Interior Point Methods for Computing Optimal Designs *

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Abstract

In this paper we study interior point (IP) methods for solving optimal design problems. In particular, we propose a primal IP method for solving the problems with general convex optimality criteria and establish its global convergence. In addition, we reformulate the problems with A-, D- and E-criterion into linear or log-determinant semidefinite programs (SDPs) and apply standard primal-dual IP solvers such as SDPT3 [21, 25] to solve the resulting SDPs. We also compare the IP methods with the widely used multiplicative algorithm introduced by Silvey et al. [18]. The computational results show that the IP methods generally outperform the multiplicative algorithm both in speed and solution quality. Moreover, our primal IP method theoretically converges for general convex optimal design problems while the multiplicative algorithm is only known to converge under some assumptions.

Key words: Optimal design, A-criterion, c-criterion, D-criterion, E-criterion, pth mean criterion, interior point methods

1 Introduction

In this paper, we consider the optimal experimental design problems on a given finite design space $\mathcal{X} = \{x_1, \ldots, x_n\}$. Suppose $p(y|x,\theta)$ is the probability density function of the response y, where $\theta = (\theta_1, \ldots, \theta_m)^T$ is some model parameter. Let A_i denote the $m \times m$ expected Fisher information matrix from per unit of x_i, whose (j,k)th entry is given by

$$A_i(j,k) = E\left[\frac{\partial \log p(y|x_i,\theta)}{\partial \theta_j}\frac{\partial \log p(y|x_i,\theta)}{\partial \theta_k}\right]$$

for $i = 1, \ldots, n$. As a function of design measure $w = (w_1, \ldots, w_n)^T$, the moment matrix is defined as

$$\mathcal{M}(w) = \sum_{i=1}^n w_i A_i$$

for $w \in \Omega := \{w : \ w_i \geq 0, \sum_{i=1}^n w_i = 1\}$. Throughout this paper, we assume that A_i's are well-defined and hence positive semidefinite, and moreover, that there exists a $w \in \Omega$ such that $\mathcal{M}(w)$ is positive definite. Therefore, we can observe that $\mathcal{M}(w)$ is positive definite for all positive $w \in \Omega$.

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Given an optimality criterion ϕ defined on the set of positive definite matrices, the optimal experimental design problem can be formulated as the following minimization problem:

$$\begin{array}{rl} f^* := \min\limits_{w} & \phi(\mathcal{M}(w)) \\ \text{s.t.} & w \in \Omega,\ \mathcal{M}(w) \text{ is positive definite.} \end{array} \tag{1}$$

Some classical optimality criteria include (see [16, Chapter 6]):

(i) A-criterion $\phi(X) := \mathrm{tr}(K^T X^{-1} K)$;

(ii) c-criterion $\phi(X) := c^T X^{-1} c$;

(iii) D-criterion $\phi(X) := \log\det(K^T X^{-1} K)$;

(iv) E-criterion $\phi(X) := \lambda_{\max}(K^T X^{-1} K)$;

(v) pth mean criterion $\phi(X) := \mathrm{tr}((K^T X^{-1} K)^{-p})$

for some $p < 0$, $c \in \Re^m$ and $K \in \Re^{m \times k}$. In addition, for (iii) and (iv), K is assumed to have full column rank. It is easy to observe that c-criterion is just a special case of A-criterion with $K = c$ and A-criterion is a special case of pth mean criterion with $p = -1$. We shall also mention that pth mean criterion can be defined more generally to include D-criterion and E-criterion as special cases (see [16] for details). In Section 3, we will show that the criteria (i)-(v) are convex, and hence, problem (1) with these criteria is a convex optimization problem.

The optimal design problems (1) with the aforementioned criteria usually do not have closed form solutions. Numerous procedures have thus been proposed to solve (1) (see, for example, [7, 27, 2, 26, 9, 23, 6, 24]). Among them, the multiplicative algorithm introduced in [18] has been widely explored. For example, Titterington [20], Pázman [15], Dette et al. [6] and Harman and Trnovská [10] studied the multiplicative algorithm for D-criterion. In addition, Fellman [8] and Torsney [22] considered the multiplicative algorithm for A-criterion under the assumption that all A_i's are rank-one. Recently, Yu [28] studied the multiplicative algorithm for more general optimality criteria and proved its global convergence under some assumptions. Nevertheless, for a general optimality criterion, some of those assumptions may not hold and hence there is no theoretical guarantee for its convergence. Indeed, as observed in [28, Section 5], one of the assumptions does not hold for pth mean criterion with $p = -2$. Moreover, for such a criterion, our numerical experiments in Section 5 demonstrate that the multiplicative algorithm appears not to converge. More details about the multiplicative algorithm for solving (1) are given in Section 2.

In this paper, we consider an alternative approach to solve problem (1). In particular, we study interior point (IP) methods for (1), which are Newton-type methods and can be efficiently applied to a broad class of optimal design problems of small or medium sizes. More specifically, we develop a primal IP method for (1) with a general convex optimality criterion and establish its global convergence. In addition, we reformulate problem (1) with A-, D- and E-criterion into linear or log-determinant semidefinite programs (SDPs) and apply the standard primal-dual IP solvers such as SDPT3 [21, 25] to solve the resulting SDPs. We also compare the IP methods with the multiplicative algorithm on both simulated and real data. The computational results show that the IP methods usually outperform the multiplicative algorithm in both speed and solution quality.

The rest of this paper is organized as follows. In Subsection 1.1, we introduce the notations that are used throughout the paper. In Section 2, we review the multiplicative algorithm and address its convergence. In Sections 3 and 4, we propose IP methods for solving problem (1) with general convex optimality criteria and classical optimality criteria, respectively. In Section 5, we conduct numerical experiments to test the performance of these methods and compare them with the multiplicative algorithm on both simulated and real data. Finally, we present some concluding remarks in Section 6.

1.1 Notations

In this paper, the symbol $\Re_{++}$ denotes the set of all positive real numbers and $\Re^n$ denotes the n-dimensional Euclidean space. For a vector $x \in \Re^n$ and $\mathcal{I} \subseteq \{1, \ldots, n\}$, $\|x\|$ denotes the Euclidean norm of x, $x_{\mathcal{I}}$ denotes the subvector of x indexed by $\mathcal{I}$ and $\mathscr{D}(x)$ denotes the diagonal matrix whose ith diagonal entry is x_i for all i. For a vector $x \in \Re^n$ with nonzero entries, x^{-1} denotes the vector whose ith entry is x_i^{-1} for all i. The letter e denotes the vector of all ones, whose dimension should be clear from the context. The set of all $m \times n$ matrices with real entries is denoted by $\Re^{m\times n}$. For any $A \in \Re^{m\times n}$, $\mathcal{I} \subseteq \{1, \ldots, m\}$ and $\mathcal{J} \subseteq \{1, \ldots, n\}$, a_{ij} denotes the (i, j)th entry of A, $A_{\mathcal{J}}$ denotes the submatrix of A comprising the columns of A indexed by $\mathcal{J}$ and $A_{\mathcal{I}\mathcal{J}}$ denotes the submatrix of A comprising the rows and columns of A indexed by $\mathcal{I}$ and $\mathcal{J}$, respectively. The space of $n \times n$ symmetric matrices will be denoted by $\mathcal{S}^n$. If $A \in \mathcal{S}^n$ is positive semidefinite (resp., definite), we write $A \succeq 0$ (resp., $A \succ 0$). The cone of positive semidefinite (resp., definite) matrices is denoted by $\mathcal{S}^n_+$ (resp., $\mathcal{S}^n_{++}$). For $A, B \in \mathcal{S}^n$, $A \succeq B$ (resp., $A \succ B$) means $A - B \succeq 0$ (resp., $A - B \succ 0$). Given matrices A and B in $\Re^{m\times n}$, $A \otimes B$ denotes the Kronecker product of A and B, while $A \circ B$ denotes the Hadamard (entry-wise) product of A and B. In addition, $\mathrm{vec}(A)$ denotes the column vector formed by stacking columns of A one by one. The trace of a real square matrix A is denoted by $\mathrm{tr}(A)$. We denote by I the identity matrix, whose dimension should be clear from the context.

A function $f : \mathcal{S}^n \to \Re$ is said to be increasing (resp., decreasing) if for any $A \succeq B$, it holds that

$$f(A) \geq f(B) \quad \text{(resp., } f(A) \leq f(B)).$$

2 The multiplicative algorithm

In this section we review the multiplicative algorithm introduced in [18] for solving problem (1) and address its convergence.

We now describe the multiplicative algorithm as follows, which is specified through a power parameter $\lambda \in (0, 1]$.

Multiplicative Algorithm:

1. **Start:** Let a positive $w^0 \in \Omega$ and $\lambda \in (0, 1]$ be given.

2. **For** $k = 0, 1, \ldots$

$$w_i^{k+1} = w_i^k \frac{(d_i(w^k))^\lambda}{\sum_{j=1}^n w_j^k (d_j(w^k))^\lambda}, \quad i = 1, \ldots, n, \tag{2}$$

where $d_i(w) = -\mathrm{tr}(\nabla\phi(\mathcal{M}(w))A_i)$ and $\nabla\phi(\mathcal{M}(w))$ is the gradient of ϕ at $\mathcal{M}(w)$.
End (for)

Remark. The above algorithm is the same as the one described in [28] which solves an equivalent maximization reformulation of problem (1), that is, both algorithms generate exactly the same sequence $\{w^k\}$ provided the initial points w^0 are identical. Also, it is not hard to observe that $d_i(w^k)$ can be of any sign for a general ϕ. Thus, it is possible that the denominator in (2) becomes zero at some iteration and then the successive iterations will not be defined. In addition, since this algorithm requires the differentiability of ϕ, it cannot be directly applied to problem (1) with E-criterion. ■

We now state a global convergence result for the above algorithm, which is an adaption of Theorem 2 recently established by Yu [28] for the multiplicative algorithm when applied to an equivalent maximization reformulation of problem (1).

Proposition 2.1. *Let $\{w^k\}$ be the sequence generated from the above multiplicative algorithm. Suppose the following assumptions hold:*

(a) *for any feasible point w of (1), $\nabla\phi(\mathcal{M}(w)) \preceq 0$ and $\nabla\phi(\mathcal{M}(w))A_i \neq 0$ for $i = 1, \ldots, n$;*

(b) *for any feasible point w of (1), if $T(w) \neq w$, then $\phi(\mathcal{M}(T(w))) < \phi(\mathcal{M}(w))$, where*

$$[T(w)]_i \;:=\; w_i \frac{(d_i(w))^\lambda}{\sum_{j=1}^n w_j (d_j(w))^\lambda}, \quad i = 1, \ldots, n;$$

(c) *ϕ is strictly convex and $\nabla\phi$ is continuous in $\mathcal{S}^m_{++}$;*

(d) *for any $\{X^k\} \subset \mathcal{S}^m_{++}$, if $X^k \to X^*$ and $\{\phi(X^k)\}$ is decreasing, then $X^* \succ 0$.*

Then $\phi(\mathcal{M}(w^k)) \to \inf_{w\in\Omega} \phi(\mathcal{M}(w))$ monotonically, and moreover, any accumulation point of $\{w^k\}$ is an optimal solution of (1).

Using Proposition 2.1 and some technical results developed in [28], one can establish the convergence of the above multiplicative algorithm when applied to problem (1) with A-, D- and pth mean criterion for $p \in (-1, 0)$ and $K = I$, which is summarized as follows.

Corollary 2.2. *Assume that $K = I$ and $A_i \neq 0$ for $i = 1, \ldots, n$. Then the multiplicative algorithm converges for any $\lambda \in (0, 1]$ when applied to problem (1) with D- and pth mean criterion for $p \in (-1, 0)$. Also, it converges for A-criterion when $\lambda \in (0, 1)$.*

As seen from Proposition 2.1 and Corollary 2.2, the multiplicative algorithm converges for a class of optimality criteria ϕ. Nevertheless, for a general convex optimality criterion, the assumptions stated in Proposition 2.1 may not hold and hence there is no theoretical guarantee for its convergence. Indeed, as observed in [28, Section 5], the assumption (b) with $\lambda = 1$ does not hold for pth mean criterion with $p = -2$. Moreover, for such a criterion, our numerical experiments in Section 5 demonstrate that the multiplicative algorithm appears not to converge.

Due to the aforementioned potential drawbacks of the multiplicative algorithm, we will propose IP methods for solving problem (1) with a broad class of optimality criteria ϕ in subsequent sections.

3 Primal IP method for a class of convex optimality criteria

In this section, we propose a primal IP method for solving (1) with a class of convex optimality criteria ϕ. We make the following assumption on ϕ throughout this section.

Assumption 1. *The optimality criterion ϕ is convex and twice continuously differentiable in $\mathcal{S}^m_{++}$, and $\phi(\mathcal{M}(\cdot))$ is bounded below in the feasible set of* (1).

The above assumption is fairly reasonable. We will show that each classical optimality criterion described in Section 1 either satisfies this assumption or can be arbitrarily approximated by one criterion that satisfies Assumption 1.

We first show that the optimality criteria described in Section 1 are convex in $\mathcal{S}^m_{++}$ by representing them as the infimum of some extended convex function. Before proceeding, we recall the following well-known result, whose proof can be found in [3, Lemma 4.2.1].

Lemma 3.1. *Let $A \in \mathcal{S}^m$, $B \in \Re^{k\times m}$ and $C \in \mathcal{S}^k$. Suppose that C is positive definite. Then the matrix $\begin{pmatrix} A & B^T \\ B & C \end{pmatrix}$ is positive semidefinite if and only if $A \succeq B^T C^{-1} B$.*

Proposition 3.2. *The A-, c-, D-, E- and pth mean criterion are convex in $\mathcal{S}^m_{++}$.*

Proof. We first show that pth mean criterion is convex by considering two cases: (i) $k \le m$ and (ii) $k > m$. For case (i), there exists a $K^0 \in \Re^{m\times k}$ with full column rank such that $K_\epsilon = K + \epsilon K^0$ has full column rank for all sufficiently small $\epsilon > 0$. For any such small ϵ, we see that $(K_\epsilon^T X^{-1} K_\epsilon)^{-1} \succ 0$ whenever $X \succ 0$. Furthermore, we have

$$\mathrm{tr}((K_\epsilon^T X^{-1} K_\epsilon)^{-p}) = \mathrm{tr}([(K_\epsilon^T X^{-1} K_\epsilon)^{-1}]^p) = \inf_U\{\mathrm{tr}(U^{2p}) :\ (K_\epsilon^T X^{-1} K_\epsilon)^{-1} \succeq U^2,\ U \succ 0\} \tag{3}$$

due to the fact that $U \mapsto \mathrm{tr}(U^p)$ is convex and decreasing (see [3, Exercise 4.7] and [4, Corollary 5.2.3]). For any $U \succ 0$, we observe that

$$(K_\epsilon^T X^{-1} K_\epsilon)^{-1} \succeq U^2 \ \Leftrightarrow\ U^{-2} \succeq K_\epsilon^T X^{-1} K_\epsilon \ \Leftrightarrow\ I \succeq (K_\epsilon U)^T X^{-1} K_\epsilon U, \tag{4}$$

which together with Lemma 3.1 and (3) implies that for any $X \succ 0$,

$$\mathrm{tr}((K_\epsilon^T X^{-1} K_\epsilon)^{-p}) = \inf_U \left\{ \mathrm{tr}(U^{2p}) :\ \begin{pmatrix} I & (K_\epsilon U)^T \\ K_\epsilon U & X \end{pmatrix} \succeq 0,\ U \succ 0 \right\}. \tag{5}$$

We now claim that $\mathrm{tr}((K_\epsilon^T X^{-1} K_\epsilon)^{-p})$ is convex in $X \in \mathcal{S}^m_{++}$. Let C_X denote the feasible region of (5) and define $C = \{(X, U) : X \succ 0, U \in C_X\}$. Then C is convex, and moreover, it follows from (5) that

$$\mathrm{tr}((K_\epsilon^T X^{-1} K_\epsilon)^{-p}) = \inf_U \{\mathrm{tr}(U^{2p}) + \delta_C(X, U)\}, \tag{6}$$

where δ_C is the indicator function of C. Since the objective function of (6) is convex in (X, U), it follows from [17, Theorem 5.7] that $\mathrm{tr}((K_\epsilon^T X^{-1} K_\epsilon)^{-p})$ is a convex function in $X \in \mathcal{S}^m_{++}$. Upon taking limit as $\epsilon \downarrow 0$, we easily conclude that $\mathrm{tr}((K^T X^{-1} K)^{-p})$ is convex in $X \in \mathcal{S}^m_{++}$ when $k \le m$. We next consider case (ii). Let $\tilde{K} = \begin{pmatrix} K^T & 0 \end{pmatrix}^T \in \Re^{k\times k}$. It is not hard to observe that

$$\mathrm{tr}((K^T X^{-1} K)^{-p}) = \mathrm{tr}\left(\left[\tilde{K}^T \begin{pmatrix} X & 0 \\ 0 & I \end{pmatrix}^{-1} \tilde{K}\right]^{-p}\right).$$

Using a similar argument as in case (i), we can easily show that $\mathrm{tr}((K^T X^{-1} K)^{-p})$ is also convex in $X \in \mathcal{S}^m_{++}$ when $k > m$. Therefore, pth mean criterion is convex in $X \in \mathcal{S}^m_{++}$.

We next show that A-, c-, D- and E-criterion are convex. Since A- and c-criterion are just special cases of pth mean criterion with $p = -1$ and a suitable choice of K, their convexity immediately follows from that of pth mean criterion. For D-criterion, since $\log\det(\cdot)$ is increasing, we observe that for any $X \succ 0$,

$$\log\det(K^T X^{-1} K) \ = \ \inf_U \left\{\log\det(U^{-2}) : \ U^{-2} \succeq K^T X^{-1} K, \ U \succ 0\right\}.$$

Using this relation, the second equivalence in (4), Lemma 3.1, and the fact $\log\det(U^{-2}) = -2\log\det(U)$, we obtain that

$$\log\det(K^T X^{-1} K) \ = \ \inf_U \left\{-2\log\det(U) : \ \begin{pmatrix} I & (KU)^T \\ KU & X \end{pmatrix} \succeq 0\right\}. \tag{7}$$

Using this relation and a similar argument as above, we can show that $\log\det(K^T X^{-1} K)$ can be represented as the infimum of some extended convex function and its convexity thus follows. Finally, for E-criterion, applying Lemma 3.1, we have, for any $X \succ 0$,

$$\lambda_{\max}(K^T X^{-1} K) \ = \ \inf_t \left\{t : \ tI \succeq K^T X^{-1} K\right\} \ = \ \inf_t \left\{t : \ \begin{pmatrix} tI & K^T \\ K & X \end{pmatrix} \succeq 0\right\}. \tag{8}$$

The convexity of E-criterion then immediately follows from this relation and a similar argument as used for D-criterion. ■

From the above discussion, we know that the optimality criteria described in Section 1 are convex in $\mathcal{S}^m_{++}$. Further, we can observe that A-, c-, D- and pth mean criterion with $p \le -2$ are twice continuously differentiable in $\mathcal{S}^m_{++}$. Moreover, when K has full column rank, the latter criterion is also twice continuously differentiable for $p \in (-2, 0)$. However, if K is not of full column rank, pth mean criterion for $p \in (-2,-1) \cup (-1, 0)$ may not be twice continuously differentiable in $\mathcal{S}^m_{++}$. In this case, using a similar argument as in the proof of Proposition 3.2, we can show that pth mean criterion can be arbitrarily approximated by a twice continuously differentiable function given by

$$\begin{cases} \operatorname{tr}((K_\epsilon^T X^{-1} K_\epsilon)^{-p}) & \text{if } k \le m, \\ \operatorname{tr}\left(\left[\tilde{K}_\epsilon^T \begin{pmatrix} X & 0 \\ 0 & I \end{pmatrix}^{-1} \tilde{K}_\epsilon\right]^{-p}\right) & \text{otherwise} \end{cases}$$

for some full column rank matrices $K_\epsilon \in \Re^{m\times k}$ and $\tilde{K}_\epsilon \in \Re^{k \times k}$. In addition, as discussed in [13, Section 4], the function $\lambda_{\max}(\cdot)$ can be uniformly approximated by an analytic convex function and hence E-criterion can also be arbitrarily approximated by a twice continuously differentiable convex function. Therefore, each classical optimality criterion described in Section 1 either satisfies Assumption 1 or can be arbitrarily approximated by one criterion which satisfies that assumption.

It is well known that IP methods are efficient tools for solving a broad class of small- or medium-sized smooth convex optimization problems (see, for example, [14]). Given that the dimension of problem (1) is typically not high and its objective function has nice smooth property, we will develop an IP method to solve it. To proceed, we first reformulate the problem by eliminating the equality constraint. And the resulting equivalent problem is given by

$$\begin{array}{rl} f^* = \min\limits_{\tilde{w}} & f(\tilde{w}) := \phi(\mathcal{M}(P\tilde{w} + q)) \\ \text{s.t.} & e^T \tilde{w} \le 1, \ \tilde{w} \ge 0, \ \mathcal{M}(P\tilde{w} + q) \succ 0, \end{array} \tag{9}$$

where $P \in \Re^{n\times(n-1)}$ and $q \in \Re^n$ are such that

$$P\tilde{w} + q = \begin{pmatrix} \tilde{w} \\ 1 - e^T\tilde{w} \end{pmatrix} \qquad \forall \tilde{w} \in \Re^{n-1}. \tag{10}$$

We next develop an IP method for solving problem (9) instead. First, we need to build a suitable barrier function for IP method. Given any $\tilde{w} > 0$ satisfying $e^T\tilde{w} < 1$, one can observe that $P\tilde{w}+q > 0$ and hence $\mathcal{M}(P\tilde{w} + q) \succ 0$. This implies that any barrier function that takes into account the first two inequality constraints of (9) is sufficient for the development of IP method. Here we naturally choose the logarithmic barrier function and then solve the barrier subproblem in the form of

$$\min_{\tilde{w}} f_\mu(\tilde{w}) := f(\tilde{w}) - \mu \sum_{i=1}^{n-1} \log(\tilde{w}_i) - \mu \log\left(1 - e^T\tilde{w}\right) \tag{11}$$

for a sequence of parameters $\mu \downarrow 0$. In view of Assumption 1, we clearly see that any level set of f_μ is compact. Moreover, f_μ is strictly convex. Thus, there exists a unique minimizer to (11) for any $\mu > 0$. Furthermore, it follows from Assumption 1 that f_μ is twice continuously differentiable and its Hessian is positive definite in its domain. Therefore, problem (11) can be suitably solved by the Newton's method with a line search whose stepsize is chosen by Armijo rule.

We are now ready to present our IP method for solving problem (9).

Primal IP Method:

1. **Start:** Let a strictly feasible $\tilde{w}^0$, $0 < \beta, \gamma, \eta, \sigma < 1$ and $\mu_1 > 0$ be given. Let $\epsilon(\mu)$ be an increasing function of μ so that $\lim_{\mu\downarrow 0} \epsilon(\mu) = 0$. Set $\tilde{w} = \tilde{w}^0$ and $k = 1$.

2. **While** $\|\nabla f_{\mu_k}(\tilde{w})\| > \epsilon(\mu_k)$ **do**

   (a) Compute the Newton direction

   $$d := -(\nabla^2 f_{\mu_k}(\tilde{w}))^{-1}\nabla f_{\mu_k}(\tilde{w}).$$

   (b) Let $\alpha_{\max}(\tilde{w}) := \max\{\alpha : \ \tilde{w}[\alpha] \geq 0, \ e^T\tilde{w}[\alpha] \leq 1\}$, where $\tilde{w}[\alpha] := \tilde{w} + \alpha d$.

   (c) Let α be the largest element of $\{\bar{\alpha}(\tilde{w}), \beta\bar{\alpha}(\tilde{w}), \beta^2\bar{\alpha}(\tilde{w}), \cdots\}$ satisfying

   $$f_{\mu_k}(\tilde{w}[\alpha]) \leq f_{\mu_k}(\tilde{w}) + \sigma\alpha(\nabla f_{\mu_k}(\tilde{w}))^T d,$$

   where $\bar{\alpha}(\tilde{w}) := \min\{1, \eta\alpha_{\max}(\tilde{w})\}$.

   (d) Set $\tilde{w} \leftarrow \tilde{w}[\alpha]$.

   End (while)

3. Set $\mu_{k+1} \leftarrow \gamma\mu_k$, $\tilde{w}^k \leftarrow \tilde{w}$, $k \leftarrow k+1$, and go to step 2.

For standard IP methods, when applied to solve convex optimization problems, the feasible sets are usually assumed to be closed and the objective functions are twice continuously differentiable in a neighborhood of the feasible sets. However, the feasible set of our problem (9) may not be closed, and moreover, the objective function of (9) may not be well-defined on the boundary of the feasible set. Thus, the existing convergence analysis for IP methods does not directly apply to the above IP algorithm. We next analyze the convergence regarding the outer iterations of our primal IP method and leave the discussion on the convergence of its inner iterations to the end of this section.

For notational convenience, in the remainder of this section, we associate with each $\tilde{w} \in \Re^{n-1}$ a unique $w \in \Re^n$ by letting $w := P\tilde{w} + q$. Analogously, we associate with each $w \in \Re^n$ a unique $\tilde{w} \in \Re^{n-1}$ by letting $\tilde{w}_i = w_i$ for $i = 1, \ldots, n-1$. Also, we let $\phi_{\mathcal{M}}(w) := \phi(\mathcal{M}(w))$.

We first observe that if problem (1) has an optimal solution w^*, then there exists a Lagrange multiplier $u^* \geq 0$ such that (w^*, u^*) satisfies the following KKT system:

$$\begin{array}{rcl} P^T(\nabla \phi_{\mathcal{M}}(w) - u) & = & 0, \\ e^T w & = & 1, \\ u \circ w & = & 0, \\ (w, u) & \geq & 0. \end{array} \tag{12}$$

Given a strictly feasible point $\tilde{w} \in \Re^{n-1}$ of problem (9), we notice that

$$\nabla f_\mu(\tilde{w}) = P^T(\nabla \phi_{\mathcal{M}}(w) - \mu w^{-1}). \tag{13}$$

Then it is not hard to observe that for each $\mu > 0$, the w associated with the approximate solution $\tilde{w}$ of (11) obtained by the Newton's method detailed in step 1 above together with $u := \mu w^{-1}$ satisfies the following perturbed KKT system:

$$\begin{array}{rcl} P^T(\nabla \phi_{\mathcal{M}}(w) - u) & = & v, \\ e^T w & = & 1, \\ u \circ w & = & \mu e, \\ (w, u) & > & 0 \end{array} \tag{14}$$

for some $v \in \Re^{n-1}$. In order to analyze the convergence of our primal IP method, we will study the limiting behavior of the solutions of system (14) as $(\mu, v) \to (0_+, 0)$, that is, $(\mu, v) \to (0, 0)$ with $\mu > 0$.

We first claim that system (14) has a unique solution for any $(\mu, v) \in \Re_{++} \times \Re^{n-1}$. Indeed, it is easy to observe that $\tilde{w} \in \Re^{n-1}$ is an optimal solution of

$$\min_{\tilde{w}} f_\mu(\tilde{w}) - v^T \tilde{w} \tag{15}$$

if and only if there exists $u \in \Re^n$ so that (w, u) is a solution of (14). Since the objective function of (15) is strictly convex and it has compact level sets, problem (15) has a unique optimal solution, which immediately implies that system (14) has a unique solution. From now on, we denote by $(w(\mu, v), u(\mu, v))$ the unique solution of (14) and by $\tilde{w}(\mu, v)$ the vector obtained from $w(\mu, v)$ by dropping the last entry for all $(\mu, v) \in \Re_{++} \times \Re^{n-1}$. It is clear that $\tilde{w}(\mu, v)$ is the unique optimal solution of (15). We next establish the limiting behavior of $w(\mu, v)$ as $(\mu, v) \to (0_+, 0)$.

Theorem 3.3. *Let $(w(\mu, v), u(\mu, v))$ be defined above for $(\mu, v) \in \Re_{++} \times \Re^{n-1}$. Then the following statements hold:*

(a) $\lim\limits_{(\mu,v) \to (0_+, 0)} \phi(\mathcal{M}(w(\mu, v))) = f^*$.

(b) *Suppose that problem* (1) *has an optimal solution. Then any accumulation point of* $w(\mu, v)$ *as* $(\mu, v) \xrightarrow[\Xi_C]{} (0,0)$, *i.e.,* $(\mu, v) \to (0,0)$ *with* $(\mu, v) \in \Xi_C := \{(\mu, v) : \ \|v\|_\infty < C\mu\}$ *for some given* $C > 0$, *is an optimal solution of* (1) *with maximum cardinality.*

(c) *Suppose that problem* (1) *has an optimal solution* w^*. *Let* u^* *be the associated Lagrange multiplier satisfying* (12). *Assume that* $|\mathcal{B}| + |\mathcal{N}| = n$, *where* $\mathcal{B} := \{i : \ w_i^* > 0\}$ *and* $\mathcal{N} := \{i : \ u_i^* > 0\}$. *Suppose further that* $[\nabla^2 \phi_{\mathcal{M}}(w)]_{\mathcal{B}\mathcal{B}} \succ 0$ *for any* $w \in \Omega$ *satisfying* $w_{\mathcal{B}} > 0$ *and* $w_{\mathcal{N}} = 0$. *Then* $w(\mu, v)$ *converges to an optimal solution of* (1) *with maximum cardinality as* $(\mu, v) \to (0_+, 0)$.

Proof. We first prove part (a). Given an arbitrary $\epsilon > 0$, there exists a strictly feasible point $\tilde{w}$ of problem (9) such that $f(\tilde{w}) < f^* + \epsilon/2$. By the definition, we know that $\tilde{w}(\mu, v)$ is the unique optimal solution of (15). Then we have that for any $v \in \Re^{n-1}$,

$$f_\mu(\tilde{w}(\mu, v)) - v^T \tilde{w}(\mu, v) \leq f_\mu(\tilde{w}) - v^T \tilde{w}. \tag{16}$$

It is easy to observe that $\tilde{w}(\mu, v)$ is strictly feasible for (9). Hence,

$$-\sum_{i=1}^{n-1} \log(\tilde{w}_i(\mu, v)) - \log\left(1 - e^T \tilde{w}(\mu, v)\right) > 0$$

and $f(\tilde{w}(\mu, v)) \geq f^*$. In view of these inequalities, (16) and the fact that $\|\tilde{w}(\mu, v)\|_1 \leq 1$ and $\|\tilde{w}\|_1 \leq 1$, one can obtain that for any $(\mu, v) \in \Re_{++} \times \Re^{n-1}$,

$$\begin{aligned}
f^* \leq f(\tilde{w}(\mu, v)) &= f_\mu(\tilde{w}(\mu, v)) + \sum_{i=1}^{n-1} \log(\tilde{w}_i(\mu, v)) + \log\left(1 - e^T \tilde{w}(\mu, v)\right) \\
&\leq f_\mu(\tilde{w}(\mu, v)) \ \leq \ f_\mu(\tilde{w}) + v^T \tilde{w}(\mu, v) - v^T \tilde{w} \\
&\leq f(\tilde{w}) - \mu \sum_{i=1}^{n-1} \log(\tilde{w}_i) - \mu \log\left(1 - e^T \tilde{w}\right) + 2\|v\|_\infty \\
&\leq f^* + \frac{\epsilon}{2} - \mu \sum_{i=1}^{n-1} \log(\tilde{w}_i) - \mu \log\left(1 - e^T \tilde{w}\right) + 2\|v\|_\infty.
\end{aligned}$$

Clearly, there exists some $\delta > 0$ such that $f^* \leq f(\tilde{w}(\mu, v)) \leq f^* + \epsilon$ whenever $\|(\mu, v)\| < \delta$, $\mu > 0$. Hence, $\phi_{\mathcal{M}}(w(\mu, v)) = f(\tilde{w}(\mu, v)) \to f^*$ as $(\mu, v) \to (0_+, 0)$.

We now show part (b) holds. Let w^* be an optimal solution of (1) with maximum cardinality and let u^* be the corresponding Lagrange multiplier, that is, (w^*, u^*) satisfies (12). Let $\tilde{w}^*$ be the vector obtained from w^* by dropping the last entry. In view of (10) and the first equation of (12) and (14), we observe that for any $(\mu, v) \in \Xi_C$,

$$\begin{aligned}
(w(\mu, v) - w^*)^T (u(\mu, v) - u^*) &= (P\tilde{w}(\mu, v) - P\tilde{w}^*)^T (u(\mu, v) - u^*) \\
&= (\tilde{w}(\mu, v) - \tilde{w}^*)^T P^T (\nabla \phi_{\mathcal{M}}(w(\mu, v)) - \nabla \phi_{\mathcal{M}}(w^*)) - (\tilde{w}(\mu, v) - \tilde{w}^*)^T v \\
&= (w(\mu, v) - w^*)^T (\nabla \phi_{\mathcal{M}}(w(\mu, v)) - \nabla \phi_{\mathcal{M}}(w^*)) - (\tilde{w}(\mu, v) - \tilde{w}^*)^T v \\
&\geq -2C\mu,
\end{aligned}$$

where the last inequality holds since ϕ is convex in $\mathcal{S}^m_{++}$, $w(\mu,v), w^* \in \Omega$ and $\|v\|_\infty < C\mu$. Using this inequality and the third equation in (12) and (14), we see that

$$w^{*T}u(\mu,v) + w(\mu,v)^T u^* \;\le\; w^{*T}u^* + w(\mu,v)^T u(\mu,v) + 2C\mu \;=\; (2C+n)\mu. \tag{17}$$

Dividing both sides of the above inequality by μ and using the third equation of (14), we obtain that

$$\sum_{i=1}^n \frac{w_i^*}{w_i(\mu,v)} + \sum_{i=1}^n \frac{u_i^*}{u_i(\mu,v)} \;\le\; 2C+n. \tag{18}$$

Since $(w^*,u^*) \ge 0$ and $(w(\mu,v),u(\mu,v)) > 0$, it follows from (18) that for all i,

$$w_i(\mu,v) \;\ge\; \frac{w_i^*}{2C+n}, \qquad u_i(\mu,v) \;\ge\; \frac{u_i^*}{2C+n}. \tag{19}$$

It immediately implies that the ith entry of any accumulation point $w^\diamond$ of $w(\mu,v)$ as $(\mu,v) \xrightarrow[\Xi_C]{} (0,0)$ must be positive whenever $w_i^* > 0$, which together with $\mathcal{M}(w^*) \succ 0$ further yields $\mathcal{M}(w^\diamond) \succ 0$. Hence, $\phi_{\mathcal{M}}$ is continuous at $w^\diamond$. Using this result and part (a), we see that $\phi_{\mathcal{M}}(w^\diamond) = f^*$ and hence, $w^\diamond$ is an optimal solution of (1), which together with the definition of w^* and the result that $w_i^\diamond > 0$ whenever $w_i^* > 0$ implies that part (b) holds.

Finally, we show that part (c) holds. By assumption, (w^*,u^*) is a solution of (12) with $|\mathcal{B}|+|\mathcal{N}| = n$. Notice from the third equation of (12) that $\mathcal{B} \cap \mathcal{N} = \emptyset$. Thus, $\mathcal{B}$ and $\mathcal{N}$ form a partition for $\{1,\ldots,n\}$. We first show that when $(\mu,v) \in \Xi_C$ and μ is sufficiently small,

$$\begin{array}{ll} w_{\mathcal{N}}(\mu,v) = O(\mu), & w_i(\mu,v) = \Theta(1),\ i \in \mathcal{B}, \\ u_{\mathcal{B}}(\mu,v) = O(\mu), & u_i(\mu,v) = \Theta(1),\ i \in \mathcal{N}. \end{array} \tag{20}$$

Since $w^*_{\mathcal{B}} > 0$ and $u^*_{\mathcal{N}} > 0$, it follows from (17) that $w_{\mathcal{N}}(\mu,v) = O(\mu)$ and $u_{\mathcal{B}}(\mu,v) = O(\mu)$ for all $(\mu,v) \in \Xi_C$. In addition, in view of (19) and the fact that $w(\mu,v) \in \Omega$, one can immediately see that $w_i(\mu,v) = \Theta(1)$ for all $i \in \mathcal{B}$ and $(\mu,v) \in \Xi_C$. We now show that when $(\mu,v) \in \Xi_C$ and μ is sufficiently small, $u_i(\mu,v) = \Theta(1)$ for all $i \in \mathcal{N}$. Indeed, using the first equation of (14), we obtain that

$$P^T \nabla\phi_{\mathcal{M}}(w(\mu,v)) - (P^T)_{\mathcal{B}}\ u_{\mathcal{B}}(\mu,v) - (P^T)_{\mathcal{N}}\ u_{\mathcal{N}}(\mu,v) = v.$$

Since $w^* \in \Omega$, we know that $|\mathcal{B}| \ge 1$, which together with the definition of P implies that $(P^T)_{\mathcal{N}}$ has full column rank. It then follows from the above equation that

$$u_{\mathcal{N}}(\mu,v) = \left([(P^T)_{\mathcal{N}}]^T (P^T)_{\mathcal{N}}\right)^{-1} [(P^T)_{\mathcal{N}}]^T \left(P^T\nabla\phi_{\mathcal{M}}(w(\mu,v)) - (P^T)_{\mathcal{B}}\ u_{\mathcal{B}}(\mu,v) - v\right). \tag{21}$$

Recall from above that $w_i(\mu,v) = \Theta(1)$ for all $i \in \mathcal{B}$ and $(\mu,v) \in \Xi_C$. Using this result and the fact that $w(\mu,v) \in \Omega$ and $\mathcal{M}(w^*) \succ 0$, it is not hard to see that $\{\mathcal{M}(w(\mu,v)) : (\mu,v) \in \Xi_C\}$ is included in a compact set in $\mathcal{S}^m_{++}$. Hence, $P^T\nabla\phi_{\mathcal{M}}(w(\mu,v))$ is bounded for all $(\mu,v) \in \Xi_C$. Further, in view of (19), (21) and the result that $u_{\mathcal{B}}(\mu,v) = O(\mu)$ for all $(\mu,v) \in \Xi_C$, we easily see that $u_i(\mu,v) = \Theta(1)$ for all $i \in \mathcal{N}$ when $(\mu,v) \in \Xi_C$ and μ is sufficiently small.

For all $(\mu,v) \in \Re_{++} \times \Re^{n-1}$, let

$$w^+(\mu,v) := \left(w_{\mathcal{B}}(\mu,v), \frac{1}{\mu} w_{\mathcal{N}}(\mu,v)\right), \qquad u^+(\mu,v) := \left(\frac{1}{\mu} u_{\mathcal{B}}(\mu,v), u_{\mathcal{N}}(\mu,v)\right), \tag{22}$$

$$I_1(\mu) = \begin{pmatrix} I & 0 \\ 0 & \mu I \end{pmatrix}, \qquad I_2(\mu) = \begin{pmatrix} \mu I & 0 \\ 0 & I \end{pmatrix}.$$

Then it follows from (14) that $(w^+(\mu,v), u^+(\mu,v))$ is the unique solution of

$$F(w,u,\mu,v) := \begin{pmatrix} P^T(\nabla\phi_{\mathcal{M}}(I_1(\mu)w) - I_2(\mu)u) - v \\ e^T(I_1(\mu)w) - 1 \\ u \circ w - e \end{pmatrix} = 0, \qquad (w,u) > 0 \tag{23}$$

for all $(\mu,v) \in \Re_{++} \times \Re^{n-1}$. In view of (20), we know that when $(\mu,v) \in \Xi_C$ and μ is sufficiently small,

$$\begin{array}{ll} w^+_{\mathcal{N}}(\mu,v) = O(1), & w^+_i(\mu,v) = \Theta(1), \ i \in \mathcal{B}, \\ u^+_{\mathcal{B}}(\mu,v) = O(1), & u^+_i(\mu,v) = \Theta(1), \ i \in \mathcal{N}. \end{array}$$

Thus, $(w^+(\mu,v), u^+(\mu,v))$ has accumulation points as $(\mu,v) \xrightarrow[\Xi_C]{} (0,0)$. Let $(w^\diamond, u^\diamond)$ be one such accumulation point. Clearly, $(w^\diamond, u^\diamond) > 0$ due to the third equation and the inequality in (23). We will show below that $(w^+(\mu,v), u^+(\mu,v)) \to (w^\diamond, u^\diamond)$ as $(\mu,v) \to (0_+, 0)$.

First, it is easy to see that $(w^\diamond, u^\diamond, 0, 0)$ satisfies (23). Since $\mathcal{M}(w^*) \succ 0$ and $w^\diamond > 0$, it is not hard to verify $\mathcal{M}(I_1(0)w^\diamond) \succ 0$. Using this result and Assumption 1, we observe that F is continuously differentiable in a neighborhood of $(w^\diamond, u^\diamond, 0, 0)$. The Jacobian matrix of F with respect to (w,u) at $(w^\diamond, u^\diamond, 0, 0)$ is given by

$$J := \begin{pmatrix} P^T\nabla^2\phi_{\mathcal{M}}(I_1(0)w^\diamond)I_1(0) & -P^T I_2(0) \\ e^T I_1(0) & 0 \\ \mathscr{D}(u^\diamond) & \mathscr{D}(w^\diamond) \end{pmatrix}.$$

We next show that the Jacobian matrix J is nonsingular. It suffices to show that the linear system $J\begin{pmatrix} \Delta w \\ \Delta u \end{pmatrix} = 0$, or equivalently,

$$\begin{aligned} P^T\nabla^2\phi_{\mathcal{M}}(I_1(0)w^\diamond)I_1(0)\Delta w - P^T I_2(0)\Delta u &= 0, \\ e^T(I_1(0)\Delta w) &= 0, \\ u^\diamond \circ \Delta w + w^\diamond \circ \Delta u &= 0, \end{aligned} \tag{24}$$

has only zero solution. Indeed, we observe that the null space of P^T is spanned by e. It then follows from the first equation of (24) that

$$\nabla^2\phi_{\mathcal{M}}(I_1(0)w^\diamond)I_1(0)\Delta w - I_2(0)\Delta u = \lambda e, \tag{25}$$

for some $\lambda \in \Re$. Multiplying both sides of (25) by $(I_1(0)\Delta w)^T$ and making use of the second equation of (24) and the fact $I_1(0)I_2(0) = 0$, we arrive at

$$\Delta w^T I_1(0)\nabla^2\phi_{\mathcal{M}}(I_1(0)w^\diamond)I_1(0)\Delta w = 0,$$

which is equivalent to

$$\Delta w_{\mathcal{B}}^T[\nabla^2\phi_{\mathcal{M}}(I_1(0)w^\diamond)]_{\mathcal{B}\mathcal{B}}\Delta w_{\mathcal{B}} = 0.$$

This together with the assumption implies that $\Delta w_{\mathcal{B}} = 0$. Using this result, the third equation of (24) and the fact $w^\diamond > 0$, we see that $\Delta u_{\mathcal{B}} = 0$. Substituting $\Delta w_{\mathcal{B}} = 0$ into (25), we obtain that $-I_2(0)\Delta u = \lambda e$, which together with the definition of $I_2(0)$ and $|\mathcal{B}| \geq 1$ implies $\lambda = 0$ and hence $\Delta u_{\mathcal{N}} = 0$. Using this result, the third equation of (24) and the fact $u^\diamond > 0$, we see that $\Delta w_{\mathcal{N}} = 0$. Thus, we have shown that $\Delta w = \Delta u = 0$. Hence, the Jacobian matrix J is nonsingular.

By applying the implicit function theorem to (23), we conclude that there exists $\epsilon > 0$, a neighborhood $\mathcal{U}$ of 0 and a continuously differentiable function $(w^\ddagger(\mu, v), u^\ddagger(\mu, v))$ defined on $(-\epsilon, \epsilon) \times \mathcal{U}$ such that

$$\begin{aligned}&F(w^\ddagger(\mu, v), u^\ddagger(\mu, v), \mu, v) = 0, \quad (w^\ddagger(\mu, v), u^\ddagger(\mu, v)) > 0 \quad \forall (\mu, v) \in (-\epsilon, \epsilon) \times \mathcal{U}, \\ &\lim_{(\mu,v)\to 0} (w^\ddagger(\mu, v), u^\ddagger(\mu, v)) = (w^\diamond, u^\diamond).\end{aligned}$$

Recall that system (23) has a unique solution $(w^+(\mu, v), u^+(\mu, v))$ for all $(\mu, v) \in \Re_{++} \times \Re^{n-1}$. Therefore, $(w^+(\mu, v), u^+(\mu, v)) = (w^\ddagger(\mu, v), u^\ddagger(\mu, v))$ for all $(\mu, v) \in (0, \epsilon) \times \mathcal{U}$. It then follows that

$$\lim_{(\mu,v)\to(0_+,0)} (w^+(\mu, v), u^+(\mu, v)) = (w^\diamond, u^\diamond).$$

Using this equality and (22), we finally conclude that

$$\begin{aligned}\lim_{(\mu,v)\to(0_+,0)} w_{\mathcal{B}}(\mu, v) &= \lim_{(\mu,v)\to(0_+,0)} w^+_{\mathcal{B}}(\mu, v) = w^\diamond_{\mathcal{B}} > 0, \\ \lim_{(\mu,v)\to(0_+,0)} w_{\mathcal{N}}(\mu, v) &= \lim_{(\mu,v)\to(0_+,0)} \mu w^+_{\mathcal{N}}(\mu, v) = 0.\end{aligned}$$

From part (b), we further see that $(w^\diamond_{\mathcal{B}}, 0)$ is an optimal solution of (1) with maximum cardinality. This proves part (c) of the theorem. ■

As an immediate consequence of Theorem 3.3, we now state a global convergence result regarding the outer iterations of our primal IP method.

Corollary 3.4. *Let $\{\mu_k\}$ and $\{\tilde{w}^k\}$ be the sequences generated in the primal IP method. Let $w^k = P\tilde{w}^k + q$ for all k. Then the following statements hold:*

(a) $\lim_{k\to\infty} \phi(\mathcal{M}(w^k)) = f^*$.

(b) *Suppose that problem (1) has an optimal solution and $\epsilon(\mu_k) = O(\mu_k)$. Then any accumulation point of $\{w^k\}$ is an optimal solution of (1) with maximum cardinality.*

(c) *Suppose that problem (1) has an optimal solution w^*. Let u^* be the associated Lagrange multiplier satisfying (12). Assume that $|\mathcal{B}| + |\mathcal{N}| = n$, where $\mathcal{B} := \{i : w^*_i > 0\}$ and $\mathcal{N} := \{i : u^*_i > 0\}$. Suppose further that $[\nabla^2 \phi_{\mathcal{M}}(w)]_{\mathcal{B}\mathcal{B}} \succ 0$ for any $w \in \Omega$ satisfying $w_{\mathcal{B}} > 0$ and $w_{\mathcal{N}} = 0$. Then $\{w^k\}$ converges to an optimal solution of (1) with maximum cardinality.*

Proof. Let $v^k = \nabla f_{\mu_k}(\tilde{w}^k)$ and $u^k = \mu_k (w^k)^{-1}$ for all k. In view of (13) and (14), we can observe that (w^k, u^k, μ_k, v^k) satisfies (14). By virtue of the definition of $(w(\mu, v), u(\mu, v))$, we then have $(w^k, u^k) = (w(\mu_k, v^k), u(\mu_k, v^k))$, which together with the fact $\mu_k \to 0$ and Theorem 3.3 implies the conclusion holds. ■

Before ending this section, we now establish a convergence result regarding the inner iterations of our primal IP method.

Proposition 3.5. *Let $\mu_k > 0$ and $\epsilon(\mu_k) > 0$ be given. Then the Newton's method detailed in step 2 of the primal IP method starting from any strictly feasible point $\tilde{w}^{\rm init}$ of (9) generates a point $\tilde{w}^k$ satisfying $\|\nabla f_{\mu_k}(\tilde{w}^k)\| \le \epsilon(\mu_k)$ within a finite number of iterations.*

Proof. It is easy to observe that all iterates generated by the Newton's method lie in the compact level set $\Upsilon := \{\tilde{w} : \ f_{\mu_k}(\tilde{w}) \le f_{\mu_k}(\tilde{w}^{\rm init})\}$. Clearly, $\tilde{w} > 0$ for all $\tilde{w} \in \Upsilon$. This together with the assumption that problem (9) has a feasible point implies that $\mathcal{M}(\Upsilon) \subset \mathcal{S}^m_{++}$. Thus ∇f_{μ_k} and $\nabla^2 f_{\mu_k}$ are continuous in Υ. Using this observation and the strong convexity of f_{μ_k} in Υ, there exist $\underline{\lambda}$, $\overline{\lambda} > 0$ such that $\underline{\lambda} I \preceq \nabla^2 f_{\mu_k}(\tilde{w}) \preceq \overline{\lambda} I$ for all $\tilde{w} \in \Upsilon$. This relation along with the continuity of ∇f_{μ_k} and $\nabla^2 f_{\mu_k}$ implies that $d = -(\nabla^2 f_{\mu_k}(\tilde{w}))^{-1}\nabla f_{\mu_k}(\tilde{w})$ is continuous in Υ. In view of this result and the definition of $\bar{\alpha}(\tilde{w})$, it is not hard to show that $\bar{\alpha}(\tilde{w})$ is positive and continuous in Υ. This fact together with the compactness of Υ yields $\underline{\alpha} := \inf\{\bar{\alpha}(\tilde{w}) : \ \tilde{w} \in \Upsilon\} > 0$. Thus, all iterates $\tilde{w}$ generated by the Newton's method satisfy $\underline{\lambda} I \preceq \nabla^2 f_{\mu_k}(\tilde{w}) \preceq \overline{\lambda} I$ and $\bar{\alpha}(\tilde{w}) \in [\underline{\alpha}, 1]$. The remaining proof follows the same arguments as in the proof of [12, Theorem 3.13]. ∎

4 IP methods for classical optimality criteria

In this section, we discuss IP methods for solving problem (1) with A-, D-, E- and pth mean criterion. In particular, we apply the primal IP method proposed in Section 3 to solve (1) with pth mean criterion. In addition, we reformulate problem (1) with A-, D- and E-criterion into linear or log-determinant SDPs which can be solved by standard primal-dual IP solvers such as SDPT3 [21, 25].

4.1 IP method for pth mean criterion

Recall from Section 1 that pth mean criterion ϕ is given by

$$\phi(X) = \mathrm{tr}((K^T X^{-1} K)^{-p}) \tag{26}$$

for some $K \in \Re^{m\times k}$ and $p < 0$. As discussed in Section 3, such ϕ either satisfies Assumption 1 or can be arbitrarily approximated by a function which satisfies that assumption. Thus problem (1) with this criterion can be suitably solved by our primal IP method proposed in Section 3. For convenience of presentation, we assume throughout this subsection that K has full column rank and hence ϕ is twice continuously differentiable in $\mathcal{S}^m_{++}$.

We now discuss applying our primal IP method to solve problem (1) for the above ϕ. Clearly, the main computational parts of this method lie in computing the gradient and Hessian of f_μ defined in (11), which can be reduced to evaluate those of ϕ. We next derive the gradient and Hessian of ϕ that is defined in (26) by using a result about the derivative of matrix-valued functions established in [5, Proposition 4.3(a)]. For convenience of reference, we state this result as follows.

Lemma 4.1. *Let $g : \Re \to \Re$ be a differentiable function and let $g^{\square} : \mathcal{S}^m \to \mathcal{S}^m$ be defined by*

$$g^{\square}(Y) := V \begin{pmatrix} g(d_1) & & & \\ & g(d_2) & & \\ & & \ddots & \\ & & & g(d_m) \end{pmatrix} V^T,$$

where $V\mathscr{D}(d)V^T$ is an eigenvalue decomposition of Y for some $d \in \Re^m$. Then the function $g^\square$ is well-defined, i.e., it is independent of the choice of V and d, and is also differentiable. Moreover, let $S^{g,d} \in \mathcal{S}^m$ be a symmetric matrix whose (i,j)th entry is given by

$$s_{ij}^{g,d} := \begin{cases} \dfrac{g(d_i) - g(d_j)}{d_i - d_j} & \text{if } d_i \neq d_j, \\ g'(d_i) & \text{otherwise.} \end{cases} \tag{27}$$

Then the directional derivative of $g^\square$ at Y along the direction $H \in \mathcal{S}^m$ is given by

$$V(S^{g,d} \circ (V^T H V))V^T. \tag{28}$$

Proposition 4.2. *Let ϕ be defined in (26). Suppose that K has full column rank. Then ϕ is twice continuously differentiable in $\mathcal{S}^m_{++}$, and its gradient and Hessian at any $X \in \mathcal{S}^m_{++}$ are given by*

$$\nabla\phi(X) = pX^{-1}K(K^TX^{-1}K)^{-p-1}K^TX^{-1}, \tag{29}$$

$$\begin{aligned}\nabla^2\phi(X) = &-p[(X^{-1}KV)\otimes(X^{-1}KV)]\mathscr{D}(\mathrm{vec}(S^{g,d}))[(X^{-1}KV)\otimes(X^{-1}KV)]^T \\ &- p\; X^{-1}\otimes G - p\; G\otimes X^{-1},\end{aligned} \tag{30}$$

respectively, where $V\mathscr{D}(d)V^T$ is an eigenvalue decomposition of $K^TX^{-1}K$ for some $d \in \Re^m$, $g(t) = t^{-p-1}$ and $G = X^{-1}K[K^TX^{-1}K]^{-p-1}K^TX^{-1}$. In particular, when $K = I$, the above gradient and Hessian reduce to

$$\nabla\phi(X) = pX^{p-1}, \tag{31}$$

$$\nabla^2\phi(X) = (V\otimes V)\mathscr{D}(\mathrm{vec}(S^{g,d}))(V\otimes V)^T, \tag{32}$$

where $g(t) = pt^{p-1}$ and $V\mathscr{D}(d)V^T$ is an eigenvalue decomposition of X for some $d \in \Re^m$.

Proof. By the assumption that K has full column rank, we evidently see that ϕ is twice continuously differentiable in $\mathcal{S}^m_{++}$. To derive the gradient of ϕ, we fix an arbitrary $X \in \mathcal{S}^m_{++}$. For all sufficiently small $H \in \mathcal{S}^m$, we then have $X + H \succ 0$ and moreover,

$$(X+H)^{-1} = X^{-1} - X^{-1}HX^{-1} + o(H). \tag{33}$$

Using (33) and Lemma 4.1 with $g(t) = t^{-p}$ and $Y = K^TX^{-1}K$, we obtain that

$$\begin{aligned}\phi(X+H) &= \mathrm{tr}((K^T[X+H]^{-1}K)^{-p}) = \mathrm{tr}((K^TX^{-1}K - K^TX^{-1}HX^{-1}K + o(H))^{-p}) \\ &= \phi(X) - \mathrm{tr}(V(S^{g,d}\circ(V^TK^TX^{-1}HX^{-1}KV))V^T) + o(H),\end{aligned} \tag{34}$$

where $V\mathscr{D}(d)V^T$ is an eigenvalue decomposition of Y. Letting $R := -K^TX^{-1}HX^{-1}K$ and using the fact that $V^TV = I$ and $s_{ii}^{g,d} = -pd_i^{-p-1}$ for all i, we further have

$$\begin{aligned}\mathrm{tr}(V(S^{g,d}\circ(V^TRV))V^T) = \mathrm{tr}(S^{g,d}\circ(V^TRV)) &= \sum_{i=1}^m s_{ii}^{g,d}\sum_{j,k} v_{ji}r_{jk}v_{ki} \\ &= -p\sum_{j,k}\left(\sum_{i=1}^m v_{ji}d_i^{-p-1}v_{ki}\right)r_{jk} \\ &= -\mathrm{tr}(p(K^TX^{-1}K)^{-p-1}R) \\ &= \mathrm{tr}(pX^{-1}K(K^TX^{-1}K)^{-p-1}K^TX^{-1}H).\end{aligned} \tag{35}$$

Combining (34) and (35), we see that (29) holds. In the case when $K = I$, it immediately follows from (29) that (31) also holds.

We next derive the matrix representation of the Hessian of ϕ at any $X \in \mathcal{S}^m_{++}$. To proceed, we first recall the following well-known results (see, for example, page 243 and Lemma 4.3.1 of [11]):

$$\mathrm{vec}(ABC) = (C^T \otimes A)\mathrm{vec}(B), \qquad (A \otimes B)^T = A^T \otimes B^T. \tag{36}$$

Consider any sufficiently small $H \in \mathcal{S}^m$ such that $X + H \succ 0$. Using (33) and Lemma 4.1 with $g(t) = t^{-p-1}$ and $Y = K^T X^{-1} K$, we have

$$\begin{aligned}
\nabla\phi(X+H) &= p(X+H)^{-1}K[K^T(X+H)^{-1}K]^{-p-1}K^T(X+H)^{-1} \\
&= p(X^{-1} - X^{-1}HX^{-1})K[K^TX^{-1}K - K^TX^{-1}HX^{-1}K]^{-p-1}K^T(X^{-1} - X^{-1}HX^{-1}) + o(H) \\
&= \nabla\phi(X) - p(X^{-1}K)V(S^{g,d} \circ (V^TK^TX^{-1}HX^{-1}KV))V^T(K^TX^{-1}) \\
&\quad - pGHX^{-1} - pX^{-1}HG + o(H),
\end{aligned} \tag{37}$$

where G is defined as above. Since X is symmetric, it follows from (36) that

$$\begin{aligned}
&\mathrm{vec}((X^{-1}KV)(S^{g,d} \circ (V^TK^TX^{-1}HX^{-1}KV))(V^TK^TX^{-1})) \\
&= [(X^{-1}KV) \otimes (X^{-1}KV)]\mathrm{vec}(S^{g,d} \circ (V^TK^TX^{-1}HX^{-1}KV)) \\
&= [(X^{-1}KV) \otimes (X^{-1}KV)]\mathscr{D}(\mathrm{vec}(S^{g,d}))\mathrm{vec}(V^TK^TX^{-1}HX^{-1}KV)) \\
&= [(X^{-1}KV) \otimes (X^{-1}KV)]\mathscr{D}(\mathrm{vec}(S^{g,d}))[(X^{-1}KV) \otimes (X^{-1}KV)]^T\mathrm{vec}(H).
\end{aligned} \tag{38}$$

In addition, since G is symmetric, we further have that

$$\mathrm{vec}(GHX^{-1} + X^{-1}HG) = \left[X^{-1} \otimes G + G \otimes X^{-1}\right]\mathrm{vec}(H). \tag{39}$$

In view of (37)-(39), we see that the matrix representation of the Hessian of ϕ is given in (30).

For the case when $K = I$, one can obtain (32) by simplifying (30). Indeed, in this case, let VDV^T be the eigenvalue decomposition of X^{-1}. Then $X^{-1}V = VD$ and the matrix G defined above becomes X^{p-1}. It then follows from (30) that

$$\nabla^2\phi(X) = -p[(VD) \otimes (VD)]\mathscr{D}(\mathrm{vec}(S^{g,d}))[(VD) \otimes (VD)]^T - pX^{-1} \otimes X^{p-1} - pX^{p-1} \otimes X^{-1}, \tag{40}$$

where $g(t) = t^{-p-1}$. Using the well-know result $(AB) \otimes (CE) = (A \otimes C)(B \otimes E)$(see, for example, [11, Lemma 4.2.10]) and (36), we obtain that

$$\begin{aligned}
[(VD) \otimes (VD)]\mathscr{D}(\mathrm{vec}(S^{g,d}))[(VD) \otimes (VD)]^T &= (V \otimes V)[D \otimes D]\mathscr{D}(\mathrm{vec}(S^{g,d}))[D \otimes D](V \otimes V)^T, \\
X^{-1} \otimes X^{p-1} + X^{p-1} \otimes X^{-1} &= [VDV^T \otimes VD^{1-p}V^T] + [VD^{1-p}V^T \otimes VDV^T] \\
&= (V \otimes V)[D \otimes D^{1-p} + D^{1-p} \otimes D](V \otimes V)^T,
\end{aligned}$$

which together with (40) implies that

$$\nabla^2\phi(X) = (V \otimes V)\mathfrak{D}(V \otimes V)^T,$$

where

$$\mathfrak{D} = -p\left([D \otimes D]\mathscr{D}(\mathrm{vec}(S^{g,d}))[D \otimes D] + [D \otimes D^{1-p} + D^{1-p} \otimes D]\right).$$

Clearly, $\mathfrak{D}$ is a diagonal matrix. Letting $\lambda = d^{-1} \in \Re^m$ and using (27) with $g(t) = t^{-p-1}$ and $Y = X^{-1}$, it is not hard to show that the $(m(k-1)+l)$th diagonal entry of $\mathfrak{D}$ equals

$$-p\left(\lambda_k^{-1}\lambda_l^{p-1} + \lambda_k^{p-1}\lambda_l^{-1} + \frac{\lambda_k^{p+1} - \lambda_l^{p+1}}{\lambda_k^{-1} - \lambda_l^{-1}}\frac{1}{\lambda_k^2\lambda_l^2}\right) = p\frac{\lambda_k^{p-1} - \lambda_l^{p-1}}{\lambda_k - \lambda_l}$$

if $\lambda_k \neq \lambda_l$; otherwise, it equals

$$-p\left(\lambda_k^{p-2} + \lambda_k^{p-2} - (p+1)\lambda_k^{p+2}\frac{1}{\lambda_k^4}\right) = p(p-1)\lambda_k^{p-2}.$$

Notice that $V\mathscr{D}(\lambda)V^T$ is an eigenvalue decomposition of X and also $\mathfrak{D} = \mathscr{D}(\mathrm{vec}(S^{g,\lambda}))$ with $g(t) = pt^{p-1}$. Thus (32) holds. ∎

Remark. Alternatively, the Hessian of ϕ for the case when $K = I$ can be directly derived as follows. We know from (31) that $\nabla\phi(X) = pX^{p-1}$. Letting $g(t) = pt^{p-1}$ and $V\mathscr{D}(d)V^T$ be an eigenvalue decomposition of X, it follows from Lemma 4.1 that

$$\nabla\phi(X+H) = \nabla\phi(X) + V(S^{g,d} \circ (V^THV))V^T + o(H). \tag{41}$$

In view of (36), one can see that

$$\begin{aligned} \mathrm{vec}(V(S^{g,d} \circ (V^THV))V^T) &= (V \otimes V)\mathrm{vec}(S^{g,d} \circ (V^THV)) \\ &= (V \otimes V)[\mathrm{vec}(S^{g,d}) \circ \mathrm{vec}(V^THV)] \\ &= (V \otimes V)(\mathrm{vec}(S^{g,d}) \circ [(V \otimes V)^T\mathrm{vec}(H)]) \\ &= (V \otimes V)\mathscr{D}(\mathrm{vec}(S^{g,d}))(V \otimes V)^T\mathrm{vec}(H), \end{aligned} \tag{42}$$

which together with (41) immediately leads to (32). ∎

Finally we are ready to compute the gradient and Hessian of f_μ at any strictly feasible point $\tilde{w}$ of (9). Let M be the matrix representation of the linear mapping $\mathcal{M}$. By the chain rule, it follows immediately that

$$\begin{aligned} \nabla f_\mu(\tilde{w}) &= P^TM^T\nabla\phi(\mathcal{M}(w)) - \mu P^Tw^{-1}, \\ \nabla^2 f_\mu(\tilde{w}) &= P^TM^T\nabla^2\phi(\mathcal{M}(w))MP + \mu P^T\mathscr{D}(w^{-1} \circ w^{-1})P, \end{aligned}$$

where $w = P\tilde{w} + q$, and $\nabla\phi$ and $\nabla^2\phi$ are given in Proposition 4.2.

4.2 IP method for A-criterion

Recall from Section 1 that problem (1) with A-criterion becomes:

$$\begin{array}{ll} \min & \mathrm{tr}(K^T\mathcal{M}(w)^{-1}K) \\ \text{s.t.} & e^Tw = 1, w \geq 0, \mathcal{M}(w) \succ 0 \end{array} \tag{43}$$

for some $K \in \Re^{m\times k}$. Since A-criterion is a special case of pth mean criterion, the primal IP method discussed in Sections 3 and 4.1 can be suitably applied to solve problem (43). Alternatively, by exploiting the special structure of this problem, we will reformulate it into a linear SDP, which can be efficiently solved by standard primal-dual IP solvers such as SeDuMi [19] and SDPT3 [21, 25].

Notice that $\mathrm{tr}(\cdot)$ is an increasing function. It then follows that (43) is equivalent to

$$\begin{array}{ll} \min & \mathrm{tr}(U) \\ \mathrm{s.t.} & U \succeq K^T \mathcal{M}(w)^{-1} K, \\ & e^T w = 1, w \geq 0, \mathcal{M}(w) \succ 0. \end{array} \tag{44}$$

Since $\mathcal{M}(w) \succ 0$, we see from Lemma 3.1 that $U \succeq K^T \mathcal{M}(w)^{-1} K$ is equivalent to

$$\begin{pmatrix} U & K^T \\ K & \mathcal{M}(w) \end{pmatrix} \succeq 0.$$

In addition, we know from assumption that the feasible set of (43) (or equivalently, (44)) is nonempty. Thus, the closure of the feasible set of (44) is given by

$$\left\{ (U, w) : \begin{pmatrix} U & K^T \\ K & \mathcal{M}(w) \end{pmatrix} \succeq 0, e^T w = 1, w \geq 0 \right\}.$$

Since $\mathrm{tr}(\cdot)$ is a continuous function, it follows that problem (44) (or equivalently, (43)) has the same optimal value as the following linear SDP problem:

$$\begin{array}{ll} \min & \mathrm{tr}(U) \\ \mathrm{s.t.} & \begin{pmatrix} U & K^T \\ K & \mathcal{M}(w) \end{pmatrix} \succeq 0, \\ & e^T w = 1, w \geq 0, \end{array} \tag{45}$$

which can be efficiently solved by standard primal-dual IP solvers such as SeDuMi and SDPT3.

4.3 IP method for D-criterion

As mentioned in Section 1, problem (1) with D-criterion is as follows:

$$\begin{array}{ll} \min & \log\det(K^T \mathcal{M}(w)^{-1} K) \\ \mathrm{s.t.} & e^T w = 1, w \geq 0, \mathcal{M}(w) \succ 0 \end{array} \tag{46}$$

for some $K \in \Re^{m \times k}$ with full column rank. As discussed in Section 3, problem (46) can be suitably solved by the primal IP method. Alternatively, we will reformulate (46) as a log-determinant SDP, which can be efficiently solved by standard primal-dual IP solvers such as SDPT3.

In view of (7), problem (46) can be equivalently written as

$$\begin{array}{ll} \min & -2\log\det(U) \\ \mathrm{s.t.} & \begin{pmatrix} I & (KU)^T \\ KU & \mathcal{M}(w) \end{pmatrix} \succeq 0, \\ & \mathcal{M}(w) \succ 0, \\ & e^T w = 1, w \geq 0. \end{array} \tag{47}$$

Moreover, we know from assumption that the feasible set of (46) (or equivalently, (47)) is nonempty. Thus, the closure of the feasible set of (47) is given by

$$\left\{(U,w):\begin{pmatrix} I & (KU)^T \\ KU & \mathcal{M}(w)\end{pmatrix}\succeq 0, e^Tw=1, w\geq 0\right\}.$$

Since the intersection of the domain of the objective function and the feasible set of (47) is nonempty, it follows that problem (47) (or equivalently, (46)) has the same optimal value as the following log-determinant SDP problem:

$$\begin{array}{ll} \min & -2\log\det(U) \\ \text{s.t.} & \begin{pmatrix} I & (KU)^T \\ KU & \mathcal{M}(w)\end{pmatrix}\succeq 0, \\ & e^Tw=1, w\geq 0, \end{array} \tag{48}$$

which can be efficiently solved by standard primal-dual IP solvers such as SDPT3.

4.4 IP method for E-criterion

As seen from Section 1, problem (1) with E-criterion is as follows:

$$\begin{array}{ll} \min & \lambda_{\max}(K^T\mathcal{M}(w)^{-1}K) \\ \text{s.t.} & e^Tw=1, w\geq 0, \mathcal{M}(w)\succ 0, \end{array} \tag{49}$$

for some $K\in\Re^{m\times k}$ with full column rank. As discussed in Section 3, problem (49) can be approximately solved by the primal IP method. Alternatively, we will reformulate (49) as a linear SDP, which can be efficiently solved by standard primal-dual IP solvers such as SeDuMi and SDPT3.

In view of (8), problem (49) is equivalent to

$$\begin{array}{ll} \min & t \\ \text{s.t.} & \begin{pmatrix} tI & K^T \\ K & \mathcal{M}(w)\end{pmatrix}\succeq 0, \\ & e^Tw=1, w\geq 0, \mathcal{M}(w)\succ 0. \end{array} \tag{50}$$

Moreover, we know from assumption that the feasible set of (49) (or equivalently, (50)) is nonempty. Thus, the closure of the feasible set of (50) is given by

$$\left\{(t,w):\begin{pmatrix} tI & K^T \\ K & \mathcal{M}(w)\end{pmatrix}\succeq 0, e^Tw=1, w\geq 0\right\}.$$

Since the objective function of (50) is continuous, it follows that problem (50) (or equivalently, (49)) has the same optimal value as the following linear SDP problem:

$$\begin{array}{ll} \min & t \\ \text{s.t.} & \begin{pmatrix} tI & K^T \\ K & \mathcal{M}(w)\end{pmatrix}\succeq 0, \\ & e^Tw=1, w\geq 0, \end{array} \tag{51}$$

which can be efficiently solved by standard primal-dual IP solvers such as SeDuMi and SDPT3.

5 Computational results

In this section, we conduct numerical experiments to test the performance of the IP methods discussed in this paper for solving problem (1) with A-, D-, E- and pth mean criterion and also compare their performance with the multiplicative algorithm on both simulated and real data.

For problem (1) with A-, D- and E-criterion, we solve their SDP reformulations (45), (48) and (51), respectively, by calling the primal-dual IP solver SDPT3 (version 4.0) [21, 25], whose basic code is written in Matlab and key subroutines are written in C. In addition, we develop a Matlab code for our primal IP method to solve (1) with pth mean criterion. Also, we implement the multiplicative algorithm in Matlab for solving (1) with A-, D- and pth mean criterion. All computations in this section are performed in Matlab version 7.7.0 (R2008b) on a Windows machine with 1.73GHz dual-core CPU and 2GB RAM.

We now address initialization and termination for the aforementioned methods. In particular, for the primal-dual IP solver SDPT3, we use the default settings. For our primal IP method, we set $\tilde{w}^0 = \frac{1}{n}e \in \Re^{n-1}$, $\mu_1 = 10$, $\beta = 0.5$, $\sigma = \gamma = 0.1$ and $\eta = 0.95$. In addition, we set

$$\epsilon(\mu) := \begin{cases} \mu & \text{if } \mu \geq 10^{-6}, \\ 10^{-6} & \text{if } \mu < 10^{-6}, \end{cases}$$

and terminate the algorithm once $\mu_k \leq 10^{-8}$. Similarly as in [28], for the multiplicative algorithm, we set $\lambda = 1$, $w^0 = \frac{1}{n}e \in \Re^n$, and terminate the algorithm when it reaches $10,000$ iterations or

$$\max_{1 \leq i \leq n} d_i(w^k) \leq (1+\delta) \sum_{i=1}^{n} w_i^k d_i(w^k)$$

holds with $\delta = 10^{-4}$, where $d_i(w)$ is defined in (2).

5.1 Computational results on simulated data

We randomly generate the data for problem (1). In particular, we generate n vectors $x_i \in \Re^m$, with each entry uniformly chosen from $[0, 1]$, and set $A_i = x_i x_i^T$ for $i = 1, \ldots, n$. We also generate a $K \in \Re^{m \times k}$ whose entries are chosen uniformly from $[0, 1]$. For convenience of the subsequent reference, we list these instances in Table 1.

Table 1: Sizes of random data

P	n	m	k
1	500	5	5
2	500	10	5
3	1000	5	5
4	1000	10	5

We now apply the aforementioned IP methods to solve problem (1) with A-, D-, E- and pth mean criterion on the above random instances and compare their performance with the multiplicative algorithm. The computational results are reported in Tables 2-4. As mentioned before, the multiplicative algorithm cannot be directly applied to solve (1) with E-criterion. Thus we only report the result by

Table 2: Computational results for A-, D- and E-criterion on random data

	A		D		E
	MUL	IPM	MUL	IPM	IPM
P	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu
1	12.2997/1.8	12.2997/1.0	0.282958/3.6	0.282954/1.2	3.76274/1.3
2	24.1093/5.5	24.1093/1.5	7.12598/3.1	7.12597/1.7	6.02139/1.6
3	8.96395/20.6	8.96395/1.1	-4.15964/3.0	-4.15969/1.3	3.30368/1.4
4	18.2381/18.8	18.2381/2.4	5.80129/15.6	5.80129/2.8	4.44196/2.7

Table 3: Computational results for pth mean criterion on random data with some $p \in (-1, 0)$

	$p = -\frac{1}{4}$		$p = -\frac{1}{2}$		$p = -\frac{3}{4}$	
	MUL	IPM	MUL	IPM	MUL	IPM
P	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu
1	5.6262/10.6	5.6262/3.5	7.04422/4.3	7.04422/3.9	9.20519/5.2	9.20519/4.2
2	7.23559/6.8	7.23559/4.3	10.6817/6.5	10.6817/4.6	15.9771/8.1	15.9771/4.9
3	4.9074/10.4	4.90741/14.7	5.72487/7.3	5.72486/16.5	7.06877/5.0	7.06875/16.4
4	6.76435/12.4	6.76436/19.6	9.31478/16.7	9.31479/21.0	12.9812/15.0	12.9812/20.7

the IP method for this criterion. In each table, we label IP methods and the multiplicative algorithm as "IPM" and "MUL", and abbreviate their objective value and CPU time as "obj" and "cpu", respectively. In addition, we only report the objective values up to six significant digits and the CPU times with one decimal place.

From Table 2, we see that the objective values given by the IP method and the multiplicative algorithm when applied to (1) with A- and D-criterion are comparable, but the former method consistently outperforms the latter one in terms of CPU time. We also observe that the IP method is capable of solving (1) with E-criterion efficiently. In addition, we observe from Table 3 that when applied to (1) with pth mean criterion for $p = -1/4$, $-1/2$ and $-3/4$, the multiplicative algorithm is usually faster than our IP method while they produce comparable objective values. However, for $p = -3/2$, -2 and $-5/2$, our IP method generally achieves much better objective values than the multiplicative algorithm especially when $p = -5/2$ (see Table 4), where the objective value for the latter method is chosen as the smallest one over all iterations. Moreover, our IP method usually substantially outperforms the multiplicative algorithm in terms of CPU time for these p's. This phenomenon is actually not surprising since the multiplicative algorithm is only known to converge for $p \in [-1, 0)$, but it may not converge when $p < -1$.

5.2 Computational results on real models

In this subsection, we consider the following three design spaces:

$$\begin{aligned} \chi_1(n) &= \{x_i = (e^{-s_i}, s_i e^{-s_i}, e^{-2s_i}, s_i e^{-2s_i})^T, 1 \le i \le n\}, \\ \chi_2(n) &= \{x_i = (1, s_i, s_i^2, s_i^3, s_i^4)^T, 1 \le i \le n\}, \\ \chi_3(n) &= \{x_{(i-1)\lfloor\sqrt{n}\rfloor + j} = (1, r_i, r_i^2, t_j, r_i t_j)^T, 1 \le i, j \le \lfloor\sqrt{n}\rfloor\}, \end{aligned} \tag{52}$$

Table 4: Computational results for pth mean criterion on random data with some $p < -1$

	$p = -\frac{3}{2}$		$p = -2$		$p = -\frac{5}{2}$	
	MUL	IPM	MUL	IPM	MUL	IPM
P	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu
1	22.8258/66.2	22.7046/4.7	52.7247/65.8	42.7616/5.5	144.979/65.3	81.1819/5.2
2	55.832/6.7	55.832/5.9	131.998/74.0	131.136/6.1	337.524/67.4	311.029/5.8
3	15.0623/130.8	15.002/22.8	30.3229/128.7	25.7169/21.1	62.4917/129.3	44.8469/22.4
4	36.5731/16.3	36.5731/24.1	75.2237/143.6	74.4299/24.8	171.505/141.4	152.829/26.9

Table 5: Computational results for A-, D- and E-criterion on real data

		A		D		E
		MUL	IPM	MUL	IPM	IPM
P	n	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu
χ_1	500	55304.1/40.3	54834.2/2.9	20.5806/20.5	20.5804/1.7	54208.4/1.9
	1000	54765/81.0	54312.3/3.0	20.5446/41.9	20.5444/2.3	53695.4/2.2
χ_2	500	580.095/42.0	568.963/1.6	1.986/21.3	1.98575/1.7	539.047/1.5
	1000	571.57/82.2	560.824/2.4	1.96597/41.7	1.96575/1.9	531.071/1.9
χ_3	400	24.6971/1.6	24.6971/1.0	5.64128/0.8	5.64115/0.8	8.82936/1.0
	900	23.3277/5.5	23.3277/1.1	5.43046/3.1	5.43033/1.2	8.24605/1.3

where $s_i = \frac{3i}{n}$, $r_i = \frac{2i}{\sqrt{n}} - 1$ and $t_i = \frac{i}{\sqrt{n}}$ for $i = 1, \ldots, n$. The space $\chi_1(n)$ represents the linearization of a compartmental model (see, for example, [1]). The space $\chi_2(n)$ corresponds to polynomial regression. The third space represents a response surface with a nonlinear effect and an interaction as mentioned in [29]. We set $A_i = x_i x_i^T$ for $i = 1, \ldots, n$, and $K = I$ for problem (1).

We now apply the aforementioned IP methods to solve problem (1) with A-, D-, E- and pth mean criterion on the above three design spaces and compare their performance with the multiplicative algorithm. The computational results are reported in Tables 5-7. For the same reason as mentioned earlier, we only report the result by the IP method for E-criterion.

From Table 5, we see that our IP method substantially outperforms the multiplicative algorithm in both objective value and CPU time when applied to (1) with A-criterion on the spaces $\chi_1(n)$ and $\chi_2(n)$, while their performances are comparable on $\chi_3(n)$. When applied to (1) with D-criterion, we observe that the objective values achieved by the IP method and the multiplicative algorithm are comparable, but the former method substantially outperforms the latter one in terms of CPU time. We also see that the IP method is capable of solving (1) with E-criterion efficiently. In addition, we observe from Table 6 that our IP method substantially outperforms the multiplicative algorithm in both objective value and CPU time when applied to (1) with pth mean criterion for $p = -1/4$, $-1/2$ and $-3/4$ on the spaces $\chi_1(n)$ and $\chi_2(n)$, while their performances are comparable on $\chi_3(n)$. Finally, for $p = -3/2$, -2 and $-5/2$, we see from Table 7 that our IP method is significantly superior to the multiplicative algorithm in both objective value and CPU time, where the objective value for the latter method is chosen as the smallest one among all iterations.

Table 6: Computational results for pth mean criterion on real data with some $p \in (-1, 0)$

		$p = -\frac{1}{4}$		$p = -\frac{1}{2}$		$p = -\frac{3}{4}$	
		MUL	IPM	MUL	IPM	MUL	IPM
P	n	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu
χ_1	500	23.4786/32.6	23.4785/3.5	263.204/25.5	263.199/4.3	3685.42/26.4	3685.31/5.2
	1000	23.4226/64.2	23.4223/15.0	261.932/59.5	261.926/18.3	3659/56.7	3658.89/18.5
χ_2	500	9.24086/34.7	9.24072/3.4	30.4681/30.0	30.4672/3.9	125.984/65.2	125.983/4.3
	1000	9.2195/67.4	9.21936/14.8	30.2796/62.9	30.2786/15.9	124.686/129.4	124.684/17.3
χ_3	400	6.89279/2.7	6.8928/2.1	10.1239/2.5	10.1239/2.3	15.5623/2.5	15.5623/2.4
	900	6.81198/7.3	6.81198/10.3	9.86735/8.7	9.86735/12.0	14.9379/8.5	14.9379/11.6

Table 7: Computational results for pth mean criterion on real data with some $p < -1$

		$p = -\frac{3}{2}$		$p = -2$		$p = -\frac{5}{2}$	
		MUL	IPM	MUL	IPM	MUL	IPM
P	n	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu	obj/cpu
χ_1	500	1.31591e7/63.2	1.26361e7/6.2	3.1057e9/63.0	2.93892e9/9.4	7.33052e11/63.0	6.84183e11/22.0
	1000	1.28053e7/121.8	1.24571e7/26.3	2.94453e9/121.9	2.88354e9/45.6	7.15523e11/122.2	6.828e11/82.5
χ_2	500	12951/64.1	12664.5/4.6	294160/64.6	291339/5.8	7.28862e6/63.3	6.75011e6/7.5
	1000	12652.3/125.8	12386.6/20.5	295777/126.0	282807/24.7	7.0093e6/125.4	6.50357e6/31.4
χ_3	400	70.9744/51.8	65.9462/2.7	196.592/50.1	183.612/2.7	593.302/51.3	521.75/2.8
	900	65.7541/111.5	60.2521/11.8	175.187/111.4	162.192/14.1	504.114/111.2	445.485/17.4

6 Concluding remarks

In this paper we study IP methods for solving optimal design problem (1). In particular, we propose a primal IP method for solving problem (1) with a general convex optimality criterion and establish its global convergence. In addition, we reformulate problem (1) with A-, D- and E-criterion into linear or log-determinant SDPs and apply standard primal-dual IP solvers such as SDPT3 to solve the resulting SDPs. Our computational results show that the IP methods usually outperform the widely used multiplicative algorithm in both speed and solution quality. The codes for this paper are available online at www.math.sfu.ca/∼zhaosong.

Though we establish the global convergence for our primal IP method, we have not studied its local convergence and iteration complexity. Also, we have not considered primal-dual IP methods for solving problem (1) with a general convex optimality criterion. These are certainly interesting topics for our future research.

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