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Computing optimal designs of multiresponse experiments reduces to second-order cone programming

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ABSTRACT

Elfving's theorem is a major result in the theory of optimal experimental design, which gives a geometrical characterization of $\boldsymbol{c}-$optimality. In this paper, we extend this theorem to the case of multiresponse experiments, and we show that when the number of experiments is finite, the $\boldsymbol{c}$-,*A*-,*T*- and *D*-optimal design of multiresponse experiments can be computed by second-order cone programming (SOCP). Moreover, the present SOCP approach can deal with design problems in which the variable is subject to several linear constraints.

We give two proofs of this generalization of Elfving's theorem. One is based on Lagrangian dualization techniques and relies on the fact that the semidefinite programming (SDP) formulation of the multiresponse $\boldsymbol{c}-$optimal design always has a solution which is a matrix of rank 1. Therefore, the complexity of this problem fades.

We also investigate a *model robust* generalization of $\boldsymbol{c}-$optimality, for which an Elfving-type theorem was established by Dette (1993). We show with the same Lagrangian approach that these model robust designs can be computed efficiently by minimizing a geometric mean under some norm constraints. Moreover, we show that the optimality conditions of this geometric programming problem yield an extension of Dette's theorem to the case of multiresponse experiments.

When the goal is to identify a small number of linear functions of the unknown parameter (typically for $\boldsymbol{c}-$optimality), we show by numerical examples that the present approach can be between 10 and 1000 times faster than the classic, state-of-the-art algorithms.

1. Introduction

An important branch of statistics is the *theory of optimal experimental designs*, which explains how to best select experiments in order to estimate a vector of parameters $\boldsymbol{\theta}$. We refer the reader to the monographs of Fedorov (1972) and Pukelsheim (1993) for a comprehensive review on the subject, and to an article of Atkinson and Bailey (2001) for more details on the early development of this theory.

The importance of Elfving's theorem (1952), which was one of the first major improvements in the field of optimal design of experiments, was illustrated in many works (Chernoff, 1999; Dette, 1993; Dette and Studden, 1993; Dette et al., 1995; Studden, 1971, 2005). This result gives a geometrical characterization of the experimental design which minimizes the variance of the best estimator for the linear combination of the parameters $\boldsymbol{c}^T\boldsymbol{\theta}$. Namely, the optimal design can be found at

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the intersection of a vectorial straight-line and the boundary of a convex set referred as *Elfving Set*. When the number of available experiments is finite, Elfving set becomes a polyhedron, and so Elfving's geometrical characterization allows one to compute $\boldsymbol{c}-$optimal designs by linear programming methods, see Harman and Jurík (2008).

An interesting case appears in the study of the design of experiments, when a single experiment is allowed to give simultaneously several observations of the parameters. This setting is referred in the literature as *multiresponse experiments*, and occurs in many practical situations. For more details on the optimal design of multiresponse experiments, the reader is referred to the book of Fedorov (1972).

In this paper, we extend Elfving's classic result (Theorem 2.1) to the optimal design of multiresponse experiments, see Theorem 3.1, and we show that the latter problem reduces to a second-order cone programming (SOCP) problem, see Theorem 3.3.

Moreover, we show in Section 4.1 that this result generalizes the Elfving-type result of Studden (1971), which characterizes geometrically the *A*-optimal design for the estimation of a multidimensional linear combination of the parameters. As a consequence, one may cast the problem of finding an *A*-optimal design on a finite regression range (for single- or multi-response experiments) as an SOCP.

In contrast to the classic algorithms for the computation of optimal designs, the flexibility of mathematical programming approaches makes it possible to add constraints in the problem *without additional effort*. We will see that the present SOCP approach can indeed handle optimal design problems subject to multiple resource constraints, see Section 4.2.

The fact that the $\boldsymbol{c}-$optimal design problem (on a finite regression space) has a semidefinite programming (SDP) formulation can be traced back to 1980, as a particular case of Theorem 4 in Pukelsheim (1980). Similarly, the classic *A*- and *D*-optimal design problems for multiresponse experiments can be formulated as SDP (Vandenberghe et al., 1998). Second-order cone programming (SOCP) is a class of convex programs which is somehow harder than linear programming (LP), but which can be solved by interior point codes like SeDuMi (Sturm, 1999) in a much shorter time that semidefinite programs (SDP) of the same size. Moreover the SOCP method takes advantage of the sparsity of the matrices arising in the problem formulation. Hence, this work shows that computing *A*- and $\boldsymbol{c}-$optimal designs actually belongs to an easier class of problems, and makes it possible to solve instances that were previously intractable.

While our proof of Theorem 3.1 is an extension of Elfving's original proof, it leaves unexplained why the SDP formulation actually reduces to an SOCP. We provide in Section 5 another proof of the present Elfving-type result based on Lagrangian relaxation, which explains why the complexity of this problem fades. The proof relies on Theorem 5.2, which shows that a certain class of semidefinite programs (packing programs with a rank-one objective function) have a rank-one solution. Theorem 5.2 appears to be a result of an independent interest, in relation with the study of semidefinite relaxations of combinatorial optimization problems, and is therefore the subject of the companion paper (Sagnol, submitted for publication).

We next show (Theorem 6.1) that *T*-optimality also admits a second-order cone programming representation, which gives another argument for saying that second-order cone programming is a natural tool for handling experimental optimal design problems. If the experimenter wishes to estimate the full vector of parameters $\boldsymbol{\theta}$, the *T*-optimal design problem is trivial. However, if he is interested in a linear subsystem $K^T\boldsymbol{\theta}$, the *T*-optimal design problem is complicated and can be handled by SOCP.

In Section 7, we consider a generalization of $\boldsymbol{c}-$optimality which was originally proposed by Läuter (1974) in order to deal with the uncertainty on the model. In this approach (called *S*-optimality by Läuter), the objective criterion takes into account the variance of several estimators, balanced in a log term with coefficients which indicate the belief of the experimenter in each model. Dette (1993) characterized by an Elfving-type result the *S*-optimal designs. We show in Theorem 7.1, which is the main result of this section, that when the number of available experiments is finite, *S*-optimal designs of multiresponse experiments can be computed efficiently by minimizing a geometric mean under some norm constraints. Moreover, we show in Theorem 7.3 that the optimality conditions of this geometric program yield an extension of Dette's theorem to the case of multiresponse experiments. As a consequence of Theorem 7.1, we obtain a SOCP for *D*-optimality (cf. Remark 7.5). The results of this section are proved in appendix.

This work grew out from an application to networks (Bouhtou et al., 2008), in which the traffic between any two pairs of nodes must be inferred from a set of measurements. This leads to a large scale optimal experimental design problem which cannot be handled by standard SDP solvers. In a companion work relying on the present reduction to an SOCP (Sagnol et al., 2010), we illustrate our method by solving within seconds optimal design problems that could not be handled by SDP. In addition, the constraints of the SOCP formulation involves the *observation matrices* A_i of the experiments, which happen to be very sparse in practice. This is in contrast with the *information matrices* involved in the SDP formulation (M_i=$A_i^TA_i$), which are not sparse in general. The present SOCP formulation takes advantage of the intrinsic sparsity of the data, and the instances can be solved very efficiently.

We present in Section 8 some numerical experiments for problems of the kind that arise in network monitoring, as well as classic polynomial regression problems. Our experiments show that the SOCP approach is well suited when the number of linear functions to estimate is *small*. For the case of $\boldsymbol{c}-$optimality (only one linear function to estimate), we will see that solving the second-order cone program is usually 10 times faster than the classic exchange or multiplicative algorithms, and up to 2000 times faster than the SDP approach for problems with multiple constraints.

Some results of this paper, including Theorem 3.1, were presented at the conference (Sagnol et al., 2009), and the technical result justifying the reduction to a SOCP was posted on arXiv (Sagnol, submitted for publication). Shortly before the time of