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Computing A-optimal and E-optimal designs for regression models via semidefinite programming

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ABSTRACT

In semidefinite programming (SDP), we minimize a linear objective function subject to a linear matrix being positive semidefinite. A powerful program, SeDuMi, has been developed in MATLAB to solve SDP problems. In this paper, we show in detail how to formulate A-optimal and E-optimal design problems as SDP problems and solve them by SeDuMi. This technique can be used to construct approximate A-optimal and E-optimal designs for all linear and non-linear regression models with discrete design spaces. In addition, the results on discrete design spaces provide useful guidance for finding optimal designs on any continuous design space, and a convergence result is derived. Moreover, restrictions in the designs can be easily incorporated in the SDP problems and solved by SeDuMi. Several representative examples and one MATLAB program are given.

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1 Introduction

Consider a regression model,

$$y_i = g(\mathbf{x}_i; \boldsymbol{\theta}) + \epsilon_i, \quad i = 1, \ldots, n, \tag{1}$$

where $g(\mathbf{x}_i; \boldsymbol{\theta})$ can be a linear or nonlinear function of $\boldsymbol{\theta} \in R^q$, $\mathbf{x}_1, \ldots, \mathbf{x}_n$ are design points in a design space $S \subset R^p$, and the errors ϵ_i's are i.i.d. having mean 0 and variance σ^2. Suppose $\hat{\boldsymbol{\theta}}$ is the least squares estimator (LSE) of $\boldsymbol{\theta}$ in the model. In optimal design of experiments, one aims at choosing optimal design points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ in S such that $\mathcal{L}\left(Var(\hat{\boldsymbol{\theta}})\right)$ is minimized, where $\mathcal{L}(\cdot)$ is a scalar function. The commonly used scalar functions include the determinant, trace, and the largest eigenvalue, which are used to define D-optimal, A-optimal and E-optimal designs, respectively.

Optimal designs have been constructed for various models and design spaces; see, for example, Fedorov (1972) and Pukelsheim (1993). However, finding optimal designs is still a very active research area and there are open problems for various regression models and design spaces. Optimal design problems are constrained optimization problems that are usually hard to solve analytically. Specific techniques are often developed for specific models and design spaces. Recent work in this area includes Papp (2012) for computing optimal designs for rational function regression models, Dette *et al.* (2007) for finding approximate optimal designs for trigonometric regression models on a full circle, Zhang (2007) for deriving optimal designs for trigonometric regression models with only cosine terms or sine terms, Chang *et al.* (2013) for deriving exact D-optimal designs for the first-order trigonometric regression models on a partial circle, Zhou (2008) for finding optimal regression designs on discrete design spaces, and Dette *et al.* (2006) for constructing locally D-optimal designs for exponential regression models.

SDP problems are a special class of convex optimization problems having a linear objective function subject to a linear matrix being positive semidefinite (PSD), *i.e.*, a linear matrix inequality constraint; see Vandenberghe and Boyd (1996) for a review of the topic. SDP has been successfully applied to various areas of applications; see Vandenberghe and Boyd (1999). The SeDuMi (Self-Dual-Minimization), developed by Jos Sturm, is a toolbox in MATLAB which can be downloaded from website *http://sedumi.ie.lehigh.edu/*. SeDuMi can be used to solve optimization problems with a linear objective function subject to a symmetric cone constraint such as linear programming, second order cone programming and SDP problems; see Sturm (1999) for a user's guide.

Over the last two decades, SDP and SeDuMi have become powerful tools for modeling and solving optimization problems. In Vandenberghe and Boyd (1999), it was pointed out that the A- and E-optimal design problems for linear regression models on discrete design spaces can be cast as SDP problems; however, the detail on how to use SeDuMi to solve those problems was not provided. In this paper, we demonstrate in detail on how to cast A-optimal and E-optimal design problems for any linear and nonlinear regression models with discrete design spaces as SDP problems and solve them by SeDuMi. Furthermore, we provide guidance for deriving optimal designs on continuous design spaces. In order to use SDP and SeDuMi, we discretize the continuous design space, solve the optimal design problems on the discrete design space, and obtain a convergence result.

The rest of the paper is organized as follows. In Section 2 we discuss the E-optimal design problem and cast it as an SDP problem. Two examples of E-optimal designs computed using SeDuMi are given. In Section 3 we work on the A-optimal design problem and cast it as an SDP problem. Examples are also presented. In Section 4 we address the continuous design space and constrained optimal design problems. A convergence result is derived. Concluding remarks are in Section 5. A MATLAB program and the proof of the convergence result are given in the Appendix.

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2 E-optimal design problem

For model (1), the LSE is defined as $\hat{\boldsymbol{\theta}} = \arg\min_{\theta} \sum_{i=1}^{n}(y_i - g(\mathbf{x}_i; \boldsymbol{\theta}))^2$. The variance-covariance matrix of $\hat{\boldsymbol{\theta}}$, approximated from its asymptotic distribution (Seber and Wild, 1989, p24), is

$$Var(\hat{\boldsymbol{\theta}}) = \frac{\sigma^2}{n}\mathbf{C}^{-1},$$

where

$$\mathbf{C} = \frac{1}{n}\sum_{i=1}^{n} \frac{\partial g(\mathbf{x}_i; \boldsymbol{\theta}^*)}{\partial \boldsymbol{\theta}} \frac{\partial g(\mathbf{x}_i; \boldsymbol{\theta}^*)}{\partial \boldsymbol{\theta}^\top}, \tag{2}$$

$\boldsymbol{\theta}^*$ is the true parameter value, and $\frac{\partial g}{\partial \theta^\top}$ is the transpose of the gradient vector $\frac{\partial g}{\partial \theta}$. Notice that the above variance is exact for linear regression models.

2.1 Exact and approximate E-optimal design

Assume the design space contains a finite number of points, and is denoted by $S = \{\mathbf{u}_1, \ldots, \mathbf{u}_N\} \subset R^p$. The exact E-optimal design problem is a constrained optimization problem,

$$(P_E) \quad \begin{cases} \min_{\mathbf{x}_1,\ldots,\mathbf{x}_n} \lambda_{max}\left(\mathbf{C}^{-1}\right) \\ \text{subject to: } \mathbf{x}_i \in S, \quad i = 1, \ldots, n, \end{cases}$$

where λ_{max} denotes the largest eigenvalue of a matrix. A solution, say $\mathbf{x}_1^*, \ldots, \mathbf{x}_n^*$, is an E-optimal design. For linear models, since matrix $\mathbf{C}$ does not depend on the true parameter value $\boldsymbol{\theta}^*$, the E-optimal designs do not depend on $\boldsymbol{\theta}^*$ either. However, for nonlinear models since the matrix $\mathbf{C}$ depends on the true parameter value $\boldsymbol{\theta}^*$, $\boldsymbol{\theta}^*$ is needed for computing the E-optimal designs and the resulting optimal designs are called locally E-optimal designs. For simplicity, we just call them E-optimal designs for both linear and nonlinear models in the paper. The same discussion applies to A-optimal designs in the next section.

Let $n_1, \ldots, n_N$ be the number of times that points $\mathbf{u}_1, \ldots, \mathbf{u}_N$ are selected, respectively, into a design ξ, where $n_i \geq 0$ and $\sum_{i=1}^N n_i = n$. Define weights $w_i = n_i/n,\ i = 1, \ldots, N$. It is clear that $\sum_{i=1}^N w_i = 1$. Then ξ can be presented as

$$\xi = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \ldots & \mathbf{u}_N \\ w_1 & w_2 & \ldots & w_N \end{pmatrix}.$$

Using ξ, we can write the expression in (2) as

$$\mathbf{C}(\xi) = \mathbf{C} = \sum_{i=1}^N w_i \frac{\partial g(\mathbf{u}_i; \boldsymbol{\theta}^*)}{\partial \boldsymbol{\theta}} \frac{\partial g(\mathbf{u}_i; \boldsymbol{\theta}^*)}{\partial \boldsymbol{\theta}^\top}, \tag{3}$$

and the optimization problem (P_E) becomes

$$(P_E') \qquad \begin{cases} \min_{w_1,\ldots,w_N} \lambda_{max}\left(\mathbf{C}^{-1}\right) \\ \text{subject to: } \sum_{i=1}^N w_i = 1, \text{ and } w_i \in \{0, 1/n, 2/n, \ldots, 1\},\ i = 1, \ldots, N. \end{cases}$$

Problems (P_E) and (P_E') are the same, and they define the exact E-optimal design. Since they are combinatorial optimization problems, they are extremely hard to solve in general.

However, we can relax the exact design problem slightly by allowing $w_i \in [0, 1]$ and consider the following approximate E-optimal design problem,

$$(P_{EA}) \qquad \begin{cases} \min_{w_1,\ldots,w_N} \lambda_{max}\left(\mathbf{C}^{-1}\right) \\ \text{subject to: } \sum_{i=1}^N w_i = 1, \text{ and } w_i \in [0, 1],\ i = 1, \ldots, N. \end{cases}$$

The corresponding optimal design is called the approximate E-optimal design. Then we can formulate the approximate E-optimal design problem as an SDP problem and solve it by SeDuMi.

2.2 SDP problem

Define $t = \lambda_{min}(\mathbf{C})$, where λ_{min} is the smallest eigenvalue of a matrix. Then minimizing $\lambda_{max}\left(\mathbf{C}^{-1}\right)$ is equivalent to maximizing t or minimizing $-t$. Since $\mathbf{C}$ is PSD and $t = \lambda_{min}(\mathbf{C})$, $\mathbf{C} - t\,\mathbf{I}_q$ is PSD and is denoted by $\mathbf{C} - t\,\mathbf{I}_q \succeq 0$, where $\mathbf{I}_q$ is the $(q \times q)$ identity matrix. Let matrices

$$\mathbf{G}(\mathbf{u}_i) = \frac{\partial g(\mathbf{u}_i;\boldsymbol{\theta}^*)}{\partial\boldsymbol{\theta}}\frac{\partial g(\mathbf{u}_i;\boldsymbol{\theta}^*)}{\partial\boldsymbol{\theta}^\top}, \quad i = 1,\ldots,N. \tag{4}$$

From (3) and $\sum_{i=1}^{N} w_i = 1$, we have

$$\mathbf{C} - t\,\mathbf{I}_q = \mathbf{G}(\mathbf{u}_N) + \sum_{i=1}^{N-1} w_i\left(\mathbf{G}(\mathbf{u}_i) - \mathbf{G}(\mathbf{u}_N)\right) - t\,\mathbf{I}_q \succeq 0. \tag{5}$$

Notice that, for a given design space S, $\mathbf{C} - t\,\mathbf{I}_q$ is a linear matrix of $w_1,\ldots,w_{N-1},t$. Define a diagonal matrix $\mathbf{W} = diag(w_1,\ldots,w_{N-1},1-\sum_{i=1}^{N-1} w_i)$, where $diag(a_1,\ldots,a_n)$ denotes the diagonal matrix of size n with the diagonal elements being $a_1,\ldots,a_n$. Then the constraints in problem (P_{EA}) are equivalent to $\mathbf{W} \succeq 0$. Construct a block diagonal matrix,

$$\mathbf{H}(w_1,\ldots,w_{N-1},t) = \left(\mathbf{C} - t\,\mathbf{I}_q\right) \oplus \mathbf{W}, \tag{6}$$

where $\oplus$ denotes the direct sum of two matrices. It is obvious that matrix $\mathbf{H}$ is a linear matrix of $w_1,\ldots,w_{N-1}$ and t, and it is PSD. Now the approximate E-optimal design problem can be transformed into an SDP problem as follows,

$$(P_{E1}) \qquad \begin{cases} \min_{w_1,\ldots,w_{N-1},t} & -t \\ \text{subject to: } & \mathbf{H}(w_1,\ldots,w_{N-1},t) \succeq 0. \end{cases}$$

It is clear that the objective function $-t$ is a linear function of $w_1,\ldots,w_{N-1}$ and t, and the constraint is a linear matrix being PSD.

In order to use SeDuMi, we write matrix $\mathbf{H}$ as

$$\mathbf{H}(w_1, \ldots, w_{N-1}, t) = \mathbf{H}_0 + w_1\mathbf{H}_1 + \cdots + w_{N-1}\mathbf{H}_{N-1} + t\mathbf{H}_N, \tag{7}$$

where $\mathbf{H}_0, \mathbf{H}_1, \ldots, \mathbf{H}_N$ are $(N + q) \times (N + q)$ constant matrices and given by

$$\begin{aligned}
\mathbf{H}_0 &= \mathbf{G}(\mathbf{u}_N) \oplus \mathbf{W}_0, \\
\mathbf{H}_i &= (\mathbf{G}(\mathbf{u}_i) - \mathbf{G}(\mathbf{u}_N)) \oplus \mathbf{W}_i, \quad i = 1, \ldots, N-1, \\
\mathbf{H}_N &= -\mathbf{I}_q \oplus \mathbf{W}_N, \\
\mathbf{W}_0 &= diag(0, \ldots, 0, 1), \\
\mathbf{W}_1 &= diag(1, 0, \ldots, 0, -1), \\
&\vdots \\
\mathbf{W}_{N-1} &= diag(0, \ldots, 0, 1, -1), \\
\mathbf{W}_N &= diag(0, \ldots, 0).
\end{aligned} \tag{8}$$

Notice that $\mathbf{W}_0, \mathbf{W}_1, \ldots, \mathbf{W}_N$ are all diagonal matrices of size N. For each design problem, we need to specify matrices $\mathbf{H}_0, \mathbf{H}_1, \ldots, \mathbf{H}_N$ to define problem (P_{E1}). Matrices $\mathbf{H}_0, \mathbf{H}_1, \ldots, \mathbf{H}_N$ depend on matrix $\mathbf{G}$, and the elements of $\mathbf{G}$ in (4) are determined by the regression model and $\mathbf{u}_i$ in design space S.

2.3 Examples

We present two examples to show how to use SeDuMi to solve problem (P_{E1}). Example 1 is a quadratic regression model with one design variable. It is used to illustrate the detailed procedure and a MATLAB program is provided. Example 2 is a quadratic regression model with two design variables.

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Example 1. Consider the quadratic regression model,

$$y_i = \theta_0 + \theta_1 x_i + \theta_2 x_i^2 + \epsilon_i, \quad i = 1, \ldots, n,$$

with the design space $S = \{u_1, \ldots, u_N\} = \{-1.0, -0.5, 0, 0.5, 1.0\}$ which contains $N = 5$ points. We construct the approximate E-optimal design by solving the SDP problem (P_{E1}). For this model, we have $q = 3$ and $p = 1$. From (4),

$$\mathbf{G}(u_i) = \begin{pmatrix} 1 & u_i & u_i^2 \\ u_i & u_i^2 & u_i^3 \\ u_i^2 & u_i^3 & u_i^4 \end{pmatrix}, \quad i = 1, \ldots, 5.$$

From (7) and (8), we get

$$\mathbf{H}_0 = \begin{pmatrix} 1 & u_N & u_N^2 \\ u_N & u_N^2 & u_N^3 \\ u_N^2 & u_N^3 & u_N^4 \end{pmatrix} \oplus \mathrm{diag}(0,0,0,0,1),$$

$$\mathbf{H}_1 = \begin{pmatrix} 0 & u_1 - u_N & u_1^2 - u_N^2 \\ u_1 - u_N & u_1^2 - u_N^2 & u_1^3 - u_N^3 \\ u_1^2 - u_N^2 & u_1^3 - u_N^3 & u_1^4 - u_N^4 \end{pmatrix} \oplus \mathrm{diag}(1,0,0,0,-1),$$

$$\mathbf{H}_2 = \begin{pmatrix} 0 & u_2 - u_N & u_2^2 - u_N^2 \\ u_2 - u_N & u_2^2 - u_N^2 & u_2^3 - u_N^3 \\ u_2^2 - u_N^2 & u_2^3 - u_N^3 & u_2^4 - u_N^4 \end{pmatrix} \oplus \mathrm{diag}(0,1,0,0,-1),$$

$$\mathbf{H}_3 = \begin{pmatrix} 0 & u_3 - u_N & u_3^2 - u_N^2 \\ u_3 - u_N & u_3^2 - u_N^2 & u_3^3 - u_N^3 \\ u_3^2 - u_N^2 & u_3^3 - u_N^3 & u_3^4 - u_N^4 \end{pmatrix} \oplus \mathrm{diag}(0,0,1,0,-1),$$

$$\mathbf{H}_4 = \begin{pmatrix} 0 & u_4 - u_N & u_4^2 - u_N^2 \\ u_4 - u_N & u_4^2 - u_N^2 & u_4^3 - u_N^3 \\ u_4^2 - u_N^2 & u_4^3 - u_N^3 & u_4^4 - u_N^4 \end{pmatrix} \oplus \mathrm{diag}(0,0,0,1,-1),$$

$$\mathbf{H}_5 = \mathrm{diag}(-1,-1,-1,0,0,0,0,0).$$

A MATLAB program is given in the Appendix to solve this SDP problem (P_{E1}) using SeDuMi. **This program can be used for the general d-th degree polynomial regression model and any design space.** Running the program gives the following result: $w_1 = 0.2, w_2 = 0.0, w_3 = 0.6, w_4 = 0.0$ and $t = 0.2$. Since $w_5 = 1 - \sum_{i=1}^{4} w_i$, we get $w_5 = 0.2$. Thus the approximate E-optimal design for the quadratic model is

$$\xi_E = \begin{pmatrix} -1 & 0 & +1 \\ 0.2 & 0.6 & 0.2 \end{pmatrix},$$

which is the same as the theoretical result on design space $[-1, 1]$ in Pukelsheim (1993, p233). Now we change the design space to $S = \{-1 + 2(j-1)/(N-1), j = 1, \ldots, N\}$ with N equally spaced points on $[-1, 1]$ and N is odd. We have computed the E-optimal design for various values of N, $21, 31, 55, 101$ and 301, and the numerical results show that the E-optimal design stays the same. In fact, if S contains the three points: $-1,\ 0,\ 1$, then the E-optimal design stays the same. Furthermore, SeDuMi is very effective and efficient. The SDP problem (P_{E1}) with N variables can be solved very fast. For instance, when $N = 301$, it only takes 12.18 seconds of CPU time on a PC with Intel(R) Core(TM)2 Quad CPU Q9550@2.583GHz to get the result.

The program also works well for higher degree polynomial models. The E-optimal designs are similar to the ones in Pukelsheim (1993, p236). Here are some representative results. For the 5th and 8th degree polynomial models and $N = 301$, it takes 20.39 and 24.03 seconds, respectively. The E-optimal designs obtained from the program are:

$$\xi_{E5} = \begin{pmatrix} -1.0 & -0.81 & -0.31 & 0.31 & 0.81 & 1.0 \\ 0.07 & 0.18 & 0.25 & 0.25 & 0.18 & 0.07 \end{pmatrix},$$

$$\xi_{E8} = \begin{pmatrix} -1.0 & -0.93 & -0.71 & -0.38 & 0 & 0.38 & 0.71 & 0.93 & 1.0 \\ 0.05 & 0.10 & 0.12 & 0.15 & 0.16 & 0.15 & 0.12 & 0.10 & 0.05 \end{pmatrix}.$$

□

Example 2. Consider the quadratic regression model with two design variables,

$$y_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} + \theta_3 x_{i1}^2 + \theta_4 x_{i2}^2 + \theta_5 x_{i1} x_{i2} + \epsilon_i, \quad i = 1, \ldots, n,$$

with the design space $S = \{\mathbf{u}_1, \ldots, \mathbf{u}_N\}$ containing the following $N = 9$ points,

$$\mathbf{u}_1 = \begin{pmatrix} -1 \\ -1 \end{pmatrix}, \ \mathbf{u}_2 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \ \mathbf{u}_3 = \begin{pmatrix} -1 \\ +1 \end{pmatrix}, \ \mathbf{u}_4 = \begin{pmatrix} 0 \\ -1 \end{pmatrix},$$
$$\mathbf{u}_5 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \ \mathbf{u}_6 = \begin{pmatrix} 0 \\ +1 \end{pmatrix}, \ \mathbf{u}_7 = \begin{pmatrix} +1 \\ -1 \end{pmatrix}, \ \mathbf{u}_8 = \begin{pmatrix} +1 \\ 0 \end{pmatrix}, \ \mathbf{u}_9 = \begin{pmatrix} +1 \\ +1 \end{pmatrix}.$$

This model is often considered to build response surface designs (Montgomery, 2013, p479), and these 9 points are from a cube. For this model, we have $q = 6$ and $p = 2$. SeDuMi gives the following result: $w_1 = 0.05, w_2 = 0.10, w_3 = 0.05, w_4 = 0.10, w_5 = 0.40, w_6 = 0.10, w_7 = 0.05, w_8 = 0.10$ and $t = 0.20$. Thus the approximate E-optimal design is

$$\xi_E = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 & \mathbf{u}_4 & \mathbf{u}_5 & \mathbf{u}_6 & \mathbf{u}_7 & \mathbf{u}_8 & \mathbf{u}_9 \\ 0.05 & 0.10 & 0.05 & 0.10 & 0.40 & 0.10 & 0.05 & 0.10 & 0.05 \end{pmatrix}.$$

□

3 A-optimal design problem

The A-optimal design minimizes the trace of $Var(\hat{\boldsymbol{\theta}})$, and the design problem can also be transformed to an SDP problem with a different transformation from the E-optimal design problem.

3.1 Exact and approximate A-optimal design

For a given regression model and a design space S, the exact A-optimal design problem is

$$(P_A) \quad \begin{cases} \min_{\mathbf{x}_1,\ldots,\mathbf{x}_n} \operatorname{trace}\left(\mathbf{C}^{-1}\right) \\ \text{subject to: } \mathbf{x}_i \in S, \quad i = 1, \ldots, n. \end{cases}$$

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If we use weights $w_1, \ldots, w_N$ to present the design, problem (P_A) becomes,

$$(P'_A) \qquad \begin{cases} \min_{w_1,\ldots,w_N} \operatorname{trace}\left(\mathbf{C}^{-1}\right) \\ \text{subject to:} \quad \sum_{i=1}^N w_i = 1, \ \text{and } w_i \in \{0, 1/n, 2/n, \ldots, 1\}, \ i = 1, \ldots, N. \end{cases}$$

The solution to problem (P_A) or $\left(P'_A\right)$ gives the exact A-optimal design, and it is also hard to find the solution in general. Similar to the approximate E-optimal design problem, the approximate A-optimal design problem can be written as

$$(P_{AA}) \qquad \begin{cases} \min_{w_1,\ldots,w_N} \operatorname{trace}\left(\mathbf{C}^{-1}\right) \\ \text{subject to:} \quad \sum_{i=1}^N w_i = 1, \ \text{and } w_i \in [0, 1], \ i = 1, \ldots, N, \end{cases}$$

which can be transformed to an SDP problem and solved by SeDuMi for any regression model.

3.2 SDP problem

Let $\mathbf{e}_i$ be the unit vector in R^q and γ_i be the ith diagonal element of $\mathbf{C}^{-1}$, $i = 1, \ldots, q$. Define $(q+1) \times (q+1)$ matrices

$$\mathbf{B}_i = \begin{pmatrix} \mathbf{C} & \mathbf{e}_i \\ \mathbf{e}_i^\top & \gamma_i \end{pmatrix}, \quad i = 1, \ldots, q. \tag{9}$$

Since $\mathbf{C} \succ 0$ and $\gamma_i - \mathbf{e}_i^\top \mathbf{C}^{-1} \mathbf{e}_i = 0$, we have $\mathbf{B}_i \succeq 0$ $(i = 1, \ldots, q)$ from Schur complement result (Boyd and Vandenberghe, 2004, Appendix A.5.5). Construct a block diagonal matrix

$$\mathbf{K}(w_1, \ldots, w_{N-1}, \gamma_1, \ldots, \gamma_q) = \mathbf{B}_1 \oplus \mathbf{B}_2 \oplus \cdots \oplus \mathbf{B}_q \oplus \mathbf{W},$$

and from the above discussion $\mathbf{K}(w_1, \ldots, w_{N-1}, \gamma_1, \ldots, \gamma_q) \succeq 0$ if and only if $\mathbf{W} \succeq 0$. In addition, from (3) and (9), $\mathbf{K}$ is a linear matrix of $w_1, \ldots, w_{N-1}, \gamma_1, \ldots, \gamma_q$. From the definition of γ_i, it is clear that $\operatorname{trace}\left(\mathbf{C}^{-1}\right) = \sum_{i=1}^q \gamma_i$, which is a linear function of $w_1, \ldots, w_{N-1}, \gamma_1, \ldots, \gamma_q$. Therefore, problem (P_{AA}) becomes the following SDP problem,

$$(P_{A1}) \qquad \begin{cases} \min_{w_1,\ldots,w_{N-1},\gamma_1,\ldots,\gamma_q} & \sum_{i=1}^{q} \gamma_i \\ \text{subject to: } & \mathbf{K}(w_1,\ldots,w_{N-1},\gamma_1,\ldots,\gamma_q) \succeq 0. \end{cases}$$

Similar to (7) and (8), we can express

$$\mathbf{K}(w_1,\ldots,w_{N-1},\gamma_1,\ldots,\gamma_q) = \mathbf{K}_0 + w_1\mathbf{K}_1 + \cdots + w_{N-1}\mathbf{K}_{N-1} + \gamma_1\mathbf{K}_N + \cdots + \gamma_q\mathbf{K}_{N+q-1},$$

where $\mathbf{K}_0,\ldots,\mathbf{K}_{N+q-1}$ are constant matrices. In Section 3.3, we use Example 3 to display all the matrices and the detailed procedure. Using SeDuMi, we can find the solution for $w_1,\ldots,w_{N-1},\gamma_1,\ldots,\gamma_q$, and the approximate A-optimal design is denoted by

$$\xi_A = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \ldots & \mathbf{u}_N \\ w_1 & w_2 & \ldots & w_N \end{pmatrix}.$$

3.3 Examples

Example 3 is presented to illustrate the SDP problem (P_{A1}) with detailed information for all the matrices involved. Example 4 gives an A-optimal design for a trigonometric regression model.

Example 3. Consider the simple linear regression model,

$$y_i = \theta_0 + \theta_1 x_i + \epsilon_i, \quad i = 1,\ldots,n,$$

and the design space $S = \{0.0, 0.6, 1.0\}$ contains $N = 3$ points. For this model $q = 2$ and $p = 1$. From (3) and (4), we have

$$\mathbf{C} = \mathbf{G}(u_3) + w_1(\mathbf{G}(u_1) - \mathbf{G}(u_3)) + w_2(\mathbf{G}(u_2) - \mathbf{G}(u_3)), \quad \text{with } \mathbf{G}(u_i) = \begin{pmatrix} 1 & u_i \\ u_i & u_i^2 \end{pmatrix}.$$

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From Section 2.2 and (9),

$$\mathbf{W} = \begin{pmatrix} w_1 & 0 & 0 \\ 0 & w_2 & 0 \\ 0 & 0 & 1 - w_1 - w_2 \end{pmatrix}, \quad \mathbf{B}_1 = \begin{pmatrix} \mathbf{C} & \mathbf{e}_1 \\ \mathbf{e}_1^\top & \gamma_1 \end{pmatrix}, \quad \mathbf{B}_2 = \begin{pmatrix} \mathbf{C} & \mathbf{e}_2 \\ \mathbf{e}_2^\top & \gamma_2 \end{pmatrix}.$$

By $\mathbf{K}(w_1, w_2, \gamma_1, \gamma_2) = \mathbf{B}_1 \oplus \mathbf{B}_2 \oplus \mathbf{W} = \mathbf{K}_0 + w_1\mathbf{K}_1 + w_2\mathbf{K}_2 + \gamma_1\mathbf{K}_3 + \gamma_2\mathbf{K}_4$, we get

$$\mathbf{K}_0 = \begin{pmatrix} \mathbf{G}(u_3) & \mathbf{e}_1 \\ \mathbf{e}_1^\top & 0 \end{pmatrix} \oplus \begin{pmatrix} \mathbf{G}(u_3) & \mathbf{e}_2 \\ \mathbf{e}_2^\top & 0 \end{pmatrix} \oplus \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\mathbf{K}_1 = \begin{pmatrix} \mathbf{G}(u_1) - \mathbf{G}(u_3) & \mathbf{0} \\ \mathbf{0}^\top & 0 \end{pmatrix} \oplus \begin{pmatrix} \mathbf{G}(u_1) - \mathbf{G}(u_3) & \mathbf{0} \\ \mathbf{0}^\top & 0 \end{pmatrix} \oplus \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$\mathbf{K}_2 = \begin{pmatrix} \mathbf{G}(u_2) - \mathbf{G}(u_3) & \mathbf{0} \\ \mathbf{0}^\top & 0 \end{pmatrix} \oplus \begin{pmatrix} \mathbf{G}(u_2) - \mathbf{G}(u_3) & \mathbf{0} \\ \mathbf{0}^\top & 0 \end{pmatrix} \oplus \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$\mathbf{K}_3 = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0}^\top & 1 \end{pmatrix} \oplus \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0}^\top & 0 \end{pmatrix} \oplus \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\mathbf{K}_4 = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0}^\top & 0 \end{pmatrix} \oplus \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0}^\top & 1 \end{pmatrix} \oplus \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

where $\mathbf{0}$ denotes a zero vector or zero matrix. Following the MATLAB program for Example 1, one can easily write a program for this example. With $u_1 = 0.0, u_2 = 0.6, u_3 = 1.0$, the solution is

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$w_1 = 0.5858, w_2 = 0.0, \gamma_1 = 1.7071, \gamma_2 = 4.1213$. Thus the approximate A-optimal design is

$$\xi_A = \begin{pmatrix} 0.0 & 0.6 & 1.0 \\ 0.5858 & 0.0 & 0.4142 \end{pmatrix}.$$

It is easy to show that the theoretical A-optimal design on $[0, 1]$ is

$$\xi_A^* = \begin{pmatrix} 0.0 & 1.0 \\ 2 - \sqrt{2} & \sqrt{2} - 1 \end{pmatrix}.$$

It is obvious that ξ_A is a good approximation of ξ_A^*. □

Example 4. Consider the first-order trigonometric regression model,

$$y_i = \theta_0 + \theta_1 \cos(x_i) + \theta_2 \sin(x_i) + \epsilon_i, \quad i = 1, \ldots, n,$$

and the design space $S = \{u_1, \ldots, u_N\} = \{-2\pi/3, -\pi/3, 0, \pi/3, 2\pi/3\}$ contains $N = 5$ equally spaced points on a partial circle. Optimal designs for trigonometric regression have been investigated by many authors including Chang *et al.* (2013), Dette *et al.* (2007), Wu (2002), and Dette *et al.* (2002). We construct the approximate A-optimal design by solving the SDP problem (P_{A1}). For this model, we have $q = 3$ and $p = 1$. SeDuMi gives the following result: $w_1 = 0.333, w_2 = 0.000, w_3 = 0.333, w_4 = 0.000, \gamma_1 = 1.000, \gamma_2 = 2.000$ and $\gamma_3 = 2.000$. Thus the approximate A-optimal design for the trigonometric model is

$$\xi_A = \begin{pmatrix} -2\pi/3 & -\pi/3 & 0 & \pi/3 & 2\pi/3 \\ 0.333 & 0.000 & 0.333 & 0.000 & 0.333 \end{pmatrix},$$

which is the same as the D-optimal design on $[-2\pi/3, 2\pi/3]$ in Dette *et al.* (2002). □

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4 Applications

There are various applications of the methods discussed in Sections 2 and 3. In this section we provide two applications: one is for continuous design spaces, and the other is for restricted designs.

4.1 Continuous design space

Although the methods in Sections 2 and 3 are for discrete design spaces, they can be applied to continuous design spaces by discretizing the design spaces. For a continuous design space S, equally spaced or uniformly distributed N points can be selected to define a discrete space, say S_N. On S_N, we can construct optimal designs using the methods in Sections 2 and 3. If N is very large, then S_N should have a good coverage of S and the optimal design on S_N should be close to that on S. In addition, if the optimal design on S is a discrete distribution with a finite number of support points, then we have the following theoretical result.

Theorem 1. *Let* $\mathbf{f}(\mathbf{x}) = \frac{\partial g(\mathbf{x};\theta^*)}{\partial \theta}$ *and assume* $\mathbf{f}(\mathbf{x})$ *is continuous and bounded on a continuous design space* S. *Suppose the A-optimal (or E-optimal) design on* S *is* ξ^* *having* m *distinct support points,* $\mathbf{x}_1^*, \ldots, \mathbf{x}_m^*$, *with probabilities* $p_1^*, \ldots, p_m^*$, *respectively. Consider a sequence of discrete design spaces* $S_l \subset S$, $l = 1, 2, \ldots$, *and assume there are design points* $\mathbf{u}_{l_i} \in S_l$ *such that* $\mathbf{u}_{l_i} \to \mathbf{x}_i^*$ *as* $l \to \infty$, *for all* $i = 1, \ldots, m$. *If* ξ^l *is the optimal design on* S_l, *then* $\mathcal{L}(\mathbf{C}^{-1}(\xi^l)) \to \mathcal{L}(\mathbf{C}^{-1}(\xi^*))$ *as* $l \to \infty$, *where function* $\mathcal{L}$ *is the trace for the A-optimal design or the largest eigenvalue for the E-optimal design.*

The proof is in the Appendix. This result is very useful to explore optimal designs on continuous design spaces. We can construct the optimal designs on discrete design spaces first, and the solutions will provide guidance for finding theoretical optimal designs on continuous design spaces. Often we have $\xi^l \to \xi^*$ as $l \to \infty$. Example 5 illustrates this result for an E-optimal design of a nonlinear regression model.

Example 5. Consider the Michaelis-Menten regression model in Dette and Wong (1999),

$$y_i = \theta_1 x_i/(\theta_2 + x_i) + \epsilon_i, \quad i = 1, \ldots, n, \quad x_i \in S = [0, 200].$$

We construct the approximate locally E-optimal design by solving the SDP problem (P_{E1}) with the true parameter values: $(\theta_1^*, \theta_2^*) = (10, 10)$. Notice that for this model, we have

$$\begin{aligned} \frac{\partial g(u_i; \boldsymbol{\theta}^*)}{\partial \boldsymbol{\theta}} &= \left(u_i/(\theta_2^* + u_i), -\theta_1^* u_i/(\theta_2^* + u_i)^2\right)^\top \\ &= \left(u_i/(10 + u_i), -10u_i/(10 + u_i)^2\right)^\top. \end{aligned}$$

Putting this in (4), we can compute matrix

$$\mathbf{G}(u_i) = \left(u_i/(10 + u_i), -10u_i/(10 + u_i)^2\right)^\top \left(u_i/(10 + u_i), -10u_i/(10 + u_i)^2\right), \ i = 1, \ldots, N.$$

The locally E-optimal design, from Dette and Wong (1999), is

$$\xi^* = \begin{pmatrix} x_1^* = 6.515 & x_2^* = 200 \\ p_1 = 0.6838 & p_2 = 0.3162 \end{pmatrix}.$$

In the following we compute E-optimal designs ξ^l for a sequence of discrete design spaces S_l and show that $\lambda_{max}(\mathbf{C}^{-1}(\xi^l)) \to \lambda_{max}(\mathbf{C}^{-1}(\xi^*))$ and $\xi^l \to \xi^*$. In order to present the numerical results clearly, each S_l is chosen to have $N = 5$ design points. However, it works for any number of design points. A sequence of design spaces is given below:

$$\begin{aligned} &S_1 = \{0, 2, 25, 199, 200\}, \quad S_2 = \{0, 2, 15, 199, 200\}, \\ &S_3 = \{0, 2, 10, 199, 200\}, \quad S_4 = \{0, 6, 7, 199, 200\}, \\ &S_5 = \{0, 6.3, 6.8, 199, 200\}, \quad S_6 = \{0, 6, 6.6, 199, 200\}, \\ &S_7 = \{0, 6, 6.55, 199, 200\}, \quad S_8 = \{0, 6, 6.53, 199, 200\}, \\ &S_9 = \{0, 6, 6.51, 199, 200\}, \quad S_{10} = \{0, 6, 6.515, 199, 200\}. \end{aligned}$$

Notice that the third points of these design spaces converge to 6.515, which is one of the support points in ξ^*. The last points of these design spaces are equal to 200, which is the other support point in ξ^*. Using SeDuMi, we get the approximate E-optimal design ξ^l on S_l,

$$\xi^l = \begin{pmatrix} x_1^l & x_2^l \\ w_1^l & w_2^l = 1 - w_1^l \end{pmatrix}, \quad l = 1, \ldots, 10.$$

Each ξ^l has two support points, and the results show that $x_2^l = 200$ for all $l = 1, \ldots, 10$. Table 1 shows the values of x_1^l and w_1^l in ξ^l, and the results indicate that $\lambda_{min}(\mathbf{C}(\xi^l))$ converges to $\lambda_{min}(\mathbf{C}(\xi^*))$ and ξ^l converges to ξ^*. □

When ξ^* is unknown, we can take equally spaced points to form S_N and compute the optimal design ξ^N. With this approach, as $N \to \infty$, there exist sequences of design points such that $\mathbf{u}_{N_i} \to \mathbf{x}_i^*$ for $i = 1, \ldots, m$. Thus, $\mathcal{L}(\mathbf{C}(\xi^N))$ converges to $\mathcal{L}(\mathbf{C}(\xi^*))$, and often ξ^N converges to ξ^* too. Here is one example.

Example 6. Consider the k-th order polynomial regression model,

$$y_i = \theta_0 + \theta_1 x_i + \cdots + \theta_k x_i^k + \epsilon_i, \quad i = 1, \ldots, n,$$

and the design space $S = [-1, 1]$ is continuous. Define a sequence of design spaces as $S_N = \{-1 + 2(i-1)/(N-1), \ \ i = 1, \ldots, N\}, \ \ N = 10, 11, \ldots$. For fixed k, using SeDuMi we compute the A-optimal design for each S_N. We have obtained numerical results for various values of k and N. The results indicate that trace($\mathbf{C}^{-1}(\xi^N)$) converges, and ξ^N converges too. Therefore, for large N, ξ^N can approximate the theoretical A-optimal design well. Two representative results are given below:

$$k = 3, \quad N = 501, \quad \xi^N = \begin{pmatrix} -1 & -0.464 & 0.464 & 1 \\ 0.1505 & 0.3495 & 0.3495 & 0.1505 \end{pmatrix},$$

$$k = 4, \quad N = 501, \quad \xi^N = \begin{pmatrix} -1 & -0.676 & 0 & 0.676 & 1 \\ 0.1042 & 0.2504 & 0.2908 & 0.2504 & 0.1042 \end{pmatrix}.$$

These results are almost the same as the theoretical A-optimal designs on S for $k = 3$ and 4, respectively; see Pukelsheim (1993, p224). □

4.2 Restricted optimal designs

Sometimes we are interested in optimal designs with special design properties, such as symmetric designs, and rotatable designs. We can achieve this goal by imposing linear constraints on weights $w_1, \ldots, w_N$, and the corresponding A-optimal and E-optimal design problems can also be transformed to SDP problems and solved by SeDuMi.

Suppose the linear constraints on the weights can be written as $\mathbf{L}\,(w_1, \ldots, w_N)^\top = \mathbf{c}$, where $\mathbf{L}$ is a $r \times N$ constant matrix with $r < N$ and rank$(\mathbf{L}) = r$, $\mathbf{c}$ is a constant vector, and the constraint $\sum_{i=1}^N w_i = 1$ is included. Because of these constraints, there are $v = N - r$ independent weights, say $w_1, \ldots, w_v$, without loss of generality. Then problems (P_{E1}) and (P_{A1}) can be modified by reducing the weights from $w_1, \ldots, w_{N-1}$ to $w_1, \ldots, w_v$. Consequently, matrices $\mathbf{W}$, $\mathbf{H}_i$ and $\mathbf{K}_i$ need to be modified in these problems.

We now use Example 1 to explain the detailed procedure. For a symmetric E-optimal design, we have $w_1 = w_5$, $w_2 = w_4$ and also $\sum_{i=1}^{5} w_i = 1$, so the linear constant matrix is

$$\mathbf{L} = \begin{pmatrix} 1 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}, \quad \text{and the constant vector is } \mathbf{c} = (0, 0, 1)^\top.$$

Since $N = 5$ and $r = \text{rank}(\mathbf{L}) = 3$, we have $v = N - r = 2$ and the problem (P_{E1}) has two weights in it, say, w_1 and w_2. Matrices $\mathbf{H}_i$ are modified as follows. From $\mathbf{L}\ (w_1, \ldots, w_N)^\top = \mathbf{c}$, we get $w_5 = w_1$, $w_4 = w_2$ and $w_3 = 1 - 2w_1 - 2w_2$. From (5), we have

$$\mathbf{C} - t\,\mathbf{I}_q = w_1(\mathbf{G}(\mathbf{u}_1) + \mathbf{G}(\mathbf{u}_5)) + w_2(\mathbf{G}(\mathbf{u}_2) + \mathbf{G}(\mathbf{u}_4)) + (1 - 2w_1 - 2w_2)\mathbf{G}(\mathbf{u}_3) - t\,\mathbf{I}_q.$$

From $\mathbf{W} = diag(w_1, w_2, 1 - 2w_1 - 2w_2)$ and (6), we get

$$\mathbf{H}_0 = \mathbf{G}(\mathbf{u}_3) \oplus diag(0, 0, 1),$$

$$\mathbf{H}_i = (\mathbf{G}(\mathbf{u}_i) + \mathbf{G}(\mathbf{u}_{6-i}) - 2\mathbf{G}(\mathbf{u}_3)) \oplus \mathbf{W}_i, \quad i = 1, 2,$$

$$\mathbf{H}_3 = -\mathbf{I}_3 \oplus diag(0, 0, 0),$$

$$\mathbf{W}_1 = diag(1, 0, -2),$$

$$\mathbf{W}_2 = diag(0, 1, -2).$$

SeDuMi gives the same E-optimal design as in Example 1, which is expected, since the result in Example 1 is already symmetric.

5 Conclusion

Approximate A-optimal and E-optimal design problems can be transformed to SDP problems, and SeDuMi is effective and powerful to compute approximate A-optimal and E-optimal designs for any linear or nonlinear regression model with a discrete design space. Furthermore, since it is hard to find theoretical optimal designs for many regression models and design spaces, we provide a method to find numerical solutions, which can shed light on deriving theoretical solutions.

Appendix: Matlab program and proof

The following MATLAB program is for Example 1, which is simple and easy to read. This program can be easily modified to compute A-optimal and E-optimal designs for other regression models and design spaces. More general and efficient programs for all the examples in the paper are available from the authors upon request.

Program for Example 1: In MATLAB, everything after the symbol % (in the same line) is designated as a comment.

```
%----------------------------------------------------------------------
% Use SeDuMi to solve the E-optimal design problem in Example 1.
% Input:
% a,b - lower and upper bounds of the design space,
% n - number of the design points in the design space,
% p=d+1, for the d-th degree polynomial regression model.
% Output:
% y - the solution for w_1, ..., w_{n-1}, t.
% info - number of iterations, CPU time, ...

clear
a=-1;    b=1;    n=5;    p=3;      %Input line

for j=1:n
      for i=2:p
            U(1,j)=1;
            U(i,j)=(a+(b-a)*(j-1)/(n-1))^ (i-1);
      end
end

H=zeros(p+n,(p+n)*(n+1));
B=U(:,n)*U(:,n)';
for j=1:p
      for i=1:p
```

```
        H(i,j)=B(i,j);
    end
end

for k=1:n-1
    B=U(:,k)*U(:,k)'-U(:,n)*U(:,n)';
    for j=k*(p+n)+1:k*(p+n)+p
        for i=1:p
            H(i,j)=B(i,j-k*(p+n));
        end
    end
end

B=-eye(p);
for j=n*(p+n)+1:n*(p+n)+p
    for i=1:p
        H(i,j)=B(i,j-n*(p+n));
    end
end

H(p+n,p+n)=1;
for j=1:n-1
    H(p+j,p+j+j*(p+n))=1;
    H(p+n,(j+1)*(p+n))=-1;
end

for i=1:n-1
    bt(i)=0;
end
bt(n)=1;
ct=vec(H(:,1:p+n));
At=zeros((p+n)^2,n);
for j=1:n
    At(:,j)=-vec(H(:,(p+n)*j+1:(p+n)*(j+1)));
end
K.s=size(-H(:,1:p+n),1);

[x,y,info]=sedumi(At,bt,ct,K)    %Call SeDuMi solver
y                                %Output – optimal solution vector
info
%————————————————————————————————————-
```

Proof of Theorem 1: We will prove the result for the A-optimal design here. For the E-optimal design, the proof is similar and omitted.

Define a design on each S_l,

$$\xi^{l*} = \begin{pmatrix} \mathbf{u}_{l_1} & \dots & \mathbf{u}_{l_m} \\ p_1^* & \dots & p_m^* \end{pmatrix}, \qquad l = 1, 2, \dots.$$

Denote the information matrices corresponding to designs ξ^*, ξ^{l*}, ξ^l, respectively, by

$$\mathbf{C}_* = \mathbf{C}(\xi^*) = \sum_{i=1}^m p_i^* \mathbf{f}(\mathbf{x}_i^*)\mathbf{f}^\top(\mathbf{x}_i^*),$$
$$\mathbf{C}_{l*} = \mathbf{C}(\xi^{l*}) = \sum_{i=1}^m p_i^* \mathbf{f}(\mathbf{u}_{l_i})\mathbf{f}^\top(\mathbf{u}_{l_i}),$$
$$\mathbf{C}_l = \mathbf{C}(\xi^l).$$

Since ξ^* is the A-optimal design on S and ξ^l is the A-optimal design on $S_l \subset S$, we must have

$$\text{trace}(\mathbf{C}_*^{-1}) \leq \text{trace}(\mathbf{C}_l^{-1}) \leq \text{trace}(\mathbf{C}_{l*}^{-1}). \tag{10}$$

Since $\mathbf{f}(\mathbf{x})$ is continuous and bounded on S and $\mathbf{u}_{l_i} \to \mathbf{x}_i^*$ as $l \to \infty$ for all $i = 1, \dots, m$, we have $\mathbf{C}_{l*} \to \mathbf{C}_*$ as $l \to \infty$. Suppose $\lambda_1(\mathbf{C}) \geq \dots \geq \lambda_q(\mathbf{C})$ are the q ordered eigenvalues of $\mathbf{C}$. From Horn and Johnson (1985, p539), we get $\lambda_i(\mathbf{C}_{l*}) \to \lambda_i(\mathbf{C}_*)$ for all $i = 1, \dots, q$. Thus

$$\text{trace}(\mathbf{C}_{l*}^{-1}) \to \text{trace}(\mathbf{C}_*^{-1}), \quad \text{as} \quad l \to \infty. \tag{11}$$

Combining (10) with (11) gives the result. □

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Table 1: Support points x_1^l and weights w_1^l in ξ^l in Example 5.

l	x_1^l	w_1^l	$t = \lambda_{min}(\mathbf{C}(\xi^l))$	l	x_1^l	w_1^l	$t = \lambda_{min}(\mathbf{C}(\xi^l))$
1	2.000	0.8351	0.012093043	6	6.600	0.6822	0.023183683
2	15.000	0.5987	0.016274986	7	6.550	0.6831	0.023185304
3	10.000	0.6358	0.021125673	8	6.530	0.6835	0.023185577
4	7.000	0.6752	0.023125637	9	6.510	0.6839	0.023185631
5	6.300	0.6879	0.023164305	10	6.515	0.6838	0.023185639

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