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Luc Pronzato, Henry P. Wynn, Anatoly A. Zhigljavsky

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Abstract We consider functionals measuring the dispersion of a d-dimensional distribution which are based on the volumes of simplices of dimension $k \leq d$ formed by $k+1$ independent copies and raised to some power δ. We study properties of extremal measures that maximize these functionals. In particular, for positive δ we characterize their support and for negative δ we establish connection with potential theory and motivate the application to space-filling design for computer experiments. Several illustrative examples are presented.

Keywords Potential theory · Logarithmic potential · Computer experiments · Space-filling design

Mathematics Subject Classification (2000) 62K05 · 31C15

1 Introduction

Let $\mathscr{X}$ be a compact subset of $\mathbb{R}^d$ and $\mathscr{M}$ be the set of probability measures on the Borel subsets of $\mathscr{X}$. We shall consider the class of functionals $\psi_{k,\delta} : \mathscr{M} \longrightarrow \mathbb{R}^+$ defined by

$$\psi_{k,\delta}(\mu) = \Psi_{k,\delta}(\mu, \ldots, \mu)\,, \tag{1}$$

where

$$\Psi_{k,\delta}(\mu_1, \ldots, \mu_{k+1}) = \int \ldots \int \mathscr{V}_k^{\delta}(x_1, \ldots, x_{k+1})\, \mu_1(\mathrm{d}x_1) \ldots \mu_{k+1}(\mathrm{d}x_{k+1})\,,$$

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Luc Pronzato
CNRS, Laboratoire I3S, UMR 7172, UNS, CNRS; 2000, route des Lucioles, Les Algorithmes, bât. Euclide B, 06900 Sophia Antipolis, France
Tel.: +33-4-92942708
Fax: +33-4-92942896
E-mail: pronzato@cnrs.fr

H.P. Wynn
London School of Economics, Houghton Street, London, WC2A 2AE, UK
E-mail: H.Wynn@lse.ac.uk

A. Zhigljavsky
School of Mathematics, Cardiff University, Senghennydd Road, Cardiff, CF24 4YH, UK
and Lobachevsky Nizhnii Novgorod State University, Russia
E-mail: ZhigljavskyAA@cf.ac.uk

for some δ in $\mathbb{R}$ and $k \in \{1, \ldots, d\}$, with $\mathscr{V}_k(x_1, \ldots, x_{k+1})$ the volume of the k-dimensional simplex (its length when $k = 1$ and area when $k = 2$) formed by the $k+1$ vertices $x_1, \ldots, x_{k+1}$ in $\mathbb{R}^d$. The volume $\mathscr{V}_k(x_1, \ldots, x_{k+1})$ can be computed by the formula

$$\mathscr{V}_k(x_1, \ldots, x_{k+1}) = \frac{1}{k!} \, |\det(A)|^{1/2} \, ,$$

with

$$A = X^\top X \, , \quad X = [(x_2 - x_1) \; (x_3 - x_1) \; \cdots (x_{k+1} - x_1)] \, , \tag{2}$$

where the matrix X has size $d \times k$. Define the potential of μ at $x \in \mathbb{R}^d$ by

$$P_{k,\delta,\mu}(x) = \Psi_{k,\delta}(\mu, \ldots, \mu, \delta_x) \, , \tag{3}$$

where δ_x is the delta-measure at x and μ appears k times on the right-hand side. Note that $\max_{x \in \mathscr{X}} P_{k,\delta,\mu}(x) \geq \psi_{k,\delta}(\mu)$ for all μ in $\mathscr{M}$ since $\int P_{k,\delta,\mu}(x) \, \mu(\mathrm{d}x) = \psi_{k,\delta}(\mu)$.

The case $\delta = 2$ corresponds to an extension of the notion of Wilk's generalized variance and is considered in [11]. In this paper we investigate properties of the functional (1) for general δ.

2 The case $\delta > 0$

When δ is positive we are interested in the maximization of the functional $\psi_{k,\delta}(\mu)$, $\mu \in \mathscr{M}$, and properties of an extremal measure μ^* where the maximum is attained.

2.1 Functionals based on powered distances: $k = 1$

For $k = 1$, the functional $\psi_{k,\delta}(\cdot)$ defined by (1) corresponds to

$$\psi_{1,\delta}(\mu) = \mathsf{E}\{\|x_1 - x_2\|^\delta\}$$

where x_1 and x_2 are supposed to be i.i.d. with the measure μ. Properties of measures that maximize $\psi_{1,\delta}(\mu)$ for $\delta > 0$ are investigated in [2]. In particular, it is shown there that for any $\delta > 0$ the mass of an optimal measure is concentrated on the boundary of $\mathscr{X}$ and that the support only comprises the extreme points of the convex hull of $\mathscr{X}$ when $\delta > 1$. Also, the optimal measure is unique for $\delta < 2$; it is supported at no more than $d + 1$ points when $\delta > 2$.

We can give a more precise statement than in Theorem 2 of [2] for $0 < \delta \leq 2$, using the concavity of $\psi_{1,\delta}(\cdot)$, which follows from results discussed in [13] and is based on the fact that $B(\lambda) = \lambda^\alpha$ is a Bernstein function for all $0 < \alpha \leq 1$. Indeed, using concavity of $\psi_{1,\delta}(\cdot)$, the measure μ^* is extremal (i.e., it maximizes $\psi_{1,\delta}(\mu)$ with respect to $\mu \in \mathscr{M}$) if and only if the directional derivative

$$F_{\psi_{1,\delta}}(\mu; \nu) = \lim_{\alpha \to 0^+} \frac{\psi_{1,\delta}[(1-\alpha)\mu + \alpha\nu] - \psi_{1,\delta}(\mu)}{\alpha}$$

satisfies $F_{\psi_{1,\delta}}(\mu_k^*; \nu) \leq 0$ for all $\nu \in \mathscr{M}$. Direct calculation gives

$$F_{\psi_{1,\delta}}(\mu; \nu) = 2 \left[\int P_{1,\delta,\mu}(x) \, \nu(\mathrm{d}x) - \psi_{1,\delta}(\mu) \right] \tag{4}$$

and we thus obtain the following.

Theorem 1 *For any $0 < \delta \leq 2$, the measure μ^* maximizes $\psi_{1,\delta}(\mu)$ with respect to $\mu \in \mathscr{M}$ if and only if*

$$\max_{x \in \mathscr{X}} P_{1,\delta,\mu^*}(x) = \psi_{1,\delta}(\mu^*)\,.$$

Equivalently, μ^* minimizes $\max_{x \in \mathscr{X}} [P_{1,\delta,\mu}(x) - \psi_{1,\delta}(\mu)]$ with respect to $\mu \in \mathscr{M}$.

In connection with the statement of the theorem, we may notice that the extremal measure μ^* does not necessarily minimize $\max_{x \in \mathscr{X}} P_{1,\delta,\mu}(x)$, see [2, Th. 14]. In the next section we show how some of the properties that hold for $k = 1$ can be generalized to the functionals $\psi_{k,\delta}(\cdot)$ with $k \geq 2$.

2.2 Functionals based on powered volumes: $k \geq 2$

2.2.1 A necessary condition for optimality

First note that the existence of an extremal measure follows from the continuity of $\mathscr{V}_k(x_1, \ldots, x_{k+1})$ in each x_i, see [2, Th. 1].

Similarly to the case $k = 1$, we can compute the second order derivative of the functional $\psi_{k,\delta}(\cdot)$. Indeed, for any μ_0, μ_1 in $\mathscr{M}$, we have

$$\begin{aligned}\left.\frac{\partial^2 \psi_{k,\delta}[(1-\alpha)\mu_0 + \alpha\mu_1]}{\partial \alpha^2}\right|_{\alpha=0} &= k(k+1)\,[\Psi_{k,\delta}(\mu_0, \ldots, \mu_0, \mu_1, \mu_1) \\ &\quad + \Psi_{k,\delta}(\mu_0, \ldots, \mu_0) - 2\Psi_{k,\delta}(\mu_0, \ldots, \mu_0, \mu_1)]\,, \\ &= k(k+1) \int\int P_{k,\delta}(x,y)\,[\mu_0 - \mu_1](\mathrm{d}x)[\mu_0 - \mu_1](\mathrm{d}y)\,,\end{aligned}$$

where $P_{k,\delta}(x,y) = \int \ldots \int \mathscr{V}_k^\delta(x_1, \ldots, x_{k-1}, x, y)\,\mu_0(\mathrm{d}x_1) \ldots \mu_0(\mathrm{d}x_{k-1})$. The proof is by direct calculation, using the symmetry of the kernel $\mathscr{V}_k^\delta(x_1, \ldots, x_{k+1})$ in (1).

For $k = 1$, $P_{1,\delta}(x,y) = \|x - y\|^\delta$, and $\psi_{1,\delta}(\cdot)$ for $\delta \leq 2$ is concave as discussed above. For $\delta = 2$, concavity of $\psi_{k,2}^{1/k}(\cdot)$ is proved in [11] for any $k \in \{1, \ldots, d\}$. We are not aware of any similar result for $k > 1$ and $\delta \neq 2$, so that we have no guarantee that $\psi_{k,\delta}(\cdot)$, even raised to some power less than 1, is concave for $\delta \neq 2$. Therefore, we can only give a necessary condition of optimality for a measure μ^* maximizing $\psi_{k,\delta}(\cdot)$. A similar result for $k = 1$ is Theorem 2 in [2].

Theorem 2 *For any $0 < \delta$, if the measure μ^* maximizes $\psi_{k,\delta}(\mu)$ with respect to $\mu \in \mathscr{M}$, then*

$$\max_{x \in \mathscr{X}} P_{k,\delta,\mu^*}(x) = \psi_{k,\delta}(\mu^*)$$

and $P_{k,\delta,\mu^*}(x) = \psi_{k,\delta}(\mu^*)$ on the support of μ^*.

The proof relies on a straightforward extension of (4) to $k \geq 1$:

$$F_{\psi_{k,\delta}}(\mu;\nu) = (k+1)\left[\int P_{k,\delta,\mu}(x)\,\nu(\mathrm{d}x) - \psi_{k,\delta}(\mu)\right]\,.$$

2.2.2 Support of extremal measures

Below we indicate some properties concerning the support of extremal measures that generalize those in Section 2.1.

Theorem 3 *For any $\delta > \max\{0, k+1-d\}$, the support of any measure μ_k^* maximizing $\psi_{k,\delta}(\mu)$ is a subset of the boundary of $\mathscr{X}$.*

Proof For $\delta > 1$, we can simply use the convexity property of the L_2 norm and multilinearity of the determinant. Indeed, from Binet-Cauchy formula, the squared volume $\mathscr{V}_k^2(x_1, \ldots, x_{k+1})$ can be written as

$$\mathscr{V}_k^2(x_1, \ldots, x_{k+1}) = \frac{1}{(k!)^2} \sum_{1 \le i_1 < i_2 < \cdots < i_k \le d} \det^2 \begin{bmatrix} \{x_1\}_{i_1} & \cdots & \{x_{k+1}\}_{i_1} \\ \vdots & \vdots & \vdots \\ \{x_1\}_{i_k} & \cdots & \{x_{k+1}\}_{i_k} \\ 1 & \cdots & 1 \end{bmatrix} . \qquad (5)$$

Each determinant in the right-hand side of (5) is linear in x_1, so that, when $\delta > 1$, $\mathscr{V}_k^\delta(x_1, \ldots, x_{k+1})$ is a strictly convex function of x_1. This implies that the potential $P_{k,\delta,\mu_k^*}(x_1)$ is strictly convex in x_1. We then follow similar arguments to those in the proof of [2, Th. 3]. Suppose that x_1 is an interior point of $\mathscr{X}$, and consider a sphere $\mathcal{S}(x_1, r)$ centered at x_1 with radius r included in $\mathscr{X}$. Strict convexity of $P_{k,\delta,\mu_k^*}(\cdot)$ implies that $P_{k,\delta,\mu_k^*}(x_1)$ is strictly smaller than the mean value of $P_{k,\delta,\mu_k^*}(x)$ on $\mathcal{S}(x_1, r)$. From Theorem 2, this mean value is less than or equal to $\psi_{k,\delta}(\mu^*)$, and x_1 cannot be support point of μ_k^*.

For $\delta \le 1$, the proof uses subharmonicity of $P_{k,\delta,\mu_k^*}(\cdot)$ as in [2, Th. 3]. We only need to prove that for fixed $x_2, \ldots, x_{k+1}$, $\mathscr{V}_k^\delta(x_1, \ldots, x_{k+1})$ is a strictly subharmonic function of x_1. From Lemma 2, see Appendix, we have

$$\sum_{i=1}^{d} \frac{\partial^2 \mathscr{V}_k^\delta(x_1, \ldots, x_{k+1})}{\partial \{x_1\}_i^2} = \delta(\delta + d - k - 1)\, \mathscr{V}_k^\delta(x_1, x_2, \ldots, x_{k+1})\, (\mathbf{1}_k^\top A^{-1} \mathbf{1}_k)\,,$$

with A defined in (2) and $\mathbf{1}_k = (1, \ldots, 1)^\top \in \mathbb{R}^k$. The right-hand side is strictly positive when $\delta > k + 1 - d$. □

Theorem 4 *For any $\delta > 1$ and any $k \in \{1, \ldots, d\}$, any measure μ_k^* maximizing $\psi_{k,\delta}(\mu)$ is supported on extreme points of the convex hull of $\mathscr{X}$.*

Proof As shown in the proof of Theorem 3, the potential $P_{k,\delta,\mu_k^*}(x)$ is a strictly convex function of x when $\delta > 1$. Suppose that $x_0 \in \mathscr{X}$ is not an extreme point of the convex hull of $\mathscr{X}$. Then, x_0 can be written as a linear combination of such points z_j with strictly positive weights summing to one. The potential $P_{k,\delta,\mu_k^*}(x_0)$ is then strictly less than the weighted sum of potentials at the z_j, which, from Theorem 2, are all less than or equal to $\psi_{k,\delta}(\mu^*)$. By the same theorem, x_0 cannot be in the support of μ_k^*. □

3 The case $\delta \le 0$

When $\delta < 0$, we are interested in the minimization of the functional $\psi_{k,\delta}(\mu) = \mathsf{E}\{\mathscr{V}_k^\delta(x_1, \ldots, x_{k+1})\}$, $\mu \in \mathscr{M}$. Equivalently, we can consider the maximization of $\psi_{k,\delta}^{1/\delta}(\mu)$, the continuous extension of which at $\delta = 0$ is $\exp\left(\mathsf{E}\{\log[\mathscr{V}_k(x_1, \ldots, x_{k+1})]\}\right)$. We thus define

$$\mathscr{D}_{k,\delta}(\mu) = \begin{cases} \left(\mathsf{E}\{\mathscr{V}_k^\delta(x_1, \ldots, x_{k+1})\}\right)^{1/\delta} & \text{for } \delta \neq 0\,, \\ \exp\left(\mathsf{E}\{\log[\mathscr{V}_k(x_1, \ldots, x_{k+1})]\}\right) & \text{for } \delta = 0\,. \end{cases}$$

The results in Sections 2 have shown that when $\delta > 0$ the support of a measure that maximizes $\mathscr{D}_{k,\delta}$ is sometimes finite and is always included in the boundary of $\mathscr{X}$ when $k \le d-1$. The situation is quite different for $\delta \le 0$, the case we investigate in this section.

In the case $k = 1$, the investigation of the properties of extremal measures $\mu_{1,\delta}^*$ and optimal values $\mathscr{D}_{1,\delta}^* = \mathscr{D}_{1,\delta}(\mu_{1,\delta}^*)$ is one of the main concerns of potential theory,

see e.g., [12]. This is equivalent to studying the asymptotic behavior of the so-called Fekete points, defined as follows. Given a natural number n and a real $\delta \leq 0$, the n points $X_n = (x_1, \ldots, x_n) \in \mathscr{X}^n$ are called Fekete points when they maximize

$$\widehat{\mathscr{D}}_{1,\delta}(X_n) = \left[\frac{2}{n(n-1)} \sum_{1 \leq i < j \leq n} \|x_i - x_j\|^{\delta} \right]^{1/\delta} \tag{6}$$

for $\delta < 0$ and

$$\widehat{\mathscr{D}}_{1,0}(X_n) = \exp\left\{ \frac{2}{n(n-1)} \sum_{1 \leq i < j \leq n} \log\left(\|x_i - x_j\|\right) \right\} \tag{7}$$

for $\delta = 0$, or equivalently minimize the s-energy, $s = -\delta$, defined by $\mathscr{E}^{(s)}(X_n) = \sum_{1 \leq i < j \leq n} \|x_i - x_j\|^{-s}$ for $s > 0$ and by $\mathscr{E}^{(0)}(X_n) = \sum_{1 \leq i < j \leq n} \log \|x_i - x_j\|^{-1}$ for $s = 0$.

We shall denote by $F_n^{(s)}$ a set of n Fekete points, $s \geq 0$. For instance, when $\mathscr{X} = [-1, 1]$, then the set $F_n^{(0)}$ is uniquely defined and coincides with the zeros of $(1 - x^2)P'_{n-1}(x)$, where P_{n-1} is the Legendre polynomial of degree $n - 1$. One may note that $F_n^{(0)}$ corresponds to the support of a D-optimal design measure for polynomial regression of degree $n - 1$ on $[-1, 1]$, see, e.g., [3, p. 89].

The (logarithmic) transfinite diameter of $\mathscr{X}$ is defined by

$$\tau^{(0)}(\mathscr{X}) = \lim_{n \to \infty} \exp\left\{ -\frac{2}{n(n-1)} \mathscr{E}^{(0)}(F_n^{(0)}) \right\} \tag{8}$$

where the convergence to the limit in (8) is monotonic (in the sense that the exponential term in non-increasing with n). The logarithmic potential associated with $\mu \in \mathscr{M}$ is $P_\mu^{(0)}(z) = \int \log(1/\|z - t\|)\, \mu(\mathrm{d}t)$, the corresponding energy is defined by

$$I^{(0)}(\mu) = \int P_\mu^{(0)}(z)\, \mu(\mathrm{d}z) = \int \int \log \frac{1}{\|z - t\|}\, \mu(\mathrm{d}t)\, \mu(\mathrm{d}z)\,.$$

Similarly, the transfinite diameter of order $s > 0$ is

$$\tau^{(s)}(\mathscr{X}) = \lim_{n \to \infty} \left\{ \frac{2}{n(n-1)} \mathscr{E}^{(s)}(F_n^{(s)}) \right\}^{-1},$$

the s-potential for μ is $P_\mu^{(s)}(z) = \int \|z - t\|^{-s}\, \mu(\mathrm{d}t)$, with associated energy

$$I^{(s)}(\mu) = \int P_\mu^{(s)}(z)\, \mu(\mathrm{d}z) = \int \int \frac{1}{\|z - t\|^s}\, \mu(\mathrm{d}t)\, \mu(\mathrm{d}z)\,.$$

The minimum energy problem involves the determination of

$$I_*^{(s)}(\mathscr{X}) = \inf\{I^{(s)}(\mu) : \mu \in \mathscr{M}\}\,.$$

The logarithmic capacity of $\mathscr{X}$, denoted by $\mathrm{cap}^{(0)}(\mathscr{X})$, is defined by $\mathrm{cap}^{(0)}(\mathscr{X}) = \exp\{-I_*^{(0)}(\mathscr{X})\}$; its s-capacity for $s > 0$ is $\mathrm{cap}^{(s)}(\mathscr{X}) = [I_*^{(s)}(\mathscr{X})]^{-1}$. If $\mathrm{cap}^{(0)}(\mathscr{X}) > 0$, then the extremal measure $\mu_{1,0}^*$ exists with $\mathrm{cap}^{(0)}(\mathscr{X}) = \mathscr{D}_{1,0}(\mu_{1,0}^*)$. Also, for any $s > 0$, if $\mathrm{cap}^{(s)}(\mathscr{X}) > 0$ then $\mu_{1,-s}^*$ exists and $\mathrm{cap}^{(s)}(\mathscr{X}) = [\mathscr{D}_{1,-s}(\mu_{1,-s}^*)]^s$. One of the main results in potential theory is that the capacity of $\mathscr{X}$ coincides with its transfinite diameter: $\mathrm{cap}^{(s)}(\mathscr{X}) = \tau^{(s)}(\mathscr{X})$ for all compact sets $\mathscr{X}$. It also coincides with $\sup_{\mu \in \mathscr{M}} \mathscr{D}_{1,0}(\mu)$ when $s = 0$ and with $\sup_{\mu \in \mathscr{M}} [\mathscr{D}_{1,-s}(\mu)]^s$ when $s > 0$. When $\mathrm{cap}^{(s)}(\mathscr{X}) > 0$, which happens in particular when $\mathscr{X}$ is a compact subset of $\mathbb{R}^d$ and $0 \leq s < d$, then $\mu_{1,-s}^*$ exists, it is called s-energy equilibrium measure and is the

weak limit of a sequence of empirical measures associated with Fekete points. Even if $\mathrm{cap}^{(s)}(\mathscr{X}) = 0$ and no measure μ exists with $I^{(s)}(\mu) < \infty$, it is still interesting to study the limiting behaviour of empirical measures of Fekete points, see [4].

Fekete point are extremely difficult to construct, except for a few particular cases. When $s = 0$, Fekete points necessarily lie on $\partial_\infty(\mathscr{X})$, the outer boundary of $\mathscr{X}$. This implies that the extreme (equilibrium) measure $\mu^*_{1,0}$ is supported on $\partial_\infty(\mathscr{X})$ too. Consequently, $\mathrm{cap}^{(0)}(\mathscr{X}) = \mathrm{cap}^{(0)}(\partial_\infty(\mathscr{X}))$. If the outer boundary $\partial_\infty(\mathscr{X})$ is a continuum, then $\mathrm{supp}(\mu^*_{1,0}) = \partial_\infty(\mathscr{X})$. In general, $\partial_\infty(\mathscr{X}) \setminus \mathrm{supp}(\mu^*_{1,0})$ has capacity zero.

Example 1: $d = 1$, $\mathscr{X} = [0, 1]$. The extremal measure $\mu^*_{1,0}$ has the arcsine density

$$\pi_0(t) = \frac{1}{\pi\sqrt{t(1-t)}}$$

on $[0, 1]$ and $\mathrm{cap}^{(0)}(\mathscr{X}) = 1/4$. More generally, the measure $\mu^*_{1,\delta}$ maximizing $\mathscr{D}_{1,\delta}(\mu)$ with $\delta \in (-1, 0]$ corresponds to the Beta distribution on $[0, 1]$ with density

$$\pi_\delta(t) = \frac{1}{B[(1-\delta)/2, (1-\delta)/2]} \frac{1}{\sqrt{[t(1-t)]^{\delta+1}}},$$

see, e.g., [14]. This distribution is uniform for $\delta = -1$, with $\mathscr{E}^{(0)}(F^{(0)}_n)$ growing as $n^2 \log n$, and, as mentioned in [4], the limiting distribution of Fekete points is uniform for every $\delta \le -1$.

Example 2: $\mathscr{X} = \mathscr{B}_d(\mathbf{0}, \rho)$. As indicated in [4], the extremal measure $\mu^*_{1,\delta}$ maximizing $\mathscr{D}_{1,\delta}(\cdot)$ is uniquely defined for $-d < \delta \le 0$ (as the $|\delta|$-energy equilibrium measure). From [6, p. 163], $-d < \delta < 2 - d$, it has the density

$$\varphi_\delta(x) = \frac{C}{(\rho^2 - \|x\|^2)^{(d+\delta)/2}}, \; x \in \mathscr{B}_d(\mathbf{0}, \rho),$$

where $C = R^\delta \pi^{-d/2} \Gamma(1 - \delta/2)/\Gamma(1 - (d + \delta)/2)$. For $2 - d \le \delta \le 0$, $\mu^*_{1,\delta}$ is uniform on the sphere $\mathcal{S}_d(\mathbf{0}, \rho)$. For $\delta \le -d$, any sequence of Fekete points is asymptotically uniformly distributed in $\mathscr{B}_d(\mathbf{0}, \rho)$, with $\mathscr{E}^{(-\delta)}(F^{(-\delta)}_n)$ growing as $n^2 \log n$ for $\delta = -d$ and as $n^{1-\delta/d}$ for $\delta < -d$, see [4].

To the best of our knowledge, no theory is available which would cover the case $k > 1$. In the next section we only present results concerning a particular example which illustrate the difference with the case $k = 1$.

4 Particular case: $\mathscr{X} = \mathscr{B}_d(\mathbf{0}, \rho)$

Take $\mathscr{X} = \mathscr{B}_d(\mathbf{0}, \rho)$, the closed ball of $\mathbb{R}^d$ centered at the origin $\mathbf{0}$ with radius ρ.

Case $\delta = 2$. Let μ_0 be the uniform measure on the sphere $\mathcal{S}_d(\mathbf{0}, \rho)$ (the boundary of $\mathscr{B}_d(\mathbf{0}, \rho)$). Then, the covariance matrix $V_{\mu_0} = \int xx^\top \mu_0(\mathrm{d}x)$ is proportional to the identity matrix I_d, $V_{\mu_0} = \rho^2 I_d/d$. Take $k = d$. We have

$$\max_{x \in \mathscr{X}} x^\top \nabla_{\psi_{d,2}}[V_{\mu_0}]x = \frac{(d+1)\rho^{2d}}{d^{d-1}d!} = \mathrm{trace}\{V_{\mu_0} \nabla_{\psi_{d,2}}[V_{\mu_0}]\},$$

where $\nabla_{\psi_{d,2}}[V_\mu] = [(d+1)/d!] \det(V_\mu) V_\mu^{-1}$ is the gradient of $\psi_{d,2}(\mu)$ considered as a function of V_μ, see [11]. From Theorem 4.1 in the same paper, this implies that μ_0 maximizes $\psi_{d,2}(\mu)$.

Let μ_d be the measure that allocates mass $1/(d+1)$ at each vertex of a d regular simplex having its $d+1$ vertices on $\mathcal{S}_d(\mathbf{0},\rho)$, with squared volume $\rho^{2d}(d+1)^{d+1}/[d^d(d!)^2]$. We also have $V_{\mu_d} = \rho^2 I_d/d$, so that μ_d also maximizes $\psi_{d,2}(\cdot)$. In view of [11, Remark 4.2], μ_0 and μ_d maximize $\psi_{k,2}$ for all k in $\{1,\ldots,d\}$.

Let now μ_k be the measure that allocates mass $1/(k+1)$ at each vertex of a k regular simplex $\mathscr{P}_k$, centered at the origin, with its vertices on $\mathcal{S}_d(\mathbf{0},\rho)$. The squared volume of $\mathscr{P}_k$ equals $\rho^{2k}\,(k+1)^{k+1}/[k^k(k!)^2]$. Without any loss of generality, we can choose the orientation of the space so that V_{μ_k} is diagonal, with its first k diagonal elements equal to ρ^2/k and the other elements equal to zero. Note that $\psi_{k',2}(\mu_k) = 0$ for $k' > k$. Direct calculations give

$$\psi_{k,2}(\mu_k) = \frac{k+1}{k!}\,\frac{\rho^{2k}}{k^k} \le \psi_k(\mu_0) = \frac{k+1}{k!}\binom{d}{k}\frac{\rho^{2k}}{d^k}\,,$$

with equality for $k=1$ and $k=d$, the inequality being strict otherwise. Figure 1 presents the efficiency $[\psi_{k,2}(\mu_k)/\psi_{k,2}(\mu_0)]^{1/k}$ as a function of k when $d=20$.

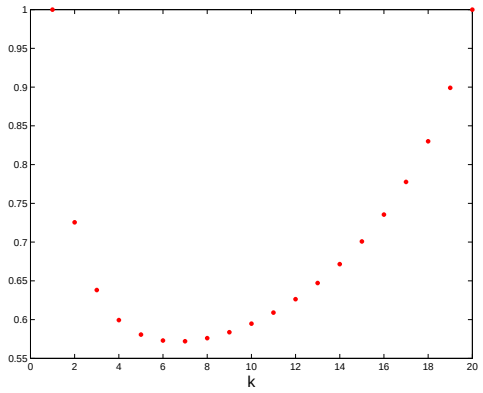

Fig. 1 Efficiency $[\psi_{k,2}(\mu_k)/\psi_{k,2}(\mu_0)]^{1/k}$ as a function of k when $d=20$

Case $\delta > 2$. We can show that for any $\delta > 2$ the measure μ maximizes $\psi_{d,\delta}(\cdot)$ if and only if it coincides with one of the measures μ_d introduces above.

The proof follows closely that of Theorem 7 in [2] which concerns the case $k=1$. We have

$$\begin{aligned}\psi_{d,\delta}(\mu) &= \int \mathscr{V}_d^{\delta-2}(x_1,\ldots,x_{d+1})\,\mathscr{V}_d^2(x_1,\ldots,x_{d+1})\,\mu(\mathrm{d}x_1)\ldots\mu(\mathrm{d}x_{d+1})\\ &\le \max_{x_1,\ldots,x_{d+1}} \mathscr{V}_d^{\delta-2}(x_1,\ldots,x_{d+1}) \int \mathscr{V}_d^2(x_1,\ldots,x_{d+1})\,\mu(\mathrm{d}x_1)\ldots\mu(\mathrm{d}x_{d+1})\,. \quad (9)\end{aligned}$$

Since $\mathscr{V}_d^* = \max_{x_1,\ldots,x_{d+1}} \mathscr{V}_d(x_1,\ldots,x_{d+1}) = \rho^d(d+1)^{(d+1)/2}/[d^{d/2}\,d!]$ and the uniform measure μ_0 on the sphere $\mathcal{S}_d(\mathbf{0},\rho)$ is extremal for $\psi_{d,2}(\cdot)$, we get

$$\psi_{d,\delta}(\mu) \le \left(\frac{\rho^{2d}(d+1)^{d+1}}{d^d(d!)^2}\right)^{\delta/2-1} \psi_{d,2}(\mu_0) = \rho^{d\delta}\,\frac{(d+1)^{(d+1)\delta/2-d}}{(d!)^{\delta-1}\,d^{d\delta/2}}\,.$$

On the other hand, this is exactly the value $\psi_{d,\delta}(\mu_d)$. Therefore, for the measure μ to be extremal we need to have equality in (9), which requires that $\mathscr{V}_d(x_1,\ldots,x_{d+1}) = \mathscr{V}_d^*$ for all $(k+1)$-tuples that contribute to the integral. This forces the extremal measure to have the form indicated.

Consider the case $d = 2$, $\rho = 1$. Figure 2 presents the potential $P_{2,\delta,\mu_2}(x(t))$ with $x(t) = (\cos(t), \sin(t))$ as a function of $t \in [0, 2\pi]$ for $\delta = 1$ (left) and $\delta = 4$ (right), with μ_2 allocating weight $1/3$ at each of the three points $(1, 0)$, $(\cos(2\pi/3), \sin(2\pi/3))$ and $(\cos(4\pi/3), \sin(4\pi/3))$. The value of $\psi_{2,\delta}(\mu_2)$ is indicated in dashed line. The figure illustrates the fact that μ_2 is extremal for $\psi_{2,4}(\cdot)$ but is not extremal for $\psi_{2,1}(\cdot)$ since the necessary condition of Theorem 2 is violated. The analytic forms for the potentials are $P_{2,1,\mu_2}(x(t)) = (\sqrt{3}/18) + (\sqrt{3}/9)\cos(t) + (1/3)\sin(t)$ for $0 \le t \le 2\pi/3$ and $P_{2,4,\mu_2}(x(t)) = 57/128 + (3/16)\cos(3t)$ for $0 \le t \le 2\pi$.

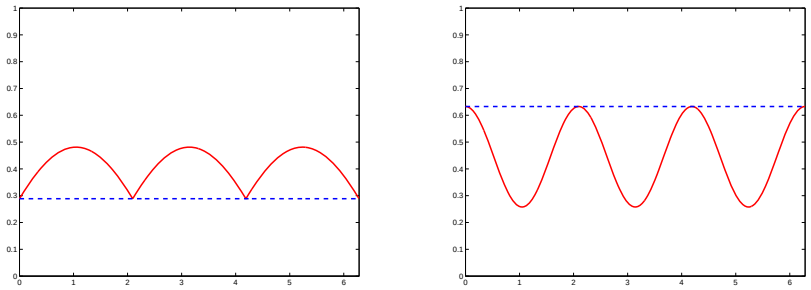

Fig. 2 Potential $P_{2,\delta,\mu_2}(x(t))$, with $x(t) = (\cos(t), \sin(t))$, as a function of $t \in [0, 2\pi]$ (solid line) and value of $\psi_{2,\delta}(\mu_2)$ (dashed line) for $\delta = 1$ (left) and $\delta = 4$ (right); μ_2 allocates weight $1/3$ at each point of an equilateral triangle with vertices on $\mathcal{S}_2(\mathbf{0}, 1)$

Uniform measure on the circle $\mathcal{S}_2(\mathbf{0}, 1)$. Assume that $k = d = 2$, $\mathscr{X} = \mathscr{B}(\mathbf{0}, 1)$, and consider the uniform measure $\mu_{\mathcal{S}}$ on $\mathcal{S}_2(\mathbf{0}, 1)$, which is optimal for $\delta = 2$.

Consider n-point sets X_n containing the points $x_j = (\cos(2\pi j/n), \sin(2\pi j/n))$, $j = 0, \ldots, n-1$, with empirical measure converging to $\mu_{\mathcal{S}}$. The empirical version of (1) is

$$\psi_{2,\delta}(X_n) = \frac{2}{(n-1)(n-2)} \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \mathscr{V}_2^{\delta}(x_0, x_i, x_j)\,.$$

Direct calculations give

$$\begin{aligned}
\psi_{2,1}(X_n) &= \frac{3\,n}{2(n-1)(n-2)}\,\cot(\pi/n) = \frac{3}{2\,\pi}\left(1 + \frac{3}{n} + O\left(n^{-2}\right)\right)\\
\psi_{2,2}(X_n) &= \frac{3\,n^2}{2^3(n-1)(n-2)}\\
\psi_{2,3}(X_n) &= \frac{35}{32\,\pi}\left(1 + \frac{3}{n} + O\left(n^{-2}\right)\right)\\
\psi_{2,4}(X_n) &= \frac{45\,n^2}{2^7\,(n-1)(n-2)}\\
\psi_{2,5}(X_n) &= \frac{3003}{2560\,\pi}\left(1 + \frac{3}{n} + O\left(n^{-2}\right)\right)\\
\psi_{2,6}(X_n) &= \frac{105\,n^2}{2^8\,(n-1)(n-2)}\\
\psi_{2,8}(X_n) &= \frac{17325\,n^2}{2^{15}\,(n-1)(n-2)}
\end{aligned}$$

Figure 3 presents $\psi_{2,\delta}(\mu_{\mathcal{S}})$ as a function of $\delta \in [0, 8]$. The stars indicate the exact values obtained from the expressions above.

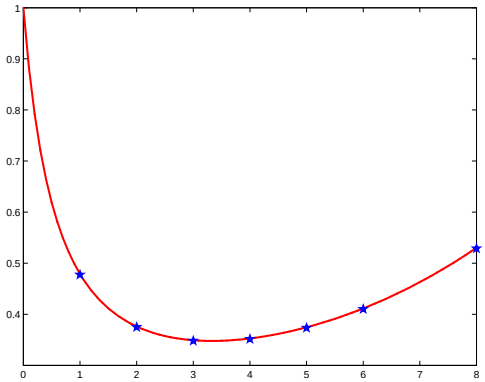

Fig. 3 $\psi_{2,\delta}(\mu_{\mathcal{S}})$ as a function of $\delta \in [0,8]$, for $\mu_{\mathcal{S}}$ uniform on $\mathcal{S}_2(\mathbf{0},1)$

By considering the potential $P_{2,\delta,\mu_{\mathcal{S}}}(\cdot)$ at the origin $\mathbf{0}$ for δ close to zero, we can show that the necessary condition of Theorem 2 for $\mu_{\mathcal{S}}$ being optimal is violated for $\delta < 0$. Indeed, we have

$$\psi_{2,\delta}(\mu_{\mathcal{S}}) = 1-(2\log 2)\,\delta+c_1\delta^2+O(\delta^3)\,, \quad P_{2,\delta,\mu_{\mathcal{S}}}(\mathbf{0}) = 1-(2\log 2)\,\delta+c_2\delta^2+O(\delta^3)\,,$$

with $c_1 \simeq 2.1946$ and $c_2 \simeq 1.3721$, so that $P_{2,\delta,\mu_{\mathcal{S}}}(\mathbf{0}) < \psi_{2,\delta}(\mu_{\mathcal{S}})$ for all $\delta \neq 0$. However, for negative δ, $\psi_{2,\delta}(\cdot)$ should be minimized, the necessary condition for optimality of μ^* becomes $P_{2,\delta,\mu^*}(x) \geq \psi_{2,\delta}(\mu^*)$ for any $x \in \mathcal{B}(\mathbf{0},1)$, and is thus violated for $\mu_{\mathcal{S}}$ at $x = \mathbf{0}$. Although $\mu_{\mathcal{S}}$ is not optimal for negative δ, $\psi_{2,\delta}(\mu_{\mathcal{S}})$ remains finite for $\delta > -2/3$. If $\mathcal{X}$ is reduced to the circle $\mathcal{S}_2(\mathbf{0},1)$, then the n-point sets X_n are Fekete points (in the usual sense, for $k=1$) and can be considered as generalized Fekete points for $k=2$. One can show that $\psi_{2,\delta}(X_n) = O(n^{-(2+3\delta)})$ for $\delta < -2/3$.

On the other hand, for $k=1$, the measure $\mu_{\mathcal{S}}$ is optimal for $0 \leq \delta \leq 2$ and $\psi_{1,\delta}(\mu_{\mathcal{S}})$ is finite for all $\delta > -1$; $\lim_{n\to\infty} \mathscr{E}^{(1)}(X_n)/(n^2\log n) = 1$ and $\mathscr{E}^{(-\delta)}(X_n)$ grows like $n^{1-\delta}$ ($\psi_{1,\delta}(X_n)$ grows like $n^{-(1+\delta)}$) for $\delta < -1$.

5 Generalized Fekete points and design criteria for computer experiments

For a n-point sample, or design, $X_n = \{x_1,\ldots,x_n\}$, $n \geq k+1$, as extensions of (6) and (7), we define

$$\widehat{\mathscr{D}}_{k,\delta}(X_n) = \left[\binom{n}{k+1}^{-1} \sum_{1\leq j_1<j_2<\cdots<j_{k+1}\leq n} \mathscr{V}_k^{\delta}(x_{j_1},\ldots,x_{j_{k+1}})\right]^{1/\delta}, \ \delta \neq 0\,,$$

and

$$\widehat{\mathscr{D}}_{k,0}(X_n) = \exp\left\{\binom{n}{k+1}^{-1} \sum_{1\leq j_1<j_2<\cdots<j_{k+1}\leq n} \log\left[\mathscr{V}_k(x_{j_1},\ldots,x_{j_{k+1}})\right]\right\}.$$

The functions $\widehat{\mathscr{D}}_{1,\delta}(\cdot)$ with $\delta \leq 0$ have been suggested as criteria to be maximized for the construction of space-filling designs for computer experiments. An optimal design $X^*_{n,1,\delta}$ maximizing $\widehat{\mathscr{D}}_{1,\delta}(X_n)$ is a set of Fekete points, as defined in Section 3. In particular, $\widehat{\mathscr{D}}_{1,-2}(\cdot)$ corresponds to the energy criterion considered in [1]; see also [8,9].

Lemma 1 *Take $\delta \le 0$, $k \in \{1,\dots,d\}$, and consider a design X_n with $\widehat{\mathscr{D}}_{k,\delta}(X_n) > 0$. Then, for any $k' \in \{1,\dots,k\}$, the projection of X_n on any $(d+1-k')$-dimensional linear subspace contains at least $\lfloor n/k' \rfloor + n(\mathrm{mod}\, k')$ distinct elements.*

Proof Take $k' \in \{1,\dots,k\}$, any $(k'-1)$-dimensional subspace of $\mathbb{R}^d$ contains k' points at most since otherwise one could find $k+1$ points in the same $(k-1)$-dimensional subspace, contradicting the property $\widehat{\mathscr{D}}_{k,\delta}(X_n) > 0$. Consider the projection p_i of one point x_i of X_n on a $(d+1-k')$-dimensional linear subspace. There are necessarily k' points at most in X_n, including x_i itself, that yield the same projection p_i. □

One may notice the difference with the usual projection properties considered in design for computer experiments, where only projections onto fixed canonical subspaces are considered. For instance, Latin hypercube design [7] ensures that all projections on coordinate axes have exactly n points; however, it does not protect against all points lying on a single line.

Letting δ tend to $-\infty$ in $\widehat{\mathscr{D}}_{1,\delta}(\cdot)$ yields maximin-distance optimal design, see [5], equivalent to the solution of a sphere-packing problem. More generally, for a given sample X_n, we define

$$\widehat{\mathscr{D}}_{k,-\infty}(X_n) = \min_{1\le j_1<j_2<\cdots<j_{k+1}\le n} \mathscr{V}_k(x_{j_1},\dots,x_{j_{k+1}})\,. \tag{10}$$

Then, $\widehat{\mathscr{D}}_{k,-\infty}(X_n) \le \widehat{\mathscr{D}}_{k,\delta}(X_n)$ for any $\delta \in \mathbb{R}$, with $\lim_{\delta\to-\infty} \widehat{\mathscr{D}}_{k,\delta}(X_n) = \widehat{\mathscr{D}}_{k,-\infty}(X_n)$. Also, if $X^*_{n,k,\delta} \in \mathscr{X}^n$ maximizes $\widehat{\mathscr{D}}_{k,\delta}(\cdot)$ and $X^*_{n,k,-\infty} \in \mathscr{X}^n$ is a maximin-optimal design that maximizes $\widehat{\mathscr{D}}_{k,-\infty}(\cdot)$, then we have the following bound on the maximin-efficiency of $X^*_{n,k,\delta}$,

$$\frac{\widehat{\mathscr{D}}_{k,-\infty}(X^*_{n,k,\delta})}{\widehat{\mathscr{D}}_{k,-\infty}(X^*_{n,k,-\infty})} \ge \binom{n}{k+1}^{1/\delta},$$

see [10, Chap. 8]. In general, $\widehat{\mathscr{D}}_{1,\delta}(\cdot)$ with δ not too small is easier to optimize than $\widehat{\mathscr{D}}_{1,-\infty}(\cdot)$, see, e.g., [1,8]; one may expect the same to be true for $k > 1$. Notice that from the discussion in Section 3, it is recommended to choose $\delta \le -d$ to obtain designs evenly spread over $\mathscr{X}$ when maximizing $\widehat{\mathscr{D}}_{1,\delta}(\cdot)$. Also note that, contrary to $\widehat{\mathscr{D}}_{1,-\infty}(X_n)$ which only depends on the relative distances between neighboring pairs of points, the value of $\widehat{\mathscr{D}}_{k,-\infty}(X_n)$ with $k > 1$ is influenced by the respective positions of points whatever their relative distances, see Lemma 1.

Example 3. We report the maximin optimal designs we have calculated for values of n between 5 and 8 for $d = 2$ and $\mathscr{X} = [0,1]^2$. Note that we have in fact equivalence classes of optimal designs, considering symmetries ($\{x\}_i \mapsto 1 - \{x\}_i$, $i = 1,2$) and a permutation of coordinates; only one representant is indicated. We represent designs as matrices, with column i corresponding to coordinates of the i-th design point. Maximin-distance optimal designs ($k = 1$) can be found for instance at `http://www.packomania.com/`. We have used the following procedure to determine maximin optimal designs for $\widehat{\mathscr{D}}_{2,-\infty}(\cdot)$: (*i*) a global random search algorithm, initialized at a random Latin hypercube design, generates a first design $X_n^{(1)}$; (*ii*) a local maximization (subgradient-type method, see Appendix) initialized at $X_n^{(1)}$, generates a second design $X_n^{(2)}$; (*iii*) the configuration of the best design obtained after several repetitions of steps (*i*) and (*ii*) is used to determine analytically the optimal design having this configuration. Although we only proved local optimality, we conjecture that the designs presented are indeed optimal for $\widehat{\mathscr{D}}_{2,-\infty}(\cdot)$.

The maximin-distance optimal design ($k = 1$) with $n = 5$ points is

$$X^*_{5,1,-\infty} = \begin{bmatrix} 0 & 1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1 & 1/2 \end{bmatrix},$$

with $\widehat{\mathscr{D}}_{1,-\infty}(X^*_{5,1,-\infty}) = \sqrt{2}/2 \simeq 0.70711$. For $k = 2$, we get $\widehat{\mathscr{D}}_{2,-\infty}(X^*_{5,1,-\infty}) = 0$ since the presence of a central point produces two alignements of three points. On the other hand, the optimal design that we have obtained for $\widehat{\mathscr{D}}_{2,-\infty}(\cdot)$ is

$$X^*_{5,2,-\infty} = \begin{bmatrix} 1/3 & 1 & 1 & 1-\sqrt{3}/3 & 0 \\ 0 & 0 & 2/3 & 1 & \sqrt{3}/3 \end{bmatrix},$$

with $\widehat{\mathscr{D}}_{1,-\infty}(X^*_{5,2,-\infty}) = \sqrt{2}(1-\sqrt{3}/3) \simeq 0.59771$ and $\widehat{\mathscr{D}}_{2,-\infty}(X^*_{5,2,-\infty}) = \sqrt{3}/9 \simeq 0.19245$.

For $n = 6$, there exists a continuum of maximin optimal designs $X^*_{6,2,-\infty}$, of the form

$$X^*_{6,2,-\infty} = \begin{bmatrix} 1/2 & 1 & 1 & 1/2 & 0 & 0 \\ 0 & 1/2-a & 1-a & 1 & 1/2+a & a \end{bmatrix}, \ a \in [0, 1/2],$$

all with $\widehat{\mathscr{D}}_{2,-\infty}(X^*_{6,2,-\infty}) = 1/8$. Notice that $X^*_{5,2,-\infty}$ and $X^*_{6,2,-\infty}$ do not contain any central point.

For $n = 7$, we have obtained

$$X^*_{7,2,-\infty} = \begin{bmatrix} 0 & 2/3 & 1 & 1 & 2/3 & 0 & 1/6 \\ 0 & 0 & 1/4 & 3/4 & 1 & 1 & 1/2 \end{bmatrix},$$

with $\widehat{\mathscr{D}}_{2,-\infty}(X^*_{7,2,-\infty}) = 1/12 \simeq 0.08333$.

The maximin optimal design for $k = 2$ and $n = 8$ is

$$X^*_{8,2,-\infty} = \begin{bmatrix} a & 1 & 1 & 1-a & 0 & 0 & c & 1-c \\ 0 & 0 & 1-b & 1 & 1 & b & 1-b & b \end{bmatrix},$$

with $a = (7-\sqrt{13})/18$, $b = (5-\sqrt{13})/6$ and $c = (7-\sqrt{13})/9$, with $\widehat{\mathscr{D}}_{2,-\infty}(X^*_{8,2,-\infty}) = (1+\sqrt{13})(7-\sqrt{13})/216 \simeq 0.072376$.

The designs $X^*_{5,2,-\infty}$ to $X^*_{8,2,-\infty}$ are presented on Figure 4. The circles centered at the design points have radius $r_n = \widehat{\mathscr{D}}_{1,-\infty}(X_n)/2$, with $r_n < \widehat{\mathscr{D}}_{1,-\infty}(X^*_{n,1,-\infty})/2$ since the designs X_n are not maximin-distance optimal. On the other hand, any triplet of design points forms a triangle with area at least $\widehat{\mathscr{D}}_{2,-\infty}(X^*_{n,2,-\infty})$. Note that for each n equality is achieved for several triplets of points. For instance, when $n = 5$, the area of the four triangles ABE, ADE, CDE and BCD on Figure 4-top-left equals $\widehat{\mathscr{D}}_{2,-\infty}(X^*_{5,2,-\infty}) = \sqrt{3}/9$, and any other five-point design contains a triangle with area $\mathcal{A} \leq \sqrt{3}/9$.

Appendix

Lemma 2 *Consider matrix A given by* (2)*. The Laplacian of* $\det^\alpha(A)$ *considered as a function of* x_1 *is*

$$\sum_{i=1}^{d} \frac{\partial^2 \det^\alpha(A)}{\partial \{x_1\}_i^2} = 2\alpha(2\alpha + d - k - 1) \det^\alpha(A) \, (\mathbf{1}_k^\top A^{-1} \mathbf{1}_k), \tag{11}$$

where $\mathbf{1}_k = (1, \ldots, 1)^\top \in \mathbb{R}^k$.

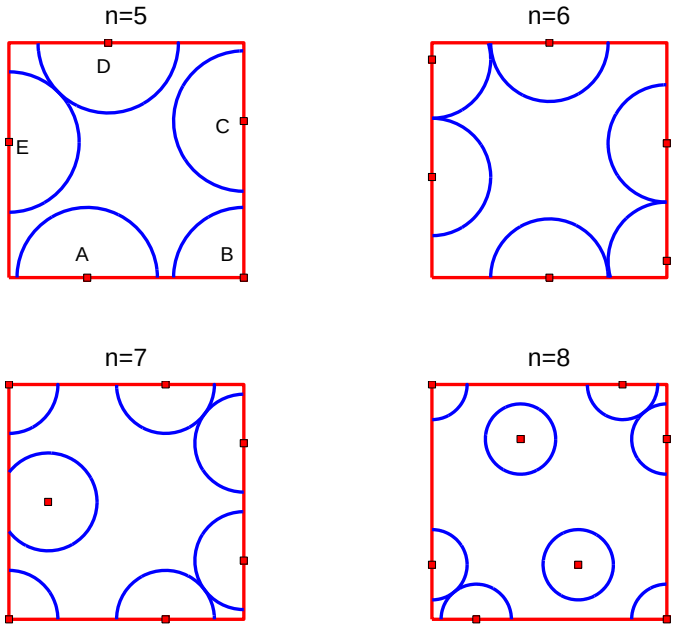

Fig. 4 Optimal designs for $\widehat{\mathscr{D}}_{2,-\infty}(\cdot)$ for n from 5 to 8; $a = 3/7$ in $X^*_{6,2,-\infty}$; the circles have radius $\widehat{\mathscr{D}}_{1,-\infty}(X_n)/2$

Proof We have

$$\begin{aligned}
\frac{\partial \det(A)}{\partial \{x_1\}_i} &= \det(A)\,\mathrm{trace}\left(A^{-1}\frac{\partial A}{\partial \{x_1\}_i}\right)\\
\frac{\partial^2 \det(A)}{\partial \{x_1\}_i^2} &= -\det(A)\,\mathrm{trace}\left(A^{-1}\frac{\partial A}{\partial \{x_1\}_i}A^{-1}\frac{\partial A}{\partial \{x_1\}_i}\right)\\
&\qquad + \det(A)\,\mathrm{trace}^2\left(A^{-1}\frac{\partial A}{\partial \{x_1\}_i}\right) + \det(A)\,\mathrm{trace}\left(A^{-1}\frac{\partial^2 A}{\partial \{x_1\}_i^2}\right),
\end{aligned}$$

where $\partial A/\partial\{x_1\}_i = -[\mathbf{1}_k \Delta_i^\top + \Delta_i \mathbf{1}_k^\top]$ and $\partial^2 A/\partial\{x_1\}_i^2 = 2\mathbf{1}_k\mathbf{1}_k^\top$, with $\Delta_i = (\{x_2 - x_1\}_i, \ldots, \{x_{k+1} - x_1\}_i)^\top \in \mathbb{R}^k$. This gives

$$\frac{\partial^2 \det(A)}{\partial \{x_1\}_i^2} = 2\,\det(A)\,\left\{\mathbf{1}_k^\top A^{-1}\mathbf{1}_k(1 - \Delta_i^\top A^{-1}\Delta_i) + (\mathbf{1}_k^\top A^{-1}\Delta_i)^2\right\}.$$

Noting that $\sum_{i=1}^d \Delta_i\Delta_i^\top = A$, we have $\sum_{i=1}^d \Delta_i^\top A^{-1}\Delta_i = \mathrm{trace}(I_k) = k$ and obtain

$$\begin{aligned}
\sum_{i=1}^d \left(\frac{\partial \det(A)}{\partial \{x_1\}_i}\right)^2 &= \det^2(A)\sum_{i=1}^d \mathrm{trace}^2\left(A^{-1}\frac{\partial A}{\partial \{x_1\}_i}\right)\\
&= \det^2(A)\sum_{i=1}^d \mathrm{trace}^2\left(A^{-1}[\mathbf{1}_k\Delta_i^\top + \Delta_i\mathbf{1}_k^\top]\right)\\
&= 4\det^2(A)\,\mathbf{1}_k^\top A^{-1}\mathbf{1}_k
\end{aligned}$$

and

$$\sum_{i=1}^d \frac{\partial^2 \det(A)}{\partial \{x_1\}_i^2} = 2\det(A)\,\mathbf{1}_k^\top A^{-1}\mathbf{1}_k\,(d + 1 - k).$$

Now,

$$\frac{\partial \det^{\alpha}(A)}{\partial \{x_1\}_i} = \alpha \det{}^{\alpha-1}(A) \frac{\partial \det(A)}{\partial \{x_1\}_i}$$
$$\frac{\partial^2 \det^{\alpha}(A)}{\partial \{x_1\}_i^2} = \alpha(\alpha-1) \det{}^{\alpha-2}(A) \left(\frac{\partial \det(A)}{\partial \{x_1\}_i} \right)^2 + \alpha \det(A)^{\alpha-1} \frac{\partial^2 \det(A)}{\partial \{x_1\}_i^2},$$

which finally gives (11). □

A subgradient-type algorithm to maximize $\widehat{\mathscr{D}}_{k,-\infty}(\cdot)$.

Consider a design $X_n = (x_1, \ldots, x_n)$, with each $x_i \in \mathscr{X}$, a convex subset of $\mathbb{R}^d$, as a vector in $\mathbb{R}^{n \times d}$. The function $\widehat{\mathscr{D}}_{k,-\infty}(\cdot)$ defined in (10) is not concave (due to the presence of min), but is Lipschitz and thus differentiable almost everywhere. At points X_n where it fails to be differentiable, we consider any particular gradient from the subdifferential,

$$\nabla \widehat{\mathscr{D}}_{k,-\infty}(X_n) = \nabla v_{j_1,\ldots,j_{k+1}}(X_n)$$

where $x_{j_1}, \ldots, x_{j_{k+1}}$ are such that $\mathscr{V}_k(x_{j_1}, \ldots, x_{j_{k+1}}) = \widehat{\mathscr{D}}_{k,-\infty}(X_n)$ and where $\nabla v_{j_1,\ldots,j_{k+1}}(X_n)$ denotes the usual gradient of the function $\mathscr{V}_k(x_{j_1}, \ldots, x_{j_{k+1}})$. Our subgradient-type algorithm then corresponds to the following sequence of iterations, where the current design $X_n^{(t)}$ is updated into

$$X_n^{(t+1)} = P_{\mathscr{X}} \left[X_n^{(t)} + \gamma_t \nabla \widehat{\mathscr{D}}_{k,-\infty}(X_n^{(t)}) \right],$$

where $P_{\mathscr{X}}[\cdot]$ denotes the orthogonal projection on $\mathscr{X}$ and $\gamma_t > 0$, $\gamma_t \searrow 0$, $\sum_t \gamma_t = \infty$, $\sum_t \gamma_t^2 < \infty$.

Direct calculation gives

$$\frac{\partial v_{j_1,\ldots,j_{k+1}}(X_n)}{\partial \{x_j\}_\ell} = \begin{cases} 0 & \text{if } j \notin \{j_1, \ldots, j_{k+1}\} \\ \frac{1}{2k!} \det{}^{1/2}(A_{j_1,\ldots,j_{k+1}}) \operatorname{trace}\left[A^{-1}_{j_1,\ldots,j_{k+1}} \frac{\partial A_{j_1,\ldots,j_{k+1}}}{\partial \{x_j\}_\ell} \right] & \text{otherwise,} \end{cases}$$

where

$$A_{j_1,\ldots,j_{k+1}} = \left(\begin{bmatrix} (x_{j_2} - x_{j_1})^\top \\ (x_{j_3} - x_{j_1})^\top \\ \vdots \\ (x_{j_{k+1}} - x_{j_1})^\top \end{bmatrix} \left[(x_{j_2} - x_{j_1}) \; (x_{j_3} - x_{j_1}) \; \cdots (x_{j_{k+1}} - x_{j_1}) \right] \right),$$

so that

$$\operatorname{trace}\left[A^{-1}_{j_1,\ldots,j_{k+1}} \frac{\partial A_{j_1,\ldots,j_{k+1}}}{\partial \{x_j\}_\ell} \right] = 2 \left\{ A^{-1}_{j_1,\ldots,j_{k+1}} \begin{bmatrix} \{(x_{j_2} - x_{j_1})\}_\ell \\ \{(x_{j_3} - x_{j_1})\}_\ell \\ \vdots \\ \{(x_{j_{k+1}} - x_{j_1})\}_\ell \end{bmatrix} \right\}_{j-1}$$

for $j \in \{j_1, \ldots, j_{k+1}\}$, $j \neq j_1$, and

$$\operatorname{trace}\left[A^{-1}_{j_1,\ldots,j_{k+1}} \frac{\partial A_{j_1,\ldots,j_{k+1}}}{\partial \{x_{j_1}\}_\ell} \right] = -2 \sum_{i=1}^{k} \left\{ A^{-1}_{j_1,\ldots,j_{k+1}} \begin{bmatrix} \{(x_{j_2} - x_{j_1})\}_\ell \\ \{(x_{j_3} - x_{j_1})\}_\ell \\ \vdots \\ \{(x_{j_{k+1}} - x_{j_1})\}_\ell \end{bmatrix} \right\}_i .$$

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