A sub-sampling algorithm preventing outliers

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August 15, 2022

Abstract

Nowadays, in many different fields, massive data are available and for several reasons, it might be convenient to analyze just a subset of the data. The application of the D-optimality criterion can be helpful to optimally select a subsample of observations. However, it is well known that D-optimal support points lie on the boundary of the design space and if they go hand in hand with extreme response values, they can have a severe influence on the estimated linear model (leverage points with high influence). To overcome this problem, firstly, we propose an unsupervised “exchange” procedure that enables us to select a “nearly” D-optimal subset of observations without high leverage values. Then, we provide a supervised version of this exchange procedure, where besides high leverage points also the outliers in the responses (that are not associated to high leverage points) are avoided. This is possible because, unlike other design situations, in subsampling from big datasets the response values may be available.

Finally, both the unsupervised and the supervised selection procedures are generalized to I-optimality, with the goal of getting accurate predictions.
1 Introduction

Recently, the theory of optimal design has been exploited to draw a subsample from huge datasets, containing the most information for the inferential goal; see for instance, [4, 9, 10, 3] among others. Unfortunately, Big Data sets usually are the result of passive observations, so some high leverage values in the covariates and/or outliers in the response variable (denoted by Y) may be present. The most commonly applied criterion is the D-optimality. It is well known that D-optimal designs tend to lie on the boundary of the design region thus in presence of high leverage values, all of them would be selected. Since this circumstance could have a severe influence on the estimated linear model (leverage points with high influence), in this study we propose an “exchange” procedure to select a “nearly” D-optimal subset which does not include the high leverage values. Avoiding high leverage points, however, does not guard from all the outliers in Y. Therefore, we also modify the previous method to exploit the information about the responses and avoid the selection of the abnormal Y-values. The first proposal is an unsupervised procedure, as it is not based on the response observations, while the latter is a supervised exchange method. Finally, both these exchange algorithms are extended to the I-criterion, which aims at providing accurate predictions in a set of covariate-values.

After introducing methodology and notation in Section 2, in Section 3 we introduce the novel modified exchange algorithm to obtain both a noninformative and an informative D-optimal sample without outliers. Moreover an approach for the initialization of the above algorithms is proposed. In Section 4 we adapt our proposal to the I-optimal criterion with the goal of selecting a subsample to get accurate predictions. Finally in Section 5 we perform some simulations which serve as motivation for the problem presented in this paper.

2 Notation and motivation of the work

Assume that N independent responses have been generated by a super-population model

\[ Y_i = \mathbf{x}_i^\top \beta + \varepsilon_i, \quad i = 1, \ldots, N, \]

where \( \mathbf{x}_i^\top \) denotes transposition, \( \beta = (\beta_0, \beta_1, \ldots, \beta_k)^\top \) is a vector of unknown coefficients, \( \mathbf{x}_i^\top = (1, \tilde{\mathbf{x}}_i^\top) \) where \( \tilde{\mathbf{x}}_i = (x_{i1}, \ldots, x_{ik})^\top \), for \( i = 1, \ldots, N \), are
The population under study is denoted by $U = \{1, \ldots, N\}$. Let $s_n \subseteq U$ denotes a sample without replications of size $n$ from $U$ (i.e. a collection of $n$ different indices from $U$). Herein we describe a new sampling method from a given dataset $D$ with the goal of selecting $n$ observations ($k < n << N$) which produce an efficient estimate of the model coefficients even in the presence of outliers.

Given a sample $s_n = \{i_1, \ldots, i_n\}$, let $X$ to be the $n \times (k+1)$ matrix whose rows are $x_i^T$, for $i \in s_n$, and let $Y = (Y_{i_1}, \ldots, Y_{i_n})^T$ be the $n \times 1$ vector of the sampled responses. We consider the OLS estimator of the coefficients of the linear model based on the sample $s_n$:

$$
\hat{\beta} = \hat{\beta}(s_n) = (X^T X)^{-1} X^T Y
$$

where

$$
I_i = \begin{cases} 
1 & \text{if } i \in s_n \\
0 & \text{otherwise} 
\end{cases}
$$

with $i = 1, \ldots, N$ denotes the sample inclusion indicator.

To improve the precision of $\hat{\beta}$, we suggest to select the sample $s_n$ according to $D$-optimality. We denote the $D$-optimum sample as

$$
s_n^* = \arg \sup_{s_n = \{I_1, \ldots, I_N\}} \left| \sum_{i=1}^{N} x_i x_i^T I_i \right|^2.
$$

Since the $D$-optimal support points usually lie in the boundary of the experimental region, when the dataset $D$ contains high leverage points, $s_n^*$ includes them and if they are associated to abnormal responses they may produce a non-reliable estimate. Example 1 shows how the outliers are selected by the $D$-optimal sample.

**Example 1.** An artificial dataset $D$ with $N = 10000$ observations has been generated from a simple linear model,

$$
Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad i = 1, \ldots, N,
$$
The left-hand side of Figure 1 displays these last 10 observations in red, while the majority of the data, generated from the first distribution, are displayed in black. The right-hand side of Figure 1 emphasises the D-optimal subsample of size $n = 100$, $s^*_n$, displaying its support points in blue. As expected, all the abnormal values in $X$ are included in $s^*_n$ because they maximize the determinant of the information matrix ($s^*_n$ has been obtained by applying the function od_KL of the R package OptimalDesign [8]).

To avoid the outliers when applying D-optimal subsampling, we propose a modification of the well known exchange algorithm. Before describing our proposal, we recall that an observation $x_i$ with $i = 1, \ldots, n$ is called a high leverage point when its leverage value $h_{ii} = x_i^\top (X^\top X)^{-1} x_i$ is greater than a threshold, i.e.

$$h_{ii} > \nu_1 \frac{k + 1}{n}$$
where $\nu_1$ is a tuning parameter usually set equal to 2 [6].

A high leverage point can be either good or bad: if its associated response is “abnormal”, it is bad because, in this case, it might alter the model fitted by the bulk of the data; otherwise, if the response is not an outlier, the high leverage point is good because it would reduce the variance of the parameters’ estimates.

3 Modified Exchange Algorithms

The common structure of the $t$-th iteration of an exchange algorithm consists in adding a point $x_{j_a}$ (chosen from a list of candidate points $C^{(t)}$) to the available sample $s_{n}^{(t-1)}$ and then delete a point from it. The choice of the augmented and deleted points is based on the achievement of some optimality criterion. For D-optimality, the augmented observation $x_{j_a}$ is the $x$-value of the unit with the largest prediction variance,

$$j_a = \arg \max_{j \in C^{(t)}} x_j^T (X^T X)^{-1} x_j,$$

and is chosen from the experimental domain, if replications are admitted, or from the complementary space of $s_{n}^{(t-1)}$, if it is not. The deleted point is that with the smallest prediction variance, i.e. with the smallest leverage value $h_{ii}$, $i = 1, \ldots, n+1$ (see Chp. 12 in [1]). Our main idea is to modify the algorithm in such a way that points with high leverage scores are not proposed for the exchange, avoiding the dangerous combination of high leverage scores and abnormal responses. This goal is reached: a) by switching the augmentation and deletion steps; b) by changing the set $C^{(t)}$ where the observation to be added is searched.

In step b), if the information about the responses is not used to identify the set $C^{(t)}$, then the modified D-optimal sample is non-informative for the parameters of interest. This unsupervised procedure is described in detail in Subsection 3.1.

Avoiding high leverage points, however, does not guard from all the outliers in $Y$; points may be present which are in the core of the data wrt the auxiliary variables but are abnormal wrt the response variable. In Subsection 3.2 we propose a supervised version of the algorithm, where in step b) we exploit the response values to remove the outliers in $Y$. Let us note that the obtained optimal sample becomes informative because it depends on the responses.
3.1 Noninformative D-optimal samples without high leverage points

Let \( s_n^{(0)} \) be an initial sample of size \( n \), which does not include high leverage points. At the end of this section we describe a method for getting such an initial sample.

Let \( C^{(t)} \) be a set of candidate points for the exchange at the current iteration and let \( X_t \) be the design matrix associated to the sample \( s_n^{(t)} \). To update \( s_n^{(t)} \), firstly we remove from it the unit \( i_m \) with the smallest prediction variance, i.e.
\[
i_m = \arg \min_{i \in s_n^{(t)}} h_{ii};
\]
let \( X_t^- \) denote the design matrix obtained by omitting the row \( x_{im} \) from \( X_t \). Subsequently, we add the unit \( j_a \in C^{(t)} \) which presents the largest prediction variance \( x_j^\top (X_t^-^\top X_t^-)^{-1}x_j \), where
\[
C^{(t)} = \left\{ j : h_{im} < h_{im} (x_j) < \nu_1 \frac{k + 1}{n}, \right\}
\]
and \( h_{im} (x_j) \) is the leverage score obtained exchanging \( x_{im} \) with \( x_j \) for \( j \in \{U - s_n^{(t)}\} \). For computational purposes, let us note that from Saerle (1982, p.153)
\[
(X_t^-^\top X_t^-)^{-1} = (X_t^\top X_t)^{-1} + (X_t^\top X_t)^{-1} \frac{x_{im} x_{im}^\top}{1 - x_{im}^\top (X_t^\top X_t)^{-1} x_{im}} (X_t^\top X_t)^{-1}
\]
in addition, the next theorem provides an analytical expression for \( h_{im} (x_j) \).

**Theorem 3.1.** Let \( \tilde{X}_t \) be the design matrix obtained from \( X_t \) exchanging \( x_{im} \) with \( x_j \), then
\[
h_{im} (x_j) = x_j^\top (\tilde{X}_t^\top \tilde{X}_t)^{-1} x_j
\]
where
\[
(\tilde{X}_t^\top \tilde{X}_t)^{-1} = (X_t^\top X_t)^{-1} - (X_t^\top X_t)^{-1} \frac{A}{d} (X_t^\top X_t)^{-1},
\]
and
\[
\nu_1, n, k, (X_t^\top X_t)^{-1}
\]
with

\[
A = x^T_{im} (X^T_t X_t)^{-1} x_j (x_j x^T_{im} + x_{im} x^T_j) + [1 - x^T_{im} (X^T_t X_t)^{-1} x_{im}] x_j x^T_j + [1 + x^T_j (X^T_t X_t)^{-1} x_j] x_{im} x^T_{im};
\]

\[
d = [1 - x^T_{im} (X^T_t X_t)^{-1} x_{im}] [1 + x^T_j (X^T_t X_t)^{-1} x_j] + [x^T_{im} (X^T_t X_t)^{-1} x_j]^2.
\]

Proof. Expression (4) can be obtained from Lemma 3.3.1 in Fedorov (1972) after some cumbersome algebra.

In force of the upper bound in (1), our proposal is to consider as candidates for the exchange only observations in \( U - s^{(t)}_n \) which are not high leverage points. In addition, to speed up the algorithm we reduce the number of exchanges by imposing the lower bound in (1). Without this lower bound, whenever \( h_{im,i} (x_j) \leq h_{im,i} \), the new observation \( j \) would be immediately removed at the subsequent step of the algorithm.

Algorithm 1 describes in detail all the steps to select a D-optimal sample without high leverage points; instead Algorithm 2 illustrates how to select an initial sample \( s^{(0)}_n \) to start Algorithm 1.

### 3.2 Informative D-optimal sample without outliers

The previous exchange algorithm can be applied whenever the response values are not observed (for instance, if it is expensive to measure \( Y \)); this selection procedure protects against potential outliers in \( Y \) that are associated with the high leverage points in the factor-space. However, if the response values are available, then this information can be exploited by the exchange algorithm to avoid all the outliers in \( Y \), obtaining an informative D-optimal subsample.

According to [2] an influential data point is an observation that strongly influences the fitted values. To identify these influential data points, Cook’s distance may be applied. In fact, Cook’s distance for the \( i \)-th observation, \( C_i \), measures how much all of the fitted values in the model change when the \( i \)-th data point is deleted:

\[
C_i = \frac{(\hat{Y} - \hat{Y}_{(i)})^T (\hat{Y} - \hat{Y}_{(i)})}{(k + 1)\hat{\sigma}^2},
\]

\[
= \frac{(Y_i - \hat{Y}_i)^2}{(k + 1)\hat{\sigma}^2} \cdot \frac{h_{ii}}{(1 - h_{ii})^2}, \quad i = 1, \ldots, n.
\]
Algorithm 1: Non-informative D-optimal sample without high leverage points

**Input:** Dataset $D$, sample size $n$, initial sample $s^{(0)}_n$, $\nu_1$

**Output:** D-optimal sample without high leverage points

1. Set $t = 0$;
2. while $t < t_{\text{max}}$ do
3. Compute the leverage scores for the current sample
   \[ h_{ii} = x_i^\top (X_t^\top X_t)^{-1} x_i, \]
   where $X_t$ is the $n \times k$ matrix whose rows are $x_i$ with $i \in s^{(t)}_n$;
4. Identify unit $i_m = \arg \min_{i \in s^{(t)}_n} h_{ii}$;
5. Compute
   \[ (X_t^{-\top} X_t)^{-1} = (X_t^\top X_t)^{-1} + \frac{x_{im} x_{im}^\top}{1 - x_{im}^\top (X_t^\top X_t)^{-1} x_{im}} (X_t^\top X_t)^{-1}; \]
6. Select randomly $\tilde{N} \leq N - n$ units from \( \{ U - s^{(t)}_n \} \). Let $x_j$ with $j = 1, \ldots, \tilde{N}$, the observations for these units;
7. From (4), compute $(\tilde{X}_t^\top \tilde{X}_t)^{-1}$ and determine the leverage scores
   \[ h_{im}^{(t)}(x_j) = x_j^\top (\tilde{X}_t^\top \tilde{X}_t)^{-1} x_j; \]
8. Identify the set of candidate points for the exchange with $i_m$:
   \[ C^{(t)} = \{ j : h_{im}^{(t)}(x_j) < h_{im}^{(t)} < \nu_1 \frac{k+1}{n} \}; \]
9. Select from $C^{(t)}$ the observation $j_a = \arg \max_{j \in C^{(t)}} x_j^\top (X_t^{-\top} X_t)^{-1} x_j$;
10. Update $s^{(t)}_n$ by replacing unit $i_m$ with $j_a$, to form $s^{(t+1)}_n$;
11. Set $t = t + 1$;
12. end

**Remark.** In step 6 it is reasonable to consider $\tilde{N} = N - n$ whenever $N$ is not too large.

where $\hat{Y} = X \hat{\beta}^\top$, $\hat{\sigma}^2$ is the residual mean square estimate of $\sigma^2$ and $\hat{Y}_{(i)} = X \hat{\beta}_{(i)}^\top$ is the vector of predicted values when the $i$-th unit is removed from the data set $D$.

A general practical rule is that any observation with a Cook’s distance larger than $4/n$ may be considered an influential point.

When the response values are available, Algorithm 1 can be improved by
Algorithm 2: Initialization step for Algorithm 1

**Input:** Dataset $D$, sample size $n$, $\nu_2$

**Output:** $s_n^{(0)}$: initial sample without high leverage points

1. From $U$ select without replacement a simple random sample of size $n$, $r_n^{(0)}$, and set $t = 0$;
2. while $t < t_{\text{max}}$ do
3.   Compute the leverage scores for the current sample $h_{ii} = x_i^\top (X_t^\top X_t)^{-1} x_i$, where $X_t$ is the $n \times k$ matrix whose rows are $x_i^\top$ with $i \in r_n^{(0)}$;
4.   Identify unit $i_m = \arg \max_{i \in s_n^{(t-1)}} h_{ii}$;
5.   if $h_{im} < \nu_2 \frac{k+1}{n} + 1$ then
6.     set $s_n^{(0)} = r_n^{(0)}$ and stop the iterative procedure;
7.   else
8.     Select randomly $\tilde{N} \leq N - n$ units from $\{U - r_n^{(t)}\}$. Let $x_j$, with $j = 1, \ldots, \tilde{N}$, the observations for these units. From (3), compute $h_{im}(x_j)$ and identify the set of points candidate for the exchange with $i_m$:
9.     $C(t) = \{ j : h_{im}(x_j) < \nu_2 \frac{k+1}{n} \}$;
10.    Select at random a unit $j_a$ from $C(t)$;
11.   Determine $r_n^{(t+1)}$ by replacing unit $i_m$ with $j_a$ in $r_n^{(t)}$;
12.   Compute $(X_{t+1}^\top X_{t+1})^{-1}$ by applying (4) which is based on $(X_t^\top X_t)^{-1}$;
13.    Set $t = t + 1$;
14. end

**Remark.** In step 8 it is reasonable to consider $\tilde{N} = N - n$ whenever $N$ is not too large.

removing the influential points from the set $C(t)$ of the data candidate for the exchange, as illustrated in Algorithm 3 (for the computation of Cook’s distance, expression [5] is used to reduce the computational burden).
Algorithm 3: Informative D-optimal sample without outliers: additional steps to be included between 9 and 10 in Algorithm 1

Input: Dataset $D$, sample size $n$
Output: Informative D-optimal sample without outliers

1. Compute Cook’s distance for unit $j_a$, $C_{j_a}$, from (5);
2. if $C_{j_a} < 4/n$ then
3. accept the exchange and go to step 10 of Algorithm 1
4. else
5. reject the exchange; remove unit $j_a$ from $C^{(t)}$ and go back to step 9 of Algorithm 1
6. endif

4 Optimal subsampling to get accurate predictions

In the previous section we aim at selecting a subsample with the goal of getting a precise estimation of the parameters. Differently, if we are interested in obtaining accurate predictions on a set of values $X_0 = \{x_{01}, \ldots, x_{0N_0}\}$, then we should select the observations minimizing the overall prediction variance. Let $\hat{Y}_{0i} = \hat{\beta}^\top x_{0i}$ be the prediction of $\mu_{0i} = E(Y_{0i}|x_{0i})$ at $x_{0i}$, $i = 1, \ldots, N_0$. The prediction variance at $x_{0i}$, also known as “mean squared prediction error” is

$$\text{MSPE}(\hat{Y}_{0i}|x_{0i}, X) = E[(\hat{Y}_{0i} - \mu_{0i})^2|x_{0i}, X].$$

If $X_0$ is the $N_0 \times k$ matrix whose $i$-th row is $x_{0i}^\top$, then a measure of the overall mean squared prediction error is the sum of the prediction variances in $X_0$:

$$\sum_{i=1}^{N_0} \text{MSPE}(\hat{Y}_{0i}|x_{0i}, X) = \sigma^2 \text{trace}[X_0(X^\top X)^{-1}X_0^\top]$$

$$= \sigma^2 \text{trace}\left(\sum_{i=1}^{N} x_i x_i^\top I_i\right)^{-1} X_0^\top X_0,$$

$I_i = \begin{cases} 1 & \text{if } i \in s_n \\ 0 & \text{otherwise} \end{cases}$ (6)

with $l = 1, \ldots, N$. In this context, the I-optimal sample should be selected, which minimizes the overall prediction variance (6):

$$s_n^I = \arg \inf_{s_n = \{I_1, \ldots, I_N\}} \text{trace}\left(\sum_{i=1}^{N} x_i x_i^\top I_i\right)^{-1} X_0^\top X_0.$$
If we also aim at preventing outliers, then we have to modify the deletion and augmentation steps of the exchange algorithm described in Section 3.1 accordingly to the $I$-criterion. By taking into account the results given in Appendix A of Meyer and Nachtsheim (1995), the current sample $s_{n}^{(t)}$ should be updated by removing the unit $i_{m}$ which minimises

$$
\tilde{h}_{ii} = \frac{x_{i}^{T}(X_{t}^{T}X_{t})^{-1}X_{0}^{T}X_{0}(X_{t}^{T}X_{t})^{-1}x_{i}}{1 - x_{i}^{T}(X_{t}^{T}X_{t})^{-1}x_{i}},
$$

where $X_{t}$ is the $n \times k$ matrix whose rows are $x_{i}^{T}$ with $i \in s_{n}^{(t)}$.

Subsequently, from a set $C^{(t)}$ of candidate points, we should add the unit

$$
j_{a} = \arg \max_{j \in C^{(t)}} \frac{x_{j}^{T}(X_{t}^{T}X_{t})^{-1}X_{0}^{T}X_{0}(X_{t}^{T}X_{t})^{-1}x_{j}}{1 + x_{j}^{T}(X_{t}^{T}X_{t})^{-1}x_{j}},
$$

where $X_{t}^{-}$ is the design matrix obtained by removing the row $x_{im}$ from $X_{t}$ and $(X_{t}^{T}X_{t})^{-1}$ can be computed from (2). The set of candidate points should be formed by units that are not immediately removed in the subsequent step of the procedure and also are not high leverage points; therefore, $C^{(t)}$ is

$$
C^{(t)} = \left\{ j : \tilde{h}_{imim}(x_{j}) > \tilde{h}_{imim} \cap \tilde{h}_{imim}(x_{j}) < \nu_{1} \frac{k + 1}{n} \right\}
$$

where

$$
\tilde{h}_{imim}(x_{j}) = \frac{x_{j}^{T}(\tilde{X}_{t}^{T}\tilde{X}_{t})^{-1}X_{0}^{T}X_{0}(\tilde{X}_{t}^{T}\tilde{X}_{t})^{-1}x_{j}}{1 - x_{j}^{T}(\tilde{X}_{t}^{T}\tilde{X}_{t})^{-1}x_{j}},
$$

$$
h_{imim}(x_{j}) = x_{j}^{T}(\tilde{X}_{t}^{T}\tilde{X}_{t})^{-1}x_{j},
$$

$\tilde{X}_{t}$ is the matrix obtained from $X_{t}$ by exchanging $x_{im}$ with $x_{j}$ and $(\tilde{X}_{t}^{T}\tilde{X}_{t})^{-1}$ can be computed from (4).

5 Numerical studies

5.1 Simulation results

In this section, we evaluate the performance of our proposals through a simulation study. We start from the random generation of $H = 30$ datasets of size $N = 10^6$, each one including $N_{2} = 500$ high leverage points/outsiders.
Algorithm 4: Non-informative I-optimal sample without high leverage points

**Input:** Dataset $D$, sample size $n$, initial sample $s_n^{(0)}$, prediction-set $X_0 = \{x_{01}, \ldots, x_{0N_0}\}$, $\nu_1$

**Output:** I-optimal sample without high leverage points

1. Set $t = 0$;
2. while $t < t_{\text{max}}$ do
3. For the current sample, compute
   $$\tilde{h}_{ii} = \frac{x_i^T (X_t^T X_t)^{-1} X_0^T X_0 (X_t^T X_t)^{-1} x_i}{1 - x_i^T (X_t^T X_t)^{-1} x_i},$$
   where $X_t$ is the $n \times k$ matrix whose rows are $x_i^T$ with $i \in s_n^{(t)}$ and $X_0$ is the $N_0 \times k$ matrix whose rows are the elements of $X_0$;

4. Identify unit $i_m = \arg\min_{i \in s_n^{(t)}} \tilde{h}_{ii}$;

5. Compute
   $$(X_t^T X_t)^{-1} = (X_t^T X_t)^{-1} + \frac{(X_t^T X_t)^{-1} x_{im}^T (X_t^T X_t)^{-1}}{1 - x_{im}^T (X_t^T X_t)^{-1} x_{im}};$$

6. Select randomly $\tilde{N} \leq N - n$ units from $\{U - s_n^{(t)}\}$. Let $x_j$, with $j = 1, \ldots, \tilde{N}$, the observations for these units;

7. From (4) compute $(\tilde{X}_t^T \tilde{X}_t)^{-1}$ and determine the leverage scores
   $$h_{im,im}(x_j) = x_j^T (\tilde{X}_t^T \tilde{X}_t)^{-1} x_j$$ and
   $$\tilde{h}_{im,im}(x_j) = x_j^T (\tilde{X}_t^T \tilde{X}_t)^{-1} X_0^T X_0 (\tilde{X}_t^T \tilde{X}_t)^{-1} x_j;$$

8. Identify the set of candidate points for the exchange with $i_m$:
   $$C^{(t)} = \left\{j : \tilde{h}_{im,im}(x_j) > \tilde{h}_{im,im} \cap h_{im,im}(x_j) < \nu_1 \frac{k+1}{n}\right\};$$

9. Select from $C^{(t)}$ the observation
   $$j_a = \arg\max_{j \in C^{(t)}} \frac{x_j^T (X_t^T X_t)^{-1} X_0^T X_0 (X_t^T X_t)^{-1} x_j}{1 + x_j^T (X_t^T X_t)^{-1} x_j};$$

10. Update $s_n^{(t)}$ by replacing unit $i_m$ with $j_a$, to form $s_n^{(t+1)}$;
11. Set $t = t + 1$;
12. end
The computation of some metrics will illustrate the validity of our procedure in selecting a D- or I-optimal subsample without outliers.

Precisely, for \( h = 1, \ldots, H \), \( N \) iid repetitions of a 10-variate explanatory variable \( h\bar{x}_i = (x_{i1}, \ldots, x_{i10})^\top \) are generated as follows:

1. for \( j = 1, \ldots, 3 \), \( x_{ij} \) are independently distributed as \( U(0,5) \);

2. for \( j = 4, \ldots, 7 \), \( x_{ij} \) are distributed as a multivariate normal r.v. with zero mean and:
   2.a) for \( i = 1, \ldots, (N - N_2) \), covariance matrix \( \Sigma_1 = \begin{bmatrix} 9 & -1 \\ -1 & 9 \end{bmatrix} \)
   2.b) for \( i = (N - N_2) + 1, \ldots, N \), covariance matrix \( \Sigma_{1,\text{out}} = \begin{bmatrix} 25 & 1 \\ 1 & 25 \end{bmatrix} \);

3. for \( j = 8, 9 \), \( x_{ij} \) are distributed as a multivariate t-distribution with 3 degrees of freedom and scale matrix \( \Sigma_2 = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix} \);

4. for \( j = 10 \), \( x_{ij} \) is distributed as a Poisson distribution \( \mathcal{P}(5) \).

For each \( N \times (k + 1) \) factor-matrix \( hX \), whose \( i \)-th raw is \( h\bar{x}_i^\top = (1, h\bar{x}_i^\top) \) \( (i = 1, \ldots, N) \), we have generated \( S = 50 \) independent \( N \times 1 \) response vectors \( hY_s \) (with \( s = 1, \ldots, S \)), whose \( i \)-th item is

\[
hY_{s,i} = h\bar{x}_i^\top \beta + \varepsilon_{si}, \quad i = 1, \ldots, N;
\]

with

i) \( \beta = (1, 1, 1, 1, 2, 2, 2, 2, 1, 1, 1) \) and \( \sigma = 3 \) for \( i = 1, \ldots, N - N_2 \)

ii) \( \beta = (1, 1, 1, 1, -2, -2, -2, -2, 1, -1, -1), \sigma = 20 \) for \( i = N - N_2 + 1, \ldots, N \).

At each simulation step \((h, s)\), with \( h = 1, \ldots, H \) and \( s = 1, \ldots, S \), we have applied the following Algorithms:

1. Non-informative I (Algorithm 4)
2. Non-informative D (Algorithm 1)
3. Informative I (Algorithm 4 and Algorithm 3)
4. Informative D (Algorithm 1 and Algorithm 3)
5. Simple random sampling (SRS): passive learning selection
to draw a different subsample from the simulated dataset:

$$hD = \{(hx_1, hys_1), \ldots, (hx_N, hys_N)\}, \quad h = 1, \ldots, H, \ s = 1, \ldots, S.$$  

To check the validity of the inferential results obtained from the distinct sub-
samples, we have generated a test set of size $$N_T = 500$$:

$$D_T = \{(x_{T1}, y_{T1}), \ldots, (x_{TN_T}, y_{TN_T})\},$$

without high leverage points and outliers (i.e. with $$N_2 = 0$$).

Finally, to implement the I-optimality procedure, we have generated a prediction region $$X_0$$ without high leverage points; in addition, to compare
the behaviour of the distinct sub-samples in $$X_0$$, we have generated also the corresponding responses (without outliers). Let

$$D_0 = \{(x_{01}, y_{01}), \ldots, (x_{0N_0}, y_{0N_0})\}$$

be the prediction set, where $$N_0 = 500$$.

Let us denote by $$s^{(h,s)}_n$$ a subsample selected from the dataset $$hD_s$$ generated at the $$(h,s)$$-th simulation step, for $$h = 1, \ldots, H$$ and $$s = 1, \ldots, S$$, and let

$$I^{(h,s)}_i = \begin{cases} 1 & \text{if } i \in s^{(h,s)}_n \\ 0 & \text{otherwise} \end{cases}, \quad i = 1, \ldots, N,$$

be the corresponding sampling indicator variable.

At each simulation step $$(h,s)$$, to evaluate the performance of the subsam-
pling techniques, we have computed:

- The average mean squared prediction error in $$X_0$$ (from (6)):

$$\text{MSPE}_{X_0}^{(h,s)} = \sigma^2 \frac{\text{trace} \left[ \left( \sum_{i=1}^N h_xi h_{x}^\top I^{(h,s)}_i \right)^{-1} X_0^\top X_0 \right]}{N_0};$$

- The logarithm of the determinant of the information matrix:

$$\log(\det)_{X_0}^{(h,s)} = \log \left| \sum_{i=1}^N h_xi h_{x}^\top I^{(h,s)}_i \right|;$$
The average squared prediction error in \( X_0 \) and in \( X_T = \{x_{T1}, \ldots, x_{TN_T}\} \):

\[
\text{SPE}(h,s)_{X_0} = \frac{1}{N_0} \sum_{i=1}^{N_0} (\hat{y}_{0i}^{(h,s)} - \mu_{0i})^2 \quad \text{and} \quad \text{SPE}(h,s)_{X_T} = \frac{1}{N_T} \sum_{i=1}^{N_T} (\hat{y}_{Ti}^{(h,s)} - \mu_{Ti})^2,
\]

where \( \hat{y}_{0i}^{(h,s)} = h\hat{\beta}_s x_{0i} \), \( \hat{y}_{Ti}^{(h,s)} = h\hat{\beta}_s x_{Ti} \), \( \mu_{0i} = \beta^\top x_{0i} \), \( \mu_{Ti} = \beta^\top x_{Ti} \) and \( h\hat{\beta}_s \) is the OLS estimate of \( \beta \) based on the subsample \( s_{ni}^{(h,s)} \).

The standard error in the prediction set \( D_0 \) and in the test set \( D_T \):

\[
\text{SE}(h,s)_{D_0} = \frac{1}{N_0} \sum_{i=1}^{N_0} (\hat{y}_{0i}^{(h,s)} - y_{0i})^2 \quad \text{and} \quad \text{SE}(h,s)_{D_T} = \frac{1}{N_T} \sum_{i=1}^{N_T} (\hat{y}_{Ti}^{(h,s)} - y_{Ti})^2.
\]

Table 1 displays the Monte Carlo averages, MSPE\(_{X_0}\) and Log(det), for the different sampling strategies: non-inf. I, non-inf. D, inf. I, inf. D and SRS, respectively. The results are obtained having setted \( n = 500, \tilde{N} = 2 \cdot n, \nu_1 = 2 \) and \( \nu_2 = 3 \).

| Algorithm  | MSPE\(_{X_0}\) | Log(det) |
|------------|----------------|----------|
| non-inf. I | 0.0857         | 93.4269  |
| non-inf. D | 0.0947         | 94.3877  |
| inf. I     | 0.0938         | 92.0869  |
| inf. D     | 0.1030         | 92.7748  |
| SRS        | 0.2056         | 82.5234  |

Table 1: Monte Carlo averages MSPE\(_{X_0}\) and Log(det) for the subsamples of size \( n = 500 \) obtained from the different Algorithms.

Accordingly to the definitions of I- and D-optimality, the minimum value of the MSPE\(_{X_0}\) is associated to the noninformative I-Algorithm, while the maximum value of the Log(Det) corresponds to the noninformative D-subsample. Therefore, Algorithms 1 and 4 provide samples that do not include high leverage points and are “nearly” D- and I-optimal (they are not exactly D- and I-optimal because of the exclusion of these high values).

Table 2 lists the following Monte Carlo averages:
SPE\(_{X_0}\) = \(\sum_{h=1}^{H} \sum_{s=1}^{S} \operatorname{SPE}^{(h,s)} / HS\), SPE\(_{X_T}\) = \(\sum_{h=1}^{H} \sum_{s=1}^{S} \operatorname{SPE}^{(h,s)} / HS\),

SE\(_{D_0}\) = \(\sum_{h=1}^{H} \sum_{s=1}^{S} \operatorname{SE}^{(h,s)} / HS\) and SE\(_{D_T}\) = \(\sum_{h=1}^{H} \sum_{s=1}^{S} \operatorname{SE}^{(h,s)} / HS\),

for the different subsamples. These Monte Carlo averages represent an empirical version of MSPE and MSE on \(X_0\) and \(X_T\), respectively. From these results, we can appreciate the prominent role of the informative procedures in selecting subsamples without outliers. In fact, when the database includes outliers in \(Y\) which are not associated with high leverage points (as in this simulation study), then only the informative procedure enables us to exclude these abnormal values from the subsample.

| Algorithm | SPE\(_{X_0}\)  | SPE\(_{X_T}\)  | SE\(_{D_0}\)  | SE\(_{D_T}\)  |
|-----------|----------------|----------------|---------------|---------------|
| non-inf. I | 6.5104         | 6.8020         | 16.0792       | 16.3538       |
| non-inf. D | 6.1011         | 6.2945         | 15.5982       | 15.7969       |
| inf. I    | 0.1464         | 0.1494         | 9.4445        | 9.5337        |
| inf. D    | 0.1594         | 0.1601         | 9.4564        | 9.5448        |
| SRS       | 0.2629         | 0.2671         | 9.5683        | 9.6594        |

Table 2: Monte Carlo averages SPE\(_{X_0}\), SPE\(_{X_T}\), SE\(_{D_0}\) and SE\(_{D_T}\) for the subsamples of size \(n = 500\) obtained from the different Algorithms.

Remark. Actually, to take into consideration the randomness of the SRS technique, we have drawn \(N_{SRS} = 50\) different independent SRSs from each dataset \(hD_s\), for \(h = 1, \ldots, H\) and \(s = 1, \ldots, S\); the Monte Carlo averages for SRS are based also on these additional observations.

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