a_k = b_k = 0$ when $c_k = 0$. Both vectors lie in the index box, and $\mathbf{a}, \mathbf{b} - \mathbf{c} \in 2\mathbb{Z}^p \subseteq \mathcal{L}$. Hence $\mathbf{a}, \mathbf{b} \in \mathcal{I}$ and

$$\|\Phi(\mathbf{b}) - \Phi(\mathbf{a})\|_2 = \left\{ \sum_{k:c_k=1} d^*(\mathcal{Y}_k)^2 \right\}^{1/2}.$$

Minimizing over $\mathbf{c}$ yields $\rho(\mathcal{D}) \leq A$. For any k with $s_k \geq 3$, choose $i \in \{1, \dots, s_k - 2\}$ attaining $\mathcal{Y}_{k(i+2)} - \mathcal{Y}_{k(i)} = d^+(\mathcal{Y}_k)$. Since $\mathcal{L}$ is standard, there exists $\mathbf{c} \in \mathcal{H}$ with $c_k \equiv i - 1 \pmod{2}$. Set

$$\mathbf{a} = \mathbf{c} + (i - 1 - c_k)\mathbf{e}_k, \quad \mathbf{b} = \mathbf{a} + 2\mathbf{e}_k.$$

Both vectors belong to $\mathcal{L}$ and the index box, since all other coordinates lie in $\{0, 1\}$ and every $s_j \geq 2$. Their images are at distance $d^+(\mathcal{Y}_k)$. This gives $\rho(\mathcal{D}) \leq B$ when some $s_k \geq 3$; otherwise $B = +\infty$. Combining the bounds proves (3.3). Here $\min_{s_k \geq 2} d^+(\mathcal{Y}_k) = B$ because every coordinate has at least two levels. The argument does not require the endpoint conditions.

Finally, we verify that the maximum is attained. Choose a feasible design satisfying the span and endpoint conditions, as constructed above, and let its separation distance be

$\delta > 0$. For any such design with separation distance at least δ and any $s_k \geq 3$, the distance formula gives

$$\delta \leq d^+(\mathcal{Y}_k) \leq \frac{2w_k}{s_k - 2}.$$

The second inequality follows by summing all $s_k - 2$ two-step gaps. Therefore, $s_k \leq 2 + 2w_k/\delta$. Only finitely many span vectors and standard ILs need be considered, and the finite-input coordinates have finitely many level-set choices.

For a continuous coordinate with s levels in $[0, w]$, we can restrict the levels further without decreasing d^* or d^+ . For $s = 2$, use the endpoints. For odd $s \geq 3$, equally spaced levels attain both bounds $d^* \leq w/(s - 1)$ and $d^+ \leq 2w/(s - 1)$, obtained by summing the adjacent gaps and the two-step gaps along the odd-numbered levels, respectively. For even $s \geq 4$, put $a = d^* > 0$ and write the adjacent gaps as $g_1, \dots, g_{s-1}$. Since

$$w \geq g_1 + (g_2 + g_3) + \dots + (g_{s-2} + g_{s-1}) \geq a + (s/2 - 1)d^+,$$

an endpoint-containing configuration with alternating gaps $a, b, a, \dots, b, a$, where $b = (2w - sa)/(s - 2) \geq a$, has $d^* = a$ and $d^+ = 2(w - a)/(s - 2)$ and weakly improves both criteria. The distance formula shows that these coordinatewise replacements cannot decrease separation distance.

For each fixed feasible lattice, span vector, and choice of finite-input levels within the preceding bounds, use these continuous-coordinate forms and temporarily allow $0 \leq a \leq w/(s - 1)$ for every even-level continuous coordinate. Each resulting parameter set is compact. The minimum distance over the fixed set of distinct index pairs is continuous, includ-

ing at boundary values with repeated coordinate levels. Maximizing over the finitely many such compact parameter sets gives an attained value $R_* \geq \delta$. By the reductions above, the separation distance of every original admissible design is at most R_* .

To show that this maximum represents an admissible ILDM, let J be the set of coordinates with repeated levels at a maximizing parameter value, and let K be its complement. If J is empty, nothing remains to prove. Otherwise, every $k \in J$ is a continuous coordinate with $s_k = 2r_k \geq 4$ and $a = 0$. Its level list consists of equal consecutive pairs with distinct values $hw_k/(r_k - 1)$, $h = 0, \dots, r_k - 1$. Because $R_* > 0$, distinct indices have distinct images. Thus, no nonzero vector of $\mathcal{H}$ is supported entirely on J , since its image would equal that of $\mathbf{0}_p$. Since $\mathcal{H}$ is closed under coordinatewise addition modulo two, its projection onto K is injective.

Let π_K denote coordinate projection and define

$$\mathcal{L}' = \{\mathbf{x} \in \mathbb{Z}^p : \mathbf{x}_K \in \pi_K(\mathcal{L})\}.$$

This is a standard IL because it contains $2\mathbb{Z}^p$, inherits the coordinate projections on K from $\mathcal{L}$, and is unrestricted on J . For $k \in J$, replace the span by r_k and the level list by $\{hw_k/(r_k - 1) : h = 0, \dots, r_k - 1\}$; leave all other spans and levels unchanged. Each feasible index on K determines exactly one admissible parity vector on J . Therefore, replacing each old index a_k by $\lfloor a_k/2 \rfloor$ for $k \in J$ gives a bijection between the old and new finite index sets. The inverse selects the uniquely prescribed parity from each consecutive pair. This map preserves every point, so the new design has the same run size and separation distance

R_* . Its coordinate levels are distinct, contain both endpoints, and have spans at least two. These spans are also the actual marginal level counts. Indeed, an even index ℓ in coordinate k is realized by $\ell \mathbf{e}_k$; an odd index is realized by $\mathbf{c} + (\ell - 1)\mathbf{e}_k$, where $\mathbf{c} \in \mathcal{L}' \cap \{0, 1\}^p$ and $c_k = 1$. The other coordinates remain in $\{0, 1\}$, within their index ranges. We have thus obtained an admissible design attaining the largest separation distance and satisfying all the stated conditions. $\square$

Proof of Theorem 6

Proof. We first show that

$$d^*(\bar{\gamma}) = w_k/(s_k - 1) = \max\{d^*(\gamma) : \gamma_i \in \mathcal{G}_k, m(\gamma) = s_k\},$$

$$d^+(\bar{\gamma}) = 2w_k/(s_k - 1) = \max\{d^+(\gamma) : \gamma_i \in \mathcal{G}_k, m(\gamma) = s_k\},$$

and there is no other γ that fulfills both properties.

On one hand, suppose there is a $\gamma \subset \mathcal{G}_k$ such that $m(\gamma) = s_k$ and $d^*(\gamma) > w_k/(s_k - 1)$. Then $\gamma_{(1)} \geq 0$ and $\gamma_{(z+1)} \geq \gamma_{(z)} + d^*(\gamma) > \gamma_{(z)} + w_k/(s_k - 1)$ for any z . From an induction, we can show that $\gamma_{(s_k)} > w_k$, which conflicts to the assumption that $\gamma \subset \mathcal{G}_k = [0, w_k]$. Therefore, $d^*(\bar{\gamma}) = w_k/(s_k - 1) = \max\{d^*(\gamma) : \gamma \subset \mathcal{G}_k, m(\gamma) = s_k\}$.

Similarly, suppose there is a $\gamma \subset \mathcal{G}_k$ such that $m(\gamma) = s_k$ and $d^+(\gamma) > 2w_k/(s_k - 1)$. Then $\gamma_{(1)} \geq 0$ and $\gamma_{(2z+1)} \geq \gamma_{(2z-1)} + d^+(\gamma) > \gamma_{(2z-1)} + 2w_k/(s_k - 1)$ for any z . From an induction, we can show that $\gamma_{(s_k)} > w_k$, which conflicts to the assumption that $\gamma \subset \mathcal{G}_k = [0, w_k]$. Therefore, $d^+(\bar{\gamma}) = 2w_k/(s_k - 1) = \max\{d^+(\gamma) : \gamma \subset \mathcal{G}_k, m(\gamma) = s_k\}$.

Finally, suppose there is a $\gamma \in \mathcal{G}_k$ such that $m(\gamma) = s_k$ and $d^*(\gamma) \geq w_k/(s_k - 1)$. Then $\gamma_{(1)} \geq 0$ and for any z , $\gamma_{(z+1)} \geq \gamma_{(z)} + d^*(\gamma) \geq \gamma_{(z)} + w_k/(s_k - 1)$ and the equality holds if and only if $\gamma_{(z+1)} = \gamma_{(z)} + w_k/(s_k - 1)$. From an induction, we can show that $\gamma_{(s_k)} \geq w_k$ and the only choice that makes $\gamma_{(s_k)} = w_k$ is $\gamma = \bar{\gamma}$. Consequently, $\bar{\gamma}$ is the only admissible choice. $\square$

Proof of Theorem 7

Proof. Fix $0 < v_1 \leq w_k/(s_k - 1)$ and let $v_2 = (2w_k - s_kv_1)/(s_k - 2)$. By construction,

$$\tilde{\gamma}_{v_1, i} - \tilde{\gamma}_{v_1, i-1} = \begin{cases} v_1, & i \text{ is even,} \\ v_2, & i \text{ is odd.} \end{cases} \quad (\text{S1.1})$$

Since $v_2 - v_1 = 2\{w_k - (s_k - 1)v_1\}/(s_k - 2) \geq 0$, we have $d^*(\tilde{\gamma}_{v_1}) = v_1$ and $d^+(\tilde{\gamma}_{v_1}) = v_1 + v_2 = 2(w_k - v_1)/(s_k - 2)$.

We next show that $d^+(\tilde{\gamma}_{v_1})$ is the largest value of $d^+(\gamma)$ among admissible level sets satisfying $d^*(\gamma) \geq v_1$. Suppose, to the contrary, that an admissible $\gamma \in \mathcal{G}_k$ with $m\{\gamma\} = s_k$ satisfies $d^*(\gamma) \geq v_1$ and $d^+(\gamma) > v_1 + v_2$. Then $\gamma_{(2)} \geq \gamma_{(1)} + v_1$ and $\gamma_{(i+2)} > \gamma_{(i)} + v_1 + v_2$ for $i = 1, \dots, s_k - 2$. Since s_k is even, it follows that $\gamma_{(s_k)} > (s_k/2 - 1)(v_1 + v_2) + v_1 = w_k$, contradicting $\gamma \subseteq [0, w_k]$. Hence $d^+(\tilde{\gamma}_{v_1}) = \max\{d^+(\gamma) : \gamma \in \mathcal{G}_k, m\{\gamma\} = s_k, d^*(\gamma) \geq v_1\}$.

Similarly, $d^*(\tilde{\gamma}_{v_1}) = \max\{d^*(\gamma) : \gamma \in \mathcal{G}_k, m\{\gamma\} = s_k, d^+(\gamma) \geq v_1 + v_2\}$. Thus, each $\tilde{\gamma}_{v_1}$ is undominated with respect to the pair (d^*, d^+) .

Now consider any admissible $\gamma \in \mathcal{G}_k$ with $m\{\gamma\} = s_k$. Since its levels are distinct,

$d^*(\gamma) > 0$, and, because s_k points lie in $[0, w_k]$, $d^*(\gamma) \leq w_k/(s_k - 1)$. Setting $v_1 = d^*(\gamma)$ therefore gives an admissible $\tilde{\gamma}_{v_1}$ with $d^*(\tilde{\gamma}_{v_1}) = d^*(\gamma)$ and $d^+(\tilde{\gamma}_{v_1}) \geq d^+(\gamma)$. Hence every admissible level set is dominated by an element of $\{\tilde{\gamma}_{v_1} : 0 < v_1 \leq w_k/(s_k - 1)\}$, while no element of this collection is dominated by another admissible level set. Therefore, $\mathcal{F}([0, w_k], s_k) = \{\tilde{\gamma}_{v_1} : 0 < v_1 \leq w_k/(s_k - 1)\}$ is a minimal sufficient collection. $\square$

Proof of Theorem 8

Proof. By the definition of the input space, $0, w_k \in \mathcal{G}_k$ and $w_k > 0$. Let $\mathcal{P} = \{\gamma \subseteq \mathcal{G}_k : m(\gamma) = s_k\}$. This collection is finite and nonempty. If $s_k = 2$, the algorithm returns $\{\{0, w_k\}\}$. Every $\gamma \in \mathcal{P}$ satisfies $d^*(\gamma) \leq w_k$ and $d^+(\gamma) = +\infty$, while $\{0, w_k\}$ attains both bounds. The returned singleton collection is therefore sufficient, its only element is undominated, and it has no sufficient proper subset. We henceforth assume $s_k \geq 3$, so both criteria are positive and finite for every $\gamma \in \mathcal{P}$.

We first justify the two optimization steps used in Algorithm 1. Replacing the smallest and largest levels of any $\gamma \in \mathcal{P}$ by 0 and w_k , respectively, preserves its cardinality and cannot decrease either criterion. Thus, restricting either subproblem to level sets containing both endpoints does not change its optimum. For fixed thresholds $a \geq 0$ and $b \geq 0$, Algorithm 2 tests whether an ordered level set exists with every adjacent gap greater than a and every two-step gap greater than b . Algorithm 3 uses the same construction, but allows adjacent gaps equal to its positive threshold a .

In either construction, each intermediate level is chosen as the smallest admissible level satisfying the constraints imposed by the preceding one or two levels. Let $g_1, \dots, g_i$ be a constructed prefix and let $h_1 < \dots < h_{s_k}$ be any feasible ordered level set containing both endpoints. Induction gives $g_j \leq h_j$ for every constructed index j . Indeed, $g_1 = h_1 = 0$, and whenever the preceding inequalities hold, h_j satisfies the lower bounds used to select g_j , so the greedy choice cannot exceed h_j . Consequently, failure to select an intermediate level or failure of the final endpoint test rules out every feasible level set. Conversely, a successful construction provides a feasible set. Each successful pass through Algorithm 2 strictly increases its current value of d^* while maintaining the prescribed lower bound on d^+ . Each successful pass through Algorithm 3 strictly increases its current value of d^+ while maintaining the prescribed lower bound on d^* . Since only finitely many criterion values are possible, both procedures terminate and return the stated constrained optima when feasible, with Algorithm 2 returning zero when its feasible set is empty. Algorithm 3 is invoked only after a positive attainable value of d^* has been found, so its initial selection and its feasible set are nonempty.

Let $b_0 = 0$. At the t th successful iteration of Algorithm 1, write

$$a_t = \max_{\gamma \in \mathcal{P}: d^+(\gamma) > b_{t-1}} d^*(\gamma),$$

$$b_t = \max_{\gamma \in \mathcal{P}: d^*(\gamma) \geq a_t} d^+(\gamma),$$

and let $\gamma^{(t)}$ be the level set returned by the second optimization step. A level set attaining

the first maximum is feasible for the second step and has $d^+ > b_{t-1}$. Hence $b_t > b_{t-1}$. Moreover, $d^*(\gamma^{(t)}) \geq a_t$ and $d^+(\gamma^{(t)}) = b_t > b_{t-1}$. The definition of a_t then gives

$$d^*(\gamma^{(t)}) = a_t, \quad d^+(\gamma^{(t)}) = b_t.$$

If a subsequent successful iteration exists, its feasible set for the first optimization is contained in the current one, so $a_{t+1} \leq a_t$. Equality would imply the existence of a level set with $d^* \geq a_t$ and $d^+ > b_t$, contradicting the definition of b_t . Thus, consecutive outputs satisfy

$$a_{t+1} < a_t, \quad b_{t+1} > b_t.$$

Because $\mathcal{P}$ is finite, the main algorithm terminates after finitely many successful iterations, say N , and no $\gamma \in \mathcal{P}$ satisfies $d^+(\gamma) > b_N$.

To prove sufficiency, take any $\gamma \in \mathcal{P}$ and let t be the first iteration for which $b_t \geq d^+(\gamma)$. Such an iteration exists by the termination property. Since $d^+(\gamma) > 0 = b_0$, we have

$$b_{t-1} < d^+(\gamma) \leq b_t.$$

Thus, γ is feasible for the first optimization at iteration t , giving $d^*(\gamma) \leq a_t = d^*(\gamma^{(t)})$. Together with $d^+(\gamma) \leq b_t = d^+(\gamma^{(t)})$, this proves that the returned collection is sufficient.

Next, suppose that an admissible γ dominates an output $\gamma^{(t)}$, so that $d^*(\gamma) \geq a_t$ and $d^+(\gamma) \geq b_t$, with at least one strict inequality. If $d^+(\gamma) > b_t$, the definition of b_t is contradicted. Otherwise, $d^+(\gamma) = b_t$ and $d^*(\gamma) > a_t$; since $b_t > b_{t-1}$, this contradicts the definition of a_t . Therefore, every output is undominated.

Finally, removing any $\gamma^{(t)}$ destroys sufficiency. Earlier outputs have $d^+ < b_t$, while later outputs have $d^* < a_t$, so none of the remaining outputs weakly dominates $\gamma^{(t)}$. Hence no proper subset of the returned collection is sufficient. The collection produced by Algorithm 1 is therefore a minimal sufficient collection. $\square$

S2 Additional Details for the Numerical Studies

ILs for $p = 3$

There are 6 distinct ILs for $p = 3$,

$$\begin{aligned} \mathbf{G}_{3,1} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & \mathbf{G}_{3,2} &= \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}, & \mathbf{G}_{3,3} &= \begin{pmatrix} 1 & 1 & 1 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \\ \mathbf{G}_{3,4} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}, & \mathbf{G}_{3,5} &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 0 & 2 \end{pmatrix}, & \mathbf{G}_{3,6} &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 2 & 0 \end{pmatrix}, \end{aligned}$$

Implementation of the MCD benchmark.

We use Construction 2 of Deng et al. (2015), in which the qualitative and quantitative components of the design are constructed from a mixed-level orthogonal array (OA). Write $D = (D_1, D_2)$, where D_1 denotes the qualitative component and D_2 denotes the quantitative component. An OA is a design matrix whose rows represent experimental runs

and whose columns represent factors, with level combinations balanced over prescribed subsets of columns (Hedayat et al., 1999). More formally, a mixed-level OA, denoted by $\text{OA}(N, s_1^{k_1} \cdots s_m^{k_m}, t)$, has N rows and k_j columns at s_j levels, $j = 1, \dots, m$, and is said to have strength t if, for every selection of t columns, all possible combinations of their levels occur equally often.

For an $n = \lambda s^2$ -run design, Construction 2 uses a strength-two mixed-level OA

$$A = \text{OA}(\lambda s^2, s^k(\lambda s), 2).$$

The array A therefore has λs^2 rows, k columns at s levels each, and one column at λs levels. Here, s is the common number of levels of the qualitative factors, and k is the number of s -level columns. Because A has strength two, every pair of columns is balanced. In particular, each pair of levels occurs λ times in any two s -level columns, whereas each possible pair consisting of one level from an s -level column and one level from the λs -level column occurs exactly once. The required columns of D_1 are selected from the s -level columns of A . To construct each column of D_2 , we randomly permute the levels of the λs -level column of A and then apply the level-replacement procedure in Construction 2 of Deng et al. (2015) to obtain a Latin hypercube column.

For the Branin experiment, we use two qualitative factors and two quantitative factors, with $s = 2$ and $\lambda = 10, 15, 20$, corresponding to $n = 40, 60, 80$. For the eight-factor mixed setting in Figure 3(d), we use four qualitative factors and four quantitative factors, with $s = 3$ and $\lambda = 2, \dots, 11$. Ordinal factors are treated as qualitative factors, and equal

coordinate weights are used.

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