Better Solution Principle: A Facet of Concordance between Optimization and Statistics

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Abstract  Many statistical methods require solutions to optimization problems. When the global solution is hard to attain, statisticians always use the better if there are two solutions for chosen, where the word “better” is understood in the sense of optimization. This seems reasonable in that the better solution is more likely to be the global solution, whose statistical properties of interest usually have been well established. From the statistical perspective, we use the better solution because we intuitively believe the principle, called better solution principle (BSP) in this paper, that a better solution to a statistical optimization problem also has better statistical properties of interest. BSP displays some concordance between optimization and statistics, and is expected to widely hold. Since theoretical study on BSP seems to be neglected by statisticians, this paper aims to establish a framework for discussing BSP in various statistical optimization problems. We demonstrate several simple but effective comparison theorems as the key results of this paper, and apply them to verify BSP in commonly encountered statistical optimization problems, including maximum likelihood estimation, best subsample selection, and best subset regression. It can be seen that BSP for these problems holds under reasonable conditions, i.e., a better solution indeed has better statistical properties of interest. In addition, guided by the BSP theory, we develop a new best subsample selection method that performs well when there are clustered outliers.

KEY WORDS: Best subsample selection; Best subset regression; Combinatorial optimization; Global optimization; Large-scale optimization; Likelihood principle; Robust estimation; Separation property; Variable selection.
1 Introduction

Many statistical methods require solutions to optimization problems. A notable example is maximum likelihood estimation, whose objective is to maximize the likelihood function. Below is a brief description of some statistical methods that rely on optimization problems in various statistical areas.

- **Maximum likelihood and related methods:** The maximum likelihood method can be used for parametric models and has good statistical properties under regularity conditions. An extension of this method is M-estimation (Huber 1981), which obtains estimators by minimizing a general class of functions with respect to the parameter. A corresponding method for nonparametric models is empirical likelihood (Owen 2001), which requires maximizing the empirical likelihood function.

- **Model fitting and selection:** In regression analysis, the parameter of the regression model needs to estimate for yielding a good fit to the data. For this purpose, methods that minimize criteria which justify the goodness of fit are used such as the least squares method. Smoothing spline regression (Wahba 1990) and local polynomial regression (Fan and Gijbels 1996) can be viewed as two variants of the least squares method in nonparametric settings. When model selection is concerned, regularized regression methods, which minimize the regularized criteria to produce sparse estimators, can be used such as best subset regression (the $\ell_0$-norm regularized method) and the lasso (the $\ell_1$-norm regularized method); see e.g., Hastie, Tibshirani, and Friedman (2008).

- **Multivariate analysis:** Many problems in multivariate statistical analysis involve projections of the data into a lower dimensional space. Principal component analysis, canonical correlation analysis, and Fisher’s discrimination are well known examples (Anderson 2003). Optimization problems over a multi-dimensional sphere need to solve to find the projections.

- **Bayesian statistics:** A method in Bayesian point estimation is to use the posterior mode,
which is the maximum of the posterior density (Gelman et al. 2004). Maximum likelihood estimation can be viewed as a special case of this method.

- **Robust estimation**: Besides the M-estimate, popular robust estimates which can be formulated as optimization problems include the least trimmed squares estimate, the S-estimate, and the minimum covariance determinant estimate, among others (Maronna, Martin, and Yohai 2006). Optimization methods are also ubiquitous in computing depth functions (Zuo and Serfling 2000), which are useful to define multivariate median and trimmed mean.

- **Design of experiments**: A number of experimental designs are constructed by optimizing certain criteria. An example is the minimum aberration criterion in fractional factorial designs (Wu and Hamada 2009). For continuous factors, optimal designs (Atkinson, Donev, and Tobias 2007) are derived by optimizing model-based criteria, and space-filling designs (Fang, Li, and Sudjianto 2006) correspond to geometric or discrepancy criteria.

- **Statistical learning**: This area seriously utilizes computation for statistical inference. Many important methods such as support vector machine (Scholkopf and Smola 2002) and boosting (Freund and Schapire 1997) are based on minimizing loss functions. In addition, (regularized) maximum likelihood estimation is commonly used for graphical models (Wainwright and Jordan 2008). Cross-validation, which minimizes the empirical prediction error, is ubiquitous in various methods to select tuning parameters (Hastie, Tibshirani, and Friedman 2008).

The above description, although far from thorough, indicates that optimization plays a vital role in modern statistics. In the meanwhile, statisticians have to face the common difficulty in the optimization community, i.e., it is often extremely hard to obtain the global solution to a nonconvex optimization problem. A number of global optimization algorithms have been proposed, including the simulated annealing algorithm (Kirkpatrick, Gelatt, and Vecchi 1983) and the genetic algorithm (Dorsey and Mayer 1995). However, they can attain
the global solution only in the probabilistic sense, and often take an unrealistically long time to approach it in practice (Lundy and Mees 1986). When handling large-scale data, the problem of multiple extrema becomes more serious. In fact, for such cases, it is also hard to obtain the solution to a convex optimization problem due to the unaffordable computational time and memory (Tibshirani et al. 2012; Ma, Mahoney, and Yu 2013). Another difficulty from the problem of multiple extrema is that we can rarely know whether a solution at hand is the global solution (Gan and Jiang 1999).

When the global solution is hard to attain and/or to verify, statisticians always take the solution whose objective value is as small as possible (for minimization problems) as the final solution. In other words, for two solutions, we always use the “better” one, where the word “better” should be understood in the sense of optimization. This seems reasonable in that the better solution is more likely to be the global solution, whose statistical properties of interest usually have been well established. From the statistical perspective, we use the better solution because we intuitively believe the principle, called better solution principle (BSP) in this paper, that a better solution to a statistical optimization problem also has better statistical properties of interest (closer statistical properties to those the global solution has). This principle shows some concordance, or monotonicity, between optimization and statistics, and is expected to widely hold. Strictly speaking, a better solution can safely be used only after the corresponding BSP is verified. However, it is surprising that statisticians seem to neglect this problem, although we have actually made decisions following BSP ever since complex optimization problems appeared in statistics. To the best of the author’s knowledge, no paper has formally discussed BSP. For example, in the maximum likelihood problem, it is not clear to us whether a better solution with greater likelihood has higher estimation accuracy. Fairly recently, Xiong (2013) introduced the better-fitting better-screening rule when discussing variable screening in high-dimensional linear models. This rule tells us that a subset with smaller residual sums of squares possesses better asymptotic screening properties, i.e., is more likely to include the true submodel asymptotically. Here such a subset can be viewed as a better solution to the $\ell_0$-norm constrained least squares problem. Therefore, the better-fitting better-screening rule is actually the BSP for this problem. Inspired by Xiong
(2013)’s work, this paper aims to establish a relatively general framework for discussing BSP in various statistical optimization problems.

The rest of the paper is organized as follows. We first present examples where BSP immediately holds in Section 2. Such examples widely exist in experimental designs. They can help us understand BSP and the reason why we introduce the theorems in the following text. In Section 3, we demonstrate several comparison theorems which state that a better solution is more likely to have good statistical properties if the optimization problem possesses certain separation properties. These theorems, which look very simple and understandable, are effective to establish BSP in a general setting. Sections 4-7 apply these results to several statistical optimization problems, including maximum likelihood estimation, best subsample selection, and best subset regression. The latter two problems are actually combinatorial optimization problems, which are more difficult to solve than continuous problems from the optimization perspective. Here best subsample selection is referred to as the method of selecting the best part of observations to make inferences in the presence of outliers, and the minimum covariance determinant estimate and least trimmed squares estimate are instances of estimates based on it. We can see that BSP for these problems holds under reasonable conditions, i.e., a better solution indeed has better statistical properties of interest. In Section 5, we develop a new best subsample selection method which can perform well when there are clustered outliers. A robust estimator based on it having consistency even under contaminated models is of independent interest in robust statistics. Section 8 concludes with some discussion.

2 Known examples where BSP holds

Obvious examples where BSP holds exist in experimental designs derived by optimizing some criteria. We take the D-optimal design for example. Consider a regression model

\[ y = \sum_{i=1}^{d} \theta_i r_i(x) + \varepsilon, \]
where the control variable $x$ lies in a subset $\mathcal{D}$ of $\mathbb{R}^p$, $r_i$’s are specified functions, $\theta = (\theta_1, \ldots, \theta_d)'$ is the vector of unknown parameters, and $\varepsilon$ is the random error. Given the sample size $n$, denote the experimental design by $\mathcal{P} = \{x_1, \ldots, x_n\}$. The information matrix of this design is $M = R' R$, where

$$
R = \begin{pmatrix}
    r_1(x_1) & \cdots & r_d(x_1) \\
    \vdots & \ddots & \vdots \\
    r_1(x_n) & \cdots & r_d(x_n)
\end{pmatrix}.
$$

The D-optimal design minimizes the generalized variance of the least squares estimate of $\theta$, i.e., it is the solution to the optimization problem

$$
\min_{x_i \in \mathcal{D}} \psi(\mathcal{P}) = (\det(M))^{-1},
$$

where “det” denotes determinant. For two designs $\mathcal{P}_1$ and $\mathcal{P}_2$ with $\psi(\mathcal{P}_1) \leq \psi(\mathcal{P}_2)$, it is clear that $\mathcal{P}_1$ leads to a better estimator whose generalized variance is smaller. Therefore, if estimation accuracy (which is justified by the amount of generalized variance) is the statistical property of interest, BSP for problem (1) holds.

The objective function in (1) itself is a statistical criterion, which does not involve any random variables. This is the reason why BSP for (1) automatically holds. The same conclusion can be drawn for other model-based optimal designs and minimum aberration designs. For criterion-based space-filling designs, the geometric or discrepancy criteria used as objective functions seem not to have clear statistical interpretation. However, most of them relate to some desirable statistical properties. For example, the criteria for constructing the minimax distance design (Johnson, Moore, and Ylvisaker 1990) and uniform design (Fang et al. 2000) can act as factors in the upper bounds of some estimation errors (Wendland 2005; Niederreiter 1992). If such estimation errors are used to evaluate the corresponding estimators, we can say that BSP holds.

Design of experiments is a pre-sampling work, and thus the objective functions used in this area do not involve the random sample (except for sequential designs that we do not
consider here). In statistical inference, we have to deal with objective functions depending on the sample, which makes the problem of BSP more complicated. From the next section, we study whether BSP holds for sample-based optimization problems through introducing new definitions and theorems.

3 The comparison theorems

Let \((\Omega, \mathcal{F}, P)\) be a probability space. For simplicity, it is assumed that all sets and maps throughout this paper are measurable (with respect to according \(\sigma\)-fields). For each \(n \in \mathbb{N}\), the sample \(X_n\) of size \(n\) is a map from \(\Omega\) to a space \(\mathcal{X}_n\). Based on \(X_n\), we make statistical decision by optimizing a objective function. In this section several comparison theorems are provided to compare the statistical properties of two decisions with different objective values. We first consider the situation where the decision space does not depend on \(n\). An application of the corresponding results is estimation for parameters, where the decision space is the set on which the parameters are valued. The second subsection discusses the situation where the decision space depends on \(n\), which covers the problem of variable selection.

3.1 When the decision space does not depend on \(n\)

Let \(\mathcal{D}\) denote the decision space that contains all statistical decisions of interest. Suppose that we need to make inferences based on the global solution to the optimization problem

\[
\min_{x \in \mathcal{D}} \psi_n(x, X_n),
\]

where the objective function \(\psi_n\) is a map from \(\mathcal{D} \times \mathcal{X}_n\) to \(\mathbb{R}\). In general, the problem in (2) is proposed because its solution can asymptotically lie in a desirable subset \(\mathfrak{A}\) of \(\mathcal{D}\) that contains all “good” decisions. This property of the global solution can be viewed as a consistency property. When the global solution is difficult to obtain, we discuss whether BSP holds, i.e., whether a better solution with a smaller objective value is more likely to lie in \(\mathfrak{A}\). Let \(\mathfrak{B}\) be another subset of \(\mathcal{D}\), which contains relatively bad decisions compared to \(\mathfrak{A}\).
Definition 3.1. We say that \( \{ \psi_n \} \) strongly separates \( \mathcal{A} \) from \( \mathcal{B} \), or \( \{ \psi_n \} \) has the strong separation property with respect of \( \mathcal{A} \) and \( \mathcal{B} \), if as \( n \to \infty \),

\[
P \left( \sup_{x \in \mathcal{A}} \psi_n(x, X_n) < \inf_{y \in \mathcal{B}} \psi_n(y, X_n) \right) \to 1. \tag{3}
\]

We say that \( \{ \psi_n \} \) (weakly) separates \( \mathcal{A} \) from \( \mathcal{B} \), or \( \{ \psi_n \} \) has the (weak) separation property with respect of \( \mathcal{A} \) and \( \mathcal{B} \), if for all \( x \in \mathcal{A}, \ y \in \mathcal{B} \),

\[
\limsup_{n \to \infty} \left[ \psi_n(x, X_n) - \psi_n(y, X_n) \right] < 0 \ (a.s.), \tag{4}
\]

where “a.s.” denotes “almost surely”.

It is worthwhile noting that the strong separation property needs not to imply the separation property. We use the word “strong” to distinguish the two properties just because the former is generally more difficult to verify and can lead to stronger results.

Remark 3.1. For convenience in asymptotic analysis, we often consider a scaled objective function. It should be pointed out that (3) holds if

\[
P \left( \sup_{x \in \mathcal{A}} \psi_n(x, X_n)/a_n < \inf_{y \in \mathcal{B}} \psi_n(y, X_n)/a_n \right) \to 1
\]

for arbitrary sequence of positive numbers \( \{a_n\} \), and that (4) holds if

\[
\limsup_{n \to \infty} \left[ \psi_n(x, X_n) - \psi_n(y, X_n) \right]/a_n < 0 \ (a.s.)
\]

for a sequence of positive numbers \( \{a_n\} \) with \( a_n^{-1} = O(1) \).

Roughly speaking, the strong separation property requires that the level set corresponding to smaller objective values is asymptotically identical to the set of good decisions. It shows the consistency of the objective function to the statistical properties of interest. We can immediately prove the following result that this property implies BSP, where the statistical properties of interest are described with the probability of locating in the set \( \mathcal{A} \) of good
Theorem 3.1 (Strong Comparison Theorem). Suppose that \( \{\psi_n\} \) strongly separates \( \mathcal{A} \) from \( \mathcal{B} \). For all \( n \in \mathbb{N} \), \( \xi_n \) and \( \eta_n \) are statistics valued in \( \mathcal{D} \) satisfying \( P(\xi_n \in \mathcal{A} \cup \mathcal{B}, \eta_n \in \mathcal{A} \cup \mathcal{B}) \to 1 \) as \( n \to \infty \). If \( \psi_n(\xi_n, X_n) \leq \psi_n(\eta_n, X_n) \) (a.s.) for all \( n \), then

\[
\lim_{n \to \infty} \inf \left[ P(\xi_n \in \mathcal{A}) - P(\eta_n \in \mathcal{A}) \right] \geq 0.
\]

Proof. For \( \omega \in \{\eta_n \in \mathcal{A}, \xi_n \in \mathcal{B}\} \subset \Omega \), if \( \omega \in \{\sup_{x \in \mathcal{A}} \psi_n(x, X_n) < \inf_{y \in \mathcal{B}} \psi_n(y, X_n)\} \cap \{\xi_n \in \mathcal{A} \cup \mathcal{B}, \eta_n \in \mathcal{A} \cup \mathcal{B}\} \), then

\[
\psi_n(\eta_n(X_n(\omega)), X_n(\omega)) \leq \sup_{x \in \mathcal{A}} \psi_n(x, X_n(\omega)) < \inf_{y \in \mathcal{B}} \psi_n(y, X_n(\omega)) \leq \psi_n(\xi_n(X_n(\omega)), X_n(\omega)),
\]

which leads to a contradiction. Therefore, \( \omega \notin \{\sup_{x \in \mathcal{A}} \psi_n(x, X_n) < \inf_{y \in \mathcal{B}} \psi_n(y, X_n)\} \cap \{\xi_n \in \mathcal{A} \cup \mathcal{B}, \eta_n \in \mathcal{A} \cup \mathcal{B}\} \), which implies \( P(\eta_n \in \mathcal{A}, \xi_n \in \mathcal{B}) \to 0 \). We have \( P(\eta_n \in \mathcal{A}) = P(\eta_n \in \mathcal{A}, \xi_n \in \mathcal{B}) + P(\eta_n \in \mathcal{A}, \xi_n \in \mathcal{A}) + P(\eta_n \in \mathcal{A}, \xi_n \notin \mathcal{A} \cup \mathcal{B}) = P(\xi_n \in \mathcal{A}) - P(\xi_n \in \mathcal{B}) + o(1) \). This completes the proof.

Recall that, for a decision \( \xi_n \), the property that \( P(\xi_n \in \mathcal{A}) \to 1 \) can be viewed as a consistency property of \( \xi_n \). The following theorem shows that the strong separation property of \( \{\psi_n\} \) is often stronger than the consistency of the minimum of \( \psi_n \).

Theorem 3.2. Suppose that \( \{\psi_n\} \) strongly separates \( \mathcal{A} \) from \( \mathcal{B} \). If \( \xi_n = \arg \min_{x \in \mathcal{D}} \psi_n(x, X_n) \) exists and \( P(\xi_n \in \mathcal{A} \cup \mathcal{B}) \to 1 \) as \( n \to \infty \), then

\[
\lim_{n \to \infty} P(\xi_n \in \mathcal{A}) \to 1.
\]

Proof. This theorem follows from \( \{\sup_{x \in \mathcal{A}} \psi_n(x, X_n) < \inf_{y \in \mathcal{B}} \psi_n(y, X_n)\} \cap \{\xi_n \in \mathcal{A} \cup \mathcal{B}\} \subset \{\xi_n \in \mathcal{A}\} \).

We next discuss BSP with the separation property. This weaker property cannot directly imply BSP, and more conditions are needed.
Theorem 3.3 ((Weak) Comparison Theorem). Suppose that \( \{ \psi_n \} \) separates \( \mathfrak{A} \) from \( \mathfrak{B} \). Denote the set of probability one where (1) holds by \( E(x,y) \) and write \( E = \cap_{x,y \in \mathfrak{B}} E(x,y) \).

For all \( n \in \mathbb{N} \), \( \xi_n \) and \( \eta_n \) are statistics valued in \( \mathfrak{D} \) satisfying \( P(\xi_n \in \mathfrak{A} \cup \mathfrak{B}, \eta_n \in \mathfrak{A} \cup \mathfrak{B}) \to 1 \) as \( n \to \infty \). If \( \psi_n(\xi_n, X_n) \leq \psi_n(\eta_n, X_n) \) (a.s.) for all \( n \), then

\[
\liminf_{n \to \infty} [P(\xi_n \in \mathfrak{A}) - P(\eta_n \in \mathfrak{A})] \geq -P(\Omega \setminus E). \tag{5}
\]

Proof. For \( \omega \in \{ \eta_n \in \mathfrak{A}, \xi_n \in \mathfrak{B} \} \subset \Omega \), if \( \omega \in E \cap \{ \xi_n \in \mathfrak{A} \cup \mathfrak{B}, \eta_n \in \mathfrak{A} \cup \mathfrak{B} \} \), then

\[
\limsup_{n \to \infty} [\psi_n(\eta_n(X_n(\omega)), X_n(\omega)) - \psi_n(\xi_n(X_n(\omega)), X_n(\omega))] < 0.
\]

This is a contradiction. Therefore, \( \omega \notin E \cap \{ \xi_n \in \mathfrak{A} \cup \mathfrak{B}, \eta_n \in \mathfrak{A} \cup \mathfrak{B} \} \) for sufficiently large \( n \), which implies \( P(\eta_n \in \mathfrak{A}, \xi_n \in \mathfrak{B}) \leq P(\Omega \setminus E) + 1 - P(\xi_n \in \mathfrak{A} \cup \mathfrak{B}, \eta_n \in \mathfrak{A} \cup \mathfrak{B}) \) for sufficiently large \( n \). It follows that \( P(\eta_n \in \mathfrak{A}) = P(\eta_n \in \mathfrak{A}, \xi_n \in \mathfrak{B}) + P(\eta_n \in \mathfrak{A}, \xi_n \in \mathfrak{A}) + P(\eta_n \in \mathfrak{A}, \xi_n \notin \mathfrak{A} \cup \mathfrak{B}) \leq P(\xi_n \in \mathfrak{A}) - P(\xi_n \in \mathfrak{A}, \eta_n \in \mathfrak{B}) + P(\eta_n \in \mathfrak{A}, \xi_n \in \mathfrak{B}) + 1 - P(\xi_n \in \mathfrak{A} \cup \mathfrak{B}) \leq P(\xi_n \in \mathfrak{A}) + P(\Omega \setminus E) + 1 - P(\xi_n \in \mathfrak{A} \cup \mathfrak{B}, \eta_n \in \mathfrak{A} \cup \mathfrak{B}) + 1 - P(\xi_n \in \mathfrak{A} \cup \mathfrak{B}) \) for sufficiently large \( n \), which completes the proof. \( \square \)

If \( P(\Omega \setminus E) \) in (5) equals zero, then we can say BSP holds. Nevertheless, it is impossible to verify this condition in practice. A way for avoiding this problem is to consider countable subsets, and we immediately obtain the following corollary.

Corollary 3.1. Suppose that \( \{ \psi_n \} \) separates \( \mathfrak{A} \) from \( \mathfrak{B} \). For \( n \in \mathbb{N} \), \( \xi_n \) and \( \eta_n \) are statistics valued in a countable subset of \( \mathfrak{D} \) satisfying \( P(\xi_n \in \mathfrak{A} \cup \mathfrak{B}, \eta_n \in \mathfrak{A} \cup \mathfrak{B}) \to 1 \) as \( n \to \infty \). If \( \psi_n(\xi_n, X_n) \leq \psi_n(\eta_n, X_n) \) (a.s.) for all \( n \), then

\[
\liminf_{n \to \infty} [P(\xi_n \in \mathfrak{A}) - P(\eta_n \in \mathfrak{A})] \geq 0.
\]

Remark 3.2. For many cases, \( \mathfrak{D} \) is a separable set. It is usually enough to consider the decisions in its countable and dense subset in practice. For example, to estimate a scalar parameter, we can always consider the estimators valued in the set of all rational numbers,
which is countable and dense in $\mathbb{R}$. In this sense, BSP follows from the separation property of $\{\psi_n\}$.

3.2 When the decision space depends on $n$

In this subsection the decision space of interest $D_n$ depends on the sample size $n$. Suppose that we need to consider the optimization problem

$$\min_{x \in D_n} \psi_n(x, X_n),$$

where the objective function $\psi_n$ is a map from $D_n \times X_n$ to $\mathbb{R}$. Different from the results in Section 3.1, we need to consider sequences of decisions. Denote $D = \prod_{n=1}^{\infty} D_n$, and let $A$ be the subset of $D$ that contains sequences of good decisions. The statistical property of a decision sequence we concern here is whether it lies in $A$. Let $B$ be another subset of $D$. Denote $D^* = A \cup B$. The definition and theoretical results are parallel to those in Section 3.1 and the proofs are almost the same. We therefore omit the proofs in this subsection.

Definition 3.2. We say that $\{\psi_n\}$ (weakly) separates $A$ from $B$, or $\{\psi_n\}$ has the (weak) separation property with respect to $A$ and $B$, if for all $\{x_n\} \in A$, $\{y_n\} \in B$,

$$\limsup_{n \to \infty} \left[ \psi_n(x_n, X_n) - \psi_n(y_n, X_n) \right] < 0 \quad (a.s.). \quad (6)$$

Furthermore, suppose that $A$ and $B$ can be written as $A = \prod_{n=1}^{\infty} A_n$ and $B = \prod_{n=1}^{\infty} B_n$, where $A_n$ and $B_n$ are subsets of $D_n$. We say that $\{\psi_n\}$ strongly separates $A$ from $B$, or $\{\psi_n\}$ has the strong separation property with respect to $A$ and $B$, if as $n \to \infty$,

$$P \left( \sup_{x \in A_n} \psi_n(x, X_n) < \inf_{y \in B_n} \psi_n(y, X_n) \right) \to 1.$$

Theorem 3.4 (Strong Comparison Theorem). Suppose that $A$ and $B$ can be written as $A = \prod_{n=1}^{\infty} A_n$ and $B = \prod_{n=1}^{\infty} B_n$, and $\{\psi_n\}$ strongly separates $A$ from $B$. For two sequences
of statistics \( \{\xi_n\} \) and \( \{\eta_n\} \) valued in \( \mathcal{D}^* \), if \( \psi_n(\xi_n, X_n) \leq \psi_n(\eta_n, X_n) \) (a.s.) for all \( n \), then

\[
\liminf_{n \to \infty} [P(\xi_n \in \mathcal{A}_n) - P(\eta_n \in \mathcal{A}_n)] \geq 0
\]

and

\[
P(\{\xi_n\} \in \mathcal{A}) \geq P(\{\eta_n\} \in \mathcal{A}).
\]

**Theorem 3.5.** Under the conditions in Theorem 3.4, if \( \xi_n = \arg \min_{x \in \mathcal{D}^*} \psi_n(x, X_n) \) exists, then

\[
\lim_{n \to \infty} P(\xi_n \in \mathcal{A}_n) \to 1.
\]

**Theorem 3.6** (Weak) Comparison Theorem. Suppose that \( \{\psi_n\} \) (weakly) separates \( \mathcal{A} \) from \( \mathcal{B} \). Denote the set of probability one where (6) holds by \( E(\{x_n\}, \{y_n\}) \) and write \( E = \cap_{(x_n)\in \mathcal{A}, (y_n)\in \mathcal{B}} E(\{x_n\}, \{y_n\}) \). For two sequences of statistics \( \{\xi_n\} \) and \( \{\eta_n\} \) valued in \( \mathcal{D}^* \), if \( \psi_n(\xi_n, X_n) \leq \psi_n(\eta_n, X_n) \) (a.s.) for all \( n \), then

\[
P(\{\xi_n\} \in \mathcal{A}) - P(\{\eta_n\} \in \mathcal{A}) \geq -P(\Omega \setminus E).
\]

Furthermore, if \( \mathcal{A} \) and \( \mathcal{B} \) can be written as \( \mathcal{A} = \prod_{n=1}^{\infty} \mathcal{A}_n \) and \( \mathcal{B} = \prod_{n=1}^{\infty} \mathcal{B}_n \), then for sufficiently large \( n \),

\[
P(\xi_n \in \mathcal{A}_n) - P(\eta_n \in \mathcal{A}_n) \geq -P(\Omega \setminus E).
\]

**Corollary 3.2.** Suppose that \( \{\psi_n\} \) weakly separates \( \mathcal{A} \) from \( \mathcal{B} \). For two sequences of statistics \( \{\xi_n\} \) and \( \{\eta_n\} \) valued in a countable subset of \( \mathcal{D}^* \), if \( \psi_n(\xi_n, X_n) \leq \psi_n(\eta_n, X_n) \) (a.s.) for all \( n \), then

\[
P(\{\xi_n\} \in \mathcal{A}) \geq P(\{\eta_n\} \in \mathcal{A}).
\]

Furthermore, if \( \mathcal{A} \) and \( \mathcal{B} \) can be written as \( \mathcal{A} = \prod_{n=1}^{\infty} \mathcal{A}_n \) and \( \mathcal{B} = \prod_{n=1}^{\infty} \mathcal{B}_n \), then for sufficiently large \( n \),

\[
P(\xi_n \in \mathcal{A}_n) \geq P(\eta_n \in \mathcal{A}_n).
\]

**Remark 3.3.** In practice, we only have the observed values of \( \xi_n \) and \( \eta_n \) for a specified \( n \). It can be assumed that they are respectively from two sequences \( \{\xi_n\} \) and \( \{\eta_n\} \) valued in a
countable subset of $\mathcal{D}_n^*$, especially when the decision space $\mathcal{D}_n$ is a finite set for each $n$. In this sense, as in Remark 3.2, the separation property of $\{\psi_n\}$ is sufficient to imply BSP.

In the rest of this paper, we omit the sample $X_n$ in $\psi_n(\cdot, X_n)$ and write $\psi_n(\cdot)$ for emphasizing the decision variable.

4 Greater likelihood principle

We have shown in Section 3 that the separation properties of an objective function can imply the corresponding BSP. Despite simplicity, these results are effective to establish BSP since many objective functions indeed possess the separation properties under reasonable conditions. From this section to Section 7, we show that BSP holds for several important statistical optimization problems by use of them. This section discusses the problem associated with maximum likelihood estimation.

4.1 Main results

Let the data $X_1, \ldots, X_n$ be i.i.d. from a probability density function (p.d.f.) $f(\cdot, \theta)$ with respect to a $\sigma$-finite measure $\mu$ on $\mathbb{R}^p$, where $\theta$ lies in the parameter space $\Theta \subset \mathbb{R}^q$. The likelihood function is

$$l_n(\theta) = \prod_{i=1}^{n} f(X_i, \theta),$$

and the maximum likelihood estimator (MLE) is the solution to the optimization problem

$$\max_{\theta \in \Theta} l_n(\theta). \quad (7)$$

For convenience, we write (7) as the problem of minimizing the negative log-likelihood

$$\min_{\theta \in \Theta} \left[ - \log \left( l_n(\theta) \right) \right]. \quad (8)$$

The MLE is commonly used due to its well-known high asymptotic efficiency. However,
when the negative log-likelihood has multiple local minima, the MLE is difficult to compute (Gan and Jiang 1999).

When estimation accuracy is concerned, it is common to use the probability of lying in a neighborhood of the true parameter to evaluate an estimator. For a consistent estimator, this probability converges to one as the sample size goes to infinity. Following this way, we define “good” decisions in discussing BSP for the MLE problem, and show that, for two estimators, the better one with greater likelihood has larger probability of lying in a sufficiently small neighborhood of \( \theta_0 \) under regularity conditions, where \( \theta_0 \) denotes the true parameter. This result, called greater likelihood principle in this paper, is a special case of BSP and can be viewed as a supplementary of the maximum likelihood principle.

By the results in Section 3, we can establish BSP via the separation properties of the objective function. Some assumptions and lemmas are needed.

Denote

\[
s(\theta, \theta_0) = -\int \log(f(x, \theta)) f(x, \theta_0) d\mu(x). \tag{9}
\]

**Assumption 4.1.** For all \( \theta_1, \theta_2 \in \Theta \), \( f(\cdot, \theta_1) = f(\cdot, \theta_2) \) (a.s.) implies \( \theta_1 = \theta_2 \).

**Assumption 4.2.** For all \( \theta \in \Theta \), \( \int |\log(f(x, \theta))| f(x, \theta) d\mu(x) < \infty \).

**Assumption 4.3.** For all \( \theta_0 \in \Theta \), \( s(\cdot, \theta_0) \) is continuous on \( \Theta \) and \( \liminf_{x \to b} s(x, \theta_0) > s(\theta_0, \theta_0) \) for all \( b \in C(\Theta) \setminus \Theta \), where \( C(\Theta) \) denotes the closure of \( \Theta \).

**Lemma 4.1.** Let \( h \) be a continuous function defined in \( D \subset \mathbb{R}^q \). Suppose that \( h \) has a unique minimum \( x_0 \), i.e., for all \( x \neq x_0 \), \( h(x) > h(x_0) \). Furthermore, for all \( b \in C(D) \setminus D \), \( \liminf_{x \to b} h(x) > h(x_0) \). Then for all \( \epsilon > 0 \), there exists \( \delta > 0 \) such that \( \{ x \in D : h(x) - h(x_0) \leq \delta \} \subset B(x_0, \epsilon) \), where \( B(x_0, \epsilon) = \{ x \in \mathbb{R}^q : \|x - x_0\| \leq \epsilon \} \).

**Proof.** For any sequence of positive numbers \( \{a_n\} \) with \( a_n \to 0 \) as \( n \to \infty \), assume that there exist \( x_n \in D \) and \( \epsilon_0 > 0 \) such that \( h(x_n) - h(x_0) \leq a_n \) but \( |x_n - x_0| > \epsilon_0 \). Therefore \( h(x_n) \to h(x_0) \). Since any limit point of \( \{x_n\} \) in \( C(D) \) cannot be \( x_0 \), this is in contradiction to the condition that \( x_0 \) is the unique minimum of \( h \). \( \square \)
Lemma 4.2. If Assumptions 4.1 and 4.2 hold, then for all $\theta_0 \in \Theta$, $s(\cdot, \theta_0)$ in (9), as a function defined on $\Theta$, attains its minimum uniquely at $\theta_0$.

The above lemma and its proof can be found in many places; see, e.g., Wald (1949) and Van der Vaart (1998).

Under Assumptions 4.1–4.3, by Lemmas 4.1 and 4.2, for all $\epsilon > 0$, there exists $\delta(\epsilon) > 0$ such that

$$\{\theta \in \Theta : s(\theta, \theta_0) - s(\theta_0, \theta_0) \leq \delta(\epsilon)\} \subset B(\theta_0, \epsilon).$$

Denote $B_s(\theta_0, \epsilon) = \{\theta \in \Theta : s(\theta, \theta_0) - s(\theta_0, \theta_0) \leq \delta(\epsilon)\}$ and consider

$$\mathcal{A}_\epsilon = B_s(\theta_0, \epsilon), \quad \mathcal{B}_\epsilon = \Theta \setminus B_s(\theta_0, \epsilon).$$

Note that for all $\theta \in \Theta$,

$$\frac{-\log(l_n(\theta))}{n} = \frac{-\log(f(X_1, \theta)) + \cdots + \log(f(X_n, \theta))}{n} \to s(\theta, \theta_0) \quad \text{(a.s.)}.$$ 

We can immediately obtain the following theorem by Definition 3.1 and Remark 3.1.

Theorem 4.1. Under Assumptions 4.1–4.3, for all $\epsilon > 0$, $\{- \log(l_n)\}$ separates $\mathcal{A}_\epsilon$ from $\mathcal{B}_\epsilon$ in (10).

Remark 4.1. The conditions for the separation property of $\{- \log(l_n)\}$ are weaker than those for the consistency of MLE in Wald (1949). Furthermore, Our results in this section neither rely on the existence of an MLE nor require that $\Theta$ is an open subset.

Although the separation property is sufficient for BSP in practical use by Remark 3.2, the strong separation property is still of theoretical interest. We next discuss it for the likelihood function, Some stronger conditions are needed.

Assumption 4.4. The family $\{f(\cdot, \theta)\}_{\theta \in \Theta}$ has a common support set $S = \{x \in \mathbb{R}^p : 0 < f(x, \theta) < \infty\}$. For all $x \in S$, $f(x, \cdot)$ is continuous on $\Theta$.

Assumption 4.5. For any $\theta \in \Theta$ and any compact subset $K$ of $\Theta$,

$$\int \sup_{\phi \in K} |\log(f(x, \phi))| f(x, \theta) d\mu(x) < \infty.$$
Take $\mathfrak{A}^\epsilon$ as in (10). Instead of $\mathfrak{B}^\epsilon$ in (10), take $\mathfrak{B}^*_\epsilon$ as any compact subset of $\Theta \setminus B_s(\theta_0, \epsilon)$.

**Theorem 4.2.** Under Assumptions 4.1, 4.3, 4.4, and 4.5, for all $\epsilon > 0$, $\{-\log(l_n)\}$ strongly separates $\mathfrak{A}^\epsilon$ from $\mathfrak{B}^*_\epsilon$.

*Proof.* Consider the Banach space of all continuous function on $B_s(\theta_0, \epsilon)$, which is separable since $B(\theta_0, \epsilon)$ is a compact subset of $\mathbb{R}^q$. By Assumption 4.4, $-\log(f(X_1, \theta)), \ldots, -\log(f(X_n, \theta))$ are i.i.d. random variables valued in this Banach space. By Assumption 4.5 and the law of large numbers in Banach spaces (see, e.g., Corollary 7.10 in Ledoux and Talagrand 1980),

$$\sup_{\theta \in \mathfrak{A}^\epsilon} \left[ -\log(l_n(\theta)) - s(\theta, \theta_0) \right] \to 0 \quad (\text{a.s.}),$$

which implies

$$\sup_{\theta \in \mathfrak{A}^\epsilon} \left[ -\log(l_n(\theta)) \right] \to \sup_{\theta \in \mathfrak{A}^\epsilon} s(\theta, \theta_0) \quad (\text{a.s.}). \quad (11)$$

Similarly, we have

$$\inf_{\theta \in \mathfrak{B}^*_\epsilon} \left[ -\log(l_n(\theta)) \right] \to \inf_{\theta \in \mathfrak{B}^*_\epsilon} s(\theta, \theta_0) \quad (\text{a.s.}). \quad (12)$$

Since $\mathfrak{B}^*_\epsilon$ is compact, there exists $\delta_1 > 0$ such that $s(\theta, \theta_0) \geq s(\theta_0, \theta_0) + \delta + \delta_1$ for all $\theta \in \mathfrak{B}^*_\epsilon$. Consequently, by (11) and (12),

$$P \left( \sup_{\theta \in \mathfrak{A}^\epsilon} \left[ -\log(l_n(\theta)) \right] < \inf_{\theta \in \mathfrak{B}^*_\epsilon} \left[ -\log(l_n(\theta)) \right] \right) \to 1,$$

which completes the proof. \qed

**Remark 4.2.** If Assumptions 4.4 and 4.5 hold, it can be proved that $s(\cdot, \theta_0)$ is continuous on $\Theta$, which is assumed in Assumption 4.3.

By the two Strong Comparison Theorems, Theorems 3.1 and 3.4, the strong separation property of the objective function provides a more strict guarantee of BSP than its weak analogue. However, at a price of this strictness, more restrictive conditions are required for verifying the strong separation property. By Theorem 3.1, for comparing two estimators $\xi_n$ and $\eta_n$ via the strong separation property stated in Theorem 4.2, we require $P(\xi_n \in \mathfrak{A}^\epsilon \cup \mathfrak{B}^*_\epsilon) \to 1$ and $P(\eta_n \in \mathfrak{A}^\epsilon \cup \mathfrak{B}^*_\epsilon) \to 1$. 16
4.2 A counter example

A prerequisite of BSP is that the global solution has desirable statistical properties. Based on examples of inconsistent MLEs, we can find counter examples of the greater likelihood principle. They are also counter examples of BSP. The example discussed here is taken from Chen and Wu (1994).

Let $X_1, \ldots, X_n$ be i.i.d. from the following distribution

$$P(X_1 = 1) = \begin{cases} \theta & \text{if } \theta \text{ is a rational number}, \\ 1 - \theta & \text{otherwise}, \end{cases}$$

$$P(X_1 = 0) = 1 - P(X_1 = 1),$$

where $\theta \in [0, 1]$ is the unknown parameter. It is not hard to show the MLE of $\theta$ is the sample mean $\bar{X}$. However, if the true parameter $\theta_0$ is an irrational number, as $n \to \infty$, $\bar{X} \to 1 - \theta_0$ (a.s.), which cannot be $\theta_0$. Consider another estimator

$$\hat{\theta} = (1 - \bar{X})I(U \leq 1/2) + \bar{X}I(U > 1/2),$$

where $U$, independent of the sample, is drawn from the uniform distribution on $[0, 1]$ and $I$ is the indicator function. We can show that, if $\theta_0$ is an irrational number, $\hat{\theta}$ has larger probability of lying in a sufficiently small neighborhood of $\theta_0$ than $\bar{X}$ asymptotically, whereas it always produces smaller value of the likelihood function.

4.3 A simulation study

In this subsection we conduct a small simulation study to verify the greater likelihood principle in finite-sample cases. Consider a Cauchy distribution with the density function

$$f(x, \mu) = \frac{1}{\pi [(x - \theta)^2 + 1]},$$

where $\theta$ is the unknown parameter we want to estimate based on the i.i.d. observations.
Table 1: MSE comparisons in Section 4.3

| n  | median   | trimmed mean | hybrid   |
|----|----------|--------------|----------|
|    | 0.3360   | 0.4929       | 0.3260   |
| 10 | 0.2056   | 0.2236       | 0.1857   |
| 15 | 0.1427   | 0.1628       | 0.1333   |
| 20 | 0.1109   | 0.1221       | 0.1001   |
| 25 | 0.0905   | 0.1027       | 0.0845   |
| 30 | 0.0804   | 0.0827       | 0.0720   |
| 35 |

\[X_1, \ldots, X_n\]. It is known that the MLE of \(\theta\) has not closed form, and iterative algorithms such as the Newton-Raphson algorithm can be used to compute it. We compare three simple methods, the sample median, the trimmed mean removing 50% extreme values, and a hybrid method that selects the better one of the two estimators with greater likelihood as the final estimator. Given the true parameter \(\theta_0 = 0\), we repeat 10,000 times to compute mean squares errors (MSEs) of the three estimators for various sample sizes, and the results are displayed in Table 1. It can be seen that the results follow the greater likelihood principle well: the hybrid estimator always yields the smallest MSEs among the three estimators.

5 Better subsample selection under contaminated models

Let \(\mathcal{F}^p\) denote the set of all cumulative distribution functions (c.d.f.) on \(\mathbb{R}^p\). Suppose that we are interested in making inferences for the unknown parameter \(\theta\) of a parametric family \(\{F_\theta\}_{\theta \in \Theta}\) based on i.i.d. observations \(X_1, \ldots, X_n\), where \(F_\theta \in \mathcal{F}^p\) for all \(\theta\) and the parameter space \(\Theta\) is a subset of \(\mathbb{R}^q\). When the observations include some outliers, a commonly used assumption for describing this situation is that the dataset is a randomly mixed batch of \(n\) “good” observations and outliers, and that each single observation with probability \(1 - \epsilon\) is a “good” one, with probability \(\epsilon\) an outlier, where \(\epsilon \in [0, 1/2]\) (Huber 1981). Under this assumption, the observations are drawn from the contaminated population, i.e.,

\[X_1, \ldots, X_n \text{ i.i.d. } \sim (1 - \epsilon)F_\theta + \epsilon G,\]  

(13)
where $G \in F^p$ is the contamination distribution. Here we consider a simplified model by removing the randomness of $X_i$ being a good observation or an outlier. Denote the set of all subsequences of $\{n\}_{n=1,2,\ldots}$ by $\mathcal{S}$, i.e.,

$$\mathcal{S} = \{\{k_n\} : k_n \in \mathbb{N}, k_1 < k_2 < \cdots\}.$$ 

Take an integer sequence $\{l_n\}$ satisfying $l_1 \leq \cdots \leq l_n \leq \cdots$ and $l_n/n \to 1 - \epsilon$ as $n \to \infty$. For $\{k_n^0\} \in \mathcal{S}$, let

$$A_{0n} = \{k_{1n}^0, \ldots, k_{ln}^0\},$$

which denotes the index set of all good observations. Assume that

$$X_1, \ldots, X_n \text{ are independently drawn as } X_i \sim F_\theta \text{ for } i \in A_{0n} \text{ and } X_i \sim G \text{ for } i \notin A_{0n}. \quad (15)$$

The model (15) is asymptotically equivalent to (13) in the sense that the two empirical distributions based on the observations generated from both of them have the identical limit $(1 - \epsilon)F_\theta + \epsilon G$ as $n \to \infty$.

**Remark 5.1.** The assumption that $A_{0n}$ is a segment of a subsequence is technical. Under this assumption, the observations can be viewed as a sequence of random variables, and thus some limit theory on sequences of random variables can be applied such as the strong law of large numbers. Otherwise, we may have to consider the observations as triangle arrays, and more restrictive conditions are required to establish the corresponding asymptotic results. On the practical aspect, this assumption is also reasonable.

The set $A_{0n}$ in (15) consists of the indices of all good observations. An ideal method for robust inferences is based on all good observations, i.e., we first correctly identify $A_{0n}$. We refer to the method of selecting $A_{0n}$ by optimizing some criteria as *best subsample selection*, parallel to best subset regression in variable selection. The minimum covariance determinant estimate (Rousseeuw 1985) and least trimmed squares estimate (Rousseeuw 1984) are instances of best subsample selection-based estimates. In general, it is impossible to exactly
select $A_{0n}$ itself since $\epsilon$ is usually unknown. A practical purpose is to select a subset of $A_{0n}$.

The estimates based on best subsample selection have high breakdown values (Hubert, Rousseeuw, and Van Aelst 2008), whereas their asymptotic properties are difficult to derive. Limited results were obtained under uncontaminated models, i.e., $\epsilon = 0$ in (13); see, e.g., Rousseeuw and Leroy (1987), Butler, Davies, and Jhun (1993), and Agulló, Croux, and Van Aelst (2008). To the best of the author’s knowledge, there is no work on the asymptotics of best subsample selection or related estimates under contaminated models such as (13) or (15). In this section we discuss whether BSP for best subsample selection (asymptotically) holds under model (15).

The statistical optimization problem in best subsample selection can be formulated as follows. For all $n$, the decision space is

$$
\mathcal{D}_n = \{A \subset \mathbb{Z}_n : |A| = m\},
$$

where $m = m_n < n$ is a pre-specified integer and $|\cdot|$ denotes cardinality. The best subsample of size $m$ is the solution to

$$
\min_{A \in \mathcal{D}_n} \psi_n(A),
$$

where $\psi_n$ is the objective function. Two types of objective functions will be discussed in Sections 5.1 and 5.2, respectively. Since (17) is actually a combinatorial optimization problem, it is difficult to attain the best subsample. In this section we prove the separation property of the two types of objective functions. This property implies that better subsamples are more likely to be subsets of $A_{0n}$ by the comparison theorems.

Denote

$$
\mathcal{G}_0 = \left\{\{k_n\} \in \mathcal{G} : \{k_1, \ldots, k_m\} \subset A_{0n} \text{ for all } n\right\},
$$

$$
\mathcal{G}_1 = \left\{\{k_n\} \in \mathcal{G} : \sum_{i=1}^{m} I(k_i \notin A_{0n})/m \to \alpha > 0 \text{ as } n \to \infty\right\},
$$

(18)
and

$$\mathfrak{A} = \{ \{ A_n \} : A_n = \{ k_1, \ldots, k_m \} \text{ for all } n, \{ k_n \} \in \mathfrak{S}_0 \}_{n \in \mathbb{N}},$$

$$\mathfrak{B} = \{ \{ A_n \} : A_n = \{ k_1, \ldots, k_m \} \text{ for all } n, \{ k_n \} \in \mathfrak{S}_1 \}_{n \in \mathbb{N}},$$

where $I$ is the indicator function. In this section $\mathfrak{A}$ serves as the space of good decisions. In fact, the asymptotic results in this section also hold if $\mathfrak{S}_0$ in (18) is replaced by $\mathfrak{S}_0 = \{ \{ k_n \} \in \mathfrak{S} : \sum_{i=1}^{m} I(k_i \notin A_{0n}) / m \to 0 \text{ as } n \to \infty \}$.

### 5.1 Selection by maximum likelihood

Suppose that $F_\theta$ and $G$ in (15) respectively have the p.d.f.’s, $f(\cdot, \theta)$ and $g(\cdot)$, with respect to a $\sigma$-finite measure on $\mathbb{R}^p$, where $\theta \in \Theta \subset \mathbb{R}^q$. A natural idea is to select the best subsample by maximum likelihood, i.e., the objective function in (17) is taken as

$$\psi_n(A) = \inf_{\theta \in \Theta} \left[ -\sum_{i \in A} \log \left( f(X_i, \theta) \right) \right].$$

(20)

If

$$\hat{\theta}_A = \arg\min_{\theta \in \Theta} \left[ -\sum_{i \in A} \log \left( f(X_i, \theta) \right) \right]$$

(21)

exists for all $A \in \mathfrak{D}_n$, then we can write

$$\psi_n(A) = -\sum_{i \in A} \log \left( f(X_i, \hat{\theta}_A) \right).$$

(22)

The minimum covariance determinant method (Rousseeuw 1985), which looks for the observations whose classical covariance matrix has the lowest possible determinant, can be viewed as an instance of the method of minimizing (22) if the underlying model is assumed to be a multivariate normal distribution.
We need several assumptions to establish the separation property of $\psi_n$. Denote

$$s_g(\theta) = -\int \log(f(x,\theta))g(x)d\mu(x).$$

**Assumption 5.1.** For sufficiently large $n$, $m \leq |A_0n|$, and as $n \to \infty$, $m/n \to \tau \in [1/2, 1-\epsilon]$.

**Assumption 5.2.** For all $\alpha \in [0, \epsilon/(1-\tau)]$, $\arg\min_{\theta \in \Theta}(1-\alpha)s(\theta, \theta_0) + \alpha s_g(\theta)$ exists, where $s$ is defined in (9).

Denote $\theta^* = \arg\min_{\theta \in \Theta}(1-\alpha)s(\theta, \theta_0) + \alpha s_g(\theta)$, and

$$\varphi(x, r) = \sup_{\theta \in C(\Theta) \setminus B(\theta^*, r)} f(x, \theta),$$

$$\varphi^*(x, r) = \begin{cases} 1, & \text{if } \varphi(x, r) \leq 1, \\ \varphi(x, r), & \text{otherwise.} \end{cases}$$

**Assumption 5.3.** The family $\{f(\cdot, \theta)\}_{\theta \in \Theta}$ has a common support set $S = \{x \in \mathbb{R}^p : 0 < f(x, \theta) < \infty\}$. For all $x \in S$, $f(x, \cdot)$ is continuous on $\Theta$, and $\lim_{\|\theta\| \to \infty} f(x, \theta) = 0$.

**Assumption 5.4.** There exists $r^* > 0$ such that $\int \log(\varphi^*(x, r^*))f(x, \theta_0)d\mu(x) < \infty$ and $\int \log(\varphi^*(x, r^*))g(x)d\mu(x) < \infty$.

**Assumption 5.5.** For all compact subset $K$ of $\Theta$,

$$\int \sup_{\phi \in K} \left| \log\left(f(x, \phi)\right) \right| f(x, \theta_0)d\mu(x) < \infty, \quad \int \sup_{\phi \in K} \left| \log\left(f(x, \phi)\right) \right| g(x)d\mu(x) < \infty.$$

**Assumption 5.6.** For all $\theta \in \Theta$ and $\alpha \in (0, \epsilon/(1-\tau)]$, $(1-\alpha)s(\theta, \theta_0) + \alpha s_g(\theta) > s(\theta_0, \theta_0)$.

**Lemma 5.1.** Under Assumptions 5.3 and 5.4, we have

$$\lim_{r \to \infty} \int \log(\varphi(x, r_0))f(x, \theta_0)d\mu(x) = -\infty, \quad (23)$$

$$\lim_{r \to \infty} \int \log(\varphi(x, r_0))g(x)d\mu(x) = -\infty. \quad (24)$$
Proof. See Wald (1949) for the proof of (23), and that of (24) is almost the same.

Theorem 5.1. Under Assumptions 5.1–5.6, \( \{ \psi_n \} \) in (20) separates \( \mathcal{A} \) from \( \mathcal{B} \) in (19).

Proof. For \( \{ A_n \} \in \mathcal{A} \),

\[
\frac{\psi_n(A_n)}{m} = \inf_{\theta \in \Theta} \left[ -\frac{1}{m} \sum_{i \in A_n} \log \left( f(X_i, \theta) \right) \right] \\
\leq -\frac{1}{m} \sum_{i \in A_n} \log \left( f(X_i, \theta_0) \right) \to s(\theta_0, \theta_0) \quad (\text{a.s.}).
\]

Consider \( \{ A_n \} \in \mathcal{B} \). By Lemma 5.1 there exists \( r_0 \) such that

\[
\int \log \left( \varphi(x, r_0) \right) f(x, \theta_0) d\mu(x) < -s(\theta^*, \theta_0), \\
\int \log \left( \varphi(x, r_0) \right) g(x) d\mu(x) < -s_g(\theta^*).
\]

By the strong law of large numbers,

\[
-\frac{1}{m} \sum_{i \in A_n} \log \left( \varphi(X_i, r_0) \right) \to -(1 - \alpha) \int \log \left( \varphi(x, r_0) \right) f(x, \theta_0) d\mu(x) \\
\quad - \alpha \int \log \left( \varphi(x, r_0) \right) g(x) d\mu(x) \quad (\text{a.s.}),
\]

\[
-\frac{1}{m} \sum_{i \in A_n} \log \left( f(X_i, \theta^*) \right) \to (1 - \alpha)s(\theta^*, \theta_0) + \alpha s_g(\theta^*) \quad (\text{a.s.}),
\]

which implies

\[
\liminf_{n \to \infty} \left[ -\frac{1}{m} \sum_{i \in A_n} \log \left( \varphi(X_i, r_0) \right) + \frac{1}{m} \sum_{i \in A_n} \log \left( f(X_i, \theta^*) \right) \right] > 0 \quad (\text{a.s.}).
\]

Note that

\[
\inf_{\theta \in C(\Theta) \setminus B(\theta^*, r_0)} \left[ -\frac{1}{m} \sum_{i \in A_n} \log \left( f(X_i, \theta) \right) \right] \geq -\frac{1}{m} \sum_{i \in A_n} \log \left( \sup_{\theta \in C(\Theta) \setminus B(\theta^*, r_0)} f(X_i, \theta) \right) \\
= -\frac{1}{m} \sum_{i \in A_n} \log \left( \varphi(X_i, r_0) \right).
\]
By (26), for sufficiently large $n$,

$$\inf_{\theta \in C \setminus B(\theta^*, r_0)} \left[ -\frac{1}{m} \sum_{i \in A_n} \log f(X_i, \theta) \right] > -\frac{1}{m} \sum_{i \in A_n} \log f(X_i, \theta^*) \quad \text{a.s.}$$

Hence, by the law of large numbers in Banach spaces,

$$\frac{\psi_n(A_n)}{m} = \inf_{\theta \in \Theta} \left[ -\frac{1}{m} \sum_{i \in A_n} \log f(X_i, \theta) \right] = \min_{\theta \in C \cap B(\theta^*, r_0)} \left[ -\frac{1}{m} \sum_{i \in A_n} \log f(X_i, \theta) \right]$$

$$\to (1 - \alpha)s(\theta^*, \theta_0) + \alpha s_g(\theta^*) \quad \text{a.s.} \quad (27)$$

Combining (25) and (27), by Assumption 5.6 we complete the proof.

If $\hat{\theta}_A$ in (21) exists for all $A \in D_n$, we can show that $\hat{\theta}_A \to \theta_0$ and $\psi_n(A_n)/m \to s(\theta_0, \theta_0)$ (a.s.) for $\{A_n\} \in A$ under regularity conditions. From the above proof, Assumption 5.6 is actually a necessary condition for the separation property of $\{\psi_n\}$. This assumption is generally strong. Consider a simple case of $\epsilon = \tau = 1/2$, where Assumption 5.6 reduces to

$$s_g(\theta) > s(\theta_0, \theta_0) \quad \text{for all } \theta \in \Theta. \quad (28)$$

For $f(x, \theta) = (2\pi)^{-1/2} \exp \left( -\frac{(x - \theta)^2}{2} \right)$ with $\theta_0 = 0$, $s(\theta_0, \theta_0) = \log(2\pi)/2 + 1/2$, and $s_g(\theta) = \log(2\pi)/2 + 1/2 \int (x - \theta)^2 g(x)dx$. Therefore, (28) holds if and only if

$$\int (x - \theta)^2 g(x)dx > 1 \quad \text{for all } \theta \in \mathbb{R},$$

which is equivalent to $\text{Var}(Z) > 1$, where $Z \sim g$. If $g$ is the p.d.f. of $N(\mu, \sigma^2)$ with $\sigma \leq 1$, then $\{\psi_n\}$ in (20) cannot separate $A$ from $B$ no matter how far away $\mu$ is from $\theta_0$. This example indicates that the selection by maximum likelihood may perform poorly when there are clustered outliers. In the next subsection we will provide another subsample selection method that still works well for this case.
5.2 Selection by minimum distance

An important class of robust estimators is the minimum distance estimator (Wolfowitz 1957), which is derived by minimizing a certain “distance” between the observations and the assumed population. This estimator usually possesses good robust properties, and has been discussed actively in the literature; see Donoho and Liu (1994), Lindsay (1994), and Wu, Karunamuni, and Zhang (2012), among others. Here we combine it with best subsample selection to provide new robust methods. Let $d_K$ denote the Kolmogorov distance between two c.d.f.’s, i.e., for $F, G \in \mathcal{F}$,

$$d_K(F, G) = \sup_{x \in \mathbb{R}^p} |F(x) - G(x)|.$$

Take the objective function in (17) as

$$\psi_n(A) = \inf_{\theta \in \Theta} d_K(\hat{H}_A, F_\theta),$$

(29)

where $\hat{H}_A$ is the empirical distribution function based on the observations $\{X_i\}_{i \in A}$. We discuss BSP for this problem under model (15) through verifying the separation property of $\{\psi_n\}$ in (29).

Assumption 5.7. For all $\alpha \in (0, \epsilon/(1 - \tau)]$, $\inf_{\theta \in \Theta} d_K((1 - \alpha)F_{\theta_0} + \alpha G, F_\theta) > 0$.

Theorem 5.2. Under Assumptions 5.1 and 5.7, $\{\psi_n\}$ in (29) separates $\mathfrak{A}$ from $\mathfrak{B}$ in (19).

Proof. For $\{A_n\} \in \mathfrak{A}$, by the Glivenko-Cantelli theorem,

$$\psi_n(A_n) = \inf_{\theta \in \Theta} d_K(\hat{H}_{A_n}, F_\theta) \leq \inf_{\theta \in \Theta} d_K(F_{\theta_0}, F_\theta) + d_K(\hat{H}_{A_n}, F_{\theta_0}) = d_K(\hat{H}_{A_n}, F_{\theta_0}) \to 0 \text{ (a.s.)}.$$

(30)

For $\{A_n\} \in \mathfrak{B}$, we have

$$\psi_n(A_n) = \inf_{\theta \in \Theta} d_K(\hat{H}_{A_n}, F_\theta) \geq \inf_{\theta \in \Theta} d_K((1 - \alpha)F_{\theta_0} + \alpha G, F_\theta) - d_K(\hat{H}_{A_n}, (1 - \alpha)F_{\theta_0} + \alpha G),$$
which implies
\[
\liminf_{n \to \infty} \psi_n(A_n) \geq \inf_{\theta \in \Theta} d_K((1 - \alpha)F_{\theta_0} + \alpha G, F_\theta) > 0 \quad \text{(a.s.}).
\] (31)

Combining (30) and (31), we complete the proof.

Compared to Assumption 5.6, Assumption 5.7 is fairly weak. For example, let \( F_\theta \) be the c.d.f. of \( N(\theta, 1) \) with \( \theta_0 = 0 \), and let \( \epsilon = \tau = 1/2 \). Suppose that \( G \) is the c.d.f. of \( N(\mu, \sigma^2) \). Assumption 5.7 holds for all \( \sigma \neq 1 \).

As a byproduct, we next prove another interesting result that, with additional conditions, the estimator based on the best subsample selected by minimizing the objective function \( \psi_n \) in (29) is consistent even under the contaminated model (15). This result provides further support of using this objective function. In addition, to the best of the author’s knowledge, this estimator is the first one that can converge to the true parameter even under the contaminated model, and may be of independent interest.

**Assumption 5.8.** For all \( \theta_1, \theta_2 \in \Theta, \ F_{\theta_1} = F_{\theta_2} \) implies \( \theta_1 = \theta_2 \).

**Assumption 5.9.** For all \( \phi \in \Theta \), \( \lim_{\theta \to \phi} d_K(F_\theta, F_\phi) = 0 \).

**Assumption 5.10.** For all \( x \in \mathbb{R}^p \) and all \( b \in C(\Theta) \setminus \Theta \), \( \lim_{\theta \to b} (F_\theta(x) - F_\theta(-x)) = 0 \).

**Assumption 5.11.** For all \( \theta \in \Theta, \ \theta \neq \theta_0, \ [(1 - \epsilon)F_{\theta_0} + \epsilon G - \tau F_{\theta_1}] / (1 - \tau) \notin \mathcal{F}_p \).

Assumption 5.11 is the key condition to guarantee that \( \theta_0 \) is estimable. Otherwise, if there exists \( \theta_1 \neq \theta_0 \) such that \( U = [(1 - \epsilon)F_{\theta_0} + \epsilon G - \tau F_{\theta_1}] / (1 - \tau) \in \mathcal{F}_p \), then
\[
\tau F_{\theta_1} + (1 - \tau)U = (1 - \epsilon)F_{\theta_0} + \epsilon G,
\]
which makes us unable to distinguish between \( \theta_0 \) and \( \theta_1 \). This assumption is stronger than Assumption 5.7.

**Assumption 5.12.** For all \( A \in \mathcal{D}_n \), \( \arg\min_{\theta \in \Theta} d_K(\hat{H}_A, F_\theta) \) exists (a.s.) for sufficiently large \( n \).
Lemma 5.2. Suppose that $F_n \in \mathcal{F}^p$ for each $n$ with $d_K(F_n, F) \to 0$ as $n \to \infty$, where $F$ is a function defined on $\mathbb{R}^p$. Then $F \in \mathcal{F}^p$.

Proof. We can prove this lemma by verifying the definition of a c.d.f.

Denote $A_n^* = \arg \min_{A \in \mathcal{A}_n} \psi_n(A)$. By Assumption [5.12], $\hat{\theta}_{A_n^*} = \arg \min_{\theta \in \Theta} d_K(\hat{H}_{A_n^*}, F_\theta)$ exists. We now present the consistency result of $\hat{\theta}_{A_n^*}$.

Proposition 5.1. Suppose that Assumption [5.1] and Assumptions [5.8]–[5.12] hold. Then

(i) $\hat{\theta}_{A_n^*} \to \theta_0$ (a.s.);
(ii) $d_K(\hat{\theta}_{A_n^*}, F_{\theta_0}) \to 0$ (a.s.).

Proof. Here we assume $\epsilon > 0$. The proof for $\epsilon = 0$ is similar and simpler. Denote $H = (1 - \epsilon)F_{\theta_0} + \epsilon G$.

Let $\{A_n\} \in \mathfrak{A}$. We have

$$d_K(\hat{H}_{A_n^*}, F_{\hat{\theta}_{A_n^*}}) \leq d_K(\hat{H}_{A_n^*}, F_{\hat{\theta}_{A_n}}) \leq d_K(\hat{H}_{A_n^*}, F_{\theta_0}) \to 0 \text{ (a.s.)}. \quad (32)$$

On the other hand, letting $Z_n$ denote $\{1, \ldots, n\}$, we have

$$d_K(\tau \hat{H}_{A_n^*} + (1 - \tau)\hat{H}_{Z_n \setminus A_n^*}, H)$$

$$\leq d_K(m \hat{H}_{A_n^*}/n + (n - m)\hat{H}_{Z_n \setminus A_n^*}/n, H)$$

$$+ d_K(\tau \hat{H}_{A_n^*} + (1 - \tau)\hat{H}_{Z_n \setminus A_n^*}, m \hat{H}_{A_n^*}/n + (n - m)\hat{H}_{Z_n \setminus A_n^*}/n)$$

$$\leq d_K(\hat{H}_{Z_n}, H) + |\tau - m/n| + |(1 - \tau) - (n - m)/n|$$

$$\to 0 \text{ (a.s.)}. \quad (33)$$

By (32) and (33),

$$d_K(\hat{H}_{Z_n \setminus A_n^*}, (H - \tau F_{\hat{\theta}_{A_n^*}})/(1 - \tau)) \to 0 \text{ (a.s.)}. \quad (34)$$

Let $E \subset \Omega$ be the set where (32) and (34) hold. For $\omega \in E$, let $b$ be a limit point of $\hat{\theta}_{A_n^*}(\omega)$.
Consider the case of \( b \in C(\Theta) \backslash \Theta \). Let \( \hat{\theta}_{A_{k_n}}(\omega) \to b \), where \( \{k_n\} \) is a subsequence of \( \{n\}_{n=1,2,...} \). For \( \epsilon > 0 \), there exist \( \delta > 0 \) and \( x_0 \in \mathbb{R}^p \) such that

\[
H(x_0) - H(-x_0) > 1 - \tau + \delta. \tag{35}
\]

By Assumption 5.10, for sufficiently large \( n \),

\[
F_{\hat{\theta}_{A_{k_n}}}(x_0) - F_{\hat{\theta}_{A_{k_n}}}(x_0) < \delta/(3\tau).
\]

By (32), for sufficiently large \( n \),

\[
\hat{H}_{A_{k_n}}(x_0) - \hat{H}_{A_{k_n}}(-x_0) < \delta/(2\tau). \tag{36}
\]

It follows from (34), (35), and (36) that for sufficiently large \( n \),

\[
\hat{H}_{Z_{n}\backslash A_{k_n}}(x_0) - \hat{H}_{Z_{n}\backslash A_{k_n}}(-x_0) > \left[ (H(x_0) - H(-x_0)) - \tau(\hat{H}_{A_{k_n}}(x_0) - \hat{H}_{A_{k_n}}(-x_0)) - \delta/2 \right]/(1 - \tau) > 1.
\]

This is a contradiction. Therefore, \( b \in \Theta \).

By Assumption 5.9

\[
d_{K}(\hat{H}_{Z_{n}\backslash A_{k_n}}(\omega), [(1 - \epsilon)F_{\theta_0} + \epsilon G - \tau F_b]/(1 - \tau)) \to 0
\]

By Lemma 5.2

\[
[(1 - \epsilon)F_{\theta_0} + \epsilon G - \tau F_b]/(1 - \tau) \in \mathcal{F}_p. \tag{37}
\]

By Assumption 5.11 \( b = \theta_0 \). This completes the proof of (i), and (ii) follows from (i) immediately.

\[\square\]

**Remark 5.2.** From the above proof, when Assumption 5.11 does not hold, any limit point
Table 2: Comparisons of different B’s in Section 5.3

|                | (I)     | (II)    |
|----------------|---------|---------|
| likelihood     | MOV     | MSE     | MOV     | MSE     |
| (B = 10)       | 0.3244  | 0.5712  | 2.1988  | 0.4447  |
| likelihood     |         |         |         |         |
| (B = 100)      | 0.1347  | 0.7862  | 1.1227  | 0.3152  |
| d_K (B = 10)   | 0.2036  | 0.1694  | 0.1565  | 0.4366  |
| d_K (B = 100)  | 0.1677  | 0.1278  | 0.1232  | 0.3780  |

\[ \hat{\theta}_{n_0}^* (\omega) \text{ satisfies (37). For small } \epsilon, \text{ such } b \text{ cannot be far way from } \theta_0 \text{ since } d_K(F_b, F_{\theta_0}) \leq \epsilon/(1 - \epsilon). \]

5.3 A simulation study

We conduct a small simulation study to compare the two subsample selection methods by likelihood and \( d_K \). Let the good observations \( X_1, \ldots, X_{n_0} \) be i.i.d. \( \sim N(\theta, 1) \) with \( \theta_0 = 0 \). We generate \( n_o \) outliers \( X_{n_0+1}, \ldots, X_{n_0+n_o} \) as

(I): \( X_{n_0+1} = \ldots = X_{n_0+n_o} = 1; \)

(II): \( X_{n_0+1}, \ldots, X_{n_0+n_o} \) i.i.d. \( \sim N(1, 3) \).

We search the solutions to (17) with the objective functions (20) and (29) through randomly generating \( B \) subsets of size \( m \). In this simulation, we fix \( n_0 = n_o = m = 10 \) and consider two values of \( B \), 10 and 100. We Repeat 10,000 times to compute the mean objective values (MOVs) and MSEs. The results are shown in Table 2.

We state at the end of Section 5.1 that Assumption 5.6 does not hold when there are clustered outliers like (I), which can make BSP fail. The simulation results are consistent to this conclusion: the likelihood-based subsample estimator performs more poorly as \( B \) increases. For this case, the behavior of the \( d_K \)-based subsample estimator follows BSP well: smaller MOV, smaller MSE. When the outliers are from (II), the two estimators both follow BSP well, and the likelihood method is better.
6 Better subsample selection in regression

This section discusses BSP for the best subsample problem in regression models. We show that the least trimmed squares (LTS) estimate (Rousseeuw 1984) is actually an estimate based on the best subsample selected by the least squares, and prove the separation property of the corresponding objective function.

6.1 Main results

Consider a linear regression model

\[ y = X\beta + \varepsilon, \]  
(38)

where \( X = (x_{ij}) \) is the \( n \times p \) regression matrix, \( y = (y_1, \ldots, y_n)' \in \mathbb{R}^n \) is the response vector, \( \beta = (\beta_1, \ldots, \beta_p)' \) is the vector of regression coefficients and \( \varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)' \) is a vector of i.i.d. random errors with zero mean and finite variance \( \sigma^2 \). The LTS estimate is a commonly used regression estimate with high breakdown value, and we describe it as follows. For any \( \beta \) in (38), denote the corresponding residuals by \( r_i(\beta) = y_i - x_i'\beta \) for \( i = 1, \ldots, n \), where \( x_i = (x_{i1}, \ldots, x_{ip})' \). For a specified integer \( m \leq n \), the LTS estimator \( \hat{\beta}_{\text{LTS}} \) is the solution to

\[
\min_{\beta} \sum_{i=1}^{m} r_{\pi_i(\beta)}(\beta)^2,
\]  
(39)

where \( r_{\pi_1(\beta)}(\beta) \leq \cdots \leq r_{\pi_n(\beta)}(\beta) \) are the ordered squared residuals. Denote \( J(\beta) = \{\pi_1(\beta), \ldots, \pi_n(\beta)\} \).

For all \( n \), let the decision space \( \mathcal{D}_n \) be the same as (16) in the previous section. Take the objective function as

\[
\psi_n(A) = \|y_A - X_{[A]}\hat{\beta}_{[A]}\|^2,
\]  
(40)

where \( y_A \) is the subvector of \( y \) corresponding to the subsample \( A \), \( X_{[A]} \) is the submatrix of \( X \) corresponding to \( A \), i.e., \( X_{[A]} \) is obtained by removing all the rows whose subscripts are
not in $A$, and $\hat{\beta}_{[A]}$ is the least squares estimator under $A$, i.e., $\hat{\beta}_{[A]} = (X'_{[A]}X_{[A]})^{-1}X'_{[A]}y_A$.

We first show that the LTS estimator defined in (39) corresponds to the solution that minimizes $\psi_n$ in (40). Denote

$$A^*_n = \arg\min_{A \in D_n} \psi_n(A).$$

Proposition 6.1. The LTS estimator $\hat{\beta}_{LTS}$ satisfies $\hat{\beta}_{LTS} = \hat{\beta}_{[A^*_n]}$ and $J(\hat{\beta}_{LTS}) = A^*_n$.

Proof. We have

$$\sum_{i=1}^m r^2_{\pi_i(\hat{\beta}_{LTS}})(\hat{\beta}_{LTS}) \leq \sum_{i=1}^m r^2_{\pi_i(\hat{\beta}_{[A^*_n]})}(\hat{\beta}_{[A^*_n]}) \leq \|y_{A^*_n} - X_{[A^*_n]} \hat{\beta}_{[A^*_n]}\|^2$$

$$\leq \|y_{J(\hat{\beta}_{LTS})} - X_{[J(\hat{\beta}_{LTS})]} \hat{\beta}_{[J(\hat{\beta}_{LTS})]}\|^2 \leq \|y_{J(\hat{\beta}_{LTS})} - X_{[J(\hat{\beta}_{LTS})]} \hat{\beta}_{LTS}\|^2 = \sum_{i=1}^m r^2_{\pi_i(\hat{\beta}_{LTS}})(\hat{\beta}_{LTS}),$$

which completes the proof.

We next discuss BSP for the optimization problem associated with LTS. Let $A_{0n}$ be the same as in (14). The contaminated regression model is assumed to be

$$y_i = \beta'x_i + \varepsilon_i \text{ for } i \in A_{0n} \text{ and } y_i = R(x_i) + \varepsilon_i \text{ for } i \notin A_{0n},$$

(41)

where $R$ is a function defined on $\mathbb{R}^p$, and $\varepsilon_1, \ldots, \varepsilon_n$ are the same as in model (38).

Some notation and assumptions are needed to prove the separation property of $\{\psi_n\}$ under model (41). Define $\mathcal{G}_0$ and $\mathcal{G}_1$ as in (18), and $\mathfrak{A}$ and $\mathfrak{B}$ as in (19). For all $A \in \mathcal{D}_n$, let $H_{[A]} = I_m - X_{[A]}(X'_{[A]}X_{[A]})^{-1}X'_{[A]}$ denote the projection matrix on the subspace $\{x \in \mathbb{R}^m : X'_{[A]}x = 0\}$, where $I_m$ is the $m \times m$ identity matrix. In this section we let $\beta$ itself denote the true parameter in model (41), and assume that $p$ and $\beta$ are fixed.

Assumption 6.1. For all $\{k_n\} \in \mathcal{G}_0 \cup \mathcal{G}_1$, $X'_{\{k_n\}}X_{\{k_n\}}/n \to a positive definite matrix as $n \to \infty$, where $X_{\{k_n\}} = (x_{k_1} \cdots x_{k_n})'$.

Assumption 6.2. For all $\{k_n\} \in \mathcal{G}_0 \cup \mathcal{G}_1$, $v' H_{\{k_n\}} v/n$ has a positive and finite limit as $n \to \infty$, where $v = (v_1, \ldots, v_n)'$ with $v_i = 0$ for $k_i \in A_{0n}$ and $v_i = R(x_{k_i}) - \beta'x_{k_i}$ otherwise, $H_{\{k_n\}} = I_n - X_{\{k_n\}}(X'_{\{k_n\}}X_{\{k_n\}})^{-1}X'_{\{k_n\}}$, and $X_{\{k_n\}}$ is the same as in Assumption 6.1.
Remark 6.1. If $x_1, \ldots, x_n$ are i.i.d. generated from a $p$-dimensional distribution with a positive definite covariance matrix, then Assumptions 6.1 and 6.2 hold (a.s.) providing $E(R(x_1) - \beta' x_1)^2$ is positive and finite.

Lemma 6.1. Let \( \{a_{nk} : k = 1, \ldots, n, n = 1, 2, \ldots\} \) be an array of numbers satisfying
\[
\sum_{k=1}^{n} a_{nk}^2 \leq 1.
\]
Then \( \sum_{k=1}^{n} a_{nk} \varepsilon_i / \sqrt{n} \to 0 \) (a.s.) as $n \to \infty$.

Proof. See Chow (1966).

Theorem 6.1. Under Assumptions 6.1 and 6.2 \( \{\psi_n\} \) in \((40)\) separates \( \mathcal{A} \) from \( \mathcal{B} \) in \((19)\).

Proof. For \( \{A_n\} \in \mathcal{A} \), we have
\[
\psi_n(A_n)/m = \|y_{A_n} - X_{[A_n]} \hat{\beta}_{[A_n]}\|^2/m \leq \|y_{A_n} - X_{[A_n]} \beta\|^2/m \to \sigma^2 \text{ (a.s.)}. \tag{42}
\]

For \( \{A_n\} \in \mathcal{B} \), denote \( A_{1n} = A_n \cap A_{0n} \) and \( A_{2n} = A_n \setminus A_{0n} \). Partition \( H_{[A_n]} \) as \( H_{[A_n]} = (H_{[A_n]}^{(1)} \ H_{[A_n]}^{(2)}) \), where \( H_{[A_n]}^{(1)} \) corresponds to \( A_{1n} \). We have
\[
\psi_n(A_n) = \|y_{A_n} - X_{[A_n]} \hat{\beta}_{[A_n]}\|^2 = \left\| H_{[A_n]} \begin{pmatrix} X_{[A_{1n}]} \beta \\ R(X_{[A_{2n}]}) \end{pmatrix} + H_{[A_n]} \varepsilon_{A_n} \right\|^2
\]
\[
= \left\| H_{[A_n]} \left[ X_{[A_n]} \beta + \begin{pmatrix} 0 \\ R(X_{[A_{2n}]} - X_{[A_{2n}]} \beta) \end{pmatrix} \right] + H_{[A_n]} \varepsilon_{A_n} \right\|^2
\]
\[
= \left\| H_{[A_n]}^{(2)} (R(X_{[A_{2n}]} - X_{[A_{2n}]} \beta) + H_{[A_n]} \varepsilon_{A_n} \right\|^2
\]
\[
= \varepsilon_{A_n}^t H_{[A_n]} \varepsilon_{A_n} + (R(X_{[A_{2n}]} - X_{[A_{2n}]} \beta)^t H_{[A_n]}^{(2)} H_{[A_n]} \varepsilon_{A_n} \right. \\
\left. + (R(X_{[A_{2n}]} - X_{[A_{2n}]} \beta)^t H_{[A_n]}^{(2)} (R(X_{[A_{2n}]} - X_{[A_{2n}]} \beta),
\]

where \( R(X_{[A_{2n}]} = (R(x_i))'_{i \in A_{2n}} \). By Assumption 6.2 \( (R(X_{[A_{2n}]} - X_{[A_{2n}]} \beta)^t H_{[A_n]}^{(2)} H_{[A_n]}^{(2)} (R(X_{[A_{2n}]} - X_{[A_{2n}]} \beta)/m \to c > 0 \), which implies \( (R(X_{[A_{2n}]} - X_{[A_{2n}]} \beta)^t H_{[A_n]}^{(2)} H_{[A_n]} \varepsilon_{A_n} /m \to 0 \) (a.s.) by Lemma 6.1. Note that \( \varepsilon_{A_n}^t H_{[A_n]} \varepsilon_{A_n} /m \to \sigma^2 \) (a.s.) by Assumption 6.1. It follows that
\[
\psi_n(A_n)/m \to \sigma^2 + c \text{ (a.s.)}. \tag{43}
\]

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Table 3: Comparisons of different $B$’s in Section 6.2

|   | (I) MOV | (I) MSE | (II) MOV | (II) MSE |
|---|---------|---------|---------|---------|
| $B$ 100 | 12.464 | 1.2738 | 6.9142 | 0.6723 |
| 200 | 9.3486 | 0.9743 | 5.7195 | 0.6589 |
| 300 | 7.9660 | 0.8057 | 5.2018 | 0.6479 |

Combining (42) and (43), we complete the proof.

6.2 A simulation study

We conduct a small simulation to verify BSP for the LTS problem in finite-sample cases. Let $p = 2$ and $\beta = (0, 0)'$ in model (38). Generate $\{x_i = (x_{i1}, x_{i2})'\}_{i=1,\ldots,n}$ i.i.d. from a multivariate normal distribution $N(0, \Sigma)$ whose covariance matrix

$$\Sigma = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}.$$  

Then we obtain the regression matrix $X = (x_1,\ldots,x_n)'$. There are $n_0$ observations that obey the linear relationship, i.e., $y_i = \beta'x_i + \varepsilon_i$ for $i = 1,\ldots,n_0$, where the random errors $\varepsilon_1,\ldots,\varepsilon_{n_0}$ i.i.d. $\sim N(0,1)$. We generate $n_o = n - n_0$ outliers as

(I): $y_i = 5 + \beta'x_i + \varepsilon_i$ for $i = n_0 + 1,\ldots,n$, where the random errors $\varepsilon_{n_0+1},\ldots,\varepsilon_n$ i.i.d. $\sim N(0,1)$,

(II): $y_i = 2x_{i1} - 2x_{i2} + 3x_{i1}^2 + \varepsilon_i$ for $i = n_0 + 1,\ldots,n$, where the random errors $\varepsilon_{n_0+1},\ldots,\varepsilon_n$ i.i.d. $\sim N(0,3)$,

We search the solutions to minimize the objective functions (40) through randomly generating $B$ subsets of size $m$. In this simulation, we fix $n = 20$, $n_0 = 15$, $m = 11$ and consider three values of $B$, 100, 200, and 300. We repeat 10,000 times to compute the MOVs and MSEs as in Section 5.3. The results are shown in Table 3. We can see that the results follow BSP well: as $B$ in increases, the MOV and MSE both decreases.
7 Better subset for variable selection

Variable selection plays an important role in high-dimensional data analysis (Bühlmann and van de Geer 2011). Classical best subset regression ($\ell_0$-norm regularized method) has been viewed as an infeasible method for moderate or large $p$, and other regularized methods with continuous penalties such as the nonnegative garrote (Breiman, 1995), the lasso (Tibshirani, 1996), SCAD (Fan and Li, 2001), and MCP (Zhang, 2010) have become very popular in this area. However, Xiong (2013) showed that, even for large $p$, best subset regression is still a valuable method since BSP for this problem, called the better-fitting better-screening rule in Xiong (2013), holds under reasonable conditions. Therefore, we do not need to find the best subset (global solution), and a sub-optimal solution is usually satisfactory in practice. In fact, Xiong (2013) proved the strong separation property of the objective function in best subset regression. In this section we continue discussing this problem for both fixed and diverging $p$ cases.

7.1 Selection for the fixed $p$ case

Consider the linear regression model in (38) with fixed $p$ and $\boldsymbol{\beta}$. Without loss of generality, assume that there is no intercept in (38), which holds after standardizing $\mathbf{X}$ and $\mathbf{y}$. In this section, we denote the full model $\{1, \ldots, p\}$ by $\mathbb{Z}_p$. For $\mathcal{A} \subset \mathbb{Z}_p$, $|\mathcal{A}|$ denotes its cardinality, and $\mathbf{X}_\mathcal{A}$ denotes the submatrix of $\mathbf{X}$ corresponding to $\mathcal{A}$. As in Section 6, let $\boldsymbol{\beta}$ denote the true parameter in model (38). Let $\mathcal{A}_0$ denote the true submodel $\{j \in \mathbb{Z}_p : \beta_j \neq 0\}$ with $d = |\mathcal{A}_0|$. The decision space $\mathcal{D}$ is the power set of $\mathbb{Z}_p$, and its two subsets are

$$\mathcal{A} = \{\mathcal{A}_0\}, \quad \mathcal{B} = \mathcal{D} \setminus \mathcal{A}. \quad (44)$$

We adopt the BIC criterion (Schwarz, 1978) to select the important variables, which corresponds to the objective function

$$\psi_n(\mathcal{A}) = (1 + |\mathcal{A}| \log(n)/n) \| \mathbf{y} - \mathbf{X}_\mathcal{A} \hat{\boldsymbol{\beta}}_\mathcal{A} \|^2, \quad (45)$$

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where $\hat{\beta}_A$ is the least squares estimator $(X'_A X_A)^{-1} X'_A y$ under the submodel $A$. It is known that minimizing the BIC criterion leads to consistent variable selection for the fixed $p$ case; see e.g., Shao (1997). Here we provide a stronger result that BSP for this optimization problem holds through proving the strong separation property of $\psi_n$ in (45). Our result indicates that, for two subsets, the better one having smaller BIC value is more likely to be the true submodel.

Some notation and an assumption are needed. For $A \in \mathcal{D}$, let $H_A = I_n - X_A (X'_A X_A)^{-1} X'_A$ denote the projection matrix on the subspace $\{x \in \mathbb{R}^n : X'_A x = 0\}$. We denote by $\lambda_{\text{min}}(\cdot)$ the smallest eigenvalue of a matrix. Let $\beta_{\text{min}}$ denote the component of $\beta_{A_0}$ that has the smallest absolute value. Define

$$
\delta_n = \min_{A_0 \setminus A \neq \emptyset} \left[ \frac{1}{n} \lambda_{\text{min}}(X'_{A_0 \setminus A} H_A X_{A_0 \setminus A}) \right].
$$

**Assumption 7.1.** As $n \to \infty$, $X'X/n \to \Sigma$, where $\Sigma$ is a positive definite matrix.

This assumption is a standard condition to handle fixed $p$ asymptotics in linear regression (Gleser 1965; Knight and Fu 2000).

**Theorem 7.1.** Under Assumption 7.1, $\{\psi_n\}$ in (45) strongly separates $\mathfrak{A}$ from $\mathfrak{B}$ in (44).

**Proof.** First we have $\psi_n(A_0)/n \to \sigma^2$ (a.s.), For $A \in \mathcal{D}$ with $A_0 \setminus A \neq \emptyset$,

$$
(1 + |A| \log(n)/n)^{-1} \psi_n(A)
= \epsilon' H_{T_n} \epsilon + 2 \beta'_{A_0} X'_{A_0} H_A \epsilon + \beta'_{A_0} X'_{A_0} H_A X_{A_0 \setminus A} \beta_{A_0}
= \epsilon' H_{T_n} \epsilon + 2 \beta'_{A_0} X'_{A_0} H_A \epsilon + \beta'_{A_0 \setminus A} X'_{A_0 \setminus A} H_A X_{A_0 \setminus A} \tau_n \beta_{A_0 \setminus A}
\geq \epsilon' H_A \epsilon + 2 \beta'_{A_0} X'_{A_0} H_A \epsilon + n \delta_n |\beta_{\text{min}}|^2.
$$

Note that $E(\beta'_{A_0} X'_{A_0} H_A \epsilon)^2/n^2 = \sigma^2 \text{tr}(\beta'_{A_0} X'_{A_0} H_A X_{A_0} \beta_{A_0})/n^2 \to 0$, $\epsilon' H_A \epsilon/n \to \sigma^2$ (a.s.), and $\delta_n$ has a positive limit point. It follows that

$$
P(\psi_n(A_0) < \psi_n(A)) \to 1. \tag{46}
$$
For $\mathcal{A} \supset \mathcal{A}_0$ with $\mathcal{A} \neq \mathcal{A}_0$,

$$
\psi_n(\mathcal{A}_0) - \psi_n(\mathcal{A}) = \varepsilon'(H_{\mathcal{A}_0} - H_{\mathcal{A}})\varepsilon + \varepsilon' H_{\mathcal{A}_0} \varepsilon |\mathcal{A}_0| \log(n)/n - \varepsilon' H_{\mathcal{A}} \varepsilon |\mathcal{A}| \log(n)/n.
$$

Note that $H_{\mathcal{A}_0} - H_{\mathcal{A}}$ converges to an idempotent matrix of rank $|\mathcal{A}| - |\mathcal{A}_0|$, which implies $\varepsilon'(H_{\mathcal{A}_0} - H_{\mathcal{A}})\varepsilon = O_p(1)$. Therefore,

$$
(\psi_n(\mathcal{A}_0) - \psi_n(\mathcal{A})) / \log(n) \to -\sigma^2(|\mathcal{A}| - |\mathcal{A}_0|) \quad \text{in probability.}
$$

Note that $\mathcal{D}$ is a finite set. By (46) and (47),

$$
P\left(\psi_n(\mathcal{A}_0) < \inf_{\mathcal{A}\in\mathcal{B}} \psi_n(\mathcal{A})\right) \\
\geq P\left(\psi_n(\mathcal{A}_0) < \inf_{\mathcal{A}_0 \setminus \mathcal{A} \neq \emptyset} \psi_n(\mathcal{A})\right) + P\left(\psi_n(\mathcal{A}_0) < \inf_{\mathcal{A} \supset \mathcal{A}_0, \mathcal{A} \neq \mathcal{A}_0} \psi_n(\mathcal{A})\right) - 1 \\
\to 1,
$$

which completes the proof.

**Remark 7.1.** With almost the same proof, Theorem 7.3 also holds for the objective function

$$
\psi_n(\mathcal{A}) = (1 + |\mathcal{A}|\lambda_n/n) \|y - X_\mathcal{A} \hat{\beta}_\mathcal{A}\|^2
$$

with $\lambda_n \to \infty$ and $\lambda_n/n \to 0$, which corresponds to the GIC criterion (Rao and Wu 1989). BIC is its special case corresponding to $\lambda_n = \log(n)$.

### 7.2 Screening for the diverging $p$ case

When $p$ increases faster than $n$, it becomes more difficult to find consistent variable selection procedures. A compromised strategy is to use a two-stage procedure (Fan and Lv 2008). In the first stage, a screening approach is applied to pick $M$ variables, where $M < n$ is specified. In the second stage, the coefficients in the screened $M$-dimensional submodel can be estimated by well-developed regression techniques. To guarantee the effectiveness
of this procedure, the first stage should possess the sure screening property, i.e., it should retain all important variables in the model asymptotically (Fan and Lv 2008). A number of screening procedures have been studied in the literature; see Fan and Lv (2008), Hall and Miller (2009), Fan et al. (2009), Wang (2009), and Li et al. (2012), among others. Following Xiong (2013), in this subsection we establish BSP for best subset regression in the screening problem.

The model and related notation are the same as in Section 7.1 except that \( p \) and the true parameter \( \beta \) can depend on \( n \). We let \( \mathcal{A}_{0n} \) denote the true submodel, which depends on \( n \) as well. For a specified \( M \) with \( d \leq M < n \), the decision space is \( \mathcal{D}_n = \{ \mathcal{A} \subset \mathbb{Z}_p : |\mathcal{A}| = M \} \), and two decision subsets are

\[
\mathfrak{A}_n = \{ \mathcal{A} \subset \mathcal{D}_n : \mathcal{A} \supset \mathcal{A}_{0n} \}, \quad \mathfrak{B}_n = \mathcal{D}_n \setminus \mathfrak{A}_n.
\]

Denote

\[
\mathfrak{A} = \prod_{n=1}^{\infty} \mathfrak{A}_n, \quad \mathfrak{B} = \prod_{n=1}^{\infty} \mathfrak{B}_n.
\]  

(48)

The objective function is

\[
\psi_n(\mathcal{A}) = \| y - X_{\mathcal{A}} \hat{\beta}_{\mathcal{A}} \|^2,
\]

(49)

where \( \hat{\beta}_{\mathcal{A}} \) is the least squares estimator \( (X_{\mathcal{A}}X_{\mathcal{A}})^{-1}X_{\mathcal{A}}y \) under the submodel \( \mathcal{A} \). Here we allow \( X_{\mathcal{A}} \) not to be of full column rank, and therefore the generalized inverse “\( ^{-1} \)” is used in \( \hat{\beta}_{\mathcal{A}} \). Similar to Section 7.1 for \( \mathcal{A} \in \mathcal{D}_n \), denote \( H_{\mathcal{A}} = I_n - X_{\mathcal{A}}(X'_{\mathcal{A}}X_{\mathcal{A}})^{-1}X'_{\mathcal{A}} \) and

\[
\delta_n = \min_{\mathcal{A} \notin \mathfrak{A}_n} \left\{ \frac{1}{n} \lambda_{\text{min}}(X'_{\mathcal{A}_{0n} \setminus \mathcal{A}} H_{\mathcal{A}} X_{\mathcal{A}_{0n} \setminus \mathcal{A}}) \right\}.
\]

Note that the objective function \( \psi_n \) in (49) is the residual sum of squares, which describes the fit of a submodel \( \mathcal{A} \). Based on this, Xiong (2013) provided the better-fitting better-screening rule for screening important variables, i.e., a better subset with better fit is more likely to include all important variables. This rule is actually the BSP for the problem of minimizing \( \psi_n \) in (49), and follows from the following strong separation property of \( \psi_n \).
proved by Xiong (2013).

**Assumption 7.2.** The random error $\varepsilon$ in (38) follows a normal distribution $N(0, \sigma^2 I_n)$.

**Assumption 7.3.** There exists a constant $C > 0$ such that $\sum_{i=1}^{n} x_{ij}^2 / n \leq C$ for any $j \in A_0$.

**Assumption 7.4.** As $n \to \infty$, $(\delta_n \beta_{\text{min}}^2)^{-1} = O(n^{\gamma_1})$, $\|\beta\|(\delta_n \beta_{\text{min}}^2)^{-1} = O(n^{\gamma_2})$, $d = O(n^{\gamma_3})$, $M = O(n^{\gamma_4})$, and $\log p = O(n^{\gamma_5})$, where $\gamma_i \geq 0$ ($i = 1, \ldots, 5$), $2\gamma_1 + \gamma_4 + \gamma_5 < 1$, and $2\gamma_2 + \gamma_3 + \gamma_4 + \gamma_5 < 1$.

**Theorem 7.2.** Under Assumptions 7.2–7.4, $\{\psi_n\}$ in (49) strongly separates $\mathfrak{A}$ from $\mathfrak{B}$ in (48).

Assumption 7.4 is strong in that $M$ cannot be too large, whereas in practice we usually use a large $M = O(n^\gamma)$ with an unrestricted $\gamma \in (0, 1)$, or even $M = O(n)$, for insurance. We next show that, under fairly weak conditions, $\{\psi_n\}$ has the weak separation property. By Theorem 3.6, Corollary 3.2, and Remark 3.3, the weak separation property suffices to imply the better-fitting better-screening rule for practice use.

**Assumption 7.5.** As $n \to \infty$, $M = o(n\delta_n \beta_{\text{min}}^2)$, and for all $\epsilon > 0$, $\sum_{n=1}^{\infty} \exp(-\epsilon n \delta_n \beta_{\text{min}}^2) < \infty$, $\sum_{n=1}^{\infty} \exp\left(-\epsilon n \delta_n \beta_{\text{min}}^2 / (d\|\beta\|^2)\right) < \infty$.

**Assumption 7.6.** As $n \to \infty$, $M/n \to \alpha \in (0, 1)$ and $\text{rank}(H_A)/n \to \lambda \in [0, 1)$ for all $A \in \mathfrak{D}_n$; for all $n$, $\delta_n \beta_{\text{min}}^2 \geq c$, where $c > 0$ is a constant; for all $\epsilon > 0$, $\sum_{n=1}^{\infty} \exp\left(-\epsilon n/(d\|\beta\|^2)\right) < \infty$.

**Lemma 7.1.** (i) Let $\xi_n \sim N(0, 1)$ for all $n$. Suppose that $b_n$ satisfies $\sum_{n=1}^{\infty} \exp(-\epsilon b_n^2) < \infty$ for all $\epsilon > 0$. Then $\xi_n/b_n \to 0$ (a.s.).

(ii) Let $\xi_n \sim \chi_{r_n}^2$, where $r_n$ is a positive integer for all $n$. Suppose that $b_n$ satisfies $r_n/b_n \to \alpha \in [0, 1]$ and $\sum_{n=1}^{\infty} \exp(-\epsilon b_n) < \infty$ for all $\epsilon > 0$. Then $(\xi_n - r_n)/b_n \to 0$ (a.s.).

**Proof.** (i) By the Borel-Cantelli lemma, it suffices to show that, for all $\epsilon > 0$,

$$\sum_{n=1}^{\infty} P(|\xi_n/b_n| > \epsilon) < \infty.$$  \hspace{1cm} (50)
Let \( \Phi \) denote the c.d.f. of \( \xi_n \). We have \( P(|\xi_n/b_n| > \epsilon) = 2[1 - \Phi(\epsilon b_n)] \leq (\epsilon b_n)^{-1} \exp(-\epsilon^2 b_n^2/2) \leq \exp(-\epsilon^2 b_n^2/2) \) for sufficiently large \( n \), which implies (50).

(ii) By Lemma 1 in Xiong (2013), for all \( \epsilon > 0 \),

\[
P(|\xi_n - r_n|/b_n > \epsilon) = P(|\xi_n/r_n - 1| > \epsilon b_n/r_n) \leq 2 \exp \left( -\frac{\epsilon^2}{4} b_n (1 + r_n/b_n)^{-1} \right).
\]

By the Borel-Cantelli lemma, we complete the proof.

**Theorem 7.3.** Under Assumption 7.2 and 7.3, if Assumption 7.5 or 7.6 holds, then \( \psi_n \) in (49) separates \( \mathfrak{A} \) from \( \mathfrak{B} \) in (48).

**Proof.** If Assumption 7.5 holds, it suffices to show that, for any \( \{A_n\} \in \mathfrak{A} \) and \( \{B_n\} \in \mathfrak{B} \),

\[
\limsup_{n \to \infty} \left[ \psi_n(A_n)/(n\delta_n \beta_{\min}^2) - \psi_n(B_n)/(n\delta_n \beta_{\min}^2) \right] < 0 \quad (a.s.) \quad (51)
\]

We have

\[
\psi_n(A_n) - \psi_n(B_n) = \epsilon^2 H_{A_n} \epsilon - (\epsilon^2 H_{B_n} \epsilon + 2\beta'_{A_{on}} X'_{A_{on}} H_{B_n} \epsilon + \beta'_{A_{on}} X'_{A_{on}} H_{B_n} X_{A_{on}} \beta_{A_{on}})
\]

\[
= \epsilon^2 (I_n - H_{A_n}) \epsilon - \epsilon^2 (I_n - H_{B_n}) \epsilon - 2\beta'_{A_{on}} X'_{A_{on}} H_{B_n} \epsilon - \beta'_{A_{on}} X'_{A_{on}} H_{B_n} X_{A_{on}} \beta_{A_{on}}
\]

\[
\leq \epsilon^2 (I_n - H_{A_n}) \epsilon - \epsilon^2 (I_n - H_{B_n}) \epsilon - 2\beta'_{A_{on}} X'_{A_{on}} H_{B_n} \epsilon - n\delta_n \beta_{\min}^2.
\]

By Lemma 7.1 (ii) and Assumption 7.5 \( [\epsilon^2 (I_n - H_{A_n}) \epsilon - \epsilon^2 (I_n - H_{B_n}) \epsilon]/(n\delta_n \beta_{\min}^2) \to 0 \) (a.s.)

Note that \( \beta'_{A_{on}} X'_{A_{on}} H_{A} \epsilon \sim N(0, v^2) \), where \( v^2 = \sigma^2 \beta'_{A_{on}} X'_{A_{on}} H_{A} X_{A_{on}} \beta_{A_{on}} \). By Assumption 7.3 \( v^2 \leq \sigma^2 \lambda_{\max}(H_{A}) \lambda_{\max}(X'_{A_{on}} X_{A_{on}}) \|\beta\|^2 \leq \sigma^2 \text{tr}(X'_{A_{on}} X_{A_{on}}) \|\beta\|^2 \leq nC \delta \sigma^2 \|\beta\|^2 \). By Lemma 7.1 (i) and Assumption 7.5 \( \beta'_{A_{on}} X'_{A_{on}} H_{A} \epsilon/(n\delta_n \beta_{\min}^2) \to 0 \) (a.s.). This completes the proof of (51).

If Assumption 7.6 holds, similar to the above proof, we can show

\[
\limsup_{n \to \infty} \left[ \psi_n(A_n)/n - \psi_n(B_n)/n \right] < 0 \quad (a.s.),
\]

39
which completes this proof.

Remark 7.2. It is worthwhile noting that there is no any restriction on \( p \) in Theorem 7.3. That is to say, if the required conditions are satisfied, then Theorem 7.3 holds no matter how large \( p \) is. This point seems interesting since almost all results on high-dimensional asymptotics in the literature require \( p = o(\exp(n)) \) (Bühlmann and van de Geer 2011).

### 7.3 A simulation study

We conduct a small simulation study to verify the better-fitting better-screening rule. In model (38), all rows of \( X \) are i.i.d. from a multivariate normal distribution \( N(0, \Sigma) \) whose covariance matrix \( \Sigma = (\sigma_{ij})_{p \times p} \) has entries \( \sigma_{ii} = 1, \ i = 1, \ldots, p \) and \( \sigma_{ij} = \rho, \ i \neq j \). The coefficients are given by \( \beta_1 = \beta_2 = \beta_3 = 3 \) and \( \beta_j = 0 \) for other \( j \). The random errors \( \varepsilon_1, \ldots, \varepsilon_n \) i.i.d. ~ \( N(0, 1) \). We fix \( n = 50 \) and \( \rho = 0.05 \), and vary \( p \) from 100 to 10000. Three screening methods with \( M = 25 \) are compared: Efron et al. (2004)’s least angle regression (LAR), Fan and Lv (2008)’s sure independence screening (SIS), and a hybrid method that uses the better results produced by LAR and SIS with smaller residual sum of squares as the final submodel. For each model, we simulate 1000 data sets and compute the coverage rates (CRs) of including the true submodel, which are displayed in Table 4. We can see that all the results follow the better-fitting better-screening rule well: the hybrid method always yields larger CRs than LAR and SIS.

| \( p \)     | 100  | 500  | 1000 | 3000 | 5000 | 10000 |
|------------|------|------|------|------|------|-------|
| LAR        | 0.999| 0.931| 0.845| 0.656| 0.552| 0.434 |
| SIS        | 0.999| 0.977| 0.955| 0.892| 0.820| 0.728 |
| hybrid     | 1    | 0.989| 0.961| 0.906| 0.832| 0.737 |
8 Discussion

In this section we end this paper with some discussion.

8.1 Summary

When the global solution to a statistical optimization problem is difficult to obtain, BSP theoretically supports to the method of using the solution whose objective value is as small as possible (for minimization problems). Interestingly, it can be studied within a simple framework based on several obvious but effective comparison theorems. These theorems tell us that a better solution with smaller objective value is more likely to be a good decision if the objective function has the (strong) separation property. Therefore, it suffices to prove the separation property of the objective function for verifying BSP. Following this way, we have discussed BSP for several statistical optimization problems, and have established the corresponding separation properties. These problems lead to basic but important statistical methods, including maximum likelihood estimation, best subsample selection in robust statistics, and best subset regression in variable selection.

Besides the usefulness in theory, BSP can provide viewpoints on the development of methodologies. In Section 5, a new best subsample selection method based on the Kolmogorov distance has been introduced. The corresponding BSP holds under fairly weak conditions. Theoretical and numerical studies both show that this method perform well when there are clustered outliers. As a byproduct, the robust estimate based on this selection method is consistent even under contaminated models. This estimate may be of independent interest in robust estimation.

Strictly speaking, the strong separation property of the objective function is needed to establish BSP. This is a strong condition and actually implies the consistency of the global solution (Theorems 3.2 and 3.5). We have proved this property only for maximum likelihood problem and best subset regression under strong conditions. If we ignore the mathematical details, the weak separation property seems enough for practical use (Remarks 3.2 and 3.3).
In general, the weak separation property is relatively easy to prove. Simulation results in this paper are consistent to the theoretical discoveries even when only the weak separation property is proved.

When computing the global solution is a problem, we should consider whether BSP holds. This principle is as important as the consistency property or other properties of the global solution. We hope that statisticians will always keep BSP in mind when handling complex optimization problems. On the other hand, BSP can be used to justify a statistical method from an optimization problem. A good objective function whose separation properties hold under mild conditions can provide us a way to combine weak methods into a stronger one. Such examples can be found in Sections 4.3 and 7.3: the hybrid method can improve weak methods through comparing their objective values.

8.2 Limitations of this paper

A prerequisite of BSP is that the global solution has, or, is at least expected to have, desirable statistical properties. Therefore, the BSP theory is not applicable to the statistical methods which are “irregularly” derived from optimization problems. An example is boosting. Some authors showed that boosting can be viewed as a steepest descent algorithm for minimizing a loss function (Breiman 1998; Friedman, Hastie, and Tibshirani 2000). It is stopped early since the minimum usually leads to overfitting. In other words, minimization here is a “pretense”, and we are really interested in the solutions along the path to the minimum, not the minimum itself. Another example is SCAD (Fan and Li 2001), which is a penalized likelihood estimate with a nonconcave penalty. Fan and Li (2001) proved that there exists a local solution of SCAD possessing the so-called oracle property. When the oracle property is concerned, the local solution with this property is prefer to the global solution, and thus BSP fails.

BSP is a general and non-specific concept, since the statistical properties of the solution to a optimization problem can be multifold. For example, besides estimation accuracy, we use the M-estimate because of its robust properties such as the minimax property (Huber
Another example is the regularized least squares method for regression models such as the lasso (Tibshirani 1996), which is used for simultaneous estimation and variable selection. Therefore, we should evaluate it in terms of both estimation and selection performance. In our comparison theorems we only focus on the statistical property described with the probability of being a “good” decision. Nevertheless, we believe that there are other reasonable frameworks to establish BSP, which describe the “better” statistical properties in different manners and/or can cover multifold statistical properties of interest.

This paper does not discuss algorithms, i.e., how to find a better solution when BSP holds. For the algorithms used in best subsample and best subset selection, we refer the reader to Rousseeuw and Van Driessen (1999), Hawkins and Olive (2002), Rousseeuw and Van Driessen (2006), Hofmann, Gatu, and Kontoghiorghes (2007), and Xiong (2013). For discussion on general global optimization algorithms in statistics, see, e.g., Fang, Hickernell, and Winker (1996).

8.3 Future directions

Besides the limitations of this paper aforementioned, a number of issues on BSP and related topics seem valuable to research in the future.

The applications of the comparison theorems presented in Sections 4-7 are selective. The range of potential applications can be much broader than presented. For example, many optimization problems listed in Section 1 can be studied using them. A number of useful theoretical results that can guide real data analysis may be obtained along this direction.

Another research direction related to BSP is to study statistical properties of sub-optimal solutions produced by certain algorithms. Recently, Ma, Mahoney, and Yu (2013) studied estimation accuracy of several leverage-based algorithms for large-scale least squares problems. For the SCAD problem aforementioned, the statistical properties of its local solutions that can be achieved by certain algorithms were discussed by Loh and Wainwright (2013), Wang, Liu, and Zhang (2013), and Xiong, Dai, and Qian (2013). Note that forward stepwise selection is a greedy algorithm for best subset regression (Miller 2002). The study on its
screening properties (Wang 2009) can be bracketed with the work of this kind. For some estimation problems, the estimators derived from only one iteration of certain iterative algorithms can also have appealing properties with good starting estimators (Bickel 1975; Fan and Chen 1999; Zou and Li 2008). Perhaps it is also valuable to study algorithm-based BSP. Recently, Big Data begins to pose significant challenges to statistics (Fan, Han, and Liu 2013; Shen 2013). For analyzing Big Data, not only statistical methodology but also statistical theory should be considered based on computation. BSP can be viewed as a part of computational ability-based statistical theory, and we expect that BSP and related methodologies will be paid more attention to in the future.

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