An unexpected connection between Bayes $A$–optimal designs and the Group Lasso

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Abstract

We show that the $A$-optimal design optimization problem over $m$ design points in $\mathbb{R}^n$ is equivalent to minimizing a quadratic function plus a group lasso sparsity inducing term over $n \times m$ real matrices. This observation allows to describe several new algorithms for $A$-optimal design based on splitting and block coordinate decomposition. These techniques are well known and proved powerful to treat large scale problems in machine learning and signal processing communities. The proposed algorithms come with rigorous convergence guarantees and convergence rate estimates stemming from the optimization literature. Performances are illustrated on synthetic benchmarks and compared to existing methods for solving the optimal design problem.

1 Introduction

We consider an optimal experimental design problem of the form

$$\min_{w \in \Delta} \Phi_{A_K} \left( \Sigma^{-1} + \frac{N}{\sigma^2} \sum_{i=1}^{m} w_i a_i a_i^T \right),$$

(1)

where $\Phi_{A_K}(M) = \text{trace} \, K^T M^{-1} K$ is the criterion of $A_K$-optimality for some matrix $K \in \mathbb{R}^{n \times r}$ depending on the quantity to be estimated, $\Sigma$ is a known

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positive definite matrix, the constants $N$, $\sigma$ and the vectors $a_i \in \mathbb{R}^n$, $i = 1, \ldots, m$, are known, and $\Delta := \{ w \in \mathbb{R}^m : w \geq 0, \sum_{i=1}^m w_i = 1 \}$ is the probability simplex. This problem arises in linear regression models with a finite design space, which we identify with $[m] := \{1, \ldots, m\}$, in which independent trials at the $i$th design points yield random measurements $Y_i$, satisfying $E[Y_i] = a_i^T \theta$, $\forall Y_i = \sigma^2$, for all $i \in [m]$. In addition, a prior noisy observation $\theta_0$ of the unknown parameter $\theta \in \mathbb{R}^n$ is available, with variance-covariance matrix $\nu[\theta_0] = \Sigma$ and expectation $E[\theta_0] = \theta$. Then, Problem (1) can be interpreted as selecting the optimal fraction $w_i$ of a total number $N$ of trials to perform on the $i$th design point (the meaning of optimal will be detailed in the next section).

This problem was first introduced in [14] under the name $\psi$-optimality, and studied in detail by Chaloner [11], who observed that this problem could also be called Bayes A-optimality, a name still used in the literature. Nevertheless, Bayes-optimal designs can also be used in a non-Bayesian context, when the experimenter is committed to a first batch of trials, and need to select an additional batch of $N$ trials, cf. [11].

We should observe that Problem (1) is in fact the continuous relaxation of the following discrete problem, which we call $N$-exact Bayes $A_K$-optimal design:

$$\minimize_{n \in \Delta_N} \Phi_A \left( \Sigma^{-1} + \frac{1}{\sigma^2} \sum_{i=1}^m n_i a_i a_i^T \right),$$

(2)

where $\Delta_N := \{ n \in \mathbb{Z}^m_{\geq 0} : \sum_{i=1}^m n_i = N \}$ is the standard discrete $N$-simplex, and $n_i$ represents the number of trials to perform at the $i$th design point. While Problem (2) is of immediate relevance for the experimenter, this problem has a hard combinatorial structure; in particular, it contains as a special case the problem of exact $c$-optimality, which was proved to be NP-hard in [10]. Therefore, it is almost impossible to certify global optimality of a design $n$, except for small instances, when a mixed integer second order cone programming solver can be used [29]. To overcome this issue, the classical machinery of approximate design theory proposes to introduce a continuous variable $w_i = \frac{N}{N} n_i$ and to relax the integer constraints “$N w_i \in \mathbb{Z}$”, which leads to the convex optimization problem (1). In practice, the solution of Problem (1) gives a lower bound on the optimal value of (2). This can be used to ascertain the quality of an exact design $n$, which can typically be computed by using heuristic methods, such as exchange algorithms (see, e.g. [11]) or, as recently proposed, with particle swarm optimization [22]. Alternatively, rounding methods can be used to turn an approximate design $w^*$ (i.e., a solution to Problem (1)) into a good exact design $n \in \Delta_N$, which works...
particularly well when the total number $N$ of trials is large \cite{26}. For more details on the subject, we refer the reader to the monographs of Fedorov \cite{16} or Pukelsheim \cite{25}.

Many different approaches have been proposed to solve Problem (1). The traditional methods are the Fedorov-Wynn type vertex-direction algorithms \cite{16,35} and the closely related vertex exchange methods \cite{6}, the multiplicative weight update algorithms \cite{32,36}, and interior point methods based on semidefinite programming \cite{15} or second-order cone programming \cite{31} formulations. Recent progress in this area has been obtained by employing hybrid methods that alternate between steps of the aforementioned algorithms (the cocktail algorithm \cite{37}), or by using randomization \cite{20}.

Contribution and Organization. The main contribution of this article is a new reformulation of Problem (1) as a convex, unconstrained optimization problem, which brings to light a strong connection with the well-studied problem of group lasso regression \cite{35}. The particular structure of the new formulation also suggests algorithmic ideas based on proximal decomposition methods, which already proved to be very useful in machine-learning and signal processing applications \cite{4,13,3}. An appealing property of these methods is that they come with rigorous convergence guarantees, and yield sparse iterates very quickly, corresponding to designs with only a few support points.

The rest of this paper is organized as follows. In Section 2 we give more background on Problem (1), and show how this problem can be reformulated as an unconstrained convex optimization problem involving a squared group lasso penalty. Then, we characterize the proximity operator of this penalty in Section 3. This makes it possible to use a new class of algorithms, described in Section 4, to solve the reformulated problem. Finally, Section 5 presents some numerical experiments comparing performances of the proposed algorithm to existing approaches.

2 Problem Reformulation

2.1 The Bayes $A_K$–optimal design problem

For the sake of completeness, we first explain the derivation of Problem (2) and its relaxation for approximate designs, Problem (1). The experimental design is specified by a vector $n = (n_1, \ldots, n_m) \in \mathbb{Z}_{\geq 0}^m$, which indicates
the number of replications at the $i$th design point. Specifically, we obtain random observations

$$y_{ij} = a_i^T \theta + \epsilon_{ij}, \quad \forall i \in [m], \forall j \in [n_i],$$

where the measurements are unbiased (i.e., $E[\epsilon_{ij}] = 0$), uncorrelated (i.e., $(i,j) \neq (k,l) \implies E[\epsilon_{ij}\epsilon_{kl}] = 0$), and the variance is known: $E[\epsilon_{ij}^2] = \sigma^2$.

We further assume that the experimental resources are limited by a budget on the total number $N$ of trials, that is, $\sum_{i=1}^m n_i = N$ must hold.

Denote by $\mathbf{y}$ the vector of $\mathbb{R}^m$ with the averaged observations at each location, that is, $y_i = \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij}$ (and $y_i$ can be set to some arbitrary constant whenever $n_i = 0$). Then, in vector notation, we have

$$\mathbf{y} = A\mathbf{\theta} + \mathbf{\epsilon},$$

where $A = [a_1, \ldots, a_m]^T \in \mathbb{R}^{m \times n}$, and the averaged random vector $\mathbf{\epsilon}$ with elements $\epsilon_i = \frac{1}{n_i} \sum_{j=1}^{n_i} \epsilon_{ij}$ satisfies $E[\mathbf{\epsilon}] = 0$, $V[\mathbf{\epsilon}] = E[\mathbf{\epsilon}\mathbf{\epsilon}^T] = \sigma^2 \text{Diag}(\mathbf{n})^{-1}$.

(We adopt the convention $\frac{1}{0} = +\infty$, so $n_i = 0$ implies that $\epsilon_i$ has an infinite variance, which is consistent with the fact that $y_i$ is basically unobserved.) Further, we recall that we have a prior observation $\mathbf{\theta}_0 = \mathbf{\theta} + \mathbf{\eta}$, for some random vector $\mathbf{\eta} \in \mathbb{R}^n$ satisfying $E[\mathbf{\eta}] = 0$, $E[\mathbf{\eta}\mathbf{\eta}^T] = \Sigma$, and $E[\mathbf{\eta}\mathbf{\epsilon}^T] = 0$.

We know from the Gauss Markov theorem (see, e.g. [25]) that the best linear unbiased estimator (BLUE) for $\mathbf{\theta}$ solves the least squares problem

$$\min_{\mathbf{\theta} \in \mathbb{R}^n} \frac{1}{\sigma^2} (A\mathbf{\theta} - \mathbf{y})^T \text{Diag}(\mathbf{n})(A\mathbf{\theta} - \mathbf{y}) + (\mathbf{\theta} - \mathbf{\theta}_0)^T \Sigma^{-1}(\mathbf{\theta} - \mathbf{\theta}_0),$$

which admits the closed-form solution $\hat{\mathbf{\theta}} := M(\mathbf{n})^{-1}(A^T \text{Diag}(\mathbf{n}) \frac{\mathbf{y}}{\sigma^2} + \Sigma^{-1} \mathbf{\theta}_0)$, where $M(\mathbf{n}) := \frac{1}{\sigma^2} A^T \text{Diag}(\mathbf{n}) A + \Sigma^{-1}$ is the information matrix of the design. For the remaining of this paper, we focus on the approximate design problem. As explained in the introduction, this simply means that we introduce the continuous variable $\mathbf{w} = \frac{1}{N} \mathbf{n} \in \Delta$, and that we ignore the restriction that $N\mathbf{w}$ should be integer. So we define the (approximate) information matrix, by $M_N(\mathbf{w}) := M(N\mathbf{w}), \forall \mathbf{w} \in \Delta$. For the sake of notation, we find convenient to introduce the symbol $\sigma_N^2 = \frac{\sigma^2}{N}$, so

$$M_N(\mathbf{w}) = \frac{1}{\sigma_N^2} A^T \text{Diag}(\mathbf{w}) A + \Sigma^{-1} = \frac{1}{\sigma_N^2} \sum_{i=1}^m w_i a_i a_i^T + \Sigma^{-1}.$$  

The Bayes $A-$optimal design problem is to select find $\mathbf{w}$ minimizing $\Phi_A(M_N(\mathbf{w}))$, where the criterion of $A-$optimality is $\Phi_A : M \mapsto \text{trace} M^{-1}$. Geometrically,
this corresponds to minimizing the diagonal of the bounding box of confidence ellipsoids for \( \hat{\theta} \) (provided \( \epsilon \) is normally distributed), cf. [31]. Also, note that we recover the standard (non-Bayesian) A-optimal design problem when no prior is available, i.e., \( \Sigma^{-1} \to 0 \).

More generally, the criterion of \( A_K \)-optimality is defined by

\[
\Phi_{A_K} : \mathbb{S}_+^n \to \mathbb{R}, \quad M \mapsto \text{trace } K^T M^{-1} K
\]

for some matrix \( K \in \mathbb{R}^{m \times r} \). Clearly, the standard criterion of \( A \)-optimality is a particular case of \( \Phi_{A_K} \), obtained by setting \( K \) to the identity matrix.

We conclude this part by mentioning another common situation that leads to a Problem of the form (2). Assume the experimenter wants to predict the quantities \( \eta(x) := \phi(x)^T \theta, \forall x \in \mathcal{X} \), where \( \mathcal{X} \) is a compact set and \( \phi : \mathcal{X} \to \mathbb{R}^n \) is a continuous map. Then, it is well known that \( \hat{\eta}(x) := \phi(x)^T \hat{\theta} \) is the best linear unbiased predictor (BLUP) for \( \eta(x) \), and its variance is \( \phi(x)^T M_N(w)^{-1} \phi(x) \). If \( \mu \) is a measure over \( \mathcal{X} \) weighing the interest of the experimenter to predict \( \eta \) at \( x \in \mathcal{X} \), a natural criterion to consider is the integrated mean squared error, IMSE\((w) := \int_{x \in \mathcal{X}} \phi(x)^T M_N(w)^{-1} \phi(x) \, d\mu(x) \)

The minimization of IMSE\((w) \) can be cast as an \( A_K \)-optimal design problem, because:

\[
\text{IMSE}(w) = \int_{x \in \mathcal{X}} \phi(x)^T M_N(w)^{-1} \phi(x) \, d\mu(x) = \text{trace } M_n(w)^{-1} KK^T = \Phi_{A_K}(M_N(w)),
\]

where \( KK^T \) is a Cholesky decomposition of the positive symmetric definite matrix \( \int_{x \in \mathcal{X}} \phi(x)\phi(x)^T \, d\mu(x) \). We point out that large scale problems involving the minimization of IMSE\((w) \) recently arose for the sequential design of computer experiments with Gaussian process as a metamodel, when a truncated Karhunen-Loève expansion is used to approximate the covariance kernel; see [18, 19, 30].

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When \( \mu \) is the uniform measure over the design space, we point out that the IMSE criterion is sometimes called I-optimality, or IV-optimality (for integrated variance).
2.2 Reformulation as an unconstrained convex problem

Now, take a linear estimator \( \hat{\zeta} = Xy + H\theta_0 \) of \( \zeta = K^T\theta \) for some matrices \( X \in \mathbb{R}^{r \times m} \) and \( H \in \mathbb{R}^{r \times n} \). This estimator is unbiased if and only if \( AX + H = K^T \), and we have \( \mathbb{V}[\hat{\zeta}] = \sigma_N^2 X \text{Diag}(w)^{-1}XT + H\Sigma H^T \).

By the Gauss Markov theorem, minimizing over \( X \) and \( H \) the quantity

\[
\sum_{i=1}^n \mathbb{V}[\hat{\zeta}_i] = \text{trace} \mathbb{V}[\hat{\zeta}] \quad \text{such that} \quad \hat{\zeta} \text{ is unbiased,}
\]

leads to the BLUE estimator, in which case we have already seen that \( \Phi_A(K_M(w)) = \sum_{i=1}^r \mathbb{V}[\hat{\zeta}_i] \).

Hence, using the computed variance estimate, the Bayes A\(_K\)-optimal design is obtained by minimizing further with respect to \( w \), i.e., it can be obtained by solving the following optimization problem

\[
\begin{align*}
\text{minimize} & \quad \text{trace} \sigma_N^2 X \text{Diag}(w)^{-1}XT + H\Sigma H^T \quad (3) \\
\text{s.t.} & \quad AX + H = K^T, \quad w \geq 0, \quad \sum_{i=1}^m w_i = 1.
\end{align*}
\]

The objective function is convex, as it can be written as \( \|H\Sigma^{1/2}\|_F^2 + \sigma_N^2 \sum_i \frac{\|x_i\|^2}{w_i} \), where \( x_i \) is the \( i \)th column of \( X \in \mathbb{R}^{r \times m} \), which is the sum of a convex quadratic and the perspective functions \( (x_i, w_i) \mapsto \frac{\|x_i\|^2}{w_i} \) of \( x_i \mapsto \|x_i\| \); see [8]. We also point out that this problem can be reformulated as a second order cone program (SOCP); see [31].

For a fixed \( X \), consider the function \( J: w \mapsto \sum_{i=1}^m \frac{\|x_i\|^2}{w_i} \) from \( \mathbb{R}^m_+ \) to \( \mathbb{R} \cup +\infty \). We use the convention that \( \|x_i\|/0 = 0 \) whenever \( \|x_i\| = 0 \) for \( i = 1, \ldots, m \) which amounts to sum over indices with nonzero numerators:

\[
J: w \mapsto \sum_{i: \|x_i\| > 0} \frac{\|x_i\|^2}{w_i} \quad \text{and ensures that } J \text{ is well defined. We also assume that } \sum_{i} \|x_i\| > 0 \text{ so that } J \text{ is not constant. In this case, } J \text{ is minimized over the probability simplex for } w_i^* = \frac{\|x_i\|}{\sum_i \|x_i\|}, \quad i = 1, \ldots, m. \text{ In other words}
\]

\[
w^* \in \arg \min \left\{ J(w), \quad \text{s.t. } w_i \geq 0, \quad i = 1, \ldots, m, \quad \sum_{i=1}^m w_i = 1 \right\}. \quad (4)
\]

Since \( J \) is convex, this can be verified by checking the first order Karush-Kuhn-Tucker (KKT) conditions: note that \( w^* \) is feasible for (4) and \( F \) is differentiable at \( w^* \) and for all \( i = 1, \ldots, m \),

\[
\frac{\partial J(w)}{\partial w_i} \bigg|_{w=w^*} = \begin{cases} 
-\frac{\|x_i\|^2}{w_i^2} = -(\sum_i \|x_i\|)^2 & \text{if } w_i^* > 0; \\
0 & \text{otherwise.}
\end{cases} \quad (5)
\]
Equation (5) is precisely KKT optimality condition at $w^*$ for Problem (4) (see e.g. [5, Example 3.4.1]). Plugging the expression of $w^*$ into (3), we obtain the following problem:

$$\min_{X,H} \|H\Sigma^{1/2}\|_F^2 + \sigma_N^2 \left( \sum_i \|x_i\| \right)^2 \quad s.t. \quad XA + H = K^T.$$  

We can eliminate the variable $H$ from this problem, which leads to an unconstrained, convex optimization problem with a nice structure. We summarize our findings in the next proposition:

**Proposition 2.1.** Consider the optimization problem

$$\rho := \min_X \|(XA - K^T)\Sigma^{1/2}\|_F^2 + \sigma_N^2 \left( \sum_i \|x_i\| \right)^2.$$  

Then, $\rho$ is equal to the optimal value of Problem (1), and if $X^* = [x_1^*, \ldots, x_m^*]$ solves Problem (6), then the design defined by $w^*_i = \frac{\|x_i^*\|}{\sum_j \|x_j\|}$ is Bayes $A_K$-optimal.

If the square was removed from $\left( \sum_i \|x_i\| \right)^2$, this last term would be similar to a group lasso penalty [38]. From a practical perspective, the main interest of this reformulation is that it paves the way toward the use of well established first order methods to tackle such problems [1, 13, 3].

Interestingly, the idea of using a group lasso to design experiments has already been proposed in [33]. However, this paper justified the group lasso approach heuristically, in order to select the support points of an exact design. Indeed, group lasso regression was designed to recover an approximate solution of an equation of the form $\sum_i A'_i x_i \simeq y'$ with only a small number of nonzero blocks $x_i$. It is widely known that optimal designs often have a small number of support points, and hence correspond to an estimator $\hat{\theta} = Xy$ with many columns of $X$ equal to 0. Therefore, group lasso regression can be used to find sparse estimators that satisfy approximately the unbiasedness property: $XA \simeq K^T$. The result of Proposition (2.1) shows that in fact, one obtains an exact reformulation of the Bayes $A_K$-optimal design problem by squaring the penalty.

### 3 Convex analysis of the squared group lasso penalty

Throughout the rest of this article, we set for all $X \in \mathbb{R}^{r \times m}$ where, for each $i = 1, \ldots, m$, $x_i \in \mathbb{R}^n$ is the $i$th column of $X$:  

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\begin{itemize}
  \item $f : X \mapsto \|(XA - K^T)\Sigma^{1/2}\|^2_F$.
  \item The norm $\Omega : X \mapsto \sum_{i=1}^m \|x_i\|$ and its dual norm, $\Omega^* : X \mapsto \max_{i=1,...,m} \|x_i\|$.
  \item $g : \mathbb{R}^{r \times m} \mapsto \mathbb{R}$ with $g(X) = \frac{1}{2} \Omega(X)^2$.
\end{itemize}

We use the usual Euclidean scalar product on matrices. With these notations, problem \((6)\) may be rewritten as
\[
\min_X \quad F(X) := f(X) + 2 \sigma^2 g(X) \tag{7}
\]

Note that the function $g$ is convex and that the outer square destroys the separability of the inner sum in $g$, unlike standard group lasso penalty. This leads to non trivial optimization developments. The reader is referred to [27, 7] for detailed exposition of convex analysis related material.

**Lemma 3.1 (Subgradient and conjugate).** Let $g : \mathbb{R}^{r \times m} \mapsto \mathbb{R}$ be such that $g(X) = \frac{1}{2} \left( \sum_{i=1}^m \|x_i\| \right)^2$ where $x_i$ is the $i$th column of $X$. Then we have the following formula for the subgradient and the Legendre transform of $g$ denoted by $g^*$:
\[
\forall X \in \mathbb{R}^{r \times m}, \quad \partial g(X) = \left( \sum_{i=1}^m \|x_i\| \right) [v_1 v_2 ... v_m], \quad v_i \in \partial \|x_i\|, \quad i = 1, ..., m.
\]
\[
\forall Z \in \mathbb{R}^{r \times m}, \quad g^*(Z) = \frac{1}{2} \max_{i=1,...,m} \left\{ \|z_i\|^2 \right\}.
\]

**Proof.** We mostly follow [3] and provide detailed arguments. We set $\Omega : X \mapsto \sum_{i=1}^m \|x_i\|$ which is a norm. Its dual norm is $\Omega^* : Z \mapsto \max_{i=1,...,m} \|z_i\|$. Fix any $Z \in \mathbb{R}^{r \times m}$, we have for any $X \in \mathbb{R}^{r \times m},$
\[
\langle X, Z \rangle - g(X) \leq \Omega^*(Z)\Omega(X) - \frac{1}{2} \Omega(X)^2 \leq \frac{1}{2} \Omega^*(Z)^2.
\]

Setting $X = \Omega^*(Z)\partial \Omega^*(Z)$, we obtain $\Omega(X) = \Omega^*(Z)$ and $\langle Z, X \rangle = \Omega^*(Z)^2$ so that the above holds with equality. This entails that $g^* = \frac{1}{2} (\Omega^*)^2$ which is precisely the claimed formula for the conjugate function. Now symmetrically, for any fixed $X \in \mathbb{R}^{r \times m}$, setting $Z = \Omega(X)\partial \Omega(X)$ we obtain $\Omega^*(Z) = \Omega(X)$ and $\langle Z, X \rangle = \Omega(X)^2 = \frac{1}{2} (\Omega(X)^2 + \Omega^*(Z)^2)$ which shows by [27, Theorem 23.5] that $Z \in \partial g(X)$. The claimed form of the subgradient follows because $\Omega$ has a structure of separable sum, see [27, Theorem 23.8]. \hfill \Box
Algorithm 1 (prox-operator)

**Input:** $t, V$

**Output:** $\text{prox}_t g(V)$

1: Order the columns of $V$ by decreasing order of norm, such that $\|v_1\| \geq \cdots \geq \|v_m\|$ (store the corresponding permutation)
2: Make a binary search to find the largest $k \leq m$ such that $\frac{t}{tk+1} \sum_{i=1}^{k} \|v_i\| \geq t\|v_k\| + 1 \sum_{i=1}^{k} \|v_i\|$
3: Set $x_i = \left(1 - \frac{t}{tk+1} \sum_{j=1}^{k} \frac{\|v_j\|}{\|v_i\|}\right) v_i$, for $i = 1, \ldots, k$.
4: Set $X = [x_1, \ldots, x_k, 0, \ldots, 0] \in \mathbb{R}^{r \times m}$, and permute the columns according to the inverse permutation obtained from the first step.
5: return $X$

Given $t > 0$, the following lemma describes how to compute the proximity operator of $X \mapsto t g(X)$:

$$\text{prox}_t g(V) := \arg\min_X t \cdot g(X) + \frac{1}{2} \|X - V\|_F^2.$$ 

**Lemma 3.2** (Proximity operator). Let $V \in \mathbb{R}^{r \times m}$ and $v_i \in \mathbb{R}^n$ be its columns for $i = 1, \ldots, m$ and $t > 0$. Then Algorithm 1 computes $\text{prox}_t g(V)$.

**Proof.** First note that $k$ is well defined since the condition obviously holds for $k = 1$. Furthermore, for all $i \leq k$ we have $\|v_i\| \geq \|v_k\| \geq \frac{t}{tk+1} \sum_{j=1}^{k} \|v_j\|$. Note also that the proposed definition for $x_i$ ensures that $i > k$ for all $i$ such that $v_i = 0$ so that there is no division by 0 and $x_i = 0$ whenever $v_i = 0$.

We just need to check that $(V - X)/t \in \partial g(X)$. We have

$$\sum_{i=1}^{m} \|x_i\| = \sum_{i=1}^{k} \|v_i\| - \frac{kt}{tk+1} \sum_{j=1}^{k} \|v_j\| = \frac{1}{tk+1} \sum_{j=1}^{k} \|v_j\|.$$ 

We now consider several cases.

- If $i > k$ and $v_i = 0$, then $x_i = 0$ and $(v_i - x_i)/t = 0 \in \partial \|x_i\|$.
- If $i > k$ and $v_i \neq 0$, then $x_i = 0$ and it holds that $\frac{v_i}{\|v_i\|} \in \partial \|v_i\|$ and $\frac{v_i - x_i}{t} = \frac{v_i}{\|v_i\|} \left(\sum_{i=1}^{m} \|x_i\|\right)$.
- If $i \leq k$, then $\left(1 - \frac{t}{tk+1} \sum_{j=1}^{k} \frac{\|v_j\|}{\|v_i\|}\right) \geq 0$ and $v_i \neq 0$ so that $\frac{v_i}{\|v_i\|} \in \partial \|x_i\|$. We also have $\frac{v_i - x_i}{t} = \frac{v_i}{\|v_i\|} \left(\sum_{i=1}^{m} \|x_i\|\right)$. 


Algorithm 2 Forward-Backward with Backtracking line search

Input: $X_0 \in \mathbb{R}^{r \times m}$, $\eta > 1$, $L_0 > 0$

1: for $k = 1, 2 \ldots$ do
2:     Find the smallest $i \in \mathbb{N}$ such that, with $\bar{L} = \eta^i L_{k-1}$ and $P = \text{prox}_{2\sigma_N g/L} \left( X_{k-1} - \frac{1}{\bar{L}} \nabla f(X_{k-1}) \right)$,

\[ F(P) \leq f(X_{k-1}) + \langle \nabla f(X_{k-1}), P - X_{k-1} \rangle + 2\sigma_N g(P) + \frac{\bar{L}}{2} \|P - X_{k-1}\|^2 \]
3:     Set $L_k = \bar{L}$ and $X_k = P$

This shows that the proposed $X$ satisfies the subdifferential characterization in Lemma 3.1 and the result follows.

4 Algorithms

4.1 Proximal decomposition methods

In this section we describe convex optimization algorithms dedicated to structured “smooth plus nonsmooth” problems with easily computable proximity operator. Further details and historical comments are found in [13, 4, 3]. On the one hand, we have $\nabla f(X) = 2(A X - K^T) \Sigma A^T$. On the other hand, Lemma 3.2 ensures that $\text{prox}_{tg}(V)$, can be computed by Algorithm 1. These are the building blocks of proximal decomposition algorithms. We describe the backtracking line search variants of the Forward-Backward algorithm and FISTA algorithm. Backtracking line search ensures minimal parameter tuning beyond the initialization. One can use a fixed step size $1/L$ instead, where $L = \text{trace}(A \Sigma A^T)$ is the Lipschitz constant of $\nabla f$.

**Forward-Backward algorithm** : This is the simplest proximal decomposition algorithm. More details can be found in [13, 4]. Known properties for this algorithm include the following:

- The sequence $(X_k)_{k \in \mathbb{N}}$ converges to a solution of problem (7) and for any $X^*$ solution of the problem, the sequence $(\|X_k - X^*\|)_{k \in \mathbb{N}}$ is non increasing.

- The objective function $F(X_k)$ is monotonically decreasing along the
Algorithm 3 Fista with Backtracking line search

\textbf{Input:} \(X_0 \in \mathbb{R}^{r \times m}, \eta > 1, L_0 > 0, Y_1 = X_0, t_1 = 1.\)

1: for \(k = 1, 2, \ldots\) do
2: Find the smallest \(i \in \mathbb{N}\) such that, with \(\bar{L} = \eta^i L_{k-1}\) and \(P = \text{prox}_{2\sigma N g/L} \left(Y_k - \frac{1}{L} \nabla f(Y_k)\right),\)

\[F(P) \leq f(Y_k) + \langle \nabla f(Y_k), P - Y_k \rangle + 2\sigma N g(P) + \frac{\bar{L}}{2} \| P - Y_k \|_F^2\]

3: Set \(L_k = \bar{L}\) and \(X_k = P\) and \(t_{k+1} = \frac{1 + \sqrt{1 + 4 t_k^2}}{2}\) and

\[Y_{k+1} = X_k + \left(1 - \frac{t_k}{t_{k+1}}\right) (X_k - X_{k-1}).\]

sequence and we have for all \(k \in \mathbb{N},\)

\[F(X_k) - \rho \leq \frac{\eta L \| X_0 - X^* \|_F^2}{2k},\]

for any \(X^*\) solution to Problem \([7]\) (see \([4]\)). Here \(L = \text{trace}(A \Sigma A^T)\) is the Lipschitz constant of the gradient of \(f\) (with respect to Frobenius norm).

- For all \(k \in \mathbb{N}\), we have \(L_k \leq \max \{ L_0, \eta L \}\)

\textbf{FISTA acceleration:} It is known since the seminal work of Nesterov \([23]\) that \(O(1/k)\) is not optimal for convex optimization with gradient methods. Accelerated methods exist with a faster \(O(1/k^2)\) convergence rate. We now describe the FISTA algorithm \([4]\) which belongs to this family of methods and is applicable to problem \([7]\). Contrary to Forward Backward algorithm, FISTA algorithm does not provide a monotonically decreasing sequence of objective values, and convergence of the sequence \((X_k)\) is not known yet for this precise version, although it is for very close variants \([12]\). The main feature of FISTA is the following complexity estimate, for any \(k \in \mathbb{N},\)

\[F(X_k) - \rho \leq \frac{2\eta L \| X_0 - X^* \|_F^2}{(k + 1)^2},\]

for any \(X^*\) solution to Problem \([7]\) (see \([4]\)). Here \(L = \text{trace}(A \Sigma A^T)\) is the Lipschitz constant of the gradient of \(f\) (with respect to Frobenius norm).
The complexity of one iteration of either Forward-Backward or FISTA algorithm is dominated by the cost of computing \( \nabla f(X) = 2(XA - KT)\Sigma A^T \) which can be done in \( O(r \times n \times m) \) operations (this is the cost of multiplication of \( X \in \mathbb{R}^{r \times m} \) and \( A \in \mathbb{R}^{m \times n} \) and multiplying the result by \( \Sigma A^T \in \mathbb{R}^{n \times m} \)). For a typical situation with \( r = n \), this is \( O(n^2 m) \). The cost of computing the proximity operator is negligible.

### 4.2 Block coordinate descent

An alternative to solve the unconstrained optimization problem (6) is to iteratively solve the problem for one particular block \( x_i \), while keeping all other blocks fixed. This idea is attractive, because optimization over a single block admits a simple closed-form solution, as the following proposition shows.

**Proposition 4.1.** Let \( i \in [m] \), and let the \( x_j \)'s be a fixed vectors in \( \mathbb{R}^n \) (\( \forall j \in [m], j \neq i \)). We consider the variant of Problem (6) in which we minimize the criterion with respect to the block of variables \( x_i \) only, that is:

\[
\min_{x_i} h_i(x_i) := \|(x_i a_i^T + R)\Sigma^{1/2} + \sigma_N^2(\|x_i\| + \beta)^2, \quad (8)
\]

where \( R := \sum_{j \neq i} x_j a_j^T - KT \) and \( \beta = \sum_{j \neq i} \|x_j\| \). The optimal solution of this problem is given by \( x_i^* = 0 \) whenever \( R \Sigma a_i = 0 \) and otherwise,

\[
x_i^* = -\frac{1}{a_i^T \Sigma a_i + \sigma_N^2} \cdot \max \left\{ 1 - \sigma_N^2 \left( \frac{\beta}{\|R \Sigma a_i\|} \right), 0 \right\} \cdot R \Sigma a_i,
\]

**Proof.** We can rewrite the function to minimize as

\[
h_i(x_i) = a_i^T \Sigma a_i \|x_i\|^2 + 2x_i^T R \Sigma a_i + \|R \Sigma^{1/2}\|^2 + \sigma_N^2(\|x_i\| + \beta)^2.
\]

Expanding the square, the subgradient sum rule [27, Theorem 23.8] gives the following expression for the subgradient \( \partial(\|x\| + \beta)^2 = 2\partial(\|x\|)(\|x\| + \beta) \)

hence the subgradient of \( h_i \) has the following form:

\[
\partial h_i(x_i) = \begin{cases} 
2[(a_i^T \Sigma a_i)x_i + R \Sigma a_i + \sigma_N^2(\|x_i\| + \beta) \frac{x_i}{\|x_i\|}] & \text{if } x_i \neq 0; \\
2[R \Sigma a_i + \sigma_N^2 u] : \|u\| \leq \beta & \text{otherwise.}
\end{cases}
\]

It remains to show that \( 0 \in \partial h_i(x_i^*) \). If \( R \Sigma a_i = 0 \) then \( x_i = 0 \) and the statement holds. Assume that \( R \Sigma a_i \neq 0 \), we distinguish two cases.
Algorithm 4 Alternating Block Coordinate Descent

Input: $X_0 \in \mathbb{R}^{r \times m}$, and denote by $x_{i0}$, $i = 1, \ldots, m$, its columns

1: for $k = 1, 2 \ldots$ do
2:     Choose an integer $i \in \{1, \ldots, m\}$ (see the main text for different possibilities).
3:     Set $x_{ik} = -\frac{1}{a_i^T \Sigma a_i + \sigma_N^2} \cdot \max \left\{1 - \sigma_N^2 \frac{\beta}{\|R \Sigma a_i\|}, 0\right\} \cdot R \Sigma a_i$ where $R := \sum_{j \neq i} x_{j(k-1)} a_j^T - K^T$ and $\beta = \sum_{j \neq i} \|x_{j(k-1)}\|$
4:     Set $x_{jk} = x_{j(k-1)}$ for all $j \in \{1, \ldots, m\}$, $j \neq i$.

- If $(1 - \sigma_N^2 \frac{\beta}{\|R \Sigma a_i\|}) > 0$, then
  
  $x_i^* = -\frac{1}{a_i^T \Sigma a_i + \sigma_N^2} \cdot (1 - \sigma_N^2 \frac{\beta}{\|R \Sigma a_i\|}) \cdot R \Sigma a_i \neq 0$.

  Substituting in the expression of $\partial h_i$, easy (though lengthy) calculations shows that $\partial h(x_i^*) = \{0\}$.

- Otherwise, we have $\|R \Sigma a_i\| \leq \sigma_N^2 \beta$ and $x_i^* = 0$. To see that $0 \in \partial h_i(x_i^*)$, we need a vector $u$ such that $R \Sigma a_i + \sigma_N^2 u = 0$ and $\|u\| \leq \beta$. This works for $u = -\frac{1}{\sigma_N} R \Sigma a_i$.

Alternating minimization: Block coordinate methods are wide spread for large scale problems, see for example [34] for a recent overview. The idea is to update only a subset of variable at each iteration. The choice of the subset could be performed in various ways: at random with replacement, in a cyclic order, using random permutations. We describe the block minimization algorithm which is well suited for our problem thanks to Proposition 4.1. Implementing the alternating minimization algorithm requires to keep track of $X A \Sigma \in \mathbb{R}^{r \times n}$ (similarly as for computing $\nabla f$). Keeping track of this quantity when changing a single column can be done in $O(nr)$ operations. A full path through the $m$ columns can be done in $O(nrm)$ operations which is the same as for gradient based methods.

To our knowledge application of this algorithm to a problem of the form of (6) is new in the optimization literature. Indeed, alternating minimization and more generally block coordinate methods are not convergent in general, their use is limited to smooth problems or problems with a separable sum structure. This is not the case because of the square in the last term of (6).
To understand why block coordinate methods do not converge to global minima in general, consider the function \( \phi : (x, y) \mapsto \max \{ x + 2y, -2x - y \} \). Taking for any \( t > 0 \), \( x = t \) and \( y = -t \) and letting \( t \to \infty \) shows that \( \inf_{\mathbb{R}^2} \phi = -\infty \). Yet it can be checked that \( 0 = \arg \min_x \phi(x, 0) = \arg \min_y \phi(0, y) \) so that the origin is actually a stationary point for the alternating minimization algorithm applied to \( \phi \).

However problem (6) has an additional structure: the subgradient of its objective is a simple Cartesian product. Furthermore, partial minimization is strongly convex. Combining these properties leads to the following result which to our knowledge is new. This guaranty is weak, indeed, convergence of alternating minimization methods is a difficult matter for which only few results are known and virtually none outside of separable nonsmoothness.

**Proposition 4.2.** The alternating minimization algorithm applied to problem (6) with blocks taken in a cyclic order or using random permutations, produces a decreasing sequence of objective function value and satisfies \( F(X_k) \to \rho \) as \( k \to \infty \).

**Proof.** Monotonicity is obvious here, we denote by \( \hat{\rho} \) the limiting value of the objective function along the sequence. The Cartesian product structure of the subgradient of \( g \) in Lemma 3.1 entails that the subgradient of the objective of (6) has the same Cartesian product structure. This implies that if all the columns of \( X \in \mathbb{R}^{r \times m} \) are blockwise optimal for problem (6), then \( X \) itself is the global optimum. This is because block optimality ensures that \( 0 \) belongs to each partial subgradients in (8) and the global subgradient of (6) is the Cartesian product of the partial subgradients [28, Corollary 10.11].

Now the partial minimization in (8) is \( 2\sigma^2_N \)-strongly convex. Hence, for all \( k \in \mathbb{N} \),

\[
F(X_k) - F(X_{k+1}) \geq \sigma^2_N \|X_{k+1} - X_k\|^2.
\]

So \( \{\|X_{k+1} - X_k\|^2\}_{k \in \mathbb{N}} \) is summable and as \( k \to \infty \), we have \( \|X_{k+1} - X_k\| \to 0 \). By monotonicity \( \{X_k\}_{k \in \mathbb{N}} \) is a bounded sequence since the objective in (6) is coercive. Let \( \bar{X} \) be any accumulation point of the sequence (there exists at least one).

For cyclic or random permutation selections, since all blocks are visited every \( m \) iteration, using the notation of Proposition 4.1, by continuity of the objective function, one must have for all \( i = 1, \ldots, m \) that the quantity

\[
x_{ik} - \arg \min_{x_i} \| (x_i a_i^T R_k) \Sigma^{1/2}_i \|_F^2 + \sigma^2_N (\|x_i\| + \beta_k)^2 \quad \to_{k \to \infty} \quad 0,
\]
where \( R_k := \sum_{j \neq i} x_{jk} a_j^T - K^T \) and \( \beta_k = \sum_{j \neq i} ||x_{jk}|| \). By continuity \( \bar{X} \) must be blockwise optimal for (6) and hence global optimal so that \( \bar{\rho} = \rho \). \( \square \)

## 5 Numerical experiments

### 5.1 Instances

As was done in [20], we report numerical experiments on two kinds of instances to test the performance of proximal decomposition methods to solve Problem (6). On the one hand, we generate random instances by sampling the elements of \( A \in \mathbb{R}^{m \times n} \) independently from a standard normal distribution. On the other hand, we compute Bayes \( A \)-optimal designs for quadratic regression over \([-1,1]^d\):

\[
y(x) = \theta_0 + \sum_{i=1}^{d} \theta_i x_i + \sum_{1 \leq i \leq j \leq d} \theta_{ij} x_i x_j + \epsilon.
\]

So in practice, to construct the matrix \( A \) we first form a regular grid \( X = \{x_1, \ldots, x_m\} \subseteq [-1,1]^d \), and for each \( k \in [m] \) the \( k \)th row of \( A \) is set to

\[
a_k^T = [1, (x_{ki})_{k=1, \ldots, d}, (x_{ki} x_{kj})_{1 \leq i \leq j \leq d}] \in \mathbb{R}^n,
\]

where \( n = 1 + d + d(d + 1)/2 \). In addition, for all our experiments, we set \( K = \Sigma = I_n \), and \( \sigma_N^2 = 0.01 \).

### 5.2 Algorithms

We present results for the two proximal decomposition methods with backtracking line search presented in Section 4.1, which we denote by FB (for Forward-Backward) and FISTA. We also used two variants of the alternating block coordinate descent algorithm of 4.2, where blocks are selected in a fixed cyclic order (ABCD-cy), or according to a new random permutation that is drawn at random every \( m \) steps (ABCD-rp).

We compare these methods to a Fedorov-Wynn type vertex-direction method (VDM), which is, in fact, an adaptation of the celebrated Frank-Wolfe algorithm for constrained convex optimization [17]. Several variants exist to compute the step sizes \( \alpha \) of this algorithm, in particular, optimal step length can be used, see [20]. However, no simple formula exists for the optimal step lengths in the case of Bayes \( A \)-optimality, so we next describe a method with backtracking line search, which also allows a more straightforward comparison with FB and FISTA.
Algorithm 5 Vertex Direction Method with Backtracking line search

**Input:** $\eta > 1$, $L_0 > 1$, $w_0 \in \Delta$

1: for $k = 1, 2 \ldots$ do
2: \hspace{1em} Compute the vector $d$ with elements $d_i = \frac{1}{\sigma_N^2} \| K^T M_N(w_{k-1})^{-1} a_i \|^2$.
3: \hspace{1em} Select $i^* \in \text{arg max}_i \{d_i\}$.
4: \hspace{1em} Find the smallest $j \in N$ such that, with $\bar{L} = \eta^j L_{k-1}$, $\alpha = \frac{1}{\bar{L}}$ and $\bar{w} = (1 - \alpha)w_{k-1} + \alpha e_{i^*}$,
\[ \Phi_{A_K}(\bar{w}) \leq \Phi_{A_K}(w_{k-1}) - d^T(\bar{w} - w_{k-1}) + \frac{\bar{L}}{2} ||\bar{w} - w_{k-1}||^2. \]
5: \hspace{1em} Set $L_k = \bar{L}$ and $w_k = \bar{w}$.

We will also compare to the multiplicative algorithm [32] (MUL), where at each iteration, we set
\[ (d_k)_i = -\frac{\partial \Phi_{A_K}(w_k)}{\partial w_i} = \frac{1}{\sigma_N^2} \| K^T M_N(w_k)^{-1} a_i \|^2, \quad (9) \]
and we perform the update $w_{k+1} = w_k \odot d_k$; here, the symbol $\odot$ is used for the Hadamard (elementwise) product of two vectors.

For both VDM and MUL, the cost of one iteration is dominated by the cost of computing $d = -\nabla \Phi$ which requires the inversion of $M_N(w)$ with computational cost $O(n^3)$ and multiplication by $A^T$ which cost is $O(n^2 \times m)$ and dominates the overall cost of this gradient computation.

For all algorithms, we used the constants $\eta = 2$ and $L_0 = 1$ for backtracking line searches. The initial designs were set to $w_0 = \frac{1}{m} 1_m$ for VDM and MUL, and we used the initial matrix $X_0 = 0 \in \mathbb{R}^{r\times m}$ for the other algorithms.

In our experiments, $K$ is taken to be the identity so that all the algorithms have iteration complexity of order $O(n^2 m)$ and thus comparing the evolution of the cost along iterations of each algorithm provides a good intuition about their comparative performances. Note that for ABCD-cy and ABCD-rp, we consider that one iteration is complete after going through a full cycle so that all the entries of $X$ are updated.

5.3 Results

To monitor the speed of convergence of the algorithms, we can compute the design efficiencies
\[ \text{eff}_{A_K}(w_k) := \frac{\rho}{\Phi_{A_K}(w_k)}, \]
where $\rho = \inf_{w^* \in \Delta} \Phi_{A_k}(w^*)$ was computed by letting the multiplicative algorithm run for a very long time. On the graphics, we plot the quantity $\log_{10}(1 - \text{eff}_{A_k}(w_k))$, so a value of $-k$ corresponds to an efficiency of $1 - 10^{-k}$.

We will also use the following optimality measure:

$$s_k = \max_{i=1,\ldots,m} (d_k)_i - w_k^T d_k,$$

where $d_k$ is the gradient of $-\Phi_{A_k}$ at $w_k$, see [9]. It is folklore (see [25]) that this expression gives a duality bound on the efficiency of the design $w_k$: $\text{eff}_{A_k}(w_k) \geq 1 - \varepsilon_k$, where $\varepsilon_k := \frac{s_k}{\Phi_{A_k}(w_k) + s_k}$. Furthermore, for any sequence $(w_k)_{k \in \mathbb{N}}$ of designs converging to an optimal design $w^*$, it is known that $s_k$ converges to 0, so the lower bound $1 - \varepsilon_k$ on the design efficiency converges to 1. The algorithms FB, FISTA and ABCD do not directly involve iterates $w_k$, but we can compute the above efficiency bound by setting $w_k = \|x_k\|/\Omega(X)$.

Another important measure of a design’s quality is its sparsity. It is well
known that optimal designs are supported by a few points only, which is a desired property for many applications. The problem formulation (6) gives a new explanation for this fact, as the penalty term $\Omega(X)$ is added in group lasso regression in order to induce block sparsity, so we expect the optimal matrix $X^*$ to have a lot of columns equal to 0 (the squared penalty term $g(X) = \frac{1}{2} \Omega(X)^2$ is also known to be block-sparsity inducing, cf. [2]).

A remarkable property of the proximal decomposition methods presented in this article is that $\text{prox}_\delta V$ acts as a thresholding operator on $V$, literally zeroing a lot of columns. The same is true for alternating block coordinate descent methods, in which whole columns are set to 0 if a certain threshold property holds. As a result, the iterates produced by FB, FISTA, ABCD-cy and ABCD-rp are expected to have a small support. To observe this fact, we measure the sparsity of a design by $\delta_{0.01}(w_k)$, the number of coordinates of
$w_k$ exceeding the value $\frac{0.01}{m}$.

The evolution of the efficiency, the duality bound $1 - \varepsilon_k$, and the support size during the 5000 first iterations of each algorithm is depicted in Figure 1 and Figure 2 for four random and quadratic regression instances of various sizes. As already mentioned, all the algorithms we compare have a complexity of $O(n^2m)$ per iteration. It is therefore possible to get a rough idea of their comparative computational efficiency from an iteration-based performance analysis. Performing a more precise time-based analysis depends on optimization of the linear algebra operations required for each algorithm and is beyond the scope of this work, so we stick to iteration-based analysis.

We observe several properties of the new algorithms on these figures. First, the effect of acceleration can clearly be seen on the figures, as FISTA always beats VDM, while the simple forward-backward algorithm FB is typically outperformed. As explained in Section 4.1, this comes at the price of FISTA not being a descent method, which can also be observed on the plots, especially for the quadratic regression instances (Figure 2). Second, MUL is performing in general better than other algorithms, closely followed by alternating minimization methods. The performance of the remaining algorithm is in general bellow. These preliminary results suggest that the group lasso formulation of the experimental design problem has the potential to help deciphering powerful algorithms for the later problem. In particular, the alternating block coordinate descents exhibit a nice linear convergence on many instances. Pushing further would requires to look more carefully at the implementation details of each algorithms and perform much larger scale experiments which is beyond the scope of this paper. Many upgrades and improvements also have to be evaluated, e.g. preconditioning, clever subsampling of the blocks to be updated at each iteration. Third, the support plots show that FISTA and ABCD quickly converge to a sparse solution. MUL also quickly identifies a design with a small support. We recall that the iterates of FISTA and ABCD are truly sparse, while for MUL, this is only a numerical sparsity, as the iterates $w_k$ remain strictly positive. On the other hand VDM always fail to identify a smaller support. Finite time identification of sparsity patterns is an active topic of research in nonsmooth optimization and we believe that this property can be exploited to yield high-performance algorithms to solve very large scale optimal design problems.
6 Conclusion

This paper presents a strong, previously unrevealed connection between two standard problems in statistics (Bayes A-optimal design and group lasso regression), hence clearing the path to a convergence of algorithms used in the communities of optimal design of experiments and machine learning. While the new methods presented in this article are not yet competitive with other algorithms for computing optimal designs over a finite design space, they certainly present interesting features, such as sparse iterates and a guaranteed speed of convergence, and we believe that there is still an important room for improvement, e.g. by using recent techniques based on subsampling oracles [21] or lazy separators [9]. Conversely, an interesting perspective is to use well established techniques of optimal experimental design, such as methods to restrict the set of potential support points of an optimal design [24], to improve algorithms that were designed to solve group lasso regressions.

Another topic for further research is whether we can reformulate other design problems (such as the D-optimal design problem, or problems with constraints on the design weights) as unconstrained convex optimization problems.

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