A Semidefinite Programming Study of the Elfving Theorem

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July 16, 2009

Abstract

The theorem of Elfving is one of the most important and earliest results that have led to the theory of optimal design of experiments. This paper presents a fresh study of it from the viewpoint of modern semidefinite programming. There is one-to-one correspondence between solutions of the derived semidefinite programming problem (SDP) and \(c\)-optimal designs. We also derive a uniqueness theorem that ensures unique optimal design without assuming the linear independence property over the largest set of supporting points. The SDP can also be cast as an \(\ell_1\)-convex programming that has recently been extensively studied and often yields sparse solutions. Our numerical experiments on the trigonometric regression model confirm that the SDP does produce a sparse optimal design.

Keywords: Elfving theorem, Semidefinite Programming, Optimal designs, Tangent cones, Constraint qualification.

1 Introduction

Elfving’s theorem (Elfving 1952) is one of the most important results that led to the theory of optimal design of experiments. Its significance, far-reaching influence on many other important results and its links to other mathematical theories such as approximation theory have been well documented, see, e.g., Chernoff (1999), Dette (1993), Dette and Melas (2003), Fellman (1999), Nordström (1999), Studden (1971, 2005), to just name a few. Detailed discussion and more references on the theorem can be found in the classical book by Pukelsheim (Reprint 2006, SIAM Classics).

In this paper, we present a semidefinite programming study on the theorem. This study not only provides new insights into this famous theorem from a modern optimization point of view, but also derives a uniqueness theorem about when the optimal design is unique. It also provides a semidefinite programming problem that can be cast as an \(\ell_1\) convex optimization. The \(\ell_1\) convex optimization has recently made significant progress in retrieving the sparsest solutions in signal processing, see Bruckstein, Donoho, Elad (2009), Candès and Tao (2005), Donoho and Tanner (2005), and Tropp (2006). A sparse solution in our case corresponds to a set of independent design points. The notation in our study largely follows the book of Pukelsheim

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(2006) with few exceptions. For example, we use $S^k_+$ to denote the set of all positive semidefinite matrices of order $k$ (vs $\text{NND}(k)$ in the book). $S^k$ is equipped with the standard trace inner product.

Suppose we have a linear model:

$$y = \theta'x + e,$$

where $y$ is a univariate response, $\theta \in \mathbb{R}^k$ is the full vector of unknown parameters, $x \in \mathcal{X} \subset \mathbb{R}^n$ is the regression vector and $\mathcal{X}$ is usually compact, and $e$ follows $N(0, \sigma^2)$. We assume that for each observation made, $e$ is mutually independent. Our main interest is to learn a scalar system $c'\theta$ with $c \in \mathbb{R}^k$ being prescribed prior to experimentation. The Elfving theorem is about to find an optimal design for $c'\theta$ (known as $c$-optimal design.) The following version is taken from [21, Theorem 2.14].

**Theorem 1.1** Assume that the regression range $\mathcal{X} \subset \mathbb{R}^k$ is compact, and that the coefficient vector $c \in \mathbb{R}^k$ lies in the regression space $\mathcal{L}(\mathcal{X})$ and Elfving norm $\rho(c) > 0$. Then a design $\xi \in \Xi$ is optimal for $c'\theta$ iff there exists a function $\epsilon$ on $\mathcal{X}$ which on the support of $\xi$ takes values 1 or $-1$ such that

$$\frac{c}{\rho(c)} = \int_{\mathcal{X}} \epsilon(x) x d\xi.$$

There exists an optimal design for $c'\theta$ in $\Xi$, and the optimal variance is $(\rho(c))^2$.

In the above theorem, $\mathcal{L}(\mathcal{X})$ is the space spanned by all the regression vectors in $\mathcal{X}$. The Elfving norm $\rho(c)$ is given by

$$\rho(c) := \inf \{ \delta \geq 0 : c \in \delta \mathcal{R} \},$$

and $\mathcal{R}$ is the convex hull of the set $\{-\mathcal{X}, \mathcal{X}\}$. A design $\xi$ has always a finite support $\text{supp}(\xi) := \{x_i \in \mathcal{X} : \xi(x_i) > 0\}$ satisfying $\sum_{x_i \in \text{supp}(\xi)} \xi(x_i) = 1$. $\Xi$ denotes the set of all possible designs. The moment matrix $M(\xi)$ of a design $\xi$ is given by

$$M(\xi) := \sum_{x_i \in \text{supp}(\xi)} \xi(x_i) x_i x_i'.$$

When no confusion is caused we often write $M(\xi)$ as $M$.

Let us recall what defines an optimal design $\xi$ for the system $c'\theta$. Let $\mathcal{A}(c)$ denote the feasibility cone

$$\mathcal{A}(c) := \left\{ A \in S^k_+ : c \in \text{range}(A) \right\},$$

and $M(\Xi)$ be the set of all moment matrices. An optimal design $\xi$ for $c'\theta$ solves the following design problem:

$$\begin{align*}
\min_{M} & \quad c' M^{-c} \\
\text{s.t.} & \quad M \in M(\Xi) \cap \mathcal{A}(c),
\end{align*}$$

(1)

where $M^{-}$ is independent of any choice of the generalized inverse of $M$. However, the problem (1) is extremely difficult to solve, not just because the generalized inverse of $M$ is involved in the objective function, but mainly because the feasible set $M(\Xi) \cap \mathcal{A}(c)$ is, though convex, neither closed nor open.
The Elfving theorem takes a completely different route deeply rooted in duality of optimization. Two important elements play a key role here. One is the supporting hyperplane that supports the convex body $R$ at $c/\rho(c)$ (recall that $c/\rho(c)$ is on the boundary of $R$ due to the Elfving norm $\rho(c)$). The supporting hyperplane given by a normalized vector $h \in \mathbb{R}^k$ satisfies
\[ z' h \leq 1 = c' h / \rho(c) \quad \text{for all } z \in R. \] (2)

The supporting points $x_i$ in any optimal design $\xi$ are contained in this hyperplane. The second element is that the matrix $hh' \in \mathcal{S}^k$ actually constitutes a rank-1 solution to the following semidefinite programming (SDP) problem:
\begin{align*}
\max_{N \in \mathcal{S}^k} & \quad \langle N, cc' \rangle \\
\text{s.t.} & \quad \langle N, x_i x_i' \rangle \leq 1, \quad \forall x_i \in \mathcal{X} \\
& \quad N \in \mathcal{S}^k_{++}.
\end{align*} (3)

It is generally true that the optimal objective value of problem (3) provides a lower bound for that of (1). In fact, there is no duality gap between them and the common value is $(\rho(c))^2$.

It is for this reason that problem (3) is regarded as the dual problem of (1) (see [21, Section 2.11].) However, finding a rank-1 solution of (3) is a nonconvex problem and hence is extremely difficult to solve. Despite its significant role in deriving the Elfving theorem, Problem (3) is less significant from a computational point of view in the sense that a rank-1 solution is needed.

To ease our presentation, let us consider the finite case where $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$. Our development will carry over to the general compact case $X$, which is to be dealt with in Section 4. We note that when $\mathcal{X}$ is finite problem (3) is a standard SDP problem, see Ben-Tal and Nemirovski (2001), Boyd and Vandenberghe (2004), Vandenberghe and Boyd (1996), and Wolkowicz, Saigal, and Vandenberghe (2000). Now let us consider its dual problem:
\begin{align*}
\min_{y \in \mathbb{R}^n} & \quad 1_n'y \\
\text{s.t.} & \quad \sum_{i=1}^n y_i (x_i x_i') \succeq cc' \\
& \quad y_i \geq 0, \quad i = 1, \ldots, n,
\end{align*} (4)

where $1_n$ is the (column) vector of all ones in $\mathbb{R}^n$, $y := (y_1, \ldots, y_n)' \in \mathbb{R}^n$ is the Lagrangian multiplier corresponding to the inequality constraints in (3), and for symmetric matrices $A, B$, $A \succeq B$ means $(A - B)$ is positive semidefinite.

It is easy to see that there always exists a positive definite matrix $N \in \mathcal{S}^k$ such that
\[ \langle N, x_i x_i' \rangle < 1, \quad \text{for all } x_i \in \mathcal{X}. \]
That is, the well-known Slater condition holds for (3). It follows from (Theorem 5.81, Bonnans and Shapiro 2000) that there is no duality gap between (3) and (4) if (4) is feasible. Since the optimal objective function value of (4) is finite (note $1_n'y \geq 0$ for feasible $y$), Theorem 5.81 again implies that an optimal solution of (4) always exists. We will see that the feasibility condition on problem (4) actually requires
\[ M(\Xi) \cap A(c) \neq \emptyset. \] (5)

Hence, the optimal objective value for (4) is also $(\rho(c))^2$.
The duality approach is getting interesting once we slightly reformulate problem (4). Let

\[ M := \text{conv} \{ x_i x'_i \mid x_i \in \mathcal{X} \} \quad \text{and} \quad \delta := 1'_n y. \]

We only consider those points that ensure \( \delta > 0 \). Then

\[ \sum_{i=1}^n y_i (x_i x'_i) = \delta \sum_{i=1}^n \frac{y_i}{\delta} (x_i x'_i) =: \delta M, \]

where \( M := \sum_{i=1}^n y_i (x_i x'_i)/\delta \) is the moment matrix associated to the design \( \xi \) with weights \( \xi(x_i) = y_i/\delta \) (note that \( \sum (y_i/\delta) = 1 \)). Therefore, problem (4) is equivalent to

\[
\begin{align*}
\min_{\delta} & \quad \delta \\
\text{s.t.} & \quad cc' \in \delta M - S^k_+ + S^k_+ = \delta (M - S^k_+) \\
& \quad \delta \geq 0.
\end{align*}
\]

Note that \( \delta \neq 0 \) as long as \( c \neq 0 \). Let \( P \) denote the penumbra defined by the set \( M \), i.e., \( P := M - S^k_+ \). We arrived at the following optimization problem:

\[
\begin{align*}
\min_{\delta} & \quad \delta \\
\text{s.t.} & \quad cc' \in \delta P \\
& \quad \delta \geq 0.
\end{align*}
\] (6)

The existence of an optimal solution of (4) implies that of (6). This recovered Theorem 4.11 in [21].

This interesting connection between (4) and (6) suggests that optimal solutions of (4) have deep relationships with optimal designs of (1). We formalize this observation in Theorem 3.2 that shows that there is one-to-one correspondence between optimal solutions of the two problems (4) and (1). We also show in Proposition 3.1 that our SDP problem (4) is solvable if and only if condition (5) holds.

Suppose \( h \in \mathbb{R}^k \) satisfying (2) defines a hyperplane \( \mathcal{H} \) that supports \( \mathcal{R} \) at \( c/\rho(c) \). Let the set of the supporting points in \( \mathcal{H} \) be

\[ \text{supp}(\mathcal{H}) := \{ x_i \in \mathcal{X} \mid x_i \in \mathcal{H} \ \text{or} \ - x_i \in \mathcal{H} \}. \] (7)

It is widely known that if the points in the set \( \text{supp}(\mathcal{H}) \) are linearly independent, then there is a unique optimal design (this result follows from the Elfving theorem.) We present a sufficient condition in Theorem 3.6 that ensures the uniqueness of optimal designs without assuming the linear independence of the design points in \( \mathcal{H} \).

The paper is organized as follows. We review some results in Section 2 for later use. Section 3 contains our main results such as the feasibility proposition 3.1, the solvability theorem 3.2, and uniqueness theorem 3.6. We also include a couple of examples to illustrate the main results. We discuss possible generalization of those results to compact set \( \mathcal{X} \) in Section 4. Numerical results reported in Section 5 confirm that SDP (4) does lead to sparse optimal designs. We conclude the paper in Section 6.
2 Preliminaries

In this section, we introduce some notation and collect some facts mainly related to the positive semidefinite cone $S^k_+$ for later use. The first of such facts is the range summation lemma ([21, Lemma 2.3]).

**Lemma 2.1** Let $A, B \in S^k_+$. The we have
\[
\text{range}(A + B) = \text{range}(A) + \text{range}(B).
\]

It is also known that every square root $U$ of a positive semidefinite matrix $V$ has the same range as $V$ (see [21, Section 1.14]), that is
\[
V = UU' \implies \text{range}(V) = \text{range}(U).
\]

It then follows Lemma 2.1 and (8) that for any $y_i \geq 0, i = 1, \ldots, n$ we have
\[
\text{range} \left( \sum_{i=1}^n y_i (x_ix_i') \right) = \sum_{i=1}^n y_i \text{range}(x_i).
\]

We also need a representation of the tangent cone of $S^k_+$ at some of its boundary points. See Rockafellar (1970) for general treatment of tangent cone. The representation is going to be used in our uniqueness theorem 3.6.

Let $A \in S^k$ have the following spectral decomposition:
\[
A = P\Lambda P',
\]
where $\Lambda$ is the diagonal matrix of eigenvalues $\lambda_1 \geq \lambda_2 \leq \ldots \geq \lambda_k$ of $A$ and $P$ is a corresponding orthogonal matrix of orthonormal eigenvectors.

Define three index sets of positive, zero, and negative eigenvalues of $A$, respectively, by
\[
\alpha := \{i : \lambda > 0\}, \quad \beta := \{i : \lambda = 0\}, \quad \gamma := \{i : \lambda < 0\}.
\]

Write
\[
\Lambda = \begin{bmatrix}
\Lambda_\alpha & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & \Lambda_\gamma
\end{bmatrix}
\quad \text{and} \quad
P = [P_\alpha, P_\beta, P_\gamma],
\]

with $P_\alpha$ being a submatrix $P$ containing the eigenvectors of positive eigenvalues, $P_\beta$ the eigenvectors of zero eigenvalues, and $P_\gamma$ the eigenvectors of negative eigenvalues. Define
\[
A_+ := P \begin{bmatrix}
\Lambda_\alpha & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix} P' \quad \text{and} \quad
A_- := P \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & -\Lambda_\gamma
\end{bmatrix} P'.
\]

Then $A_+, A_- \in S^k_+$. The tangent cone of $S^k_+$ at $A_-$, denoted by $T_{S^k_+}(A_-)$, is given by (see Arnold 1971, Alizadeh et.al. (1997), and Bonnans and Shapiro (2000))
\[
T_{S^k_+}(A_-) = \left\{ B \in S^k : [P_\alpha, P_\beta]' B [P_\alpha, P_\beta] \succeq 0 \right\}.
\]
The orthogonal space of \( \text{span}(A_+) \) is given by
\[
A_+^\perp = \left\{ B \in S^k : P'_\alpha B P_\alpha = 0 \right\}.
\]

Therefore, we have
\[
T_{S^k_k} (A_-) \cap A_+^\perp = \left\{ B \in S^k : P'_\alpha B P_\alpha = 0, \ P'_\beta B P_\beta \succeq 0 \right\}.
\] (13)

Let \( C \) be a cone in a Hilbert space \( S \). Its polar cone \( C^0 \) is defined by
\[
C^0 := \left\{ u \in S : \langle u, v \rangle \leq 0, \text{ for all } v \in C \right\}.
\]

If \( C_1 \) and \( C_2 \) are two cones in \( S \), then (see [5, Eq. 2.31])
\[
(C_1 + C_2)^0 = C_1^0 \cap C_2^0.
\] (14)

3 Optimal Designs via SDP (4)

Our first result is about the solvability of SDP (4). Recall the fact that condition (5) holds iff \( c \in L(X) \), where \( L(X) = \text{span}\{x_1, \ldots, x_n\} \) (see [21, Section 2.8].) Associated with the subspace \( L(X) \) is a face of \( S^k_\perp \) defined by (see Barker and Carlson 1975)
\[
\mathcal{F} := \left\{ A \in S^k_\perp : \text{range}(A) \subseteq L(X) \right\}.
\]

Suppose the dimension of \( L(X) \) is \( \ell \), i.e., \( \ell := \dim(L(X)) \). Then there exists an orthonormal matrix \( P \in \mathbb{R}^{k \times k} \) such that
\[
\mathcal{F} = \left\{ P \begin{bmatrix} U & 0 \\ 0 & 0 \end{bmatrix} P' \mid U \in S^\ell_+ \right\}.
\] (15)

Let \( C(X) \) be the cone generated by all the design points in \( X \) by the following way:
\[
C(X) := \left\{ \sum_{i=1}^n y_i(x_i x'_i) \mid x_i \in X \text{ and } y_i \geq 0, \ i = 1, \ldots, n \right\}.
\]

Then for any \( A \in C(X) \), there exists \( y_i \geq 0 \) such that
\[
\text{range}(A) = \text{range} \left( \sum_{i=1}^n y_i(x_i x'_i) \right)
\]
\[
= \sum_{i=1}^n y_i \text{range}(x_i) \quad \text{(by (9))}
\]
\[
\subseteq \sum_{i=1}^n \text{range}(x_i) \quad \text{(some } y_i \text{ may be zero)}
\]
\[
= L(X).
\]
Therefore,
\[ \mathcal{C}(\mathcal{X}) \subseteq \mathcal{F}. \] (16)

We emphasize that the inclusion may be strict. For example, take \( \mathcal{X} = \{x_1, x_2\} \) with \( x_1 = [1, 0]' \) and \( x_2 = [0, 1]' \). The constraints in (4) boil down to a single constraint:
\[ cc' \in \mathcal{C}(\mathcal{X}). \]

We have the following solvability result.

**Proposition 3.1** The SDP problem (4) is feasible iff \( c \in \mathcal{L}(\mathcal{X}) \).

**Proof.** Sufficiency. Suppose \( c \in \mathcal{L}(\mathcal{X}) \). It is well known ([21, Section 2.14]) that there exists a design \( \xi \) and \( 0 \neq h \in \mathcal{L}(\mathcal{X}) \) such that
\[ \frac{c}{\rho(c)} = M(\xi)h \quad \text{and} \quad h'x \leq 1 \quad \forall \, x \in \mathcal{X}. \] (17)

Then we have the following chain of equalities and inequalities: For any \( d \in \mathbb{R}^k \),
\[
d'(cc')d = (c'd)^2 = (\rho(c))^2(h'Md)^2 \quad \text{(by (17))}
= (\rho(c))^2 \left[ h' \left( \sum_{x \in \text{supp}(\xi)} \xi(x)xx' \right) d \right]^2
= (\rho(c))^2 \left[ \sum_{x \in \text{supp}(\xi)} \xi(x)(h'x)(x'd) \right]^2
\leq (\rho(c))^2 \left[ \sum_{x \in \text{supp}(\xi)} \xi(x)h'x^2 \right] \left[ \sum_{x \in \text{supp}(\xi)} \xi(x)x'd^2 \right]
\leq (\rho(c))^2 \left[ \sum_{x \in \text{supp}(\xi)} \xi(x) \right] \left[ \sum_{x \in \text{supp}(\xi)} \xi(x)(x'd)^2 \right]
= (\rho(c))^2 \left[ \sum_{x \in \text{supp}(\xi)} \xi(x)(x'd)^2 \right]
= \sum_{i=1}^n y_i(x_i'd)^2 = d' \left( \sum_{i=1}^n y_i(x_i'x_i) \right) d, \tag{18}
\]
where
\[ y_i := \begin{cases} (\rho(c))^2 \xi(x_i), & \text{if } x_i \in \text{supp}(\xi) \\ 0, & \text{otherwise.} \end{cases} \]

The first inequality is by the Cauchy-Schwarz Inequality. Because of the arbitrary choice of \( d \) above, we proved that
\[ \sum_{i=1}^n y_i(x_i'x_i) \geq cc'. \]

This finishes the sufficiency part.
Necessity. Suppose \( c \notin \mathcal{L}(\mathcal{X}) \). That is, \( \text{range}(c) \cap \mathcal{L}(\mathcal{X}) = \emptyset \). This is equivalent to
\[
\text{range}(cc') \cap \mathcal{L}(\mathcal{X}) = \emptyset,
\]
which implies \( cc' \notin \mathcal{F} \). Let the matrix \( P \) be such defined as in (15). Then we must have
\[
P'(cc')P = \begin{bmatrix} U_1 & U_2 \\ U'_2 & U_3 \end{bmatrix} \succeq 0,
\]
with \( U_1 \in \mathcal{S}_+^\ell \) and \( 0 \neq U_3 \in \mathcal{S}_+^{k-\ell} \) (if \( U_3 = 0 \) we would have \( U_2 = 0 \) by the positive semidefiniteness of \( cc' \), leading to \( cc' \in \mathcal{F} \).)

It follows from (16) and (15) that for any \( A \in \mathcal{C}(\mathcal{X}) \) there exists \( U \in \mathcal{S}_+^\ell \) such that
\[
A - cc' = P \begin{bmatrix} U & 0 \\ 0 & 0 \end{bmatrix} P' - P(P'(cc')P)P' = P \begin{bmatrix} U - U_1 & -U_2 \\ -U'_2 & -U_3 \end{bmatrix} P' \notin \mathcal{S}_+^k,
\]
as \( -U_3 \) is not positive semidefinite. This shows
\[
cc' \notin \mathcal{L}(\mathcal{X}).
\]
This proves the necessity part. \( \square \)

Because of Proposition 3.1, we always assume that \( c \in \mathcal{L}(\mathcal{X}) \), which is also required by (1) to ensure estimability. Our next major result is on one-to-one correspondence between optimal solutions of (1) and that of (4).

**Theorem 3.2** Suppose \( \xi \) is an optimal design of (1). Then \( y \in \mathbb{R}^n \) defined by
\[
y_i := \begin{cases} (\rho(c))^2 \xi(x_i), & x_i \in \text{supp}(\xi) \\ 0, & \text{otherwise}, \end{cases} \quad i = 1, \ldots, n \tag{19}
\]
is an optimal solution of (4).

Conversely, if \( y \in \mathbb{R}^n \) is an optimal solution of (4). Then the design \( \xi \) defined by
\[
\xi(x_i) := \frac{y_i}{\sum_{i=1}^n y_i}, \quad i = 1, \ldots, n \tag{20}
\]
is an optimal design of (1).

**Proof.** Suppose \( \xi \) is a given optimal design of (1). We need to prove that the vector \( y \) defined by (19) is not only feasible, but also optimal to problem (4). We note that for any optimal design \( \xi \) there exists (see [21, Section 2.14]) \( 0 \neq h \) such that
\[
\frac{c}{\rho(c)} = M(\xi)h \quad \text{and} \quad (h'x)^2 = 1 \quad \text{for any} \ x \in \text{supp}(\xi).
\]
We can follow the proof in (18) to claim that
\[ \sum_{i=1}^{n} y_i(x_ix'_i) \succeq cc'. \]

Hence \( y \) defined by (19) is feasible. The optimality follows easily from the fact
\[ 1_n' y = (\rho(c))^2 \sum_{i=1}^{n} \xi(x_i) = (\rho(c))^2, \]
which means that \( y \) in (19) achieves the optimal objective value \( (\rho(c))^2 \) of (4) as pointed out in introduction.

Now we come to the converse part. Suppose \( y \) is an optimal solution of (4) and \( \xi \) is defined as in (20). We note that \( 1_n' y = (\rho(c))^2 \). There also exists a vector \( h \) satisfying (2) and \( N := hh' \) is an optimal solution of (3). Since (4) and (3) are a pair of dual problems, \( y \) and \( N \) must satisfy the Karush-Kuhn-Tucker condition:
\[ \langle xx', N \rangle \leq 1 \quad \forall \, x \in \mathcal{X} \]
\[ y_i(1 - \langle xx', N \rangle) = 0, \quad i = 1, \ldots, n \]
\[ \sum_{i=1}^{n} y_i(x_ix'_i) \succeq cc' \]
\[ \left( \sum_{i=1}^{n} y_i(x_ix'_i) - cc' \right) N = 0. \]
(22)

It follows from (21) that
\[ \langle x_ix'_i, N \rangle = 1 \quad \forall \, x_i \in \text{supp}(\xi) = \{x_i \mid y_i > 0\}, \]
which implies
\[ (x'_ih)^2 = 1 \quad \forall \, x_i \in \text{supp}(\xi). \]
(23)

It follows from (22) that
\[ M(\xi)N - \frac{1}{(\rho(c))^2} cc'N = 0. \]
Postmultiplying it by \( h/(h'h) \) we have
\[ M(\xi)h - \frac{1}{(\rho(c))^2} cc'h = 0, \]
which combines with (2) yields
\[ M(\xi)h = \frac{c}{\rho(c)}. \]
That is
\[ \sum_{x \in \text{supp}(\xi)} \xi(x)(xx')h = \frac{c}{\rho(c)}. \]
Noticing (23), we let \( \epsilon(x) := x'h \in \{1, -1\} \). Hence
\[
\frac{c}{\rho(c)} = \sum_{x \in \text{supp}(\xi)} \xi(x) \epsilon(x)x \quad \text{with} \quad \epsilon(x) \in \{1, -1\}.
\]
By the Elfving theorem 1.1, \( \xi \) defined by (20) is an optimal design \( \Box \).

Now let us look at an example

Example 3.3 ([21, Section 2.21]) Consider the parabola fit model:
\[
Y_{ij} = \theta_0 + \theta_1 t_i + \theta_2 t_i^2 + e_{ij},
\]
with the experimental domain \( t \in [-1, 1] \). Choose a special regression space
\[
X := \left\{ \begin{bmatrix} 1 & t & t^2 \end{bmatrix} : t \in \{-1, 0, 1\} \right\} \quad \text{and} \quad c = \begin{bmatrix} -1 \\ 0 \\ 2 \end{bmatrix}.
\]

The SDP problem (4) becomes
\[
\begin{align*}
\min & \quad y_1 + y_2 + y_3 \\
\text{s.t.} & \quad y_1 \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix} + y_2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + y_3 \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \succeq \begin{bmatrix} 1 & 0 & 2 \\ 0 & 0 & 0 \\ -2 & 0 & 4 \end{bmatrix},
\end{align*}
\]
\( y_1 \geq 0, \ y_2 \geq 0, \ y_3 \geq 0. \)

It is not hard to find that the (unique) optimal solution is:
\( y_1 = 5, \ y_2 = 15, \ y_3 = 5. \)

Hence the optimal design \( \xi \) is given by (20):
\[
\xi(x_1) = \frac{1}{5}, \ \xi(x_2) = \frac{3}{5}, \ \xi(x_3) = \frac{1}{5}.
\]

Let \( X' \) be the matrix whose \( i \)-th column is \( x_i \). It is then straightforward to verify that
\[
y_i = \left( \sum_{i=1}^{3} |u_i| \right) |u_i|, \quad i = 1, 2, 3
\]
where \( u_i, \ i = 1, 2, 3 \) are the components of the vector \( u = (XX')^{-1}Xc \). In fact, the thus defined vector \( y \) is always an optimal solution of (4) as long as the regression vectors are linearly independent. This is proved by the following result.

Corollary 3.4 Suppose \( x_1, \ldots, x_n \) are linearly independent. Then the vector
\[
y := \left( \sum_{i=1}^{n} |u_i| \right) |u| \quad \text{(24)}
\]
is the unique optimal solution of (4). Here \( u_1, \ldots, u_n \) are the components of the vector \( u := (XX')^{-1}Xc \) and \( |u| = (|u_1|, \ldots, |u_n|)' \).
Proof. In order to give a short proof for this result, we make use of [21, Corollary 8.9], where it is stated that under the linear independence condition, the unique optimal design $\xi$ is given by

$$\xi(x_i) = \frac{|u_i|}{\sum_{i=1}^{n} |u_i|}, \quad i = 1, \ldots, n.$$ 

Moreover

$$(\rho(c))^2 = \left(\sum_{i=1}^{n} |u_i|\right)^2.$$ 

It follows (19) that $y$ defined by (24) is the unique optimal solution of (4).

Suppose $0 \neq h \in \mathbb{R}^k$ defines a hyperplane $\mathcal{H}$ that supports $\mathcal{R}$ at $c/\rho(c)$. Then $h$ satisfies

$$\frac{c'h}{\rho(c)} = 1 \quad \text{and} \quad (x'h)^2 = 1 \quad \forall \ x \in \text{supp}(\mathcal{H}). \quad (25)$$

We already mentioned that $N := hh'$ defines an optimal solution of the problem (3). Suppose $y$ is an optimal solution of the problem (4).

When the linear independence condition holds for $x_i \in \text{supp}(\mathcal{H})$, $y$ is a unique optimal solution. However, there are potentially many hyperplanes (see [21, Exhibit 2.4]) that supports $\mathcal{R}$ at $c/\rho(c)$ and supporting hyperplanes may include regression vectors $x_i$ that have no contribution (i.e., $\xi(x_i) = 0$) to any optimal design and are linearly dependent on those that make contributions. We demonstrate such a possibility by taking a look at the following example.

**Example 3.5** Let

$$\mathcal{X} = \left\{ \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \right\} \quad \text{and} \quad c = \begin{bmatrix} 1 \\ 1 \\ 1/2 \end{bmatrix}.$$ 

It is easy to see that $\rho(c) = 1$ and $h = [0, 1, 0]'$ defines a hyperplane $\mathcal{H}$ that supports $\mathcal{R}$ at $c$. $\mathcal{H}$ contains all the regression points, which are apparently linearly dependent. However, there is a unique optimal design.

We will present a sufficient condition which explains the above situation under no linear independence assumption. Let

$$Z := \sum_{i=1}^{n} y_i(x_i x_i') - cc' \quad \text{and} \quad A := Z - N. \quad (26)$$

We assume that $A$ has the spectral decomposition (10) and the index sets $\alpha, \beta$ and $\gamma$ are defined by (11). Then the matrix $A_+$ and $A_-$ in (12) are given by $A_+ = Z$ and $A_- = N$. We need one more index set $\mathcal{I}$ of indices in $\mathcal{H}$, i.e.,

$$\mathcal{I} := \{ i : x_i \in \text{supp}(\mathcal{H}) \}.$$
It is easy to see by (25) and (21) that $\mathcal{I}$ is actually the index set of active constraints in (3), that is
\[ \mathcal{I} = \{ i : \langle x_i, x'_i, N \rangle = 1, \ i = 1, \ldots, n \} \quad \text{and} \quad \mathcal{I} = \{ 1, \ldots, n \} \setminus \mathcal{I}. \]

Split $\mathcal{I}$ into two disjoint sets:
\[ \mathcal{I}_0 := \{ i \in \mathcal{I} : y_i = 0 \} \quad \text{and} \quad \mathcal{I}_+ := \{ i \in \mathcal{I} : y_i > 0 \}. \]

We have the following sufficient condition that ensures uniqueness of an optimal solution of (4) without requiring the linear independence condition.

**Theorem 3.6** Let $y$ be an optimal solution of (4) and $h$ satisfy (25). Define $N := hh'$. Let $A$ be defined by (26) and have the spectral decomposition (10). Moreover, the index sets $\alpha$, $\beta$, and $\gamma$ are defined by (11). Then $y$ is unique provided the following implication holds:
\[
\begin{aligned}
\sum_{i \in \mathcal{I}} z_i \langle x_i, x'_i \rangle x_i &= 0 \\
& \quad z_i \geq 0 \quad \forall \ i \in \mathcal{I}_0 \\
& P_\beta \left( \sum_{i \in \mathcal{I}} z_i \langle x_i, x_i \rangle \right) P_\beta \preceq 0 \\
\end{aligned}
\]  
\[ \implies \ z_i = 0, \ \forall \ i \in \mathcal{I}. \quad (27) \]

**Proof.** To facilitate our proof, we define a linear operator $L : S^k \mapsto \mathbb{R}^n$ by
\[
L(S) = \begin{bmatrix}
\langle x_1, x'_1, S \rangle \\
\vdots \\
\langle x_n, x'_n, S \rangle
\end{bmatrix}, \quad \forall \ S \in S^k,
\]
and $I : S^k \mapsto S^k$ be the identity operator from $S^k$ to $S^k$. Hence, the adjoint operator $L^* : \mathbb{R}^n \mapsto S^k$ is given by
\[
L^*(z) := \sum_{i=1}^{n} z_i \langle x_i, x'_i \rangle, \quad \forall \ z \in \mathbb{R}^n.
\]

Let $v \in \mathbb{R}^n$ denote
\[
v_i := \langle x_i, x'_i, N \rangle - 1, \quad i = 1, \ldots, n.
\]

That is, $v_i$ denotes the slack value of the constraint $\langle x_i, x'_i, N \rangle \leq 1$ in (3). Let $\mathbb{R}^n_-$ denote the nonpositive orthant in $\mathbb{R}^n$. Then the tangent cone of $\mathbb{R}^n_-$ at $v$ is given by
\[
T_{\mathbb{R}^n_-}(v) = \{ z \in \mathbb{R}^n : z_i \leq 0, \ i \in \mathcal{I} \}.
\]

Note that
\[
\{ y \}^\perp = \left\{ z \in \mathbb{R}^n : \sum_{i \in \mathcal{I}_+} y_i z_i = 0 \right\}.
\]

Therefore
\[
T_{\mathbb{R}^n_-}(v) \cap \{ y \}^\perp = \{ z \in \mathbb{R}^n : z_i = 0 \ \forall \ i \in \mathcal{I}_+ \text{ and } z_i \leq 0 \ \forall \ i \in \mathcal{I}_0 \}. \quad (28)
\]
We claim that the implication (27) is equivalent to the following condition

\[
\left( \begin{array}{l} L(\cdot) \\
I
\end{array} \right) S^k + \left( \begin{array}{l} T_{\text{Re}}(v) \cap \{y\}^\perp \\
T_{S^k}(N) \cap \{Z\}^\perp
\end{array} \right) = \left( \begin{array}{l} \mathbb{R}^n \\
S^k
\end{array} \right).
\]

(29)

It is easy to see that condition (29) is equivalent to

\[
L(T_{S^k}(N) \cap \{Z\}^\perp) + T_{\text{Re}} \cap \{y\}^\perp = \mathbb{R}^n,
\]

which in turn is equivalent to (both sets on the left hand side are cones and use (14))

\[
\left\{ L(T_{S^k}(N) \cap \{Z\}^\perp) \right\}^0 \cap \left\{ T_{\text{Re}}(v) \cap \{y\}^\perp \right\}^0 = \{0\}.
\]

(30)

We first characterize the first set in (30).

\[
z \in \left\{ L(T_{S^k}(N) \cap \{Z\}^\perp) \right\}^0 \\
\iff \langle z, L(B) \rangle \leq 0 \quad \forall \ B \in T_{S^k}(N) \cap \{Z\}^\perp \\
\iff \langle L^*(z), B \rangle \leq 0 \quad \forall \ B \in T_{S^k}(N) \cap \{Z\}^\perp \\
\iff \left( \sum_{i=1}^n z_i(x_i x'_i), B \right) \leq 0 \quad \forall \ B \in T_{S^k}(N) \cap \{Z\}^\perp \\
\iff \left\{ P^\prime \left( \sum_{i=1}^n z_i(x_i x'_i) \right) P, P^\prime B P \right\} \leq 0 \quad \forall \ B \in T_{S^k}(N) \cap \{Z\}^\perp
\]

(31)

By looking at the structure of \( T_{S^k}(N) \cap \{Z\}^\perp \) in (13) (note that \( N = A_- \) and \( Z = A_+ \)), we see (31) is equivalent to

\[
P^\prime \left( \sum_{i=1}^n z_i(x_i x'_i) \right) P_\gamma = 0 \quad \text{and} \quad P^\prime \left( \sum_{i=1}^n z_i(x_i x'_i) \right) P_\beta \preceq 0
\]

(32)

Since \( N \) is a rank-1 matrix,

\[
P_\gamma = \left\{ \frac{h}{\|h\|} \right\}.
\]

Premultiplying the first equation in (32) by \( P \) yields

\[
0 = \sum_{i=1}^n z_i(x_i x'_i) h = \sum_{i \in \overline{I}} z_i(x_i x'_i) h + \sum_{i \in I} z_i(x_i x'_i) h.
\]

(33)

We also note that (by making use of (28))

\[
\left\{ T_{\text{Re}}(v) \cap \{y\}^\perp \right\}^0 = \left\{ z \in \mathbb{R}^n : \ z_i = 0 \ \forall \ i \in \overline{I} \ \text{and} \ z_i \geq 0 \ \forall \ i \in I_0 \right\}.
\]

(34)
Combination of (30), (33) and (34) means

\[ \sum_{i \in I} z_i (x_i x_i' h) = 0 \quad \text{and} \quad z_i \geq 0 \quad \forall \ i \in I_0, \tag{35} \]

which together with the second condition in (32) implies that condition (29) is equivalent to the implication (27).

Furthermore, it is known in optimization that condition (29) is the strict constraint qualification for problem (3) at \((N, y)\). And the presence of this qualification implies that the optimal solution of the dual problem (4) is unique (see [5, Proposition 4.47] for a general statement on this implication). This proves our result. \(\square\)

We now use Theorem 3.6 to explain the situation in Example 3.5.

**Example 3.7** (Example 3.5 Cont’d) For this example, we know

\[ h = [0, 1, 0]', \ I = \{1, 2, 3, 4\}, \ I_0 = \{3, 4\}, \ \text{and} \ \beta = \emptyset. \]

The left side system in (27) becomes

\[ z_1 \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + z_2 \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} + z_3 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + z_4 \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} = 0 \]

and

\[ z_3 \geq 0, \ z_4 \geq 0. \]

Clearly, this system has a unique zero solution. Hence Theorem 3.6 implies that the optimal design is unique.

4 Generalization to Compact Set \(\mathcal{X}\)

The results for finite set \(\mathcal{X}\) can be extended to compact set, but in a more general and abstract way. We just illustrate this possibility below.

Suppose \(\mathcal{X}\) is a compact set that contains infinitely many elements. Let \(C(\mathcal{X})\) denote the Banach space of continuous function on \(\mathcal{X}\). The dual space, denote by \(C(\mathcal{X})^*\), of the space \(C(\mathcal{X})\) is the space of finite signed Borel measures on \(\mathcal{X}\), with the norm given by the total variation of the corresponding measure, and that for \(y \in C(\mathcal{X})\) and \(\mu \in C(\mathcal{X})^*\)

\[ \langle \mu, y \rangle = \int_{\mathcal{X}} y(x) d\mu(x). \]

If \(\mu\) is a discrete measure, say \(\mu = \sum_{i=1}^{m} \lambda_i \delta(x_i)\) where \(\delta(x)\) is the (Dirac) measure of mass one at the point \(x \in \mathcal{X}\), then

\[ \|\mu\| = \sum_{i=1}^{m} |\lambda_i| \quad \text{and} \quad \langle \mu, y \rangle = \sum_{i=1}^{m} \lambda_i y(x_i). \]
The Lagrangian of problem (3) is

\[ L(N, \mu) := -\langle N, cc' \rangle + \int_X g(N, x)d\mu(x), \]

where \((N, \mu) \in S^k \times C(\mathcal{X})^*\) and

\[ g(N, x) = \langle N, xx' \rangle - 1, \quad \forall x \in \mathcal{X}. \]

Because \(\mathcal{X}\) is compact, the Slater condition is satisfied for problem (3). Therefore, no duality gap exists and the dual of problem (3) can be written in the form

\[
\max_{\mu \geq 0} \left\{ \inf_{N \in S^k_+} L(N, \mu) \right\}, \quad \mu \in C(\mathcal{X})^*, \tag{36}
\]

where \(\mu \geq 0\) means that the measure \(\mu\) is nonnegative.

Note that

\[
L(N, \mu) = -\int_X d\mu(x) - \langle N, cc' \rangle + \int_X \langle N, xx' \rangle d\mu(x) = -\int_X d\mu(x) + \langle N, \int_X \langle N, xx' \rangle d\mu(x) - cc' \rangle.
\]

Therefore

\[
\inf_{N \in S^k_+} L(N, \mu) = \begin{cases} -\int_X d\mu(x), & \text{if } \int_X \langle N, xx' \rangle d\mu(x) - cc' \geq 0 \\ -\infty, & \text{otherwise.} \end{cases}
\]

Consequently the dual problem (36) becomes

\[
\min_{\mu \geq 0} \int_X d\mu(x) \quad \text{s.t. } \int_X \langle N, xx' \rangle d\mu(x) - cc' \geq 0. \tag{37}
\]

If \(\mu\) is a discrete measure, the above problem becomes (4).

With (37) in hand, we can deal with issues such as feasibility (Proposition 3.1), solvability (Theorem 3.2), and uniqueness (Theorem 3.6). However, such a development would be more involved and a large part of the development would be simple generalizations of what have been developed. We hence omit the details here.

Another possible way of studying (37) is to discretize it and the resulting problem would be in the form of (4), returning to results reported in Section 3.

5 Numerical Experiment

We have seen that there is an one-to-one correspondence between optimal designs \(\xi\) of (1) and optimal solutions of (4). Moreover, we also pointed out that (4) can be cast as an \(\ell_1\)-convex optimization, which often leads to sparse solutions.

It is known (see [21, Section 8.3]) that for any scalar optimality there always exists an optimal design \(\xi\) for \(c'\theta\) in \(\Xi\) such that

\[
1 \leq |\text{supp}(\xi)| \leq k, \tag{38}
\]
where $|\text{supp}(\xi)|$ denotes the number of supporting design points in $\xi$. We also note that in most typical situations $k \ll n$. We therefore regard $\xi$ satisfying (38) sparse. The main purpose of this section is to demonstrate that (4) does lead to a sparse optimal solution.

We use the trigonometric regression of degree $d$ as an example:

$$E(y) = \theta_1 + \sum_{i=1}^{d} \theta_{2i} \sin(it) + \sum_{i=1}^{d} \theta_{2i+1} \cos(it).$$

The regression vector is

$$x = [1, \sin(t), \cos(t), \ldots, \sin(dt), \cos(dt)]'$$

with $t \in [-\tau, \tau]$ for some $\tau > 0$.

The model of trigonometric regression has received much attention in the optimal design literature, see, Pázman (1986), Pukelsheim (2006), Kitsos et al. (1988), Dette et al. (2002), Dette and Melas (2002), Wu (2002). Harman and Jurík (2008) also proposed a Simplex method that applies to this model. More comments on this method are to follow.

Our main purpose, as mentioned at the beginning of the section, is to demonstrate that the SDP problem (4) is likely to lead to a sparse design in the sense also mentioned above. We visualize the sparsity by plotting the final solution $y$ of (4). We have 15 such plots.

In our experiments, we set $d = 3$, $\tau = \frac{\pi}{2}$ (hence $k = 7$).

One may set $\tau$ other values, the performance is quite similar. We discretize the interval $[-\tau, \tau]$ by $n = 1001$ equidistant points starting from $(-\tau)$ (experiments with $n = 2001, 3001$ are similar). We would like to see sparse patterns for individual parameters $\theta_i$, corresponding to vector $c$ (in Matlab notation)

$$c = \text{zeros}(k,1), \quad c(s) = 1.$$

We would like to see the sparse pattern for scalar system that is sum of some parameters

$$\sum_{i=1}^{s} \theta_i, \quad s = 2, \ldots, 7 \quad (\text{i.e., } c = \text{zeros}(k,1), \text{ for } i=1:s; c(i) = 1; \text{ end}).$$

Finally, we consider the scalar system $\theta_2 + \theta_6$ and $\theta_2 + \theta_4 + \theta_6$, making a total of 15 scalar systems in our study.

We solve SDP (4) by SDPT3-4.0-beta [25] with the default parameter setting. All calculations were done on a desktop (Inter Core with 2 Duo CPU, 3.16GHz, 3.25GB of RAM). All tests took about 10 seconds to find the solution. Since SDPT3 use Cholesky factorization or LU factorization to solve the underlying linear equations in the solver, the largest problem that we can solve on our computer is up to $n \leq 4000$. When $n \geq 4000$ we have to use other SDP solver which uses iterative methods to solve system of linear equations (e.g., SDPNAL in [30]). It certainly remains a research area when a large number of design points is involved. We have several observations to make regarding the graphs in this section.
(i) For individual parameter $\theta_s$ estimation, $s = 1, \ldots, 7$, the supporting points are symmetric around 0. This confirms the fact that in some literature it is enough to consider the half line $[0, \alpha]$ when $\theta_s$ is to be estimated.

(ii) For each of individual parameters, the number of supporting points found is $k = 7$.

(iii) (ii) is still true for the scalar system $\sum_{i=1}^{s} \theta_i$, $s = 2, \ldots, 7$. But the supporting points are not symmetric anymore. In this case, we cannot just consider the half line $[0, \alpha]$ in order to find an optimal design.

(iv) It is possible to find an optimal design whose supporting points are strictly less than the dimension of the system $k = 7$. For example, for the scalar system $\theta_2 + \theta_6$ and $\theta_2 + \theta_4 + \theta_6$, we each found an optimal design which has 5 supporting points. Such optimal designs are known to be singular in literature.

(v) One can verify that those supporting points are linearly independent. Therefore, we can use formula (24) in Corollary 3.4 to cross verify the solution found.

Harman and Jurík [17] recently proposed a Simplex method for $c$-optimal design. While it is very efficient when estimating individual parameters $\theta_s$, it remains to be seen whether it can effectively find optimal designs that have less than $k$ supporting points. In terms of computational complexity, SDPT3, being a primal-dual interior-point method, is polynomial, whereas the worst complexity for Simplex methods is known to be exponential. Anyway, it would be interesting to compare two computational approaches on a large set of problems and this is beyond the scope of this paper.
6 Conclusion

SDP has found many applications over the past decade and efficient software are already available to use. This paper took advantage of such development and represents a contribution to optimal design theory from SDP.

The main theoretical results of this paper are the theorem of one-to-one correspondence between optimal solutions of (4) and optimal designs of (1) and the uniqueness theorem which does not need the linear independence condition. To our best knowledge, it is the first nontrivial condition that addresses the uniqueness of optimal designs. The results in this paper are easy to use, especially when it is used to demonstrate the geometric properties of the Elfving theorem. For example, [21, P.198] claims that the optimal weights for $c^T \theta$ with $k = 2$ is

$$w_1 = \frac{|c_1 - c_2|}{|c_1 - c_2| + |c_1 + c_2|} \quad \text{and} \quad w_2 = \frac{|c_1 + c_2|}{|c_1 - c_2| + |c_1 + c_2|},$$

where $c \neq 0$ and the regression space is

$$X = \left\{ x_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \ x_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right\}.$$  

We can verify this easily from (4), which, after some elementary linear algebra, gives the (unique) optimal solution:

$$y_1 = \frac{1}{8}(|c_1 - c_2| + |c_1 + c_2|)^2 - \frac{1}{2} c_1 c_2,$$

$$y_2 = \frac{1}{8}(|c_1 - c_2| + |c_1 + c_2|)^2 + \frac{1}{2} c_1 c_2.$$

By (20) of Theorem 3.2, we have

$$w_1 = \frac{1}{2} - \frac{c_1 c_2}{2 \max\{c_1^2, c_2^2\}} \quad \text{and} \quad w_1 = \frac{1}{2} + \frac{c_1 c_2}{2 \max\{c_1^2, c_2^2\}}.$$
This is just a different representation of (39). As a matter of fact, a large number of examples and exercises in [21] can be answered by our results.

Computationally, (4) is likely to lead to sparse designs, as demonstrated by experiments on the trigonometric regression model. Such sparse property seems to have related to casting (4) as an $\ell_1$-linear programming, which has been extensively studied recently because of the sparsity property of its solutions. However, no theoretical results have been available as (4) is not a conventional linear programming (LP), but an LP with a positive semidefinite constraint (the type of $\succeq 0$). This certainly needs further investigation.

Acknowledgments. The author would like to thank the optimization team in National University of Singapore: Prof. Defeng Sun, Prof. Kim-Chuan Toh, and Xinyuan Zhao for their help in using SDPT3 and SDPNAL.

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