



HAL
open science

Approximate D-optimal design and equilibrium measure

*

Didier Henrion, Jean Bernard Lasserre

► **To cite this version:**

Didier Henrion, Jean Bernard Lasserre. Approximate D-optimal design and equilibrium measure *. 2024. hal-04688534

HAL Id: hal-04688534

<https://hal.science/hal-04688534>

Preprint submitted on 5 Sep 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Approximate D-optimal design and equilibrium measure*

Didier Henrion^{1,2}, Jean Bernard Lasserre^{2,3}

Draft of September 5, 2024

Abstract

We introduce a variant of the D-optimal design of experiments problem with a more general information matrix that takes into account the representation of the design space S . The main motivation is that if $S \subset \mathbb{R}^d$ is the unit ball, the unit box or the canonical simplex, then remarkably, for every dimension d and every degree n , the equilibrium measure of S (in pluripotential theory) is an optimal solution. Equivalently, for each degree n , the unique optimal solution is the vector of moments (up to degree $2n$) of the equilibrium measure of S . Hence finding an optimal design reduces to finding a cubature for the equilibrium measure, with atoms in S , positive weights, and exact up to degree $2n$. In addition, any resulting sequence of atomic D-optimal measures converges to the equilibrium measure of S for the weak-star topology, as n increases. Links with Fekete sets of points are also discussed. More general compact basic semi-algebraic sets are also considered, and a previously developed two-step design algorithm is easily adapted to this new variant of D-optimal design problem.

1 Introduction

In this paper we consider the approximate D-optimal design problem

$$\max_{\phi \in \mathcal{P}(S)} \log \det \mathbf{M}_n(\phi), \quad (1)$$

where $S \subset \mathbb{R}^d$ is compact, $\mathcal{P}(S)$ is the set of probability measures on S , and with $\mathbf{v}_n(\mathbf{x}) := (\mathbf{x}^\alpha)_{\alpha \in \mathbb{N}_n^d}$,

$$\mathbf{M}_n(\phi) := \int_S \mathbf{v}_n(\mathbf{x}) \mathbf{v}_n(\mathbf{x})^T d\phi(\mathbf{x})$$

¹CNRS; LAAS; Université de Toulouse, France.

²Faculty of Electrical Engineering, Czech Technical University in Prague, Czechia.

³Toulouse School of Economics (TSE), Toulouse, France.

*The second author was supported by the AI Interdisciplinary Institute ANITI funding through the french program "Investing for the Future PI3A" under the grant agreement number ANR-19-PI3A-0004. This research is also part of the programme DesCartes and is supported by the National Research Foundation, Prime Minister's Office, Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) programme.

denotes the degree- n moment matrix of ϕ .

We restrict to three specific sets S , namely the Euclidean unit ball, the unit box, and the canonical simplex. We introduce the following slight variant of (1):

$$\max_{\phi \in \mathcal{P}(S)} \log \det(\mathbf{M}_n(\phi)) + \sum_{g \in G} \log \det(\mathbf{M}_{n-d_g}(g\phi)) \quad (2)$$

where $G \subset \mathbb{R}[\mathbf{x}]$ is an appropriate set of generators of S , $g\phi$ is the measure which is absolutely continuous with respect to ϕ with density g , and $d_g = \lceil \deg(g)/2 \rceil$. For instance if S is the Euclidean unit ball then G is the singleton $\mathbf{x} \mapsto g(\mathbf{x}) := 1 - \|\mathbf{x}\|^2$, and (2) reads:

$$\max_{\phi \in \mathcal{P}(S)} \log \det(\mathbf{M}_n(\phi)) + \log \det(\mathbf{M}_{n-1}(g\phi)).$$

That is, one has replaced the information matrix $\mathbf{M}_n(\phi)$ with the new information matrix

$$\begin{bmatrix} \mathbf{M}_n(\phi) & 0 \\ 0 & \mathbf{M}_{n-1}(g\phi) \end{bmatrix}.$$

Notice that the boundary ∂S of S is now clearly involved via the polynomial g in the measure $g\phi$.

In the univariate case $S = [-1, 1]$ and $x \mapsto g(x) := 1 - x^2$, our framework shares some similarities with the generalization of D-optimal design proposed in [10, 17, 25]. In [10, 25], with a so-called *efficiency* function of the form $\lambda(x) := (1+x)^u(1-x)^v$ with $u, v \in \{0, 1\}$, $\beta_{n-1} = n/(2n+1)$, $\beta_n = n+1/(2n+1)$, one minimizes the criterion

$$\frac{\beta_{n-1} \log \det(\mathbf{M}_{n-1}(\lambda\phi))}{n} + \frac{\beta_n \log \det(\mathbf{M}_n(\lambda\phi))}{n+1},$$

which is different from that in (2). That is, in [10, 25] the authors consider the product of information matrices related to $n+1$ different regressions models and with *same* efficiency function λ , whereas in (2) one also considers several regression models but each with a specific efficiency function. In fact the matrix $\mathbf{M}_{n-1}(g\phi)$ is associated with a regression model of the form

$$y = v_n(\mathbf{x})^T \theta + \frac{\varepsilon}{\sqrt{g(\mathbf{x})}},$$

i.e., when the noise explodes close to the boundary of S^1 .

Contribution

We show that for every degree n and every dimension d , the *equilibrium measure* ϕ^* of S (in pluripotential theory [20]) is an optimal solution of the variant (2) of the D-optimal design problem (1). This variant (2) takes into account explicitly the boundary of S and its criterion tends to favor points in the interior of S (as points in ∂S do not contribute to some of the information matrices $\mathbf{M}_{n-d_g}(g\phi)$). The resulting optimality conditions link the variant (2) with a generalized (polynomial) Pell's equation investigated in [22, 23]. Hence for such design spaces S :

¹The authors thank Y. de Castro and F. Gamboa for providing such a simple interpretation

The variant (2) of the D-optimal design problem (1) reduces to finding a cubature for the equilibrium measure ϕ^* of S , with positive weights, atoms in S , and exact up to degree $2n$.

In addition, if ν_n^* is any atomic probability measure, optimal solution of (2) (hence whose support is a degree- n optimal design), then the resulting sequence $(\nu_n^*)_{n \in \mathbb{N}}$ converges weak-star to the equilibrium measure ϕ^* of S , as does any sequence of probability measures equi-supported on so-called *Fekete* points of S . However, as already noted in the literature linking approximation theory with the D-optimal design problem, probability measures supported on Fekete points are rarely optimal solutions to the standard D-optimal design problem (1); see e.g. [4, 5].

Last but not least, for the univariate case $S = [-1, 1]$, the atomic probability measure ν_n^* supported on the $n + 1$ roots of the degree- $(n + 1)$ Chebyshev polynomial of first kind (and with equal weights) is optimal for (2). Hence the support of the celebrated Gauss-Chebyshev quadrature is an optimal solution of the variant (2) of (1). We emphasize that ν_n^* cannot be an optimal solution of the standard D-optimal design problem (1). A tensorized version of this result holds for the unit box $[-1, 1]^d$. Interestingly, a design on Chebyshev points of $[-1, 1]$ has been shown to be \mathbf{c} -optimal² in [14]; see also [29] for optimal design on Chebyshev points.

Finally, we extend the variant (2) to the case of arbitrary compact basic semi-algebraic sets $S \subset \mathbb{R}^d$. Of course for such general sets S , an optimal solution $\phi^* \in \mathcal{P}(S)$ of (2) is not available in closed form any more. However links with the equilibrium measure are still available asymptotically as the degree n increases. Moreover the two-step design algorithm provided in [8] to solve (1) can be easily adapted. In the convex relaxation defined in step 1 of the algorithm, it suffices to replace the log-det criterion of (1) with that of (2). Then step 2 of the algorithm remains exactly the same.

So in summary, for the three special geometries (unit ball, unit box, and simplex), and for every dimension d and every degree n , the equilibrium measure of S is an optimal solution of the variant (2) of D-optimal design. Moreover, for more general semi-algebraic sets S , this variant also provides (asymptotically) connections with the equilibrium measure of S . It still remains to investigate how this variant compares with the classical version (1) from a statistical point of view.

2 Notation, definitions and preliminaries

2.1 Notation and definitions

Let $\mathbb{R}[\mathbf{x}]_n \subset \mathbb{R}[\mathbf{x}]$ denote the space of polynomials in the variables $\mathbf{x} = (x_1, \dots, x_d)$, of total degree at most n . Let $\Sigma[\mathbf{x}]_n \subset \mathbb{R}[\mathbf{x}]_{2n}$ be the subset of sum-of-squares (SOS) polynomials of total degree at most $2n$. Let \mathbb{N} be the set of natural numbers and $\mathbb{N}_n^d := \{\boldsymbol{\alpha} \in \mathbb{N}^d : |\boldsymbol{\alpha}| (=$

²Given a vector \mathbf{c} , a design $\boldsymbol{\xi}$ is \mathbf{c} -optimal if it minimizes $\mathbf{x} \mapsto V(\mathbf{c}, \mathbf{x}) := \sup_{\mathbf{v}} \mathbf{c}^T \mathbf{v} / \mathbf{v}^T \mathbf{M}_n(\mathbf{x}) \mathbf{v}$ where $\mathbf{M}_n(\mathbf{x})$ is the information matrix associated with a design \mathbf{x} ; see e.g. [29].

$\sum_i \alpha_i) \leq n\}$, and $s_n := \binom{d+n}{d}$. A polynomial $p \in \mathbb{R}[\mathbf{x}]_n$ reads

$$\mathbf{x} \mapsto p(\mathbf{x}) = \sum_{\alpha \in \mathbb{N}_n^d} p_\alpha \mathbf{x}^\alpha,$$

where $\mathbf{p} = (p_\alpha) \in \mathbb{R}^{s_n}$ is the vector of coefficients of p in the monomial basis $\mathbf{v}_n(\mathbf{x}) := (\mathbf{x}^\alpha)_{\alpha \in \mathbb{N}_n^d}$ with $\mathbf{x}^\alpha := \prod_{i=1}^d x_i^{\alpha_i}$. With $S \subset \mathbb{R}^d$ compact, denote by $\mathcal{M}(S)_+$ the convex cone of Borel (positive) measures on S and $\mathcal{P}(S) \subset \mathcal{M}(S)_+$ its subset of probability measures on S . Denote also by $\mathcal{C}(S)$ the space of continuous functions on S . With a given real sequence $\phi = (\phi_\alpha)_{\alpha \in \mathbb{N}^d}$ is associated the linear functional $\phi \in \mathbb{R}[\mathbf{x}]^*$ defined by

$$p \mapsto \phi(p) := \sum_{\alpha \in \mathbb{N}^d} p_\alpha \phi_\alpha, \quad \forall p \in \mathbb{R}[\mathbf{x}].$$

Given a set of s_n points $\{\mathbf{x}_1, \dots, \mathbf{x}_{s_n}\} \subset S$ denote by $\text{VDM}(\mathbf{x}_1, \dots, \mathbf{x}_{s_n}) \in \mathbb{R}^{s_n \times s_n}$ the Vandermonde matrix associated with $\{\mathbf{x}_1, \dots, \mathbf{x}_{s_n}\}$.

Moment and localizing matrix

Given a real sequence $\phi = (\phi_\alpha)_{\alpha \in \mathbb{N}^d}$, the moment matrix $\mathbf{M}_n(\phi)$ associated with ϕ is the real symmetric matrix with rows and columns indexed by \mathbb{N}_n^d , and with entries

$$\mathbf{M}_n(\phi)(\alpha, \beta) := \phi_{\alpha+\beta}, \quad \alpha, \beta \in \mathbb{N}_n^d.$$

If ϕ has a representing measure ϕ then we can write $\mathbf{M}_n(\phi)$ or $\mathbf{M}_t(\phi)$ with no ambiguity, and in addition $\mathbf{M}_n(\phi) \succeq 0$. Conversely $\mathbf{M}_n(\phi) \succeq 0$ is a necessary (but not sufficient) condition for ϕ to have a representing measure on \mathbb{R}^d .

Given a polynomial $g \in \mathbb{R}[\mathbf{x}]$, $\mathbf{x} \mapsto g(\mathbf{x}) := \sum_{\beta} g_\beta \mathbf{x}^\beta$, and a real sequence $\phi = (\phi_\alpha)_{\alpha \in \mathbb{N}^d}$, the localizing matrix $\mathbf{M}_n(g\phi)$ associated with g and ϕ is the moment matrix associated with the linear functional $g\phi$ defined by:

$$(g\phi)_\alpha := \sum_{\beta \in \mathbb{N}^d} g_\beta \phi_{\beta+\alpha}, \quad \forall \alpha \in \mathbb{N}^d,$$

and so $(g\phi)(p) = \phi(gp)$ for all $p \in \mathbb{R}[\mathbf{x}]$.

Christoffel-Darboux kernel and Christoffel function

Given a compact set $S \subset \mathbb{R}^d$ and a Borel measure ϕ on S such that $\mathbf{M}_n(\phi) \succ 0$ for all n , let $(P_\alpha)_{\alpha \in \mathbb{N}^d} \subset \mathbb{R}[\mathbf{x}]$ be a family of polynomials that are orthonormal w.r.t. ϕ , i.e.:

$$\int_S P_\alpha P_\beta d\phi = \delta_{\alpha=\beta}, \quad \forall \alpha, \beta \in \mathbb{N}^d,$$

which is guaranteed to exist. Then for every n , the kernel

$$(\mathbf{x}, \mathbf{y}) \mapsto K_n^\phi(\mathbf{x}, \mathbf{y}) := \sum_{\alpha \in \mathbb{N}_n^d} P_\alpha(\mathbf{x}) P_\alpha(\mathbf{y}), \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^d,$$

is called the Christoffel-Darboux (CD) kernel, the polynomial $\mathbf{x} \mapsto K_n^\phi(\mathbf{x}, \mathbf{x})/s_n$ is called the (normalized) CD polynomial, and the rational function

$$\mathbf{x} \mapsto \Lambda_n^\phi(\mathbf{x}) = 1/K_n^\phi(\mathbf{x}, \mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^d,$$

is called the Christoffel function. Alternatively

$$\begin{aligned} \Lambda_n^\phi(\mathbf{x}) &= (\mathbf{v}_n(\mathbf{x})^T \mathbf{M}_n(\phi)^{-1} \mathbf{v}_n(\mathbf{x}))^{-1} \\ &= \min_{p \in \mathbb{R}[\mathbf{x}]_n} \left\{ \int_S p^2 d\phi : p(\mathbf{x}) = 1 \right\}, \quad \forall \mathbf{x} \in \mathbb{R}^d. \end{aligned}$$

Equilibrium measure

The notion of equilibrium measure associated with a given set originates from logarithmic potential theory (working with a compact set $E \subset \mathbb{C}$ in the univariate case). It minimizes the energy functional

$$I(\phi) := \int \int \log \frac{1}{|z-t|} d\phi(z) d\phi(t), \quad (3)$$

over all Borel probability measures ϕ supported on E . For instance if E is the interval $[-1, 1] \subset \mathbb{C}$ then the arcsine (or Chebyshev) distribution $\mu = \mathbb{1}_E/\pi\sqrt{1-x^2}$ is an optimal solution. Generalizations have been obtained in the multivariate case via pluripotential theory in \mathbb{C}^d . In particular, if $E \subset \mathbb{R}^d \subset \mathbb{C}^d$ is compact then its equilibrium measure (let us denote it by μ) is equivalent to the Lebesgue measure on compact subsets of $\text{int}(E)$. It has an even explicit expression if E is convex and symmetric about the origin; see e.g. [2, Theorems 1.1 and 1.2]. Several examples of sets E with its equilibrium measure given in explicit form can be found in [1]. Importantly, the appropriate approach to define the (intrinsic) equilibrium measure μ of a compact subset of \mathbb{R}^d with $d > 1$, is to consider \mathbb{R}^d as a subset of \mathbb{C}^d and invoke pluripotential theory with its tools from complex analysis (in particular, plurisubharmonic functions (and their regularization) and the Monge-Ampère operator). For more details on equilibrium measures and pluripotential theory, the interested reader is referred to [1, 2, 20], the discussion in [19, Section 6.8, p. 297] as well as [28, Appendix B], [26], and the references therein. In the sequel, when we speak about the equilibrium measure of a compact subset $E \subset \mathbb{R}^d$, we refer to that in pluripotential theory (i.e., with E considered as a subset of \mathbb{C}^d).

Background on approximate D-optimal design

The approximate D-optimal design problem is well-known and originates in statistics. Let $S \subset \mathbb{R}^d$ be a compact set with nonempty interior, and let $n \in \mathbb{N}$ be fixed. For a design $\boldsymbol{\xi} = (\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_r)$ with positive weights (frequencies) $\boldsymbol{\gamma} = (\gamma_i)_{i \leq r}$, the matrix $\mathbf{M}_n(\boldsymbol{\xi}) = \sum_{i=1}^r \gamma_i \mathbf{v}_n(\boldsymbol{\xi}_i) \mathbf{v}_n(\boldsymbol{\xi}_i)^T$ is called the information matrix of the design $\boldsymbol{\xi}$. Among several statistical criteria in parameter estimation, maximizing the logarithm of the determinant of the information matrix (now over all probability measures on S) is a popular one which yields problem (1). As one optimizes over $\mathcal{P}(S)$, an optimal solution is called an *approximate* D-optimal design. For a general overview on optimal experimental design the interested reader is referred to the recent tutorial [15].

If S has nonempty interior then it is shown in [9] that (1) has an optimal (not necessarily unique) atomic measure supported on m points $\mathbf{x}_j \in S$, $j = 1, \dots, m$, where $s_n \leq m \leq s_{2n}$. That is, there exists a weight vector $0 < \boldsymbol{\gamma} \in \mathbb{R}^m$ such that

$$\phi^* = \sum_{j=1}^m \gamma_j \delta_{\mathbf{x}_j}, \quad \sum_{j=1}^m \gamma_j = 1,$$

and with $K_n^{\phi^*}(\mathbf{x}, \mathbf{y})$ the CD kernel associated with ϕ^* ,

$$s_n - K_n^{\phi^*}(\mathbf{x}, \mathbf{x}) \geq 0, \quad \forall \mathbf{x} \in S \tag{4}$$

$$s_n - K_n^{\phi^*}(\mathbf{x}_j, \mathbf{x}_j) = 0, \quad \forall j = 1, \dots, m. \tag{5}$$

While an optimal atomic measure is not necessarily unique, the resulting optimal moment matrices \mathbf{M}_n are all identical (by strict concavity of the criterion). It turns out that from (4)-(5) one may also link (1) with approximation theory, orthogonal polynomials, Fekete points and Fejér points.

A set of s_n points $\{\mathbf{x}_1^*, \dots, \mathbf{x}_{s_n}^*\} \subset S$ is a Fekete set if it maximizes $\det(\text{VDM}(\mathbf{x}_1, \dots, \mathbf{x}_{s_n}))$ (the Vandermonde determinant) among all sets of s_n points of S . Observe that if μ is the s_n -atomic measure with equal weights $\frac{1}{s_n} \sum_{i=1}^{s_n} \delta_{\mathbf{x}_i}$, then one obtains

$$\mathbf{M}_n(\mu) = \frac{1}{s_n} \text{VDM}(\mathbf{x}_1, \dots, \mathbf{x}_{s_n}) \text{VDM}(\mathbf{x}_1, \dots, \mathbf{x}_{s_n})^T,$$

and $\log \det(\mathbf{M}_n(\mu)) = 2 \log \det(\text{VDM}(\mathbf{x}_1, \dots, \mathbf{x}_{s_n}))$.

Fekete points are in turn connected with the so-called *equilibrium measure* in pluri-potential theory [20]. For instance the sequence of discrete probability measures $(\nu_n)_{n \in \mathbb{N}}$ equi-supported on s_n Fekete points converges to the equilibrium measure of S for the weak-star topology on the space of signed measures on S . See e.g. [3], [24, Theorem 4.5.1], and the references therein.

A set of s_n points $\{\mathbf{x}_1, \dots, \mathbf{x}_{s_n}\} \subset S$ is a Fejér set if $\max_{\mathbf{x} \in S} \sum_{j=1}^{s_n} \ell_j(\mathbf{x}) = 1$, where $\ell_1, \dots, \ell_{s_n}$ are the Lagrange interpolation polynomials at the points $\mathbf{x}_1, \dots, \mathbf{x}_{s_n}$, and it turns out that a set of Fejér points is also a set of Fekete points. Hence it is natural to ask when a set of Fekete points is also the support of an atomic measure ϕ^* in (4)-(5), with equal weights. In fact, an s_n -atomic measure is D-optimal in (1) if and only if it is equally weighted and its support is a Fejér set. See for instance [4, 5]. However, and as noted in [5], such a situation is rather exceptional and not to be expected.

3 Main result

As we next see, the main result of this paper is obtained from [22, 23] and it is detailed for each of the three cases considered (unit ball, unit box, canonical simplex). What we emphasize here is the significance of such results for the D-optimal design problem. Namely, results from [23] show that our proposed variant of the D-optimality criterion for optimal design reveals quite strong links with the equilibrium measure ϕ^* of S . In this variant

appears a term which involves the boundary ∂S of the design space S . As a result, for three important sets $S \subset \mathbb{R}^d$, and for all dimensions d and all degrees n , ϕ^* is an optimal solution and therefore an optimal design can be computed from any cubature associated with ϕ^* , provided that it has positive weights, atoms in S , and is exact up to degree $2n$.

3.1 The unit ball

Let $S := \{ \mathbf{x} \in \mathbb{R}^d : \|\mathbf{x}\| \leq 1 \}$ with associated equilibrium measure

$$\phi^* = \frac{A_{d-1} d\mathbf{x}}{\sqrt{1 - \|\mathbf{x}\|^2}} \quad \text{on } S \quad (6)$$

where A_d is the surface area of the unit sphere of dimension d , satisfying $A_0 = 2$, $A_1 = 2\pi$, $A_n = A_{n-2}2\pi/(n-1)$, $n > 1$. Let $\mathbf{x} \mapsto g(\mathbf{x}) := 1 - \|\mathbf{x}\|^2$, and with $n \in \mathbb{N}$ fixed, instead of (1), consider now the related problem:

$$\rho_n = \max_{\phi \in \mathcal{P}(S)} \log \det \mathbf{M}_n(\phi) + \log \det \mathbf{M}_{n-1}(g\phi), \quad (7)$$

or equivalently,

$$-\rho_n = \min_{\phi \in \mathcal{P}(S)} \log \det \mathbf{M}_n(\phi)^{-1} + \log \det \mathbf{M}_{n-1}(g\phi)^{-1}. \quad (8)$$

When comparing (7) with (1) observe that we have simply replaced the information matrix $\mathbf{M}_n(\phi)$ with the new block-diagonal information matrix

$$\begin{bmatrix} \mathbf{M}_n(\phi) & 0 \\ 0 & \mathbf{M}_{n-1}(g\phi) \end{bmatrix},$$

associated with the measures ϕ and $g\phi$. The latter information matrix takes into account the distance to the boundary $\partial S = \{ \mathbf{x} : \|\mathbf{x}\| = 1 \}$ of the design space S . Indeed, for a design $\boldsymbol{\xi} = (\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_r)$ with weights $\boldsymbol{\gamma} = (\gamma_i)_{i \leq r}$, the information matrix $\mathbf{M}_{n-1}(g\nu_{\boldsymbol{\xi}})$ (with $\nu_{\boldsymbol{\xi}} = \sum_i \gamma_i \delta_{\boldsymbol{\xi}_i}$) reads

$$\mathbf{M}_{n-1}(g\nu_{\boldsymbol{\xi}}) = \sum_{i=1}^r \gamma_i (1 - \|\boldsymbol{\xi}_i\|^2) \mathbf{v}_{n-1}(\boldsymbol{\xi}_i) \mathbf{v}_{n-1}(\boldsymbol{\xi}_i)^T,$$

and so points $\boldsymbol{\xi}_i \in \partial S$ do *not* contribute to $\mathbf{M}_{n-1}(g\nu_{\boldsymbol{\xi}})$. So the criterion in (7) put more weight on points in $\text{int}(S)$ than on points in ∂S .

We also consider the convex optimization problem :

$$\begin{aligned} \rho_n^* = \max_{\mathbf{A}_0, \mathbf{A}_1 \succeq 0} \{ & \log \det \mathbf{A}_0 + \log \det \mathbf{A}_1 : \\ & s_n + s_{n-1} = \mathbf{v}_n(\mathbf{x})^T \mathbf{A}_0 \mathbf{v}_n(\mathbf{x}) \\ & + \mathbf{v}_{n-1}(\mathbf{x})^T \mathbf{A}_1 \mathbf{v}_{n-1}(\mathbf{x}) (1 - \|\mathbf{x}\|^2), \forall \mathbf{x} \in \mathbb{R}^d \}. \end{aligned} \quad (9)$$

As proved in [22, Theorem 6, p. 945], (8) is a dual of (7), that is, weak duality $\rho_n^* \leq -\rho_n$ holds, and in fact even strong duality holds³, i.e., $\rho_n^* = -\rho_n$.

³In the present context, the condition $\mathbf{1} \in Q_n(G)$ in [22, Theorem 6] is satisfied as soon as the constraint in (9) is satisfied for some matrices $\mathbf{A}_0, \mathbf{A}_1 \succ 0$.

Theorem 1 *Let $n \in \mathbb{N}$ be fixed, arbitrary. Then*

(i) *The equilibrium measure ϕ^* of S in (6) is an optimal solution of (7) (and the optimal moment matrices $\mathbf{M}_n(\phi^*)$ and $\mathbf{M}_{n-1}(g\phi^*)$ are unique).*

(ii) *The unique optimal solution $(\mathbf{A}_0^*, \mathbf{A}_1^*)$ of problem (9) satisfies $\mathbf{A}_0^* = \mathbf{M}_n(\phi^*)^{-1}$, $\mathbf{A}_1^* = \mathbf{M}_{n-1}(g\phi^*)^{-1}$, and therefore*

$$\begin{aligned} s_n + s_{n-1} &= \Lambda_n^{\phi^*}(\mathbf{x})^{-1} + g(\mathbf{x}) \Lambda_{n-1}^{g\phi^*}(\mathbf{x})^{-1}, \\ &= K_n^{\phi^*}(\mathbf{x}, \mathbf{x}) + g(\mathbf{x}) K_{n-1}^{g\phi^*}(\mathbf{x}, \mathbf{x}), \end{aligned} \quad (10)$$

for all $\mathbf{x} \in \mathbb{R}^d$.

(iii) *There are $s_n \leq m \leq s_{2n}$ points $\mathbf{x}_j^* \in S$, and a positive vector $\boldsymbol{\gamma} \in \mathbb{R}_+^m$ such that the atomic probability measure $\nu_n^* := \sum_{j=1}^m \gamma_j \delta_{\mathbf{x}_j^*}$ has same degree- $2n$ moments as ϕ^* . The normalized CD polynomial*

$$\mathbf{x} \mapsto K_n^{\phi^*}(\mathbf{x}, \mathbf{x}) / (s_n + s_{n-1}), \quad (11)$$

attains its maximum 1 on S at all points \mathbf{x} of the boundary ∂S .

(iv) *With ν_n^* as in (iii), the sequence $(\nu_n)_{n \in \mathbb{N}}$ converges to ϕ^* for the weak-star topology of $\mathcal{M}(S)$, i.e.,*

$$\lim_{n \rightarrow \infty} \int_S f d\nu_n^* = \int_S f d\phi^*, \quad \forall f \in \mathcal{C}(S).$$

Proof: For (i) and (ii) see [22, 23]. For (iii) see e.g. [9] and the many references therein. Next, observe that by (16) one obtains

$$s_n + s_{n-1} - K_n^{\phi^*}(\mathbf{x}, \mathbf{x}) = g(\mathbf{x}) K_{n-1}^{g\phi^*}(\mathbf{x}, \mathbf{x}) \geq 0, \quad \forall \mathbf{x} \in S,$$

and so $K_n^{\phi^*}(\mathbf{x}, \mathbf{x}) = s_n + s_{n-1}$ for every $\mathbf{x} \in \partial S$, which yields the result.

Finally for (iv), as S is compact, there exists a subsequence $(n_k)_{k \in \mathbb{N}}$ and a probability measure ψ on S such that $\lim_{k \rightarrow \infty} \int_S f d\nu_{n_k}^* = \int_S f d\psi$ for all $f \in \mathcal{C}(S)$. In particular, by definition of ν_n^* ,

$$\phi_{\boldsymbol{\alpha}}^* = \lim_{k \rightarrow \infty} \int_S \mathbf{x}^{\boldsymbol{\alpha}} d\nu_{n_k}^* = \int_S \mathbf{x}^{\boldsymbol{\alpha}} d\psi, \quad \forall \boldsymbol{\alpha} \in \mathbb{N}^d,$$

and so as S is compact, $\psi = \phi^*$. But this also implies that the whole sequence $(\nu_n^*)_{n \in \mathbb{N}}$ converges to ϕ^* . \square Theorem

1 states that when S is the unit ball, its equilibrium measure ϕ^* is an optimal solution of (7) for *all* degrees n . Therefore the support of any available cubature for ϕ^* , with atoms in S , positive weights, and exact up to degree $2n$, provides an optimal design. Concerning the construction of such atomic-measures in Theorem 1(iii), the interested reader is referred to [12] which proposed several cubature formula for the unit ball and unit sphere for various weight functions, including the Chebyshev weight $1/\sqrt{1 - \|\mathbf{x}\|^2}$ in (6).

Incidentally, by Theorem 1, the couple of nonnegative polynomials $(K_n^{\phi^*}(\mathbf{x}, \mathbf{x}), g(\mathbf{x}) K_{n-1}^{\phi^*}(\mathbf{x}, \mathbf{x})) / (s_n + s_{n-1})$ provides S with a partition of unity.

Example 1 *In the case $n = 2$ (degree 4) and $d = 2$ (disk) let us compare the D -optimal designs obtained with the approach described in [9], solving original problem (1), and with the approach described in this paper, solving variant problem (2).*

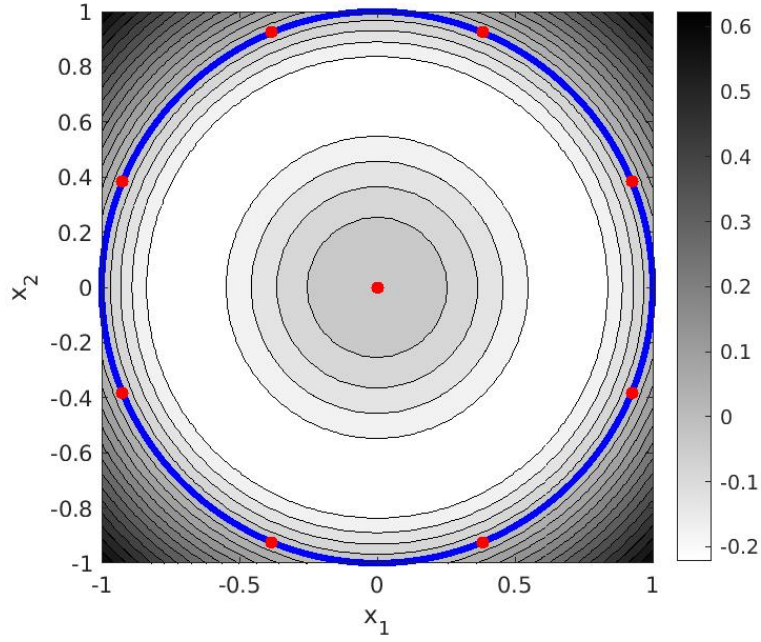


Figure 1: Degree 4 D-optimal design on the disk solving problem (1). The optimal points (red) are located on the CD polynomial unit level set (blue).

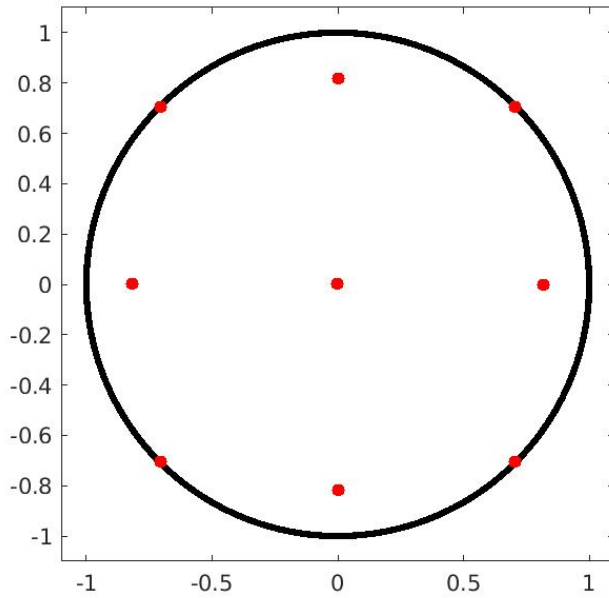


Figure 2: Degree 4 D-optimal design on the disk (black) with points (red) solving variant problem (2).

In solving original problem (1), at step-1 of our moment-SOS algorithm [9], a moment vector⁴

$$\boldsymbol{\mu}_4^* := \int_S \mathbf{v}_4(\mathbf{x}) d\mu(\mathbf{x}) \in \mathbb{R}^{15}$$

⁴The unique solution $\boldsymbol{\mu}_4^*$ is not guaranteed to come from a measure $\mu^* \in \mathcal{P}(S)$, but in our numerical

is computed numerically. Its non-zero entries are $\mu_{00}^* = 1$, $\mu_{20}^* = \mu_{02}^* = 0.4167$, $\mu_{40}^* = \mu_{04}^* = 0.3125$, $\mu_{22}^* = 0.1042$ (to 4 significant digits). In step-2, an atomic measure supported at 9 points is computed at relaxation order 5, i.e. by extending the moment vector up to degree 10. The points are displayed in red on Figure 1. They are located on the unit level set (blue) of the CD polynomial. Other level sets (gray) are represented in logarithmic scale.

In solving variant problem (1), the moment vector $\phi_4^* \in \mathbb{R}^{15}$ of the equilibrium measure ϕ^* of S is computed, either in closed form or numerically as above in step-1. Its non-zero entries read $\phi_{00}^* = 1$, $\phi_{20}^* = \phi_{02}^* = 1/3$, $\phi_{40}^* = \phi_{04}^* = 1/5$, $\phi_{22}^* = 1/15$. In step-2, an atomic measure supported on 9 points of S is computed at relaxation order 5, i.e. by extending the moment vector ϕ_4^* up to degree 10. The points are displayed in Figure 2. As expected, we observe that 5 out of 9 points are in the interior of the disk, whereas only a single point (the origin) is in interior of the disk for original problem (1).

3.2 The unit box

Let $S = [-1, 1]^d$ with associated equilibrium measure

$$\phi^* = \frac{d\mathbf{x}}{\pi^d \prod_{j=1}^d \sqrt{1-x_j^2}} \quad \text{on } S, \quad (12)$$

and for every $\varepsilon \in \{0, 1\}^d$, introduce the polynomial

$$\mathbf{x} \mapsto g_\varepsilon(\mathbf{x}) := \prod_{j=1}^d (1-x_j^2)^{\varepsilon_j}, \quad \forall \mathbf{x} \in \mathbb{R}^d,$$

and the sets $\Delta_n := \{\varepsilon \in \{0, 1\}^d : |\varepsilon| \leq n\}$, $n \in \mathbb{N}$.

From the generalized Pell's equation in [22, 23], for every n :

$$\sum_{\varepsilon \in \Delta_n} g_\varepsilon(\mathbf{x}) \Lambda_{n-|\varepsilon|}^{g_\varepsilon \phi^*}(\mathbf{x})^{-1} = \sum_{\varepsilon \in \Delta_n} s_{n-|\varepsilon|}, \quad \forall \mathbf{x} \in \mathbb{R}^d. \quad (13)$$

In view of (13), the analogue for the unit box of the D-optimal design variant (7) reads

$$\max_{\phi \in \mathcal{P}(S)} \sum_{\varepsilon \in \Delta_n} \log \det \mathbf{M}_{n-|\varepsilon|}(g_\varepsilon \phi), \quad (14)$$

with associated dual problem

$$\begin{aligned} \max_{\mathbf{A}_\varepsilon \succeq 0} \{ & \sum_{\varepsilon \in \Delta_n} \log \det \mathbf{A}_\varepsilon : \\ & \sum_{\varepsilon \in \Delta_n} s_{n-|\varepsilon|} = \sum_{\varepsilon \in \Delta_n} g_\varepsilon(\mathbf{x}) \mathbf{v}_{n-|\varepsilon|}(\mathbf{x})^T \mathbf{A}_\varepsilon \mathbf{v}_{n-|\varepsilon|}(\mathbf{x}) \\ & \text{for all } \mathbf{x} \in \mathbb{R}^d \}. \end{aligned} \quad (15)$$

experiments in [9], it does.

Theorem 2 Let $n \in \mathbb{N}$ be fixed, arbitrary. Then

(i) The equilibrium measure ϕ^* of S in (12) is an optimal solution of (14) (and the optimal moment matrices $(\mathbf{M}_{n-|\varepsilon|}(g_\varepsilon\phi^*))_{\varepsilon \in \Delta_n}$ are unique).

(ii) The unique optimal solution $(\mathbf{A}_\varepsilon^*)_{\varepsilon \in \Delta_n}$ of the dual problem (15) satisfies $\mathbf{A}_\varepsilon^* = \mathbf{M}_{n-|\varepsilon|}(g_\varepsilon\phi^*)^{-1}$, and (13) holds, or equivalently,

$$\sum_{\varepsilon \in \Delta_n} s_{n-|\varepsilon|} = \sum_{\varepsilon \in \Delta_n} g_\varepsilon(\mathbf{x}) K_{n-|\varepsilon|}^{g_\varepsilon \cdot \phi^*}(\mathbf{x}, \mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^d. \quad (16)$$

(iii) There are $s_n \leq m \leq s_{2n}$ points $\mathbf{x}_j^* \in S$, and a positive vector $\boldsymbol{\gamma} \in \mathbb{R}_+^m$ such that the atomic probability measure $\nu_n^* := \sum_{j=1}^m \gamma_j \delta_{\mathbf{x}_j^*}$ has same degree- $2n$ moments as ϕ^* . The normalized CD polynomial

$$\mathbf{x} \mapsto K_n^{\phi^*}(\mathbf{x}, \mathbf{x}) / \sum_{\varepsilon \in \Delta_n} s_{n-|\varepsilon|} \quad (17)$$

attains its maximum 1 on S , at every vertex of S .

(iv) With ν_n^* as in (iii), the sequence $(\nu_n)_{n \in \mathbb{N}}$ converges to ϕ^* for the weak-star topology of $\mathcal{M}(S)$, i. e.,

$$\lim_{n \rightarrow \infty} \int_S f d\nu_n^* = \int_S f d\phi^*, \quad \forall f \in \mathcal{C}(S).$$

Proof: The proof mimics that of Theorem 1. In particular, if \mathbf{v} is vertex of S then $g_\varepsilon(\mathbf{v}) = 0$ whenever $\varepsilon \neq 0$, and so $K_n^{\phi^*}(\mathbf{v}, \mathbf{v}) = \sum_{\varepsilon \in \Delta_n} s_{n-|\varepsilon|}$, the desired result. \square

The univariate case $S = [-1, 1]$

Let $\phi^* = dx/\pi\sqrt{1-x^2}$ and $x \mapsto g(x) = 1-x^2$. Then (13) reads:

$$s_n + s_{n-1} = \Lambda_n^{\phi^*}(x)^{-1} + (1-x^2)\Lambda_{n-1}^{g \cdot \phi^*}(x)^{-1}, \quad (18)$$

for all $x \in \mathbb{R}$, or, equivalently:

$$s_n + s_{n-1} = K_n^{\phi^*}(x, x) + (1-x^2)K_{n-1}^{g \cdot \phi^*}(x, x), \quad (19)$$

for all $x \in \mathbb{R}$. Next, the Gauss-Chebyshev quadrature for the equilibrium measure ϕ^* is supported on the zeros of the degree- $(n+1)$ Chebyshev polynomial of first kind, and reads $\nu_n = \frac{1}{n+1} \sum_{i=1}^{n+1} \delta_{x_i}$ with

$$x_i = \cos\left(\frac{2i-1}{2(n+1)}\pi\right) \in (-1, 1), \quad i = 1, \dots, n+1, \quad (20)$$

and is exact up to degree $2n+2-1 = 2n+1$, i. e.,

$$\int_{-1}^1 p d\nu_n = \int_{-1}^1 p d\phi^*, \quad \forall p \in \mathbb{R}[x]_{2n+1}.$$

Moreover it turns out that

$$K_n^{\phi^*}(x_i, x_i) = \Lambda_n^{\phi^*}(x_i)^{-1} = \Lambda_n^{\nu_n}(x_i)^{-1} = n + 1 = s_n,$$

and by (18), $(1 - x_i^2) \Lambda_{n-1}^{g \cdot \mu^*}(x_i)^{-1} = s_{n-1}$, for all $i = 1, \dots, n + 1$.

So the distinguished equidistributed atomic probability measure ν_n is an optimal solution of (7). Moreover

$$\frac{\text{VDM}(x_1^*, \dots, x_{n+1}^*) \text{VDM}(x_1^*, \dots, x_{n+1}^*)^T}{n + 1} = \mathbf{M}_n(\nu_n).$$

However, its support (zeros of the degree- $(n + 1)$ Chebyshev polynomial) is *not* a set of Fekete points because

$$\phi^* \neq \arg \max_{\mu \in \mathcal{P}(S)} \det(\mathbf{M}_n(\mu)),$$

(i.e., ϕ^* does not solve the D-optimal design⁵ (1)). Indeed $\max_{x \in S} K_n^{\phi^*}(x, x) > s_n$ because by (18)

$$K_n^{\phi^*}(x, x) (= s_n + s_{n-1}) > s_n \text{ for } x = \pm 1.$$

So the points $(x_i)_{i \leq n+1}$ have the remarkable property that the equidistributed measure ν_n (supported on $\text{int}(S)$) is an optimal solution of (7) for every n . And of course, again, $(\nu_n)_{n \in \mathbb{N}}$ converges weakly to the equilibrium measure ϕ^* as does any sequence of probability measures equi-distributed on Fekete points (see e.g. [3, 24]).

However, even for S being the unit ball or the unit sphere, cases (d, n) where a D-optimal measure $\mu \in \mathcal{P}(S)$ is equi-supported on Fekete points are exceptional; see e.g. Bos [4, p. 134]. The univariate atomic measure ν_n in (20) has an immediate extension to the multivariate $S = [-1, 1]^d$ case.

Corollary 1 *Let ν_n be the Gauss-Chebyshev atomic (univariate) measure in (20). Then the multivariate atomic product measure $\nu_n^* := \underbrace{\nu_n \otimes \dots \otimes \nu_n}_{d \text{ times}}$ on $S = [-1, 1]^d$ is an optimal solution of (14). Moreover ν_n^* converges to ϕ^* for the weak-star topology of $\mathcal{M}(S)$.*

Proof: As $\phi^* = \prod_{j=1}^d dx_j / (\pi \sqrt{1 - x_j^2})$ is an optimal solution of (14), ν_n^* provides with a cubature for ϕ^* , exact up to maximum degree $2n + 1$ in *each* variable, and hence also exact for total degree $2n$. The final statement on weak-star convergence is due to the product structure of ϕ^* and ν_n^* . \square

Example 2 *In the case $d = 1$ (interval) and $n = 8$ (degree 16) let us compare the D-optimal designs obtained with the approach described in [9] for solving original problem (1), and with the approach described in this paper for solving variant problem (2).*

In solving original problem (1), at step-1 of our moment-SOS algorithm, one obtains a CD polynomial of degree $2n = 16$ (black curve) whose local maxima (located on the unit level set) are the optimal 9 points (red dots), see Figure 3. These points are also optimal Fekete points

⁵An approximate D-optimal design for (1) is equally supported on the zeros of $(1 - x^2)P'(x)$ where P_n is the degree- n Legendre polynomial; see [13]. It is also a set of Fekete points [5].

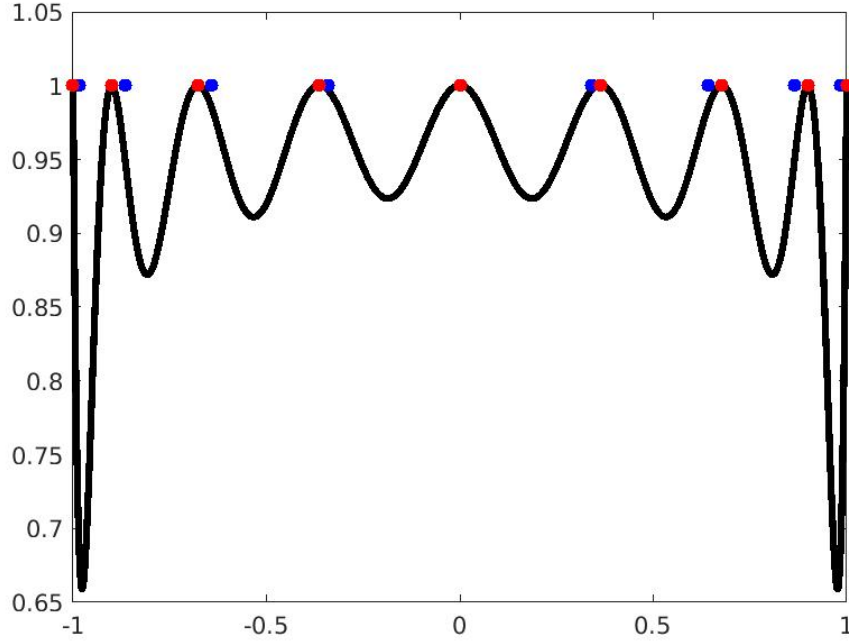


Figure 3: Degree 16 D-optimal design on unit interval: CD polynomial unit level set points (red) solve problem (1), whereas roots of the degree 9 Chebyshev polynomials (blue) solve variant problem (2).

and roots of $\mathbf{x} \mapsto (1 - \mathbf{x}^2)p'_n(\mathbf{x})$ where p_n is the degree n Legendre polynomial [5, 13]. Also represented (blue dots) are the roots of the degree 9 Chebyshev polynomial, which cannot be optimal Fekete points, as discussed above.

In solving variant problem (2), as $\phi^* = dx/(\pi\sqrt{1-x^2})$, the roots of the degree 9 Chebyshev polynomial provide the support of an optimal atomic probability measure. (Step-1 of our moment-SOS algorithm [9] also provide the moment vector ϕ_{18}^* of ϕ^* , rounded to 4 significant digits.)

3.3 The canonical simplex

Let $S = \{\mathbf{x} \in \mathbb{R}_+^d : \sum_{i=1}^d x_i \leq 1\}$, with associated equilibrium measure

$$\phi^* = \frac{d\mathbf{x}}{\pi^{d+1} \sqrt{x_1 \cdot x_2 \cdots x_d \cdot (1 - \sum_i x_i)}}, \quad (21)$$

and with $\varepsilon \in \{0, 1\}^{d+1}$ and $|\mathbf{x}| = \sum_{i=1}^d x_i$, define

$$\mathbf{x} \mapsto g_\varepsilon(\mathbf{x}) := x_1^{\varepsilon_1} \cdots x_d^{\varepsilon_d} \cdot (1 - |\mathbf{x}|)^{\varepsilon_{d+1}}, \quad \forall \mathbf{x} \in \mathbb{R}^d. \quad (22)$$

For every n , let $\Delta_n := \{\boldsymbol{\varepsilon} \in \mathbb{R}^{d+1} : |\boldsymbol{\varepsilon}| \in 2\mathbb{N}; |\boldsymbol{\varepsilon}| \leq n\}$, and introduce the vector $\mathbf{1} := (1, 1, \dots, 1) \in \mathbb{N}^{d+1}$. By [23], for every $n \in \mathbb{N}$:

$$\sum_{\boldsymbol{\varepsilon} \in \Delta_n} g_{\boldsymbol{\varepsilon}}(\mathbf{x}) \Lambda_{n-|\boldsymbol{\varepsilon}|/2}^{g_{\boldsymbol{\varepsilon}}\phi^*}(\mathbf{x})^{-1} = \sum_{\boldsymbol{\varepsilon} \in \Delta_n} s_{n-|\boldsymbol{\varepsilon}|/2}, \quad \forall \mathbf{x} \in \mathbb{R}^d. \quad (23)$$

As an example, for $d = 2$ the identity (23) reads:

$$\begin{aligned} \Lambda_n^{\phi^*}(\mathbf{x})^{-1} + x_1 x_2 \Lambda_{n-1}^{x_1 x_2 \phi^*}(\mathbf{x})^{-1} + x_1 x_3 \Lambda_{n-1}^{x_1 x_3 \phi^*}(\mathbf{x})^{-1} \\ + x_2 x_3 \Lambda_{n-1}^{x_2 x_3 \phi^*}(\mathbf{x})^{-1} = (n+1)(2n+1), \end{aligned}$$

for all $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$ and $x_3 = 1 - x_1 - x_2$.

In view of (23), the analogue for the simplex of the D-optimal design variant (7) reads

$$\max_{\phi \in \mathcal{P}(S)} \sum_{\boldsymbol{\varepsilon} \in \Delta_n} \log \det \mathbf{M}_{n-|\boldsymbol{\varepsilon}|/2}(g_{\boldsymbol{\varepsilon}} \cdot \phi), \quad (24)$$

with associated dual problem

$$\begin{aligned} \max_{\mathbf{A}_{\boldsymbol{\varepsilon}} \succeq 0} \left\{ \sum_{\boldsymbol{\varepsilon} \in \Delta_n} \log \det \mathbf{A}_{\boldsymbol{\varepsilon}} : \sum_{\boldsymbol{\varepsilon} \in \Delta_n} s_{n-|\boldsymbol{\varepsilon}|/2} \right. \\ = \sum_{\boldsymbol{\varepsilon} \in \Delta_n} g_{\boldsymbol{\varepsilon}}(\mathbf{x}) \mathbf{v}_{n-|\boldsymbol{\varepsilon}|/2}(\mathbf{x})^T \mathbf{A}_{\boldsymbol{\varepsilon}} \mathbf{v}_{n-|\boldsymbol{\varepsilon}|/2}(\mathbf{x}), \\ \left. \text{for all } \mathbf{x} \in \mathbb{R}^d. \right\} \end{aligned} \quad (25)$$

Theorem 3 *Let $n \in \mathbb{N}$ be fixed, arbitrary. Then*

(i) *The equilibrium measure ϕ^* of S in (21) is an optimal solution of (24) (and the optimal moment matrices $\mathbf{M}_{n-|\boldsymbol{\varepsilon}|}(g_{\boldsymbol{\varepsilon}}\phi^*)$ are unique).*

(ii) *The unique optimal solution ($\mathbf{A}_{\boldsymbol{\varepsilon}}^*$) of the dual problem (25) satisfies $\mathbf{A}_{\boldsymbol{\varepsilon}}^* = \mathbf{M}_{n-|\boldsymbol{\varepsilon}|/2}(g_{\boldsymbol{\varepsilon}}\phi^*)^{-1}$, and (23) holds, or equivalently,*

$$\sum_{\boldsymbol{\varepsilon} \in \Delta_n} s_{n-|\boldsymbol{\varepsilon}|/2} = \sum_{\boldsymbol{\varepsilon} \in \Delta_n} g_{\boldsymbol{\varepsilon}}(\mathbf{x}) K_{n-|\boldsymbol{\varepsilon}|/2}^{g_{\boldsymbol{\varepsilon}}\phi^*}(\mathbf{x}, \mathbf{x}), \quad (26)$$

for all $\mathbf{x} \in \mathbb{R}^d$.

(iii) *There are $s_n \leq m \leq s_{2n}$ points $\mathbf{x}_j^* \in S$, and a positive vector $\boldsymbol{\gamma} \in \mathbb{R}_+^m$ such that the atomic measure $\nu_n^* := \sum_{j=1}^m \gamma_j \delta_{\mathbf{x}_j^*}$ has same degree- $2n$ moments as ϕ^* . The normalized CD polynomial*

$$\mathbf{x} \mapsto K_n^{\phi^*}(\mathbf{x}, \mathbf{x}) / \sum_{\boldsymbol{\varepsilon} \in \Delta_n} s_{n-|\boldsymbol{\varepsilon}|/2} \quad (27)$$

attains its maximum 1 on S , at every vertex of S .

(iv) *With ν_n^* as in (iii), the sequence $(\nu_n)_{n \in \mathbb{N}}$ of probability measures on S , converges to ϕ^* for the weak-star topology of $\mathcal{M}(S)$, i.e.,*

$$\lim_{n \rightarrow \infty} \int_S f d\nu_n^* = \int_S f d\phi^*, \quad \forall f \in \mathcal{C}(S).$$

The proof of Theorem 3 mimics that of Theorem 1. Therefore finding an optimal design again reduces to finding a cubature for ϕ^* with positive weights, atoms in S , and exact up to degree $2n$. Examples of optimal atomic measures in Theorem 3(iii) can be obtained from [5].

Example 3 *With $d = 2$ and $2n = 4$, in solving the standard D-optimal design (1) one obtains 6 points (the three vertices and the mid-points on each facet). On the other hand in solving (2) one obtains a cubature for the equilibrium measure, supported on 8 points on the boundary and one point inside.*

3.4 Comparison with the original formulation

An optimal atomic solution μ^* of (1) is such that the degree- $2n$ SOS normalized CD polynomial $\mathbf{x} \mapsto K_n^{\mu^*}(\mathbf{x}, \mathbf{x})/s_n$ satisfies

$$0 \leq K_n^{\mu^*}(\mathbf{x}, \mathbf{x})/s_n \leq 1, \quad \forall \mathbf{x} \in S,$$

and μ^* is supported on r points $\mathbf{z}_i \in S$, $i = 1, \dots, r$, with $s_n \leq r \leq s_{2n}$, and $K^{\phi^*}(\mathbf{z}_i, \mathbf{z}_i) = s_n$ for all $i = 1, \dots, r$. If $r = s_n$ then the points $\{z_1, \dots, z_r\}$ form a set of Fekete points and are also Fejér points. However this case is not to be expected in general and even in special cases as the ones considered in this paper; see e.g. [4, 5]. Notice that an optimal measure $\mu^* \in \mathcal{P}(S)$ of (1) is not provided explicitly and in view of Theorem 1(iii), μ^* cannot be the equilibrium measure ϕ^* of S . Only the optimal moment matrix $\mathbf{M}_n(\mu^*)$ is obtained and is unique (while μ^* is not unique).

On the other hand, if one considers the proposed variants (7), (14) and (24) of the D-optimal design problem for the unit ball, the unit box and the simplex, respectively, then remarkably:

- For every degree n and every dimension d , the associated equilibrium measure ϕ^* of S is an optimal solution.
- every cubature of ϕ^* with positive weights, atoms in S , and exact up to degree $2n$, provides with a D-optimal atomic measure ν_n^* , and its support is an optimal design.
- The sequence $(\nu_n^*)_{n \in \mathbb{N}}$ converges to ϕ^* for the weak-star topology of $\mathcal{M}(S)$.

3.5 Computing an optimal atomic measure

As we have seen, it reduces to that of searching for *any* degree- $2n$ cubature with positive weights and atoms in S , for the (known) equilibrium measure ϕ^* of S . For the unit box $[-1, 1]^n$, the (tensorized) Gauss-Chebyshev cubature already provides a D-optimal design with no computation; see Corollary 1. For the Euclidean ball and the simplex, some cubatures for ϕ^* are also known in some cases. Otherwise one may also easily adapt the two-step procedure described in [8] to solve (1), to now solve the variants (7) and (24).

- Step-1 of the procedure now reduces to computing the vector ϕ_{2n}^* of moments up to degree $2n$ of ϕ^* , and they can be obtained in closed form with no need to invoke a numerical procedure.

– In Step-2 one solves a hierarchy of semidefinite programs. The unknowns are pseudo-moments $(\psi_\alpha)_{\alpha \in \mathbb{N}_{2t}^d}$ with $t > n$ and $\psi_\alpha = \phi_\alpha^*$ for all $|\alpha| \leq 2n$. If a (flat extension) sufficient condition on $\mathbf{M}_t(\psi)$ is satisfied then one may extract r points of S , which provide a D-optimal design (the support of a D-optimal atomic measure ν_n^*). For more details the interested reader is referred to [9].

4 More general semi-algebraic sets

The infinite-dimensional problem (7) is also equivalent to solving the single finite-dimensional convex problem:

$$\begin{aligned} \max_{\phi = (\phi_\alpha) \in \mathbb{R}^{s_{2n}}} \quad & \{ \log \det \mathbf{M}_n(\phi) + \log \det \mathbf{M}_{n-1}(g \cdot \phi) : \\ & \phi_0 = 1; \\ & \mathbf{M}_n(\phi) \succeq 0; \mathbf{M}_{n-1}(g \cdot \phi) \succeq 0 \}, \end{aligned} \quad (28)$$

where $\mathbf{M}_n(\phi)$ (resp. $\mathbf{M}_{n-1}(g \cdot \phi)$) is the moment matrix (resp. localizing matrix) associated with the sequence $\phi = (\phi_\alpha)_{\alpha \in \mathbb{N}_{2n}^d}$ of *pseudo-moments*. Notice that (28) is a relaxation of (7) as one now considers a vector ϕ of pseudo-moments (up to degree $2n$) rather than the vector of moments up to degree $2n$ of a measure ϕ on S . However and remarkably, Problem (28) has a unique optimal solution, the sequence ϕ_{2n}^* of moments (up to degree $2n$) of the equilibrium measure ϕ^* of S (uniqueness is due to strict concavity of the criterion).

Theorem 4 ([23]) *With $n \in \mathbb{N}$ fixed, the semidefinite program (28) has a unique optimal solution $\phi_{2n}^* = (\phi_\alpha^*) \in \mathbb{R}^{s_{2n}}$ which satisfies*

$$\phi_\alpha^* = \int_S \mathbf{x}^\alpha d\phi^*, \quad \forall \alpha \in \mathbb{N}_{2n}^d, \quad (29)$$

where ϕ^* is the equilibrium measure of S (optimal solution of (7)).

So while the equilibrium measure ϕ^* is not the unique optimal solution of (7) (any probability measure on \mathbb{R}^d with same degree- $2n$ moments as ϕ^* is also optimal), its vector ϕ_{2n}^* of moments up to degree $2n$, is the unique optimal solution of (28).

Basic semi-algebraic sets S

Of course for the special geometries of S (unit box, ball or simplex), we know ϕ^* (and so ϕ_{2n}^* as well) and there is no need to solve (28). But for other geometries, e.g., if $S \subset \mathbb{R}^d$ is the compact semi-algebraic set

$$S = \{ \mathbf{x} \in \mathbb{R}^d : g_j(\mathbf{x}) \geq 0, j = 1, \dots, m \} \quad (30)$$

for some $g_j \in \mathbb{R}[\mathbf{x}]$ of degree d_j , $j = 1, \dots, m$, then inspired by (28), we propose the following analogue of the D-optimal variants (2), (14), (24):

$$\max_{\phi \in \mathcal{P}(S)} \sum_{j=0}^m \log \det \mathbf{M}_{n-r_j}(g_j \cdot \phi), \quad (31)$$

where $g_0 = \mathbf{1}$, and $r_j = \lceil \deg(g_j)/2 \rceil$, $j = 0, \dots, m$.

Theorem 5 *Let $S \subset \mathbb{R}^d$ in (30) be compact with nonempty interior. Then every optimal solution $\mu \in \mathcal{P}(S)$ of (31) satisfies*

$$\sum_{j=0}^m s_{n-r_j} - \sum_{j=0}^m g_j(\mathbf{x}) K_n^{g_j \cdot \mu}(\mathbf{x}, \mathbf{x}) \geq 0, \quad \forall \mathbf{x} \in S \quad (32)$$

$$\sum_{j=0}^m s_{n-r_j} - \sum_{j=0}^m g_j(\mathbf{x}) K_{n-r_j}^{g_j \cdot \mu}(\mathbf{x}, \mathbf{x}) = 0, \quad \mu\text{-a.e.} \quad (33)$$

In addition, if $\mu = f d\mathbf{x}$ with $f > 0$ on S , is an optimal solution then

$$\sum_{j=0}^m s_{n-r_j} = \sum_{j=0}^m g_j(\mathbf{x}) K_{n-r_j}^{g_j \cdot \mu}(\mathbf{x}, \mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^d. \quad (34)$$

Proof: Introduce

$$\begin{aligned} \mathcal{C}_n &:= \left\{ \phi = (\phi_\alpha)_{\alpha \in \mathbb{N}_{2n}^d} : (\phi_\alpha) = \left(\int_S \mathbf{x}^\alpha d\phi \right) \right. \\ &\quad \left. \text{for some } \phi \in \mathcal{M}(S)_+ \right\} \\ \mathcal{P}_n &:= \{ p \in \mathbb{R}[\mathbf{x}]_{2n} : p \geq 0 \text{ on } S \}. \end{aligned}$$

It turns out that $\mathcal{C}_n = \mathcal{P}_n^*$ and $\mathcal{C}_n^* = \mathcal{P}_n$. For every $j \leq m$, let the real symmetric matrices \mathbf{B}_α^j be defined by

$$\sum_{j=0}^m g_j(\mathbf{x}) \mathbf{v}_{n-r_j}(\mathbf{x}) \mathbf{v}_{n-r_j}(\mathbf{x})^T = \sum_{\alpha \in \mathbb{N}_{2n}^d} \mathbf{B}_\alpha^j \mathbf{x}^\alpha, \quad \forall \mathbf{x} \in \mathbb{R}^d.$$

Then (31) also reads:

$$\max_{\phi \in \mathcal{C}_n} \left\{ \sum_{j=0}^m \log \det \mathbf{M}_{n-r_j}(g_j \cdot \phi) : \phi_0 = 1 \right\}, \quad (35)$$

which is a convex conic program. Let μ^* be an optimal solution of (31) and let $\boldsymbol{\mu}^* \in \mathcal{C}_n$ be its vector of moments up to degree $2n$. Then the necessary KKT-optimality conditions imply that there exists some scalar λ^* and some polynomial $q^* \in \mathcal{P}_n$ such that

$$\lambda^* \mathbf{1}_{\alpha=0} - \sum_{j=0}^m \langle \mathbf{M}_{n-r_j}(g_j \cdot \boldsymbol{\mu}^*)^{-1}, \mathbf{B}_\alpha^j \rangle = q_\alpha^*, \quad \forall \alpha \in \mathbb{N}_{2n}^d$$

and $\langle \boldsymbol{\mu}^*, q^* \rangle = 0$. Multiplying by μ_α and summing up yields $\lambda^* = \sum_{j=0}^m s_{n-r_j}$, and multiplying by \mathbf{x}^α and summing up yields the desired result (32)-(33). To get (34) observe that with $f > 0$ on S , and $q^* \in \mathcal{P}_n$

$$0 = \int_S q^* d\mu = \int_S q^* f d\mathbf{x} \quad \Rightarrow \quad q^* = 0 \text{ a.e. on } S,$$

and since S has nonempty interior, $q^* = 0$ for all $\mathbf{x} \in \mathbb{R}^d$. \square Of course as (31) is not solvable in general, we also introduce its convex relaxation

$$\max_{\boldsymbol{\mu}=(\mu_\alpha)} \left\{ \sum_{j=0}^m \log \det \mathbf{M}_{n-r_j}(g_j \cdot \boldsymbol{\mu}) : \mu_0 = 1; \right. \\ \left. \mathbf{M}_{n-r_j}(g_j \cdot \boldsymbol{\mu}) \succeq 0, \forall j \leq m \right\}, \quad (36)$$

where $\boldsymbol{\mu}$ is a vector of pseudo-moments up to degree $2n$.

In step-1 of the algorithm described in [9] to solve (1), one solves almost the same problem as (36) except that the criterion is simply $\log \det(\mathbf{M}_n(\boldsymbol{\mu}))$. So it is straightforward to adapt step-1 for solving (36). Then step-2 (whose input is the output $\boldsymbol{\mu}_{2n}^*$ of step-1), remains exactly the same. Its goal is to extract the support of an atomic probability measure on S with same moments as $\boldsymbol{\mu}_{2n}^*$, that is, an optimal design. Equivalently, (36) reduces to

$$\rho_n = \min_{\boldsymbol{\mu}=(\mu_\alpha)} \left\{ - \sum_{j=0}^m \log \det \mathbf{M}_{n-r_j}(g_j \cdot \boldsymbol{\mu}) : \phi_0 = 1; \right. \\ \left. \mathbf{M}_{n-r_j}(g_j \cdot \boldsymbol{\mu}) \succeq 0, \forall j \leq m \right\} \quad (37)$$

whose optimal value ρ_n is minus that of (36). Consider the convex optimization problem:

$$\rho_n^* = \max_{\mathbf{A}_j \succeq 0} \left\{ \sum_{j=0}^m \log \det(\mathbf{A}_j) : \right. \\ \sum_{j=0}^m s_{n-r_j} = \sum_{j=0}^m g_j(\mathbf{x}) \mathbf{v}_{n-r_j}(\mathbf{x})^T \mathbf{A}_j \mathbf{v}_{n-r_j}(\mathbf{x}), \\ \left. \text{for all } \mathbf{x} \in \mathbb{R}^d \right\}. \quad (38)$$

Under some condition⁶ it has been shown in [22, 23] that (38) is a dual of (37), and strong duality holds, i.e., $\rho_n = \rho_n^*$. Moreover (37) (resp. (38)) has an optimal solution $\boldsymbol{\mu}_{2n}^*$ (resp. (\mathbf{A}_j^*)), and $\mathbf{A}_j^* = \mathbf{M}_{n-r_j}(g_j \cdot \boldsymbol{\mu}_{2n}^*)^{-1}$ for all $j = 0, \dots, m$, and therefore

$$\sum_{j=0}^m s_{n-r_j} = \sum_{j=0}^m g_j(\mathbf{x}) K_{n-r_j}^{g_j \cdot \boldsymbol{\mu}_{2n}^*}(\mathbf{x}, \mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^d. \quad (39)$$

The difference with the above three special cases of S , is that now the linear functional $\boldsymbol{\mu}_{2n}^* \in \mathbb{R}[x]_{2n}^*$ is not guaranteed to have a representing measure μ^* on S (step-1 of the algorithm in [9] and in its adaptation proposed for (2) assumes that it is the case), let alone μ^* being the equilibrium measure of S . However as shown in [22], each accumulation point of the sequence $(\boldsymbol{\mu}_{2n}^*)_{n \in \mathbb{N}}$ is a probability measure μ^* on S .

Remark 1 Suppose that (31) has an optimal solution $\mu \in \mathcal{P}(S)$ such that $\mu = f d\mathbf{x}$ with $f > 0$ on S . If S has nonempty interior then by Theorem 5

$$\sum_{j=0}^m s_{n-r_j} = \sum_{j=0}^m g_j(\mathbf{x}) K_{n-r_j}^{g_j \cdot \mu}(\mathbf{x}, \mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^d,$$

and so $\boldsymbol{\mu}_{2n} := (\mu_\alpha)_{\alpha \in \mathbb{N}_{2n}^d}$ is an optimal solution of the relaxation (36). In other words, the relaxation (36) (or (37)) is exact.

⁶If $\mathbf{1} \in \text{int}(Q_n(g))$ with $Q_n(g) \subset \mathbb{R}[\mathbf{x}]$ being the truncated quadratic module generated by g_1, \dots, g_m in the definition of S .

Link between μ_{2n}^* and the equilibrium measure of S

With ϕ^* being the equilibrium measure of S , consider the polynomial $p_n^* \in \mathbb{R}[\mathbf{x}]_{2n}$ defined by:

$$\mathbf{x} \mapsto \left(\sum_{j=0}^m s_{n-r_j} \right) p_n^*(\mathbf{x}) := \sum_{j=0}^m g_j(\mathbf{x}) K_{n-r_j}^{g_j \cdot \phi^*}(\mathbf{x}, \mathbf{x}), \quad (40)$$

for all $\mathbf{x} \in \mathbb{R}^d$. Again under some regularity properties of S and ϕ^* , it turns out that

$$\lim_{n \rightarrow \infty} \int_S f(\mathbf{x}) p_n^*(\mathbf{x}) d\phi^*(\mathbf{x}) = \int_S f d\phi^*, \quad \forall f \in \mathcal{C}(S),$$

i.e., $p_n^* \phi^* \Rightarrow \phi^*$ as $n \rightarrow \infty$ (for the weak convergence of probability measures), and

$$\lim_{n \rightarrow \infty} p_n^*(\mathbf{x}) = 1 \quad (41)$$

uniformly on compact subsets of $\text{int}(S)$; for conditions ensuring (41) the interested reader is referred to e.g. [21]. Comparing (39) with (40)-(41) show that even if the linear functional μ_{2n}^* does not have a representing measure, asymptotically it is strongly connected to the equilibrium measure ϕ^* of S . Indeed, for sufficiently large degree n and for every $\mathbf{x} \in \text{int}(S)$:

$$\begin{aligned} \sum_{j=0}^m g_j(\mathbf{x}) K_{n-r_j}^{g_j \cdot \phi^*}(\mathbf{x}, \mathbf{x}) &\approx \sum_{j=0}^m s_{n-r_j} \\ &= \sum_{j=0}^m g_j(\mathbf{x}) K_{n-r_j}^{g_j \cdot \mu_{2n}^*}(\mathbf{x}, \mathbf{x}). \end{aligned}$$

Hence this asymptotic property supports our claim that the variant (31) of the D-optimal design problem still has a strong connection with the equilibrium measure of S .

5 Conclusion

We have introduced a variant of the D-optimal design problem with a more general information matrix which takes into account the geometry of the design space $S \subset \mathbb{R}^d$. One main reason to introduce such a variant is that remarkably, for the three cases where S is the Euclidean ball, the unit box and the canonical simplex (in any dimension), the equilibrium measure ϕ^* of S (in pluripotential theory) provides an optimal solution for every degree n . Therefore finding a D-optimal design (for this variant) reduces to finding a cubature for ϕ^* , with positive weights, atoms in S , and exact up to degree $2n$. Moreover and trivially, the associated resulting sequence of atomic probability measures $(\nu_n^*)_{n \in \mathbb{N}}$ converges to ϕ^* for the weak-star topology.

If the link between statistics and approximation theory has been largely invoked in the literature since the pioneer works [18] and [16], this new variant makes it even stronger and striking, at least for the three specific cases of S . Hence such a remarkable property suggests that one might use the log-det criterion of this new information matrix, even for more general compact basic semi-algebraic sets $S \subset \mathbb{R}^d$. In particular, the two-step algorithm proposed in [9] is easily adapted to this new variant of the D-optimal design problem.

Acknowledgments

The authors are grateful to Saroj Prasad Chhatoi and Srecko Durasinovic, as well as Yohann de Castro and Fabrice Gamboa for useful discussions.

References

- [1] M. Baran. Complex equilibrium measure and Bernstein type theorems for compact sets in \mathbb{R}^n , Proc. Amer. Math. Soc. 123(2), pp. 485–494, 1995.
- [2] E. Bedford, B.A. Taylor. The complex equilibrium measure of a symmetric convex set in \mathbb{R}^n , Trans. Amer. Math. Soc. 294(2), pp. 705–717, 1986.
- [3] R.J. Berman, S. Boucksom, D.W. Nyström. Fekete points and convergence towards equilibrium measures on complex manifolds, Acta. Math. **207**(1), pp. 1–27, 2011
- [4] L. Bos. Some remarks on the Fejér Problem for Lagrange interpolation in several variables. J. Approx. Theory **60**, pp. 133–140, 1990.
- [5] L. Bos. On Fekete points for a real Simplex. Indagationes Mathematicae **34**(2), pp. 274–293, 2023.
- [6] L. Bos, N. Levenberg, S. Waldron. On the spacing of Fekete points for a sphere, ball or simplex, Indag. Math. (N.S.) 19(2), pp. 163–176, 2008.
- [7] M. Briani, A. Sommariva, M. Vianello. Computing Fekete and Lebesgue points: simplex, square, disk. J. Comput. Appl. Math. **236**, pp. 2477–2486, 2012
- [8] Y. de Castro, F. Gamboa, D. Henrion, R. Hess, J. B. Lasserre. Approximate optimal designs for multivariate polynomial regression. Annals of Statistics, 47(1):127-155, 2019.
- [9] Y. De Castro, F. Gamboa, D. Henrion, J. B. Lasserre. Dual optimal design and the Christoffel-Darboux polynomial. Optimization Letters, 15(1):3-8, 2021.
- [10] H. Dette. A generalization of D - and D_1 -optimal designs in polynomial regression, Ann. Stat. **18**(4), pp. 1784–1804, 1990.
- [11] C. Dunkl, Y. Xu. *Orthogonal polynomials of several variables*, Cambridge Univ. Press, Encyclopedia of Mathematics and its Applications 155, 2014, 2nd edition.
- [12] S. Heo, Y. Xu. Constructing cubature formula for spheres and balls, J. Approx. Theory **112**(1-2), pp. 95–119, 1999.
- [13] P.G. Hoel. Efficiency in polynomial estimation. Ann. Math. Statist. **29**, pp. 1134–1145, 1958.
- [14] P.G. Hoel, A. Levine. Optimal spacing and weighing in polynomial prediction, Ann. Math. Statist. **35**, pp. 1553–1560, 1964.

- [15] Xun Huan, J. Jagalur, Y. Marzouk. Optimal experimental design: Formulations and computations, *Acta Num.* **33**, pp. 1–129, 2024
- [16] S. Karlin, W.J. Studden. *Tchebycheff Systems: With Applications in Analysis and Statistics*, Interscience, New York, 1966.
- [17] J. Kiefer. Optimum designs in regression problems II, *Ann. Math. Statist.* **32**, pp. 298–325, 1961.
- [18] J. Kiefer, J. Wolfowitz. The equivalence of two extremum problems. *Canad. J. Math.* **12**, pp. 363–366, 1960.
- [19] S. Kirsch. Transfinite Diameter, Chebyshev Constant and Capacity, Chapter 6 in *Handbook of Complex Analysis: Geometric Function Theory*, volume 2, R. Kühnau ed., Elsevier B.V., 2005, pp. 243–305.
- [20] M. Klimek. *Pluripotential Theory*, Clarendon Press, UK, 1992
- [21] A. Kroó, D.S. Lubinsky. Christoffel functions and universality in the bulk for multi-variable orthogonal polynomials, *Canad. J. Math.* **65**(3), pp. 600–620, 2012.
- [22] J.B. Lasserre. Pell’s equation, sum-of-squares and equilibrium measures on a compact set, *Comptes Rendus Mathématique* **361**, pp. 935–952, 2023
- [23] J.B. Lasserre, Yuan Xu. A generalized Pell’s equation for a class of multivariate orthogonal polynomials. To appear in *Trans. Amer. Math. Soc.*, 2024
- [24] J.B. Lasserre, E. Pauwels, M. Putinar. *The Christoffel-Darboux Kernel for Data Analysis*, Cambridge University Press, Cambridge, UK, 2022.
- [25] E. Läuter. Experimental design in a class of models, *Math. Oper. Statist.* **5**, pp. 379–398, 1974.
- [26] N. Levenberg. Approximation in \mathbb{C}^N , *Surveys in Approximation Theory* **2**, pp. 92–140, 2006
- [27] F. Piazzon. Pluripotential numerics. *Constr. Approx* **49**, pp. 227–263, 2019.
- [28] E.B. Saff, V. Totik. *Logarithmic Potentials with External Fields*, Springer, Berlin, Heidelberg, 2010.
- [29] W.J. Studden. Optimal designs on Tchebycheff points, *Ann. Math. Stat.* **39**(5), pp. 1435–1447, 1968.