THE GROUP LASSO FOR DESIGN OF EXPERIMENTS

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Abstract

We introduce an application of the group lasso to design of experiments. We show that the problem of constructing an optimal design matrix can be transformed into a problem of the group lasso. We also give a numerical example that we can obtain several orthogonal arrays as the solutions of the group lasso problems.

Keywords: design of experiments, group lasso, A-optimality, second order cone programming, symmetry.

1 Introduction

Design of experiments is widely used in a variety of fields such as agriculture, quality control, and simulation. One of the purpose of design of experiments is to construct the optimal experimental design with respect to a criterion under some constraints reflecting real problem. However, it is sometimes hard to obtain the optimal designs theoretically. Recently, several computer-based approaches have been developed for this problem. Especially, mixed integer programming is used to construct balanced incomplete block designs (Yokoya and Yamada [7]), orthogonal designs (Vieira et al. [8]) and nearly orthogonal nearly balanced
mixed designs (Vieira et al. [4]). Additionally, Jones and Nachtsheim [2] gives randomized algorithm to obtain preferable designs for screening with factors having three levels. Interestingly, Xiao et al. [6] theoretically gives the optimal designs for the same problem of Jones and Nachtsheim [2], using conference matrices (Belevitch [1]).

In this paper, we propose a new machine learning approach to obtain an optimal experimental design. In our approach, we consider that a design which has fewer design points and smaller variances for what we want to estimate is preferable. In general, the fewer the design points, the larger the variances of estimates. Therefore, there exists a trade-off between the number of design points and the variances of estimators. This means that the optimality depends on how much we emphasis on the number of design points or the variances of estimators. First, to construct an optimal design, we enumerate the candidate design points. In many cases, it is difficult to conduct the experiments at every candidate design points from the aspect of the cost. Therefore, it is necessary to choose the subset of design points among them with minimum loss of information. As described in Section 2.2, this procedure corresponds to a method of variable selection for regression analysis and can be formulated as a problem of the group lasso.

The organization of this paper is as follows. In Section 2 we review the formulation of the group lasso (Section 2.1) and apply it to the problem of constructing an optimal design (Section 2.2). Section 3 is devoted to the numerical examples of our approach. In Section 4 we summarize the features of our approach.

2 An application of the group lasso to design of experiments

2.1 The group lasso

The method of the group lasso (Yuan and Lin [8]) which is a kind of generalization of the lasso (Tibshirani [5]) has become a popular method of variable selection for linear regression. Let us consider the usual linear regression: we have continuous outputs $y \in \mathbb{R}^N$ and a $N \times D$ design matrix $X$, where $N$ is the sample size and $D$ is the number of input variables. The estimator of the group lasso $\hat{\beta} \in \mathbb{R}^D$ is defined as

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^D} ||y - X\beta||_2^2 + \sum_{g=1}^G \lambda_g ||\beta_{I_g}||_2,$$

(1)

where $\lambda_1, \ldots, \lambda_G$ are tuning parameters, $||\cdot||_2$ stands for the Euclidean norm (not squared), $I_1, \ldots, I_G$ are disjoint subsets of $\{1, \ldots, D\}$ and $\beta_{I_g} = (\beta_{i_1}, \ldots, \beta_{i_g})$ for $I_g = \{i_1, \ldots, i_g\}$. If $I_1, \ldots, I_G$ are all singletons, then the group lasso of (1) coincides with the lasso. The group lasso has the property that it does variable selection at the group level, i.e., an entire group of input variables
may drop out of the model. The group lasso problem of (1) can be formulated as a second order cone programming and solved by the interior point methods. Furthermore, there are some specialized algorithms which solves the group lasso problem faster than the interior point methods.

2.2 Design of experiments

Assume that there are $F$ factors $a_1, \ldots, a_F$ and the relation between the response variable $R$ and the factors is formulated as

$$R = \sum_{f \in \mathcal{F}} \gamma_f a^f + \epsilon$$

(2)

where $\mathcal{F}$ is a finite subset of $\mathbb{Z}_{\geq 0}^F$, $a^f = \prod_{i=1}^F a^f_i$ for $f = (f_1, \ldots, f_F) \in \mathcal{F}$ and $\epsilon$ is the error with mean zero and variance $\sigma^2$. Here the set of the parameters we want to estimate is a subset of $\{\gamma_f \in \mathbb{R} | f \in \mathcal{F}\}$. For simplicity, in this paper, we only consider the case where each factor has finite fixed levels and assume that the $f$-th factor has $l_f$ levels $a_{f1}, \ldots, a_{fl_f}$. Let $A$ be the set of all candidate design points. If we consider all combinations of the levels of the factors without repetition as the candidate design points, then

$$A = \{ (a_{1i_1}, \ldots, a_{Fi_F})^T | i_f \in \{1, \ldots, l_f\} \}$$

where $T$ stands for transpose and $A$ has $\prod_{f=1}^F l_f$ elements. Let $G$ be the number of elements of $A$ and $A = \{a_1, \ldots, a_G\}$ sorting the elements of $A$, in an arbitrary order. The design matrix $C$ of the candidate points is defined such that the $g$-th column is $a_g$, i.e., $C = [a_1 \ldots a_G]$.

**Example 1.** Let us consider the case where $F = 3$ and each factor has two levels $-1$ or $1$. If we consider all combinations of the levels of the factors without repetition as the candidate design points, then there are $G = 2^3 = 8$ candidate design points and a design matrix of them is defined as follows:

$$C = \begin{bmatrix}
-1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\
-1 & 1 & -1 & 1 & -1 & 1 & 1 & 1
\end{bmatrix}.$$  

(3)

Let $|\mathcal{F}|$ be the number of elements in $\mathcal{F}$ and $\mathcal{F} = \{f_1, \ldots, f_{|\mathcal{F}|}\}$ sorting the elements of $\mathcal{F}$ in an arbitrary order. For each $a_g$, let $\tilde{a}_g = (a_g^f, \ldots, a_g^{|\mathcal{F}|})^T$. Then a model matrix $M$ of the candidate points is defined such that the $g$-th column is $\tilde{a}_g$, i.e., $M = [\tilde{a}_1 \ldots \tilde{a}_G]$.

**Example 2.** As in Example 1, we consider the case where $F = 3$ and each factor has two levels $-1$ or $1$. Furthermore, we assume that the relation between the response variable and the factors is formulated as

$$R = \gamma_{000} + \gamma_{100}a_1 + \gamma_{010}a_2 + \gamma_{001}a_3 + \epsilon.$$  

(4)
This is called the main effect model. Then $\mathcal{F} = \{(0,0,0), (1,0,0), (0,1,0), (0,0,1)\}$ and a model matrix of candidate design points is defined as follows:

$$M = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & -1 & -1 & -1 & 1 & 1 & 1 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 \\
-1 & 1 & -1 & 1 & -1 & 1 & 1
\end{bmatrix}. \tag{5}$$

Note that, for simplicity, we may also write $\gamma_0, \gamma_1, \gamma_2$ and $\gamma_3$ instead of $\gamma_{000}, \gamma_{100}, \gamma_{010}$ and $\gamma_{001}$.

Let $e_j = e_{f_j}$ be a column vector with length equal to $|\mathcal{F}|$ such that $e_j$ has an entry 1 in the row corresponding to $j$ and 0 otherwise. Furthermore, for $j \in \{1, \ldots, |\mathcal{F}|\}$, let $\gamma_j = \gamma_{f_j}$ as in Example 2 and $\gamma = (\gamma_1, \ldots, \gamma_{|\mathcal{F}|})^T$. Let $R_g$ and $\epsilon_g$ be the response variable and the error respectively when the factors $a_g^j, \ldots, a_g^{j|x}$ are given. Let $R = (R_1, \ldots, R_G)^T$ and $\epsilon = (\epsilon_1, \ldots, \epsilon_G)^T$. We use the following proposition to formulate the problem of constructing an optimal design matrix as a problem of mathematical programming.

**Proposition 3.** If there exists $\beta_j = (\beta_{j1}, \ldots, \beta_{jG})$ such that $\beta_j \hat{a}_1 + \cdots + \beta_{jG} \hat{a}_G = e_j$, then $\gamma_j = \beta_j R_1 + \cdots + \beta_{jG} R_G$ is an unbiased estimator of $\gamma_j$. The variance of $\gamma_j$ is $\text{Var}[\gamma_j] = \sigma^2 \|eta_j\|_2^2$.

**Proof:** Note that $R = M^T \gamma + \epsilon$ and $M \beta_j = e_j$ from the assumption. Then we obtain

$$E[\gamma_j] = E[\beta_j R_1 + \cdots + \beta_{jL} R_G] = E[R^T \beta_j] = E[(M^T \gamma + \epsilon)^T \beta_j] = E[\gamma^T M \beta] + E[\epsilon^T \beta_j] = E[\gamma^T e_j] = \gamma_j.$$

The variance is

$$\text{Var}[\gamma_j] = \beta_j^2 \text{Var}[R_1] + \cdots + \beta_{jL}^2 \text{Var}[R_G] = \sigma^2 \|eta_j\|_2^2.$$

As our design criterion, we use A-optimality in which the sum (or the “A”verage) of the variances of the estimators is minimized. At the same time, we consider the problem to choose the bare minimum of design points to save the cost. Assume that the parameters in the set $\gamma_J = \{\gamma_j \mid j \in J\}$ are what we want to estimate where $J \subseteq \{1, \ldots, |\mathcal{F}|\}$. For each $\gamma_j \in \gamma_J$, we consider a linear estimator $\hat{\gamma}_j = \beta_j R_1 + \cdots + \beta_{jG} R_G = R^T \beta_j$. From Proposition 3, the sum of the variances of the estimators for $\{\gamma_j \mid j \in J\}$ is $\sum_{j \in J} \|eta_j\|_2^2$. Then based on A-optimality criterion, we need to minimize the sum $\sum_{j \in J} \|eta_j\|_2^2$ under the condition of the unbiasedness: $M \beta_j = e_j$ for $j \in J$. Next, we consider the sparseness of the estimator. Let $\beta_{t_a}$ be a column vector whose entries are $\{\beta_{gj} \mid j \in J\}$. If $\beta_{t_a} = 0$, then the response $R_g$ at the $g$-th design point is not used for the estimators $\{\gamma_j \mid j \in J\}$. Therefore, using the spirit of the group lasso, the following penalized least square gives the solution which minimizes the
sum of the variances of the estimators under the condition of the unbiasedness with consideration of the sparseness.

\[
\min \left\{ \beta_j | j \in J \right\} \sum_{j \in J} ||\beta_j||^2 + \sum_{g=1}^{G} \lambda_g ||\beta_I_g|| \\
\text{s.t. } M\beta_j = e_j, \ (j \in J).
\]

Here, \(\lambda_1, \ldots, \lambda_G\) are tuning parameters. The problem of (6) is a second order cone programming and can be solved by the interior point methods. However, the formulation of (6) contains constraints and some specialized algorithms which solves the group lasso problem may not applicable. We can also consider the Lagrangian relaxation problem of (6) as follows:

\[
\min \left\{ \beta_j | j \in J \right\} \sum_{j \in J} (||\beta_j||^2 + \kappa_j ||M\beta_j - e_j||^2) + \sum_{g=1}^{G} \lambda_g ||\beta_I_g|| \tag{7}
\]

where, \(\kappa_j, \ (j \in J)\) is a tuning parameter. The formulation of (7) is the same as the group lasso and thus the specialized algorithms for the group lasso is applicable. In particular, the solution of the problem of (7) does not accurately satisfy the constraints of the unbiasedness when \(\kappa_j\)'s are not so large. This means that, from the problem of (7), we can obtain the solution when we allow confounding among the factors. Therefore, the formulation of (7) works even when the number of the elements of \(J\) is larger than \(G\) or the number of non-zero \(\beta_I_g\)'s.

As the following example shows, in the formulation of (6) or (7), we have to determine the values of \(\lambda_g\)'s and \(\kappa_j\)'s carefully to obtain the sparse solution.

**Example 4.** We assume that there are \(F = 3\) factors and each factor has two levels \(-1\) or \(1\). Furthermore, we assume that the candidate design points consist of all combinations of the levels of the factors as in (3). We consider the main effect model: \(R = \gamma_0 + \sum_{j=1}^{3} \gamma_j a_j + \epsilon\). Then the model matrix is given by (5). Suppose that we want to estimate \(\gamma_1, \gamma_2\) and \(\gamma_3\). To this model,

| Run | 1  | 2  | 3  | 4  |
|-----|----|----|----|----|
| \(a_1\) | -1 | -1 | 1  | 1  |
| \(a_2\) | -1 | 1  | -1 | 1  |
| \(a_3\) | -1 | 1  | 1  | -1 |

Table 1: \(L_4\) orthogonal array

| Run | 1  | 2  | 3  | 4  |
|-----|----|----|----|----|
| \(a_1\) | 1  | 1  | -1 | -1 |
| \(a_2\) | 1  | -1 | 1  | -1 |
| \(a_3\) | 1  | -1 | -1 | 1  |

Table 2: The orthogonal array \((-1) \times L_4\)

traditional design of experiments shows that \(L_4\) orthogonal array in Table 7 is optimal. Note that Table 7 is transposed against the traditional notation of \(L_4\) orthogonal array, i.e., each column corresponds to a run of the experiment and the rows indicate the levels of \(a_1, a_2\) and \(a_3\). The feasible solution of (6) which
corresponds to \( L_4 \) orthogonal array is

\[
\beta_1 = \frac{1}{4}(-1, 0, 0, 1, 0, -1, 0)^T, \\
\beta_2 = \frac{1}{4}(-1, 0, 0, 1, 0, -1, 1, 0)^T, \\
\beta_3 = \frac{1}{4}(-1, 0, 0, -1, 0, 1, 1, 0)^T.
\]

From Gauss-Markov theorem, the feasible solution (8) can be obtained by least squares of \( \gamma_1, \gamma_2 \) and \( \gamma_3 \) for the experiment which has exactly four design points: 1st, 4th, 6th and 7th columns of (3). However, as shown below, if we set \( \lambda_1 = \cdots = \lambda_8 = \lambda \) for any non-negative real number \( \lambda \), then we can not obtain \( L_4 \) orthogonal array as the optimal solution of (6). Let us consider the following feasible solution:

\[
\beta_1 = \frac{1}{4}(0, -1, -1, 0, 0, 1, 1, 0)^T, \\
\beta_2 = \frac{1}{4}(0, -1, 1, 0, -1, 0, 0, 1)^T, \\
\beta_3 = \frac{1}{4}(0, 1, -1, 0, -1, 0, 0, 1)^T.
\]

This solution corresponds to the orthogonal array in Table 2. It can be easily seen that the value of the objective function of (6) for (8) and that for (9) is the same. Furthermore, note that the problem of (6) is strictly convex and the minimum is unique. Therefore, the feasible solution of (8) is not the optimal solution.

The above example shows that the presence of the symmetries in the formulation of (6) or (7) prevent the sparseness of the solution. In Section 3, we give a method to construct \( \lambda_1, \ldots, \lambda_G \) which produces asymmetries in (6) and enables us to obtain the orthogonal arrays in several situations.

3 Numerical examples

In this section, we only consider the case where each factor has two levels \(-1, +1\) and the candidate design points consist of all combinations of the levels of the factors. We denote the set of candidate design points by \( C = [a_1 \ldots a_G] \) as in Section 2.2, where \( G = 2^F \) and assume \( a_1 = (-1, \ldots, -1)^T \). As Example 4 shows, we need to carefully determine the values of \( \lambda_1, \ldots, \lambda_G \) to obtain the sparse solution. In the following numerical examples, we used Algorithm 1 to construct the values of \( \lambda_1, \ldots, \lambda_G \). For \( a \in \mathbb{R}^{|\mathcal{F}|} \) and a subspace \( S \) of \( \mathbb{R}^{|\mathcal{F}|} \), let \( \text{dist}(a, S) = \min_{s \in S} ||a - s||_2 \).

Example 5. As in Example 4, we consider the case where \( F = 3 \), the model and the model matrix is given by (4) and (5) respectively. Suppose that we want to estimate \( \gamma_1, \gamma_2 \) and \( \gamma_3 \). By solving (6), we obtained the optimal \( \beta_i \)'s. Table 3
Algorithm 1 An algorithm for constructing $\lambda_1, \ldots, \lambda_G$.

1. $t = 1$, $N_1 = \{1\}$

2. Repeat the following steps (a)-(d) while $t \leq |F|$.
   
   (a) Let $S_t = \{\sum_{i \in N_t} \nu_i \tilde{a}_i \in \mathbb{R}^{|F|} \mid \nu_i \in \mathbb{R}, i \in N_t\}$ be a subspace of $\mathbb{R}^{|F|}$.
   
   (b) Calculate $l_{gt}$ as follows:
   
   $$l_{gt} = \begin{cases} 
   0 & (g \in N_t) \\
   \{||\tilde{a}_g||^2_2 - (\text{dist}(\tilde{a}_g, S_t))^2\} & (g \notin N_t). 
   \end{cases}$$
   
   (c) Select one of $g_{t+1} \in \{1, \ldots, G\} \setminus N_t$ from the following set:
   
   $$\arg\min_{g \in \{1, \ldots, G\} \setminus N_t} \{||\tilde{a}_g||^2_2 - (\text{dist}(\tilde{a}_g, S_t))^2\}.$$ 
   
   (d) $N_{t+1} = \{g_{t+1}\} \cup N_t$, $t \leftarrow t + 1$

3. Calculate $\lambda_g = \sum_{t=1}^{|F|} l_{gt}$ for $g = 1, \ldots, G$.

Table 3: The optimal design matrix for the model of (4)

| Run | 1  | 2  | 3  | 4  |
|-----|----|----|----|----|
| $a_1$ | 1  | 1  | -1 | -1 |
| $a_2$ | 1  | -1 | 1  | -1 |
| $a_3$ | 1  | -1 | -1 | 1  |

is the optimal design matrix whose columns are the selected design points such that $\beta_{I_g} \neq 0$. Note that Table 3 is equivalent to the $L_4$ orthogonal array.

Example 6. Assume that there are $F = 4$ factors $a_1, a_2, a_3, a_4$ and each factor has two levels $-1$ or $1$. We consider all $G = 2^4 = 16$ combinations of the levels of the factors as the candidate design points. Furthermore, we assume that the relation between the response variable and the factors is formulated as

$$R = \gamma_0 + \gamma_1 a_1 + \gamma_2 a_2 + \gamma_3 a_3 + \gamma_4 a_4 a_5 a_6 + \gamma_5 a_1 a_2 + \gamma_6 a_1 a_4 + \epsilon. \tag{10}$$

Suppose that we want to estimate $\gamma_1, \ldots, \gamma_7$. Then, by solving (6), we obtained the optimal $\beta_{I_g}$’s. Table 4 shows the optimal design matrix. Note that Table 4 is equivalent to the $L_8$ orthogonal array.

Example 7. Assume that there are $F = 4$ factors $a_1, a_2, a_3, a_4$ and each factor has two levels $-1$ or $1$. We consider all $G = 2^4 = 16$ combinations of the levels of the factors as the candidate design points. Furthermore, we assume that the
Table 4: The optimal design matrix for the model of (10)

| Run | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  |
|-----|----|----|----|----|----|----|----|----|
| a1  | 1  | 1  | 1  | -1 | -1 | -1 | -1 | -1 |
| a2  | 1  | 1  | -1 | -1 | 1  | 1  | -1 | -1 |
| a3  | 1  | -1 | 1  | -1 | 1  | 1  | -1 | -1 |
| a4  | 1  | -1 | -1 | 1  | 1  | 1  | -1 | -1 |

Table 5: The optimal design matrix for the model of (11)

| Run | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  |
|-----|----|----|----|----|----|----|----|----|----|
| a1  | 1  | 1  | 1  | -1 | -1 | -1 | -1 | -1 | 1  |
| a2  | 1  | 1  | -1 | -1 | 1  | 1  | -1 | -1 | 1  |
| a3  | 1  | -1 | 1  | -1 | 1  | 1  | -1 | -1 | 1  |
| a4  | 1  | -1 | -1 | 1  | 1  | 1  | -1 | -1 | 1  |

relation between the response variable and the factors is formulated as

\[ R = \gamma_0 + \gamma_1 a_1 + \gamma_2 a_2 + \gamma_3 a_3 + \gamma_4 a_4 + \gamma_5 a_1 a_2 + \gamma_6 a_1 a_6 + \gamma_7 a_1 a_4 + \gamma_8 a_2 a_3 + \epsilon. \] 

Suppose that we want to estimate \( \gamma_1, \ldots, \gamma_8 \). Then, by solving (6), we obtained the optimal \( \beta_I \)'s. Table 5 shows the optimal design matrix. Note that the first 8 columns of Table 5 are similar to Table 4.

4 Concluding remarks

We apply the group lasso to the problem of constructing an optimal design matrix. Though we mainly treat the case where each factor has two levels and the set of candidate design points consists of all combinations of the levels of the factors without repetition in the examples, our approach, described in Section 2.2, has the following features.

- Each factor can have two or more levels.
- By duplicating the columns of the design matrix, we can treat the case of repeated measurements.
• By solving the problem of (7), we can obtain the optimal design matrix when we allow confounding among the factors.

• Assume that we have already observed the responses at the design points \(a_{g_1}, \ldots, a_{g_Q}\). Then, by setting \(\lambda_{g_1} = \cdots = \lambda_{g_Q} = 0\), we can choose additional design points given \(R_{g_1}, \ldots, R_{g_Q}\).

Furthermore, we do not need to consider all combinations of the levels of the factors as the candidate design points. If the number of the levels or the factors increases, then the number of the combinations increases explosively. This means that the number of the variables in the formulation of (6) or (7) increases explosively, and hence it becomes difficult to solve the problem. Therefore, if the number of the levels or the factors is large, then it is needed to reduce the number of the candidates in advance to bound the number of variables in (6) or (7). For future work, we will investigate how to choose the candidate design points in advance. We will also investigate how to determine the values of \(\lambda_g\)’s and \(\kappa_j\)’s.

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