PROJECTION-BASED AFFINE EQUIVARIANT MULTIVARIATE LOCATION ESTIMATORS WITH THE BEST POSSIBLE FINITE SAMPLE BREAKDOWN POINT

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Abstract: The sample mean has long been used as an estimator of a location parameter in statistical data analysis and inference. Though attractive from many viewpoints, it suffers from an extreme sensitivity to outliers. The median has been adopted as a more robust location estimator in one dimension, it will not break down even if up to half of the data points are "bad". Another desirable property of the median is that it does not depend on the underlying measurement scale and coordinate system. Clearly, multivariate analogues of the univariate median are practically desirable and theoretically interesting. Among proposed analogues, only the spatial median (the L_1-median) and the coordinate-wise median have a breakdown point as high as that of the univariate median. These estimates, however, lack the affine equivariance property. Affine equivariant analogues exist, but their breakdown points decrease as dimension increases. We propose a class of projection-based affine equivariant multivariate location estimators. There are estimators in this class that possess a breakdown point (with respective to a definition slightly weaker than the usual one) as high as that of the univariate median, free of dimension. Compared with the existing best breakdown point affine equivariant location estimators, these estimators can, in some cases, resist up to 10% more contamination in a data set without break down. Computing issues are briefly addressed.

Key words and phrases: Affine equivariance, breakdown point, location estimator, multivariate median, projection pursuit methodology, robustness.

1. Introduction

The sample mean is a well-known estimator of a location parameter or the center of a data cloud. It possesses many attractive properties but can be fooled by a single outlier, which may be due to the measurement or recording error, instrument failure, etc. To overcome the extreme sensitivity to unusual observations, the median has been adopted as a robust estimator of location in one dimension. The univariate median will not break down even if up to half the data points are contaminated - the univariate median has the highest breakdown point. The notion of breakdown point was introduced in Donoho and Huber

(1983), and has become the most prevalent quantitative assessment of robustness of estimators. Let $X^n = \{X_1, \ldots, X_n\}$ be a sample of size n in $\mathbb{R}^d$ ($d \geq 1$). The *replacement breakdown point* (RBP) of an estimator T at the given sample X^n is defined as

$$\text{RBP}(T, X^n) = \min\{\frac{m}{n} : \sup_{X_m^n} \|T(X_m^n) - T(X^n)\| = \infty\},$$

where X_m^n denotes a contaminated sample from X^n by replacing m points of X^n with an arbitrary m points in $\mathbb{R}^d$, $\|\cdot\|$ is the Euclidian norm. In other words, the RBP of an estimator is the minimum replacement fraction which could drive the the estimator beyond any bound. It is readily seen that the RBP of the sample mean and the univariate median are $1/n$ and $\lfloor (n+1)/2 \rfloor /n$ respectively. ($\lfloor x \rfloor$ is the largest integer no larger than x.)

In addition to robustness against extreme observations, it is desirable that location estimators be independent of the underlying measurement scale and coordinate system. Such estimator is said to be *affine equivariant*, for example the univariate median. (Strictly speaking, T is affine equivariant if $T(AX^n + b) = AT(X^n) + b$ for any $d \times d$ nonsingular matrix A and $b \in \mathbb{R}^d$, where $AX^n + b = \{AX_1 + b, \ldots, AX_n + b\}$.)

High-dimensional analogues of the univariate median are desirable. Indeed, for years, constructing *affine equivariant* multivariate location estimators with *high breakdown point* has been a primary robustness goal. The task, however, turns out to be non-trivial. Among existing multivariate analogues, only the spatial median and the coordinate-wise median have a breakdown point as high as that of the univariate median, but they lack the affine equivariance property. Affine equivariant location estimators with high breakdown points include the Stahel-Donoho location estimator (Stahel (1981), Donoho (1982)), the MVE estimators (Lopuhaä and Rousseeuw (1991)), the S-estimators (Davies (1987), Lopuhaä and Rousseeuw (1991)), and the location estimators in Tyler (1994). Many papers discuss both location and scatter estimators. Careful examination, however, reveals that none of location components of these estimators has a breakdown point as high as that of the univariate median. Furthermore, the breakdown points of these location estimators decrease as dimension d increase (indeed the RBP of these estimators is $\leq \lfloor (n - d + 1)/2) \rfloor /n$). What is the best possible breakdown point of affine equivariant location estimators in high dimension? Can one construct a multivariate analogue of the univariate median that is affine equivariant with an RBP as high as its univariate counterpart, free of the dimension? Attempts to answer these questions have been made (see Donoho (1982, pages 10 and 16), Lopuhaä and Rousseeuw (1991, pp.232-235), for example) but they have remained open.

The objective here is to answer these questions. Following Maronna and Yohai (1995) and Juan and Prieto (1995), we adopt the worst case contamination model, that is, putting all m contaminating points at the same site or within a bounded ball. Hence we have a slightly weaker version of the usual breakdown point definition.

The rest of the paper is organized as follows. Section 2 shows that there are estimators in a class of affine equivariant projection-based location estimators that can have an RBP as high as that of the univariate median. These estimators are optimal in the sense that their breakdown points are the highest among all existing affine equivariant multivariate location estimators (and, in some cases, can resist 10% more contamination in a data set without breakdown) and the best that one can obtain. Computing issues are addressed briefly in Section 3. It turns out that these best breakdown point estimators can be computed by exact algorithms. The proof of the main result is in the Appendix.

2. Projection-based Location Estimators

In this section, a class of projection-based affine equivariant multivariate location estimators is proposed. There are estimators in this class that can have a breakdown point as high as that of the univariate median.

2.1. Outlyingness of points

Given univariate location and scale estimators $\mu(\cdot)$ and $\sigma(\cdot)$, the outlyingness of a point $x \in \mathbb{R}^1$ with respect to a data set X^n in $\mathbb{R}^1$ can be measured by $|x - \mu(X^n)|/\sigma(X^n)$, the deviation of x from the center $\mu(X^n)$ standardized by scale $\sigma(X^n)$; see p.205 of Mosteller and Tukey (1977), for example. Typical choices of the pair (μ, σ) include (mean, standard deviation), (median, median absolute deviation) and, more generally, (M-estimator of location, M-estimator of scale); see Huber (1981). Throughout our discussion, we assume that $\mu(sX^n + b) = s\mu(X^n) + b$ and $\sigma(sX^n + b) = |s|\sigma(X^n)$ for any data set X^n and scalars s and b in $\mathbb{R}^1$, where $sX^n + b = \{sX_1 + b, \cdots, sX_n + b\}$.

Stahel (1981) and Donoho (1982) extended the univariate outlyingness measure to high dimension and defined, independently, the outlyingness of a point $x \in \mathbb{R}^d$ $(d \geq 1)$ with respect to a data set X^n in $\mathbb{R}^d$ as

$$O(x, X^n) = \sup_{u \in S^{d-1}} \left\{ \frac{|u'x - \mu(u'X^n)|}{\sigma(u'X^n)} \right\}, \tag{1}$$

where $S^{d-1} = \{u : \|u\| = 1\}$ and $u'X^n = \{u'X_1, \ldots, u'X_n\}$. When $|u'x - \mu(u'X^n)| = \sigma(u'X^n) = 0$, we define $|u'x - \mu(u'X^n)|/\sigma(u'X^n) = 0$ (see Remark 3.5 of Zuo (2003) for some explanations).

In virtue of the affine equivariance of μ and σ, it is readily seen that $O(x, X^n)$ is *affine invariant*. That is, $O(x, X^n) = O(Ax + b, AX^n + b)$ for any nonsingular $d \times d$ matrix A and vector $b \in \mathbb{R}^d$. Based on the outlyingness of data points, Stahel (1981) and Donoho (1982) introduced a multivariate location estimator

$$T_w(X^n) = \sum_{i=1}^{n} w\left(O(X_i, X^n)\right) X_i \Big/ \sum_{i=1}^{n} w\left(O(X_i, X^n)\right),$$

where $w(x)$ is a weight function which downweights outlying observations. It is readily seen that T_w is affine equivariant since $O(x, X^n)$ is affine invariant.

For X^n *in general position* (i.e., no more than d points of X^n lie in any $(d-1)$-dimensional subspace), Donoho (1982) studied the breakdown point of T_w, where μ and σ are the median (Med) and the median absolute deviation (MAD) with $\mathrm{Med}(Y^n) = (Y_{(\lfloor (n+1)/2 \rfloor)} + Y_{(\lfloor (n+2)/2 \rfloor)})/2$ and $\mathrm{MAD}(Y^n) = \mathrm{Med}\{|Y_i - \mathrm{Med}(Y^n)|\}$, where Y^n is in $\mathbb{R}^1$ and $Y_{(1)} \leq Y_{(2)} \leq \cdots \leq Y_{(n)}$ are ordered values of $Y_1, \cdots, Y_n$. His result implies that the RBP of T_w is $\lfloor (n - 2d + 2)/2) \rfloor / n$, see Davies (1987) and Zuo (2001), which is less than $\lfloor (n+1)/2 \rfloor / n$, the RBP of the univariate median. The Stahel-Donoho multivariate location estimator, however, is the first one that can combine affine equivariance with high breakdown point. It has stimulated a lot of follow-up work seeking affine equivariant location estimators with higher breakdown points. Tyler (1994) modified the MAD in the definition of T_w (and a corresponding scatter estimator) so that the RBP of the resulting estimator is increased to $\lfloor (n - d + 1)/2 \rfloor / n$ for X^n in general position (Tyler's breakdown point result is stated for the location and scatter estimators jointly). Gather and Hilker (1997) and Zuo (2000) also modified MAD in T_w and obtained the same RBP $\lfloor (n - d + 1)/2 \rfloor / n$ for X^n in general position. This RBP, however, is still less than $\lfloor (n+1)/2 \rfloor / n$ and decreases with increasing d.

Other affine equivariant location estimators have been introduced, but none of them has a RBP higher than $\lfloor (n - d + 1)/2 \rfloor / n$. The first affine equivariant location estimator that can break this RBP barrier is the "projection median" defined via the outlyingness or "depth functions" studied in Zuo (2003), with a RBP of $\lfloor (n - d + 2)/2 \rfloor / n$. (For general discussions on depth functions, see Liu (1990) and Zuo and Serfling (2000a, b).) The questions in Section 1, however, are still not completely answered by this result.

For a translation equivariant location estimator T (i.e., $T(X^n + b) = T(X^n) + b$ for any $b \in \mathbb{R}^d$), Lopuhaä and Rousseeuw (1991) proved that the upper bound of RBP is $\lfloor (n+1)/2 \rfloor / n$. In the next subsection, we propose a class of affine equivariant (hence necessarily translation equivariant) location estimators and

show that there are estimators in the class that can attain this RBP upper bound. Hence we provide answers to the open questions in Section 1.

2.2. A class of projection based location estimators

Closely related to the Stahel-Donoho estimator T_w is a location estimator called the "projection median" (PM). Instead of considering the outlyingness-weighted *mean*, the projection *median* is the average of sample points which possess minimum outlyingness among all sample points. That is,

$$PM(X^n) = \text{ave}\Big\{X_i \in X^n : O(X_i, X^n) = \min_{X_j \in X^n}\{O(X_j, X^n)\}\Big\}, \qquad (2)$$

where $O(\cdot, X^n)$ is defined at (1). Since $O(x, X^n)$ is affine invariant, it is readily seen that PM is affine equivariant. Clearly, PM and its characteristics depend on the choices of μ and σ that define $O(\cdot, X^n)$. A class of μ and σ corresponds to a class of PM. In one dimension PM is μ and hence is the median when μ is. For general μ we still use the phrase "projection median" in one and more dimensions for convenience.

The location estimator in (2) has not been proposed and studied in the literature but is a variant of the projection medians introduced and discussed in Tyler (1994) and in Zuo and Serfling (2000c) and Zuo (2003). Depth functions, called "projection depths", are associated with the medians in Zuo (2003). It turns out that the medians in Zuo (2003), with RBP $\lfloor(n - d + 2)/2\rfloor/n$ for X^n in general position, are the first type of affine equivariant location estimators that can break the RBP barrier $\lfloor(n - d + 1)/2\rfloor/n$ that existed in the literature.

In practice the restriction "in general position" on X^n can be severe. In our discussion, we drop this restriction and allow more than d sample points to lie in a $(d - 1)$-dimensional hyperplane. Following Tyler (1994), let $c(X^n)$ be the maximum number of points of X^n contained in any $(d - 1)$-dimensional hyperplane. Then $c(X^n) \geq d$. We do assume that X^n is *in non-special position* in the sense that the convex hull formed by any $k \geq \lfloor n+2\rfloor/2$ points of X^n does not contain all k points on its boundary. This of course is true almost surely for large n if the population distribution is absolute continuous. We now propose a class of affine equivariant projection medians (2) and show that there are projection medians that can have RBP as high as $(\lfloor(n + 1)/2\rfloor)/n$ for any sample X^n in non-special position. In view of Lopuhaá and Rousseeuw (1991), this is the best possible RBP for any affine equivariant multivariate location estimator.

Take μ to be any affine equivariant univariate location estimator with a RBP $\lfloor(n + 1)/2\rfloor/n$. This includes some M-estimators of location; see Huber (1981). Take σ to be any affine equivariant univariate scale estimator that has very high *implosion* RBP (higher than that of MAD). Note that the implosion

RBP of a scale estimator is the minimum replacement fraction that can force the estimator to be zero. It is readily seen that the implosion RBP of MAD is $(\lfloor (n+2)/2 \rfloor - c(X^n))/n$ for an arbitrary data set X^n in $\mathbb{R}^1$. Examples of σ's that have higher implosion RBP than that of MAD include the median of differences $\text{MOD}(X^n) = \text{Med}_{i<j}\{|X_i - X_j|\}$, the sum of differences $\text{SOD}(X^n) = \sum_{i<j}\{|X_i - X_j|\}$, and the sum of absolute deviations $\text{SAD}(X^n) = \sum_i |X_i - \mu^*(X^n)|$ for X^n in $\mathbb{R}^1$, where μ^* can be any affine equivariant location estimators such as Mean and Med. It is not difficult to see that the implosion RBP's of MOD, SOD, and SAD are $(\lfloor (3 + \sqrt{2n^2 - 2n + 1})/2 \rfloor - c(X^n))/n$, $(n - c(X^n))/n$, and $(n - c(X^n))/n$, respectively. Other desirable σ's include the standard deviation (SD) and the partial sum of absolute deviations: $\text{PSAD}(X^n) = Y_{(i_0)} + \cdots + Y_{(i_1)}$ with $1 \leq i_0 \leq i_1$, $\lfloor (n+2)/2 \rfloor < i_1 \leq n$, where $Y_i = |X_i - \mu^*(X^n)|$. Note that all these σ's are affine equivariant.

With different μ's and σ's in (1), the resulting projection medians in (2) are still denoted by *PM* for the sake of simplicity. Obviously, these projection medians are affine equivariant. They can also possess the best possible breakdown point.

Theorem 2.1. *Let μ be any affine equivariant univariate location estimator with the best possible* RBP *and σ be the largest absolute deviation from μ, hence with the best possible implosion* RBP. *Then for any X^n in non-special position in $\mathbb{R}^d$, the corresponding projection median PM defined by (2) is affine equivariant with $RBP(PM, X^n) = \lfloor (n+1)/2 \rfloor/n$.*

Remark 2.1. Theorem 2.1 answers the questions of Section 1. It also has some practical merit. The breakdown point, $\lfloor (n-d+1)/2 \rfloor/n$, of estimators introduced earlier and the breakdown point, $\lfloor (n+1)/2 \rfloor/n$, of our estimators both approach $1/2$ as $n \to \infty$ for fixed d, but they differ for a finite sample size n. How big can the difference between the two breakdown points be? To answer this question, consider the case that X^n is in general position for convenience. Let $n = 5d$, then $\lfloor (n+1)/2 \rfloor/n - \lfloor (n-d+1)/2 \rfloor/n > 10\%$. That is, in this case the estimators discussed in the theorem can resist at least 10% more contamination in the original data set than the other estimators in use do. This has practical *significance*. (A justification for $n = 5d$ is given on p.326 of Juan and Prieto (1995).)

3. Computing the Projection Based Estimators

We now briefly address computing issues − a large concern for all high breakdown point affine equivariant estimators in high dimensions. Although many of these estimators can be computed by polynomial-time algorithms in theory, in

practice almost none of these estimators are computed in high dimensions in exactly the way they are defined. Instead, they are ordinarily computed via faster approximate algorithms.

For projection-based estimators, the practical difficulty lies in computing $O(X_i, X^n)$ defined by (1). In the light of this equation computing the outlyingness seems hopeless since we need to consider projection to all directions. This is a long-standing problem. But approximate procedures for the outlyingness, such as those based on "sub-sampling" and "pigeon hole" principles (Stahel (1981) and Rousseeuw (1993)), have been proposed and used in practice. There are concerns as to how accurate these procedures are, and whether or not the approximate procedures have the same desirable properties of the exact procedures. The best way to meet the concerns, of course, is exact computing.

It turns out that the projection-based estimators discussed in this paper can actually be computed exactly in low and high dimensions for appropriate μ and σ. A primary study indicates that one actually needs only consider projection to a linear (in n) number of fixed directions to obtain the *exact* outlyingness of the sample points. We outline an exact algorithm − a detailed discussion of the algorithm is beyond the scope (and the focus) of this paper and will be pursued elsewhere. For simplicity, we assume that n is odd and consider only bivariate data, with $\mu =$Med and $\sigma=$SAD, with μ^* the Med (see Section 2.2).

1. For each data point, connect it with each of the other $n - 1$ data points, find a direction (usually there are two) among the $n - 1$ directions that bisects the data set in the sense that the closed half-planes with this direction as their boundaries contain at least $n/2$ data points. Totally there are $O(n)$ such directions.

2. Project data points to the directions u_i perpendicular to one of the $O(n)$ directions in Step 1 and, along u_i, calculate the outlyingness of each of the projected points. Define the outlyingness of each of the projected points along u_i as that of the corresponding point and update it when it becomes larger along any other direction u_j.

3. Find the data point with minimum outlyingness among the n sample points. Take an average if there is more than one minimum outlyingness point.

The worst case time complexity is $O(n^2)$, $O(n^2)$ and $O(n)$ for Steps 1, 2 and 3, respectively and consequently is $O(n^2)$ for the exact algorithm, in theory.

With exact algorithms, one can develop faster and practical approximate algorithms for the outlyingness of high dimensional data points and the corresponding projection median. Any concern that the estimator from an approximate procedure might lack the desirable high breakdown point property of the theoretical counterpart becomes unnecessary when the approximate estimator

is within some bounded neighborhood of the exact estimator. For projection medians in this paper, the breakdown point property holds true for estimators obtained from an exact algorithm, or from any approximate algorithm that identifies an uncontaminated data point as the minimum outlyingness point.

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Appendix. Proof of Theorem 2.1

The projection depth median PM is affine equivariant, hence necessarily translation equivariant. In the light of the upper bound of RBP of translation equivariant location estimators given in Lopuhaä and Rousseeuw (1991), one can break down PM if the number m of contaminating points is as large as $\lfloor (n+1)/2 \rfloor$. To prove the theorem we need only show that one cannot break down PM when m, the number of contaminating points, is $\leq \lfloor (n+1)/2 \rfloor - 1$. This is trivially true when $d = 1$ since in this case PM is just the univariate median. In the following $d \geq 2$.

Assume that the number of contaminating points $m \leq \lfloor (n+1)/2 \rfloor - 1$. We also assume, without loss of generality, that $\mu =$Med and focus on the worst case contamination scenario: putting all contaminating points in the same site; see Maronna and Yohai (1995) and Juan and Prieto (1995) for related discussions about this model. (The proof can be slightly modified to cover the case that all contaminating points are placed within a bounded ball.) Since X^n is in non-special position, then $m + c(X^n) < n$. With such m, μ and σ it is readily seen that

$$0 < \inf_{X_m^n} \inf_{u \in S^{d-1}} \sigma(u'X_m^n) \ \text{ and } \ \sigma(u'X_m^n) < \infty$$

$$\text{for any fixed } u \in S^{d-1} \text{ and any given } X_m^n, \quad (3)$$

$$\sup_{X_m^n} \sup_{u \in S^{d-1}} \mu(u'X_m^n) < \infty, \quad (4)$$

where X_m^n is any contaminated data set resulting from replacing m of the original points in X^n by an arbitrary m points (they are at the same site) in $\mathbb{R}^d$. Write $Z = \{Z_1, \cdots, Z_n\}$ for the contaminated data set X_m^n for simplicity.

Assume that $PM(X_m^n)$ can become unbounded even if the number m of contaminating points is $\leq \lfloor (n+1)/2 \rfloor - 1$. Hence, there exists a sequence

of contaminated data sets (with m original points of X^n being contaminated) $\{Z_t\} = \{Z_{t1}, \cdots, Z_{tn}\}$ such that

$$\|PM(Z_t)\| \to \infty, \quad \text{as } t \to \infty. \tag{5}$$

Write y_t for $PM(Z_t)$ for convenience. Then the outlyingness of y_t is no greater than the minimum outlyingness of points from Z_t. Hence there are at least $n - m$ uncontaminated points from $X^n \cap Z_t$ for any fixed t whose outlyingness is no less than $O(y_t, Z_t)$. Note that there are m points of Z_t at y_t. We now seek a contradiction to (5).

Since n is fixed and finite, assume that $X_1, \ldots, X_{n-m}$ are the uncontaminated points from X^n for all t (by taking subsequences of subsequences if necessary, this is without loss of generality). Note that $O(X_i, Z_t) \geq O(y_t, Z_t)$ for $1 \leq i \leq n - m$.

Since $\|y_t\| \to \infty$, $\sigma(u'Z_t) = \|y_t\| - \mu(u'Z_t)$ for sufficiently large t and $u = y_t/\|y_t\|$ by (4). Hence $O(y_t, Z_t) \geq 1$. On the other hand, since $n - m \geq \lfloor n+2 \rfloor/2$ and X^n is in non-special position, there is at least one point X_i from the $n - m$ uncontaminated points $\{X_1, \cdots, X_{n-m}\}$ that is an interior point of the convex hull formed by the $n - m$ points. Hence, $|u'X_i - \mu(u'Z_t)| < \sigma(u'Z_t)$ for any $u \in S^{d-1}$ and any t. That is, $O(X_i, Z_t) < 1$. This, however, is a contradiction to the assumption that y_t is the point with the minimum outlyingness among all the points of Z_t, which completes the proof.

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