TESTING A NORMAL SAMPLE FOR MULTIPLE OUTLIERS. (U)

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TESTING A SOIL SAMPLE FOR MULTIPLE OUTLIERS

TECHNICAL REPORT

DOUGLAS P. HURKINS

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Testing a Normal Sample For Multiple Outliers

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Outlier, Slippage, Power, Linear Model, Regression

Test statistics G and M for two outliers due to Murphy and Grubbs are compared with a test statistic R based on applying a single-outlier test to the sample with the most extreme observation removed. It is shown that G is generally most effective. The G and R procedures are shown to be equivalent when the number of outliers is unknown, and to give satisfactory performance for one or two outliers. An extension to the linear hypothesis is outlined.
Testing a Normal Sample for Multiple Outliers*

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SUMMARY

Test statistics $G$ and $H$ for two outliers due to Murphy and Grubbs are compared with a test statistic $R$ based on applying a single-outlier test to the sample with the most extreme observation removed. It is shown that $G$ is generally most effective. The $G$ and $R$ procedures are shown to be equivalent when the number of outliers is unknown, and to give satisfactory performance for one or two outliers. An extension to the linear hypothesis is outlined.

Key Words: Outlier, slippage, power, linear model, regression.

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Introduction

The problem of identifying outliers in a sample is a very old one, but is nevertheless not yet solved entirely. A considerable amount of work has been devoted to the situation in which the underlying distribution is normal, and at most one outlier is believed to be present. It is known (Paulsen 1952, Kado 1956) that if this outlier is known a priori to be on the right, then the optimal test statistic is the largest studentized deviation. An early paper by Pearson and Chandrasekar (1936) highlighted a severe problem associated with the use of this statistic - the 'masking effect.' This effect occurs when in fact more than one outlier is present. The additional outliers mask each other's presence by so inflating the sample variance as to reduce the power of the test severely - in some cases driving it to zero as the outliers move further to the right.

This masking effect has led to the development of several outlier test statistics aimed at testing specifically for the presence of \( K > 1 \) outliers in the sample (Grubbs 1950, Murphy 1951, Ferguson 1961, Dixon 1950). These \( K \)-outlier statistics are competitors to the recursive procedure: Compute the single-outlier statistic for the full sample, and for each of the subsamples obtained by deleting the \( 1, 2, 3, \ldots, K \) most extreme observations, and decide on the basis of some rule using this sequence whether outliers are present, and how many and which observations they are.

The object of this paper is to propose a modification to this recursive procedure, and to compare its performance with that of the Grubbs
and Murphy statistics.

**Notation**

Let $X_1, X_2, \ldots, X_n$ be $n$ observations believed to come from a normal distribution $N(\xi, \sigma^2)$, \( \xi, \sigma \) unknown, and let $Y_1 \geq Y_2 \geq \ldots \geq Y_n$ be the corresponding order statistics. We will also suppose that there is at hand some additional information on $\sigma^2$ in the form of an independent $\sigma^2 X_0^2$ variate $W$. If there is no such $W$, then set $W = v = 0$.

Define

\[
\bar{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i/n
\]

\[
\bar{Y}_1 = \frac{1}{n} \sum_{i=2}^{n} Y_i/(n-1)
\]

\[
\bar{Y}_{12} = \frac{1}{n} \sum_{i=3}^{n} Y_i/(n-2)
\]

\[
S = W + \sum_{i=1}^{n} (Y_i - \bar{Y})^2
\]

\[
S_1 = W + \sum_{i=2}^{n} (Y_i - \bar{Y}_1)^2
\]

\[
S_{12} = W + \sum_{i=3}^{n} (Y_i - \bar{Y}_{12})^2
\]

Initially make the somewhat artificial assumption that it is known a priori that, if outliers are present, there are exactly two, one a $N(\xi + \lambda \sigma, \sigma^2)$ and the other a $N(\xi + \delta \sigma, \sigma^2)$ variable with $\lambda, \delta > 0$.

The two-outlier test statistics to be considered are $G = S_{12}/S$, $M = (Y_1 + Y_2 - 2\bar{Y})/\sqrt{S}$ and $R = (Y_2 - \bar{Y}_1)/\sqrt{S_1}$. 
The statistic \( G \) is a slight generalization of one proposed by Grubbs (1950) (in the original definition, \( W = \nu = 0 \)). It seems to have no proven optimality properties, but corresponds to the \( F \) test of the Anova model for comparing the three "samples" \( Y_1, Y_2 \) and \( \{Y_3, \ldots, Y_n\} \). For this reason, it seems likely to be effective when it is not known a priori that \( \lambda = 6 \).

Murphy (1951) defined the statistic \( M \) for the case \( W = \nu = 0 \), and proved its optimality when it is known a priori that \( \lambda = 6 \). We note that this statistic is equivalent to the Anova test for comparing the two "samples" \( \{Y_1, Y_2\} \) and \( \{Y_3, \ldots, Y_n\} \), which in turn is equivalent to the two-sample \( t \) statistic. Of course neither \( G \) nor \( M \) has a distribution which can be derived from the conventional Anova distributions, since the "samples" are obtained by ranking the \( X_i \).

Both statistics are extensions of the single-outlier statistic \( B = (Y_1 - \bar{Y})/\nu S \) to the two-outlier situation. For the single-outlier case, Grubbs proposed the statistic \( S_1/S = (1 - nB^2/(n-1)) \).

The recursive statistic \( R \) is clearly not optimal since it does not use the sufficient statistics \( Y_1, Y_2, \nu_{12} \) and \( S_{12} \), but is a natural one to consider since, if \( Y_1 \) is an outlier, it corresponds to the Paulson optimal statistic for the subsample \( \{Y_2, Y_3, \ldots, Y_n\} \).

The three test statistics are related, in that \( G \) and \( M \) may be expressed as functions of \( B \) and \( R \). The relationships may be established by use of some algebraic identities from Quesenberry and David (1961) and are
\[
G = \{1 - nb^2/(n-1)\} \{1 - (n-1)R^2/(n-2)\}
\]
\[
H = (n-2)B/(n-1) + R\{1 - nb^2/(n-1)\}^{1/2}.
\] (1)

The null joint distribution of \(R\) and \(B\) is given in Hawkins (1973), where it is shown that if \(F_{n,v}(\cdot)\) denotes the cumulative distribution function of \(B\) based on a sample of size \(n\), then the probability

\[
Pr[(b < B < b+db) \cap (x \in B)] = nf(b)[F_{n-1,v}(t(b)) - F_{n-1,v}(x)]db + o(db) \tag{2}
\]

where

\[
t(b) = nb/[(n-1)\{1 - nb^2/(n-1)\}^{1/2}]
\]

and

\[
f(b) = \frac{\Gamma\{\frac{1}{2}(n+m-1)\}}{\Gamma\{\frac{1}{2}(n+m-2)\}} \frac{1}{(n-1)m^{1/2}(1 - nb^2/(n-1))^{1/2(m+n-4)}}.
\]

The range is \(0 \leq x \leq t(b) \leq ((n-1)/n)^{1/2}\), the constraints \(R \leq B\) and \(x \leq t(b)\) being imposed by the condition \(Y_1 \geq Y_2\).

The Grubbs test has critical region \(G < G_0\), whose size is

\[
Pr[G < G_0] = Pr[\{1 - nb^2/(n-1)\} \{1 - (n-1)R^2/(n-2)\} < G_0] \nonumber = Pr[\{1 - nb^2/(n-1)\} < G_0 \{1 - (n-1)R^2/(n-2)\}^{-1}] \tag{3}
\]

For any \(G_0\), we may integrate (2) over the region defined by (3), and so get this probability. In this way, the distribution function of \(G\) may be found and fractiles deduced. For the case \(W = v = 0\), fractiles were found by Grubbs, who found the density of \(G\) directly, though in terms of a multiple integral over a complicated region.

The Murphy test has critical region \(H > H_0\), whose size is

\[
Pr[H > H_0] = Pr[(n-2)B/(n-1) + R\{1 - nb^2/(n-1)\}^{1/2} > H_0] \tag{4}
\]
and so the null distribution of $M$ may be found in the same way.

Finally, the size of the region $R > R_0$ may be found from (2), and its fractiles deduced.

Some fractiles of $G$, $M$ and $R$ are listed in Table 1. Those fractiles listed both here and in Grubbs (1950) agree. So far as this author is aware, this is the first table of exact fractiles of $M$ and $R$.

Figure 1 shows the critical regions of each of these tests for the case $n = 10$, $v = 0$, $a = .05$. Recalling that a large value of $B$ suggests that $Y_1$ is aberrant, while a large value of $R$ indicates that $Y_2$ is aberrant, we can interpret these regions as follows:

i) Each test is best in some region of $(B,R)$ in the sense of rejecting the null hypothesis, while both other tests accept it.

ii) If $Y_1 \rightarrow \infty$ while $\{Y_2, Y_3, \ldots, Y_n\}$ remain constant, then $B$ ultimately $(B,R)$ falls in the acceptance region of the test based on $M$, and the critical region of that based on $G$. This means that $G$ tends to be significant when in fact only a single outlier is present. This may be a shortcoming in the use of $G$. The fact that $M$ may become non-significant when $Y_1$ becomes more aberrant is interesting, and possibly surprising. In fact, if we let $Y_1 \rightarrow \infty$, $\{Y_2, Y_3, \ldots, Y_n\}$ remaining fixed, it can be shown quite easily that $M + C = (n-2)/(n(n-1))^{1/2}$. Thus if the fractile $M_0 > C$, then $M$ will ultimately become non-significant. This means that $M$ suffers from a type of masking effect, in that if $M_0 > C$,
it is not effective for finding two outliers whose means are markedly dissimilar.

iii) By contrast, the critical region of $R$ is specific for two outliers, and is not affected by the relative magnitude of $B$ and $R$.

Performance of the tests.

In this section, measures of the performance of the three tests in locating exactly two outliers are considered. The best criterion would be the probability of a correct decision — that is the probability that the two contaminants are the first two order statistics of the sample, and that $(B,R)$ falls in the critical region. The evaluation of this probability however seems to involve some rather difficult distributional problems, familiar from the single-outlier case (David and Paulson 1965), and so an approximation similar to that of David and Paulson is proposed.

As a preliminary, suppose that

$$T_1 \sim N(\beta,1)$$
$$T_2 \sim N(\gamma,1)$$
$$V \sim \chi^2_{11}$$

all three terms being mutually independent. Let

$$U = \frac{T_1}{\sqrt{V}}$$
$$Z = \frac{T_2}{(V+U^2)^{\frac{1}{4}}}.$$
Standard transformation methods then show that the joint density of $U$ and $Z$ is

$$f(u,z) = 4K \sum_{n=0}^{\infty} \frac{(\beta/2)^n u^n}{n!(1+u^2)^{\frac{1}{2}(n+1)}} \sum_{m=0}^{\infty} \frac{m^{1/2} I_{1/2}(\gamma i+m+2)}{m!(1+2^{1/2})^{1/2}(m+1+2)}$$

where $K = \exp -\frac{1}{2}(\beta^2 + \gamma^2)/(4\pi \Gamma(i))$.

From this $\Pr[(U>b) \cap \{Z > a(v)\}]$ is

$$K \int_{v=0}^{(1+b^2)^{-1}} \sum_{n=0}^{\infty} (\beta/2)^n \sqrt{i(n-2)} (1-v) \frac{\Gamma(1/2)(n+1)}{n!} \sum_{i=0}^{\infty} \frac{(\sqrt{v})^i \Gamma(i+1)}{\Gamma(i+1)} \{1+a^2(v)^{-1} \}^{-1/2} \{1+a^2(v)^{-1}\}^{-1} \{i+1\}^{i+1} dv \tag{5}$$

where $I_x(a,b)$ denotes the incomplete beta ratio, and the variable of integration $v = (1 + u^2)^{-1}$.

Returning to the problem at hand, suppose that

$$X_1 \sim N(\xi + \delta \sigma, \sigma^2)$$
$$X_2 \sim N(\xi + \lambda \sigma, \sigma^2)$$
$$X_i \sim N(\xi, \sigma^2) \quad i = 3, \ldots, n$$
$$W \sim X^2_v.$$ 

Let

$$\overline{X} = \frac{1}{n} \sum_{i=1}^{n} X_i/n$$
$$\overline{X}_1 = \frac{1}{n-1} \sum_{i=2}^{n} X_i/(n-1).$$

Make the Helmert orthogonal transformation, defining

$$T_1 = \{n/(n-1)\}^{1/2}(\overline{X}_1 - \overline{X}) \sim N(\alpha \sigma, \sigma^2)$$
$$T_2 = \{(n-1)/(n-2)\}^{1/2}(\overline{X}_2 - \overline{X}_1) \sim N(\alpha \sigma, \sigma^2)$$
where
\[ \beta = \left\{ \frac{n}{(n-1)} \right\}^{\frac{1}{2}} \delta - \left\{ \frac{n(n-1)}{n} \right\}^{\frac{1}{2}} \lambda \]
\[ \gamma = \left\{ \frac{(n-2)}{(n-1)} \right\}^{\frac{1}{2}} \lambda \]

Letting
\[ S = n + \sum_{i=1}^{n} (x_i - \bar{x})^2 \]
we identify \( T_1 \) and \( T_2 \) with the \( T_1 \) and \( T_2 \) of the preceding theory, \( V \) with \( S - T_1^2 - T_2^2 \), and \( N \) with \( n + v - 2 \).

Then
\[ U = T_2 / (S - T_1^2 - T_2^2)^{\frac{1}{2}} \]
\[ Z = T_1 / (S - T_1^2)^{\frac{1}{2}} \]
\[ T_1 / S^{\frac{1}{2}} = Z / (1 + Z^2)^{\frac{1}{2}} \]
\[ T_2 / (S - T_1^2)^{\frac{1}{2}} = U / (1 + U^2)^{\frac{1}{2}} \]

Now
\[ B' = \left\{ \frac{(n-1)}{n} \right\}^{\frac{1}{2}} T_1 / S^{\frac{1}{2}} \]
\[ R' = \left\{ \frac{(n-2)}{(n-1)} \right\}^{\frac{1}{2}} T_2 / (S - T_1^2)^{\frac{1}{2}} \]

are simply the \( B \) and \( R \) statistics obtained by substituting \( X_1 \) for \( Y_1 \) and \( X_2 \) for \( Y_2 \).

Let \( C \) be the critical region for any particular test, and let

\[ H(\delta, \lambda) = \Pr[(B', R') \in C] \]

This differs from \( \Pr[\{(B', R') \in C \} \cap \{X_1 = Y_1, X_2 = Y_2\}] \) by the factor

\[ \Pr[\{X_1 = Y_1\} \cap \{X_2 = Y_2\}|(B', R') \in C] \] (6)

Now we may argue, as in Anscombe (1960) that if \( \delta > \lambda >> 0 \), this conditional probability is close to 1. Alternatively, we may note as in David and Paulson that if \( B' \geq \left\{ \frac{(n-2)}{2n} \right\}^{\frac{1}{2}} \), \( R' \geq \left\{ \frac{(n-3)/(2n-2)} \right\}^{\frac{1}{2}} \).
\[ \Pr[(X_1=Y_1) \cap (X_2=Y_2) \mid (B', R')] = 1. \]

Either reasoning shows that the probability of a correct decision:

\[ \Pr[(X_1=Y_1) \cap (X_2=Y_2) \cap (B', R') \in C] + \Pr[(X_1=Y_2) \cap (X_2=Y_1) \cap (B', R') \in C] \]

is well-approximated by \( H(\delta, \lambda) + H(\lambda, \delta) \).

Table 2 shows the values of \( H(\delta, \lambda) + H(\lambda, \delta) \) for the case \( n = 10, v = 0, \alpha = 0.05 \) whose critical regions were sketched in Figure 1.

These values confirm the impressions given by Figure 1. If \( \delta=\lambda \), \( H \) is the best test statistic, but its power deteriorates if \( \delta \) is markedly different from \( \lambda \). Of interest is the good performance of \( G \); however its power when \( \lambda=0 \) is a warning of the possibility of rejecting \( H_0 \) when in fact only one outlier is present. The recursive test is never best, but is never poor when, in fact, two outliers are present.

**Extension to an unknown number of outliers**

Suppose now that it is not known a priori whether the sample contains 0, 1 or 2 outliers. A question then arises of how to adapt the test procedures.

The Grubbs statistic is equivalent to an Anova for the three groups \( Y_1, Y_2 \) and \( \{Y_3, \ldots, Y_n\} \). It might be adapted by setting up the Anova for comparing \( Y_1 \) with \( \{Y_2, \ldots, Y_n\} \) whose test statistic is equivalent to \( S_1/S = (1 - nB^2/(n-1)) \). Then \( S_1 \) is further partitioned for testing \( Y_2 \) against \( \{Y_3, \ldots, Y_n\} \) yielding a test statistic equivalent to \( S_{12}/S_1 = (1 - (n-1)R^2/(n-2)) \). The decision as to the number of outliers would then be equivalent to a sequential test based on \( B \) and \( R \).
The recursive test which has received most attention (Mcilliian 1971, Hawkins 1973) is:

i) Compute $B$. If this is non-significant, conclude that there are no outliers.

ii) Otherwise compute $R$, and depending on its significance, conclude that there are one, or two outliers.

It is now well-known that this procedure is defective because of the masking effect. However, this type of problem is very familiar in other contexts — for example deciding by what order polynomial to detrend a time series (Anderson 1971), and may be resolved very simply by reversing the order of testing. This yields the procedure:

i) Compute $R$. If it is significant conclude that there are two outliers.

ii) Otherwise, compute $B$, and depending on its significance, conclude that there are one, or no outliers.

The fractiles needed for this procedure may be computed by integrating (2) over the two regions: $C_2 : R>R_0$ and $C_1 : R<R_0, R>B_0$. The test procedure is not fully defined until one makes a decision as to how to partition $\alpha$, the overall probability of type I error, between these two regions. One reasonable partition is to let each have size $\alpha/2$.

A sample calculation for the case $n=10$, $\nu=0$, $\alpha=.05$ yields the fractiles $B_0 = 0.7434; B = 0.7596$. Let $H_1(\delta,\lambda)$ denote $Pr[(B',R') \in C_1] \ i = 1,2$ when in fact outliers are present, then

$H_1(\delta,\lambda) + H_1(\lambda,\delta)$ approximates the probability of identifying two outliers ($i=2$) or one outlier ($i=1$).
Table 3 lists these approximations for this sample case, and shows that the performance of the recursive procedure is indeed satisfactory.

The recursive procedure extends in a natural way to test for the possibility of 1, 2, ..., K outliers. The sequence of recursive statistics omitting the most aberrant 0, 1, 2, ..., K-1 observations is computed, and tested for significance in reverse order. No fractiles for the case K>2 are as yet available, though it is likely that the approach used in Hawkins (1973) could be extended. It will be shown below that conservative fractiles may be obtained by the use of the Bonferroni inequality.

The Murphy statistic extends in an obvious way to accommodate an unknown number of outliers: For k = 1, 2, ..., K, find the two-sample t statistic for comparing \( \{Y_1, \ldots, Y_k\} \) with \( \{Y_{k+1}, \ldots, Y_n\} \). If the largest of these, corresponding to \( k = k_0 \), say, is significant, then conclude that \( k_0 \) outliers are present. This statistic, in the case \( k=n \), corresponds to a test statistic used in Automatic Interaction Detection (see for example Kass 1975, Scott and Knott 1976).

However since Table 2 suggests that \( M \) is never markedly superior to \( G \), and may in fact be markedly inferior, no attempt has been made to study the performance of this procedure. Note that for \( K=2 \) its fractiles could be deduced from the basic joint distribution (2).

Extension to the linear model

Suppose now that under \( H_0 \) the \( X_i \) are generated by a linear model
where $\beta$ is a $p \times 1$ vector of unknown regression coefficient and $\sigma^2$ is unknown. The alternative model that outliers are present may be formulated as

$$x_i \sim N[\gamma_i \beta, \sigma^2]$$

where $\lambda_i = 0$ for the good observations. The sign of $\lambda_i$ may, or may not be fixed a priori, depending on circumstances.

The model 7 may be rewritten in terms of an indicator vector as follows: Let $\mathbf{w}_i^* = (w_i: 0, 0 \ldots 0, 1, 0 \ldots 0)$, the 1 occurring in position $i$ of the indicator vector, and let

$$\mathbf{w}^* = (\beta', \lambda_1, \lambda_2, \ldots, \lambda_n)$$

Then

$$x_i \sim N[\mathbf{w}_i^* \beta^*, \sigma^2].$$

Given this equivalence of the two methods, it is convenient for present purposes to work in terms of the second formulation.
In matrix form the model is

\[ Y \sim \mathcal{N}(\mathbf{X} \beta, \sigma^2 I_n). \]

In solving to find regression coefficients, form

\[
(W: X; I_n)'(W: X; I_n) = \begin{bmatrix}
W'W & W'X & W' \\
X'W & X'X & X' \\
X' & X & I
\end{bmatrix}
\]

Introducing \( Y \) into the regression by sweeping on the first \( p \) rows and columns transforms this matrix to

\[
\begin{bmatrix}
-\mathbf{W}'\mathbf{W}^{-1} & \mathbf{W}'\mathbf{W}^{-1}X & \mathbf{W}'\mathbf{W}^{-1}Y \\
X'W\mathbf{W}^{-1} & \mathbf{X}'\mathbf{A} & \mathbf{X}' \\\n\mathbf{W}'\mathbf{W}^{-1} & \mathbf{A} & \mathbf{A}
\end{bmatrix}
\]

where \( \mathbf{A} = I_n - \mathbf{X}'\mathbf{X}^{-1}\mathbf{X} \), so that \( S^2 = \mathbf{X}'\mathbf{A} \) is the residual sum of squares of the regression of \( \mathbf{X} \) on \( Y \) and \( \mathbf{e} = \mathbf{A} \) is the vector of residuals.

Let \( a_{ij} \) denote the \( i,j \)th element of \( \mathbf{A} \), and \( e_i \) the \( i \)th element of \( \mathbf{e} \). Then questions about the introduction of one or more \( \lambda_i \) into the regression focus on the matrix

\[
\begin{pmatrix}
S^2 & e'_i \\
e_i & \mathbf{e}'
\end{pmatrix}
\]

The single-outlier test would be based on the maximum of \( r_{X_i} \) — the partial correlation between \( X \) and indicator variable \( i \). This is

\[ r_{X_i} = e_i / (a_{ii}S)^{1/2} \]

a well-known outlier statistic (Ellenberg 1973). In the case \( w_i = 1 \),
$p=1$, $r_n = n/(n-1)^{1/2}$, so this statistic generalizes $B$.

Unlike the case $p=1$, the case $p>1$ poses difficulties for testing for the presence of two or more outliers: the very difficulties that beset the regression subset problem, namely that the best subset of size $k$ to include in the regression does not necessarily contain the best subset of size $k-1$.

If the number of outliers $k$ is specified a priori, then no conceptual difficulty arises. The best subset of $k$ predictors amongst the $\lambda_i$ is found by using a branch and bound multiple regression algorithm. The analysis of variance then yields a test statistic equivalent to $C$.

The use of the recursive procedure is equivalent to a stepwise regression in which one introduces $k$ of the $\lambda_i$ in order of significance, and then proceeds to eliminate them. As in stepwise regression, a conservative test may be set up by concluding that there are fewer than $k$ outliers if the partial correlation corresponding to the $k$th is not significant at the $\alpha/(K(n-k+1))$ level. Experience with multiple regression shows that there is no guarantee that this procedure will identify the correct outliers, especially since $A$ has rank only $n-p$, and so is highly multicollinear.

For the case $W_i = 1$, $p=1$, the Bonferroni bound is conservative — for example in the test case considered earlier, the .05 fractile of $R$ corresponds to a Bonferroni fractile with $\alpha = .1$. Considerable experience is still needed to establish whether this procedure is effective.
REFERENCES


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FIGURE 1. CRITICAL REGIONS.