NATIONAL BUREAU OF STANDARDS REPORT

1626

HOW TO DECIDE OBJECTIVELY WHETHER AN OUTLYING OBSERVATION SHOULD BE REJECTED

by

Frank Proschan

NBS

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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FOREWORD

A perennial problem vexing the experimenter is that of rejection of suspected data. For one hundred years attempts at the solution of this problem have been advanced, most of them to be themselves rejected as suspect. Fortunately modern statistical theory has proposed useful, reliable methods for objectively rejecting deviant values. However the solution is far from complete at present.

This report describes for the experimenter two of the modern statistical tests available for possible rejection of outlying observations. These two methods have been selected because they apply in a majority of the actually occurring situations, and because they are so easy to apply. The report was originally motivated by Mr. Proschan's consultative work in the Ordnance Development Division, National Bureau of Standards. However it is applicable more generally to the scientific and engineering work at the National Bureau of Standards.

It should be borne in mind that this report, although intended for practical every-day use in our laboratories, is not the final word on the subject of rejection of suspected observations.

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1.1 PROBLEM: Here is a very common problem facing experimenters at the National Bureau of Standards. The typical scientist, call him X. Perry Menter, makes a number (say five) of repeated measurements of some unknown quantity. One of the values (say the largest) is so far removed from the other four that he suspects that it may be in error. However, Perry has no specific knowledge that a mistake actually did occur. Let us assume, too, that he has no previous data from which to estimate the precision of measurement. How can he decide, from the values themselves, whether the suspected value is in error or not?

The answer seems clear: He should consider the suspected value as in error when it seems too far from the other four values. But how can he judge when it is "too far from the other four values"?

1.2 LOGICAL APPROACH: Here is a simple, logical, objective criterion. Suppose Perry could somehow make millions of sets of five observations each. Suppose, too, that he could guarantee that none of these observations had any mistakes. Call a typical set x_1, x_2, x_3, x_4, x_5, where the x's are arranged in order of size, so that $x_1 \leq x_2 \leq x_3 \leq x_4 \leq x_5$. Now a logical

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

measure of the distance between the largest value and the other four values is

$$r_1 = \frac{x_5 - x_4}{x_5 - x_1} \qquad (1)$$

i.e., the proportion of the total range, that the distance between the suspected value and its adjacent value, is.

Now Perry records with what frequency, among his millions of sets of five values each, different values of r_1 occur. He finds that a value of r_1 larger than .780 occurs one time in one hundred. He then reasons this way:

"I have found that among sets of five observations each (containing no mistakes) a value of r_1 larger than .780 is quite unlikely (occurs only once in one hundred). If now, in my future experiments I get a set of five observations for which r_1 is larger than .780 I will conclude that my largest observation is in error."

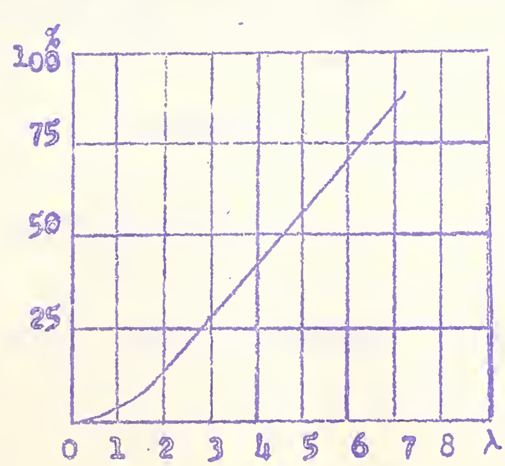
1.3 CONFIDENCE IN THE TEST: This seems reasonable. But what confidence can Perry have in such a procedure? How often will he consider as mistaken a perfectly good observation? How often will he consider acceptable an incorrect observation?

Clearly from the way he derived the test, he will classify a perfectly good largest observation as mistaken once among one hundred sets of five each, on the average. But there is no general answer to the question of how often he will let

pass a mistaken observation. This depends on how "mistaken" the mistaken observation is. If a very large error were made, his test would tend to reject the observation almost certainly. If a very small error were made, his test would tend to reject the observation with a small probability.

The following chart [1] gives some idea of the performance of r_1 in detecting mistaken observations. It is based on a sampling experiment in which samples of five from a normal population with mean μ, standard deviation σ were contaminated with values drawn from a normal population with mean $\mu + \lambda\sigma$ and standard deviation σ. The ordinate shows the percent discovery of contaminators (the proportion of the time the contaminating population provides an extreme value and the test discovers this value) while the abscissa shows λ, the magnitude of the shift (error) of the contaminator in standard deviations.

Performance of r-test



(From Dixon's article [1])

We said above that once in every 100 sets of values (on the average) Perry would consider as mistaken a perfectly good observation. If he were to reject this observation, and then compute the mean and standard deviation of the remaining values, these would be biased estimates. Also when a good observation is rejected, any further statistical tests of significance will become less reliable. This is the price that he must pay for improving the data in the cases where a mistaken observation is removed.

1.4 MATHEMATICAL DERIVATION: Of course, .780, the value of r_1 exceeded by chance 1 percent of the time (called the 1 percent level of significance of r_1), is not determined by actually making millions of sets of five observations each. Rather it may be calculated mathematically [2] with even greater accuracy than if millions of sets of five observations had been used. The basic assumption is that repeated measurements would follow the normal distribution.

Smallest Observation Suspected. What if Perry suspects the smallest observation in a set (of five, say)?

In this case, he computes

$$r_s = \frac{x_2 - x_1}{x_5 - x_1} \qquad (2)$$

He compares it with .780, as before. Exactly the same reasoning applies.

<u>1.5 Table I.</u> Let us now define r as either r_1 or r_s depending on whether the largest or smallest of a set is being tested. Table I at the end of the paper gives R, the value of r at various significance levels, α, for sample size n from 3 to 30.

Thus for example, for $n = 8$ and $\alpha = .05$, the table gives $R = .468$. This means that in 100 sets of 8 observations each free of mistakes, five values of r_1 will be larger than .468 and 5 values of r_s will be larger than .468 (on the average).

Why are various significance levels given? The reason is that no one significance level is appropriate to all problems. For example consider these two cases:

(a) Additional observations are not possible.

(b) Additional observations are possible.

In case (a) for many problems it might be appropriate to compute r and test it at the 1 percent level of significance. If the observed value of r is larger than the table value for $\alpha = 1$ percent, it might then be a good idea to exclude the responsible observation.

In case (b), for many situations a reasonable procedure might be to test r at the 5 percent level. If the sample value of r is significant at the 5 percent level, one or more additional observations would be taken. If the observation originally suspected remained outlying, it would be tested again, using the combined set of observations. This time, however, the r test would be performed at the <u>1 percent</u> level

of significance. If the outlier were significantly deviant at the 1 percent level, it would be rejected. It should be noted that among many sets tested this way, the proportion of perfectly good largest values rejected this way will be less than 1 percent. This is because the observation has a "second chance" before it is finally rejected.

1.6 SUMMARY: A set of n observations is made. No previous data are available from which to estimate the variability of a measurement. What is a rational procedure for testing whether the largest (or smallest) of the set is too deviant to be explained by the ordinary errors of measurement?

Consider the n observations in order of size,

$$x_1 \leq x_2 \leq \cdots \leq x_n$$

Compute

$$r = \frac{x_n - x_{n-1}}{x_n - x_1} \quad \text{(if } x_n \text{ is suspected)}$$

or

$$r = \frac{x_2 - x_1}{x_n - x_1} \quad \text{(if } x_1 \text{ is suspected).} \qquad (3)$$

Table I may use to determine how likely it is to get as large a value of r as actually obtained, simply by chance. A procedure that might be appropriate for many problems is as follows:

(a) No additional observations possible: In this case, compare the computed r with the Table I value at the 1 percent level. If the computed value of r is larger than the

Table I value, exclude the deviant observation. Otherwise, do not.

(b) Additional observations possible: In this case, compare the computed r with the table value of r at the 5 percent level. If the computed value of r is larger than the table value, take one or more additional observations (depending on convenience, cost of observations, etc.). Otherwise accept the suspected value without taking additional observations.

In in the enlarged set (containing all the original and the additional observation(s)), the previously suspected value remains outlying, compute r for the enlarged set. This time compare it with the Table I value at the 1 percent level. If the computed value exceeds the table value, exclude the outlier; otherwise do not.

1.7 EXAMPLES: 1. Anna List, chemist, determines five values for the iron content of an unknown solution by a new process: 7.42, 7.48, 7.39, 7.61, 7.44 (in percent). She suspects 7.61 as being mistaken, since it is so much larger than the other values. However she cannot determine additional values because no more samples are available. How can she decide whether to exclude 7.61 or not?

Since no previous data are available from which to compute the precision of measurement, the r test is appropriate. The first step is to arrange the five values in order of size:

7.39, 7.42, 7.44, 7.48, 7.61

Then

$$r = \frac{x_5 - x_4}{x_5 - x_1} = \frac{7.61 - 7.48}{7.61 - 7.39} = \frac{.13}{.22} = .591$$

Since this is less than .780, the .01 point of r for n = 5, Anna List retains the suspected value, 7.61.

2. N. G. Neer fires projectiles from a gun under constant conditions. Here are the distances in feet (in order of size):

6801	7683
7424	7720
7502	7799
7544	

He suspects 6801 as being inconsistent with the other values. What shall he do?

He computes

$$r = \frac{x_2 - x_1}{x_7 - x_1} = \frac{7424 - 6801}{7799 - 6801} = \frac{623}{998} = .624$$

This valuelies between the .01 and the .05 points of r for n = 7. Hence N. G. Neer fires an additional round and gets a new value of 7603.

Since 6801 remains outlying in the enlarged set of eight, he computes r for this set of eight. Obviously r remains .624. This time it is larger than the .01 point of r <u>for n = 8</u>. Hence N. G. Neer rejects 6801 and uses only the remaining seven values.

2 Estimate of Measurement Variability Available.

In a great many laboratory situations, past data are available for estimating the undertainty of a measurement. Thus if a laboratory makes routine analysis in triplicate of incoming specimens, there will be sets of triplicate values from which to estimate the precision of measurement. It is clear that where such information is available, it should be used, in deciding whether an outlier is mistaken or not. This will make the decision more reliable than if only the one set containing the suspected value is used.

2.1 u Test. The test ratio used now is

$$u = \frac{x_n - \bar{x}}{s_d} \qquad \text{(if } x_n \text{ is the suspected value)} \qquad (4)$$

or

$$u = \frac{\bar{x} - x_1}{s_d} \qquad \text{(if } x_1 \text{ is the suspected value)}$$

where

s_d = standard deviation of an individual measurement, based on d degrees of freedom.

2.2 Calculating s_d. To determine s_d from a single set of measurements we would first calculate the sum of the squares of the deviations of the observations from their mean. Then we would divide by one less than the number of observations. This would give us s_d^2. Thus

$$s_d^2 = \frac{\sum_{i=1}^{d} (x_i - \bar{x})^2}{d-1} \qquad (5)$$

On the other hand, suppose a number of sets of observations were available:

SETS	OBSERVATIONS	MEAN
1	$x_{11}, x_{12}, \ldots, x_{1n_1}$	$\bar{x}_1$
2	$x_{21}, x_{22}, \ldots, x_{2n_2}$	$\bar{x}_2$
...	....	...
k	$x_{k1}, x_{k2}, \ldots, x_{kn_k}$	$\bar{x}_k$

Now we could calculate s_d^2 from

$$s_d^2 = \frac{\sum_{i=1}^{n_1}(x_{1i}-\bar{x}_1)^2 + \sum_{i=1}^{n_2}(x_{2i}-\bar{x}_2)^2 + \ldots + \sum_{i=1}^{n_k}(x_{ki}-\bar{x}_k)^2}{(n_1-1) + (n_2-1) + \ldots + (n_k-1)} \quad (6)$$

d, the number of degrees of freedom for estimating the uncertainity of measurement, is $(n_1-1) + (n_2-1) + \ldots + (n_k-1)$.

2.3 EXAMPLE: An example will make the whole procedure clear:

Dr. Kem Mist has just run a set of three determinations on the yield of an ore-refining process. His values are:

39.35, 39.30, 39.00, with mean, $\bar{x} = 39.22$.

He wishes to test whether the "39.00" is unusually deviant. He has past data to estimate the precision of measurement:

Analysis

Set	1	2	3
1	36.51	36.57	36.70
2	30.27	30.35	30.19
3	35.00	35.53	35.36
4	43.51	43.65	43.65
5	51.06	51.17	51.00
6	48.03	38.19	48.31
7	39.27	39.51	39.36
8	33.46	33.21	33.28

Although we could calculate s_d^2 from (6), it is generally more convenient (especially with a computing machine available) to use (7):

$$s_d^2 = \left[\sum_{i=1}^{n_1} x_{1i}^2 - \frac{\left(\sum_{i=1}^{n_1} x_{1i} \right)^2}{n_1} + \sum_{i=1}^{n_2} x_{2i}^2 - \frac{\left(\sum_{i=1}^{n_2} x_{2i} \right)^2}{n_2} + \dots + \sum_{i=1}^{n_k} x_{ki}^2 - \frac{\left(\sum_{i=1}^{n_2} x_{ki} \right)^2}{n_k} \right] \Big/ \{(n_1-1)+(n_2-1)+\dots+(n_k-1)\} \qquad (7)$$

It can easily be shown that (7) is algebraically equivalent to (6). Thus substituting values into (7) yields:

$$s_d^2 = [36.51^2 + 36.57^2 + 36.70^2 - \frac{(36.51+36.57+36.70)^2}{3} + 30.27^2 + 30.35^2 + 30.19^2 - \frac{(30.27+30.35+30.19)^2}{3} + \dots + 33.46^2 + 33.21^2 + 33.28^2 - \frac{(33.46+33.21+33.28)^2}{3}\Big] \Big/ \Big[(3-1)+(3-1)+\dots+(3-1)\Big] = \frac{.3082}{16} = .019263$$

Hence $s_d = .139$

The u-ratio defined by (4) gives:

$$u = \frac{\bar{x} - x_1}{s_d} = \frac{39.22 - 39.00}{.139} = 1.58$$

He now uses Table II which gives the 5 percent and 1 percent levels of u for various values of n and d. n is the size of the sample which contains the suspected value, while d is the number of degrees of freedom on which s_d is based. In the present case n = 3 and d = 16.

The observed value of u, 1.58, is considerably less than the table value of u at the 5 percent level, 1.90. Hence he concludes that the suspected value 39.00 is not significantly outlying. In other words the deviation of 39.00 from the mean of the set of three measurements is easily explainable in terms of the precision of the measurement process. Hence, 39.00 is accepted into the fold of good measurements.

2.4 TABLE 2. When past data are available, the u-ratio may be computed and Table 2 used just as the r-ratio and Table I were used for the case where no past data were available. The procedure outlined in paragraph 1.5 for the two cases (a) and (b) may be followed just as before (using u and Table 2 instead of r and Table I).

III. Cautions and Comments. a. Obviously, if the experimeter knows that a mistake has occurred he should reject the observation. The tests of this paper are used only if he doesn't know that a mistake has occurred.

b. If the experimenter uses this technique for a certain routine type of measurement, he should apply it, implicitly or explicity, every time he makes that type of measurement. After several explicit applications of this technique, he will probably be able to perform the r(or u) test in all but the most doubtful cases without actually explicitly doing the arithmetic, since he will have the critical value of r(or u) in mind. He should not, however, reject outliers by the r test in some cases, and accept others just as badly deviating, simply because he did not apply the test in these latter cases.

c. Both the r and u tests are based on the assumption that repeated measurements of the same unknown follow the <u>normal frequency distribution</u>. If, in actual practice, the distribution of repeated measurements is markedly different from the normal curve, then the use of these tests will lead to different risks than originally intended.

d. The use of the .01 and .05 points is arbitrary. The individual experimenter should use whatever <u>levels of significance</u> are most appropriate.

e. Suppose the type of measurement is such that the suspected value is practically always the smallest in the set (for example, a chemical analysis where some of the material may be washed out), or practically always the largest. Then as stated above, 1 percent of the time a perfectly good

observation will be rejected in case (a) of paragraph 1.5. Suppose however the type of measurement is such that the suspected value may be either the largest or the smallest. In this case about 2 percent of the time a perfectly good observation will be rejected. The appropriate tabular point should be selected with this in mind.

f. Other tests for rejection of suspected values are available [1]. However, the r and u tests have been selected because of their ease of application.

g. The whole question of rejection of suspected values is a difficult one, and has given rise to quite a bit of discussion. [See references.] If the scientist or engineer at the National Bureau of Standards is in doubt about any assumption, procedure, or conclusion involved in a specific practical problem, we suggest that he consult the Statistical Engineering Laboratory (11.3).

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TABLE I

$Pr(r > R) = \alpha$

n \ α	.005	.01	.02	.05	.10	.20	.30	.40	.50	.60	.70	.80	.90	.95
3	.994	.988	.976	.941	.886	.781	.684	.591	.500	.409	.316	.219	.114	.059
4	.926	.889	.846	.765	.679	.560	.471	.394	.324	.257	.193	.130	.065	.033
5	.821	.780	.729	.642	.557	.451	.373	.308	.250	.196	.146	.097	.048	.023
6	.740	.698	.644	.560	.482	.386	.318	.261	.210	.164	.121	.079	.038	.018
7	.680	.637	.586	.507	.434	.344	.281	.230	.184	.143	.105	.068	.032	.016
8	.634	.590	.543	.468	.399	.314	.255	.208	.166	.128	.094	.060	.029	.014
9	.598	.555	.510	.437	.370	.290	.234	.191	.152	.118	.086	.055	.026	.013
10	.568	.527	.483	.412	.349	.273	.219	.178	.142	.110	.080	.051	.025	.012
11	.542	.502	.460	.392	.332	.259	.208	.168	.133	.103	.074	.048	.023	.011
12	.522	.482	.441	.376	.318	.247	.197	.160	.126	.097	.070	.045	.022	.011
13	.503	.465	.425	.361	.305	.237	.188	.153	.120	.092	.067	.043	.021	.010
14	.488	.450	.411	.349	.294	.228	.181	.147	.115	.088	.064	.041	.020	.010
15	.475	.438	.399	.338	.285	.220	.175	.141	.111	.085	.062	.040	.019	.010
16	.463	.426	.388	.329	.277	.213	.169	.136	.107	.082	.060	.039	.019	.009
17	.452	.416	.379	.320	.269	.207	.165	.132	.104	.080	.058	.038	.018	.009
18	.442	.407	.370	.313	.263	.202	.160	.128	.101	.078	.056	.036	.018	.009
19	.433	.398	.363	.306	.258	.197	.157	.125	.098	.076	.055	.036	.017	.008
20	.425	.391	.356	.300	.252	.193	.153	.122	.096	.074	.053	.035	.017	.008
21	.418	.384	.350	.295	.247	.189	.150	.119	.094	.072	.052	.034	.016	.008
22	.411	.378	.344	.290	.242	.185	.147	.117	.092	.071	.051	.033	.016	.008
23	.404	.372	.338	.285	.238	.182	.144	.115	.090	.069	.050	.033	.016	.008
24	.399	.367	.333	.281	.234	.179	.142	.113	.089	.068	.049	.032	.016	.008
25	.393	.362	.329	.277	.230	.176	.139	.111	.088	.067	.048	.032	.015	.008
26	.388	.357	.324	.273	.227	.173	.137	.109	.086	.066	.047	.031	.015	.007
27	.384	.353	.320	.269	.224	.171	.135	.108	.085	.065	.047	.031	.015	.007
28	.380	.349	.316	.266	.220	.168	.133	.106	.084	.064	.046	.030	.015	.007
29	.376	.345	.312	.263	.218	.166	.131	.105	.083	.063	.046	.030	.014	.007
30	.372	.341	.309	.260	.215	.164	.130	.103	.082	.062	.045	.029	.014	.007

TABLE II

Upper per cent points of the studentized extreme deviate
$(x_n - \bar{x})/s_d$ or $(\bar{x} - x_1)/s_d$

d \ n	α = .05							α = .01						
	3	4	5	6	7	8	9	3	4	5	6	7	8	9
10	2.02	2.29	2.49	2.63	2.75	2.85	2.93	2.76	3.05	3.25	3.39	3.50	3.59	3.67
11	1.99	2.26	2.44	2.58	2.70	2.79	2.87	2.71	3.00	3.19	3.33	3.44	3.53	3.61
12	1.97	2.22	2.40	2.54	2.65	2.75	2.83	2.67	2.95	3.14	3.28	3.39	3.48	3.55
13	1.95	2.20	2.38	2.51	2.62	2.71	2.79	2.63	2.91	3.10	3.24	3.34	3.43	3.51
14	1.93	2.18	2.35	2.48	2.59	2.68	2.76	2.60	2.87	3.06	3.20	3.30	3.39	3.47
15	1.92	2.16	2.33	2.46	2.56	2.65	2.73	2.57	2.84	3.02	3.16	3.27	3.35	3.43
16	1.90	2.14	2.31	2.44	2.54	2.63	2.70	2.55	2.81	3.00	3.13	3.24	3.32	3.39
17	1.89	2.13	2.30	2.42	2.52	2.61	2.68	2.52	2.79	2.97	3.10	3.21	3.29	3.36
18	1.88	2.12	2.28	2.41	2.51	2.59	2.66	2.50	2.77	2.95	3.08	3.18	3.27	3.34
19	1.87	2.11	2.27	2.39	2.49	2.58	2.65	2.49	2.75	2.92	3.06	3.16	3.24	3.31
20	1.87	2.10	2.26	2.38	2.48	2.56	2.63	2.47	2.73	2.91	3.04	3.14	3.22	3.29
24	1.84	2.07	2.23	2.35	2.44	2.52	2.59	2.43	2.68	2.85	2.97	3.07	3.15	3.22
30	1.82	2.04	2.20	2.31	2.40	2.48	2.55	2.38	2.62	2.79	2.91	3.01	3.08	3.15
40	1.80	2.02	2.17	2.28	2.37	2.44	2.51	2.34	2.57	2.73	2.85	2.94	3.02	3.08
60	1.78	1.99	2.14	2.25	2.33	2.41	2.47	2.30	2.52	2.68	2.79	2.88	2.95	3.01
120	1.76	1.97	2.11	2.21	2.30	2.37	2.43	2.25	2.48	2.62	2.73	2.82	2.89	2.95
∞	1.74	1.94	2.08	2.18	2.27	2.33	2.39	2.22	2.43	2.57	2.68	2.76	2.83	2.88

THE NATIONAL BUREAU OF STANDARDS

Functions and Activities

The National Bureau of Standards is the principal agency of the Federal Government for fundamental and applied research in physics, mathematics, chemistry, and engineering. Its activities range from the determination of physical constants and properties of materials, the development and maintenance of the national standards of measurement in the physical sciences, and the development of methods and instruments of measurement, to the development of special devices for the military and civilian agencies of the Government. The work includes basic and applied research, development, engineering, instrumentation, testing, evaluation, calibration services, and various scientific and technical advisory services. A major portion of the NBS work is performed for other government agencies, particularly the Department of Defense and the Atomic Energy Commission. The functions of the National Bureau of Standards are set forth in the Act of Congress, March 3, 1901, as amended by Congress in Public Law 619, 1950. The scope of activities is suggested in the listing of divisions and sections on the inside of the front cover.

Reports and Publications

The results of the Bureau's work take the form of either actual equipment and devices or published papers and reports. Reports are issued to the sponsoring agency of a particular project or program. Published papers appear either in the Bureau's own series of publications or in the journals of professional and scientific societies. The Bureau itself publishes three monthly periodicals, available from the Government Printing Office: the Journal of Research, which presents complete papers reporting technical investigations; the Technical News Bulletin, which presents summary and preliminary reports on work in progress; and Basic Radio Propagation Predictions, which provides data for determining the best frequencies to use for radio communications throughout the world. There are also five series of nonperiodical publications: the Applied Mathematics Series, Circulars, Handbooks, Building Materials and Structures Reports, and Miscellaneous Publications.

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