SCREENING OUTLIERS IN PROCESS CONTROL REGRESSION DATA WITH UNIFORM RESIDUALS, II

Charles P. Quesenberry
North Carolina State University, Raleigh, NC 27695-8203

Methods for screening outliers in univariate normal data using uniform residuals obtained from conditional probability integral transformations (CPIT's) were proposed in Quesenberry (1986). The methods of that paper are here extended to screen outliers in normal regression process data by using the corresponding CPIT uniform residuals from the normal regression model. As for univariate data, the exact distribution theory of these statistics allows a precise control of the number of cases incorrectly rejected when the data are generated by a regression model with independent normal errors.

Introduction

Regression models with normal errors are useful for modeling data obtained in many problems in quality control and, more generally, in applied statistics. In a recent paper Quesenberry (1988) used a simple linear regression model to design a compensator for a machining process for which tool wear is an important source of variation. For this particular example and for many other applications in process control the data for a regression analysis become available sequentially in time. For such data, analysis methods that can be applied sequentially as the data become available are needed. In this paper, uniform residuals from normal regression models are proposed to screen outliers from the data. Although primary interest here is in sequential process data, the technique proposed using uniform residuals can also be used for data that are not naturally ordered, and when used for such data offers some advantages over presently available techniques.

The outliers literature is large. See Quesenberry (1986a) for references to literature related to outliers in normal errors models. Most of the discussion in that paper for univariate normal data applies also for normal errors regression data.

Uniform Residuals from Regression Models

The problem of screening outliers from a simple linear regression model is considered first because it is possibly the most important case, and it can be treated without the use of

matrix algebra and will therefore be useful to a broader audience of readers. Univariate multiple regression models will be considered below.

Let a sequence of observations be denoted by $(x_1, y_1), \cdots, (x_i, y_i), \cdots$ and consider the simple linear regression model

$$y_i = \alpha + \beta x_i + \epsilon_i \qquad i = 1, 2, \cdots \tag{1}$$

where x_i is the value of a variable at time i and y_i is a random variable. If the ϵ_i's are independently and identically distributed (iid) as normal random variables with common mean zero and variance σ^2, then the y_i's are themselves independent normal random variables with means $\alpha + \beta x_i$ and common variance σ^2. The data point (x_i, y_i) is sometimes called a "case". A screen for outliers is a technique to decide if each case can be considered to have arisen from this regression model. The screening technique proposed here is basically the same as the method proposed for normal data in Quesenberry (1986a), Q86a, but is here applied to uniform residuals from regression models.

We define a number of (sequential) statistics as follows.

$$\bar{x}_i = \frac{1}{i}\sum_{j=1}^{i} x_j\,,\ \bar{y}_i = \frac{1}{i}\sum_{j=1}^{i} y_j\,,\ S_{xy}^{(i)} = \sum_{j=1}^{i}(x_j - \bar{x}_i)(y_j - \bar{y}_i)$$

$$S_{xx}^{(i)} = \sum_{j=1}^{i}(x_j - \bar{x}_i)^2\,,\ S_{yy}^{(i)} = \sum_{j=1}^{i}(y_j - \bar{y}_i)^2$$

$$b_i = \frac{S_{xy}^{(i)}}{S_{xx}^{(i)}}\,,\ a_i = \bar{y}_i - b_i\bar{x}_i\,,\ K_i = \frac{i\,S_{xx}^{(i)}}{(i-1)S_{xx}^{(i-1)}} \tag{2}$$

$$SSE_i = S_{yy}^{(i)} - S_{xy}^{(i)} b_i\,,\ B_i = \frac{\sqrt{i-3}(y_i - a_{i-1} - b_{i-1}x_i)}{\sqrt{(SSE_{i-1})K_i}}$$

$$u_i = G_{i-3}(B_i) \text{ for } i = 4, 5, \cdots$$

Here $G_\nu(\cdot)$ is a Student-t distribution function with ν degrees of freedom.

The actual computations are conveniently made using the following updating formulas.

$$\begin{aligned}
&\bar{x}_i = \tfrac{1}{i}\left[(i-1)\,\bar{x}_{i-1} + x_i\right], \quad \bar{y}_i = \tfrac{1}{i}\left[(i-1)\,\bar{y}_{i-1} + y_i\right] \\
&S_{xy}^{(i)} = S_{xy}^{(i-1)} + \tfrac{i-1}{i}(x_i - \bar{x}_{i-1})(y_i - \bar{y}_{i-1}) \\
&S_{xx}^{(i)} = S_{xx}^{(i-1)} + \tfrac{i-1}{i}(x_i - \bar{x}_{i-1})^2 \\
&S_{yy}^{(i)} = S_{yy}^{(i-1)} + \tfrac{i-1}{i}(y_i - \bar{y}_{i-1})^2
\end{aligned} \tag{3}$$

From the conditional probability integral theory (CPIT) of O'Reilly and Quesenberry (1973), when the linear regression model with independent normal errors is correct the values $u_1, u_2, \cdots$ are independent uniform random variables on the unit interval (0, 1). We sometimes denote this by saying they are U(0, 1) random variables. By considering B_i in display (2), it can be observed that its numerator is essentially a residual of y_i from a least squares fitted model from the preceding $i - 1$ cases, even though least squares estimation plays no role in the CPIT distribution theory. The u's are called uniform residuals. These uniform residuals have theoretical properties corresponding to the properties 1 - 4 of the uniform residuals for the iid normal model of Quesenberry (1986a). Briefly stated, in addition to the distributional properties stated above, the sequence of u's is independent of the usual least squares estimates of the model parameters, is a maximal invariant for the problem, and most powerful tests to detect mean shifts from the nominal model can be based on it alone.

Screening Outliers in Sequential Data

We propose using the same screening rule for uniform residuals computed using the above formulas as that in Q86a, equation (7). The presentation of this screening rule and the discussion of its properties in this and the next section are similar to that in Q86a, but with the modifications necessary to treat the regression models considered here. The rule is as follows. Suppose that we are willing to incorrectly decide that residuals are too large at an average rate of 1 in N_L and to incorrectly decide that they are too small at an average rate of 1 in N_S, when the nominal normal errors regression model is actually correct. Then we use the

following rejection (identification) rule:

$$\text{Declare } y_i \text{ of the } i^{th} \text{ case a left outlier if } u_i < \frac{1}{N_S},$$
$$\text{Declare } y_i \text{ of the } i^{th} \text{ case a right outlier if } u_i > \frac{N_L - 1}{N_L}. \tag{4}$$

The overall rejection rate for this rule is $\alpha = (N_S + N_L)/N_L N_S$ when the model is correct. The average run length between incorrectly declared outliers when the model is correct is $\text{ARL} = \alpha^{-1} - 1$.

A case is called a left outlier if y_i is too small and its uniform residual is too near zero, and it is called a right outlier if y_i is too large and its uniform residual is too near one. From the formula for B_i, this means that a case is declared a left or right outlier, respectively, when compared with the fitted regression function from the preceding cases. Thus, as for the simple random sample model, it is reasonable to call these values *sequential outliers.*

From the formula for u_i in display (2) it is seen that no residuals are obtained for the first three cases in each sequence of data. The reason that there are no residuals for these first three cases is that there are three parameters in the regression model that are, in effect, estimated before any residuals can be computed. These first cases for which no residuals are available are called the *basis* of the transformations. The above screening rule is designed to detect outliers that occur after the basis set. If outliers occur in the basis set it will result in an overestimate of the variance and bias, either positive or negative, in the estimate of the regression mean. Actually, outliers that occur anywhere in the data sequence will have these effects on subsequent observations. The resultant effect is to mask subsequent outliers and make them more difficult to detect. Therefore, when an outlier is detected it is necessary to carefully consider what action to take. If it is not removed from the computations of the residuals for subsequent cases its effect will be largest on the residuals of the cases immediately following it. We feel that it is almost always preferable to remove the identified outliers from the subsequent computations. When uniform residuals are computed in this manner, deleting outliers with a deletion rate of α, we call them $100\alpha\%$ *deleted uniform residuals.* Even when the normal errors regression model is correct these residuals are no longer exactly independent U(0, 1) random variables, however, if the deletion rate α is small, as it will be in most cases, the disturbance to the distribution theory should be of little consequence. Some users may

wish to choose $\alpha = 0.00270$ corresponding to the familiar 3-σ control limits.

Screening Outliers in Sequential or Nonsequential Samples of Past Data

Thus far we have considered screening a sequence of cases for outliers as the individual cases appear. We consider next a sequence of ordered past data (x_1, y_1), (x_2, y_2), $\cdots$, (x_n, y_n) with uniform residuals $u_1, u_2, \cdots, u_N$ where $N = n - 3$. In order for the distribution theory for the uniform residuals to hold it is not necessary for the cases to be analyzed in their original order. This point will be discussed further below.

Let $u_{(1)} \leq u_{(2)} \leq \ldots \leq u_{(N)}$ denote the ordered values of $u_1, \ldots, u_N$. That is, $u_{(1)}$ is the smallest value among $u_1, \cdots, u_N$; $u_{(2)}$ is the second smallest value, and so on. Now, if we apply the rejection rule in (4) to detect right outliers, then, by direct evaluation, the probability of rejecting at least one u_i when the model assumptions are correct is $1 - \left[(N_L - 1)/N_L\right]^N$. However, the event that at least one right outlier is declared occurs if and only if $u_{(N)} > (N_L - 1)/N_L$. Moreover, if P_L and P_S denote the observed significance levels or p-values for testing whether $u_{(N)}$ and $u_{(1)}$ are too large and too small, respectively; from the theory of uniform order statistics we have

$$P_S = 1 - (1 - u_{(1)})^N, \; P_L = 1 - u_{(N)}^N. \tag{5}$$

It should be observed that the quantity P_S is a p-value for testing a null hypothesis of *no left outliers* against an alternative hypothesis that there is *at least one left outlier.* The probability P_L is interpreted similarly for right outliers. Also, these values can be used to judge if the smallest and largest order statistics are "inliers," as will sometimes be the case. The smallest order statistic is an inlier if it is too large, and the largest order statistic is an inlier if it is too small. An inlier on either end of the sample may be caused, for example, by having an error distribution with a tail that is thinner than the tail of a normal distribution.

When the rejection rule (4) is applied to a sample of N uniform residuals, then, under the null hypothesis, the number, say R, of values rejected is a binomial random variable with probability function

$$b(r; N, \alpha) = \binom{N}{r} \alpha^r (1 - \alpha)^{N-r}; \; r = 0, 1, \cdots, N. \tag{6}$$

Since α will usually be chosen quite small, for N large the binomial probability function can be accurately approximated by a Poisson probability function with parameter $\lambda = \alpha N$. That is, by

$$p(r; \lambda) = \frac{\lambda^r e^{-\lambda}}{r!}, \quad \lambda = \alpha N, \quad r = 0, 1, 2, \cdots \tag{6'}$$

Thus for a given sample size $n = N + 3$, by our choice of α we can control the distribution of the number of false rejections under the null hypothesis.

When a past sample is screened as described above, then the power for detecting an outlier will be less if it occurs early in the observation sequence than if it occurs late in the sequence. This can be seen from the formula for B_t of (2) by noting that a_{r-1}, b_{r-1} and SSE_{r-1} are, of course, based on $r - 1$ observations. One strategy that can be used is to compute the unform residuals and screen the data for different permutations of the observations. One obvious choice of permutation is to take the data in the exact reverse order. If the forward and reverse orderings of the sample identify the same (or nearly the same) set of outliers, then clearly order is not an important factor to the analysis. Of course, this analysis also gives protection against outliers in the basis set.

To consider the basis for this analysis, recall that the distribution of the uniform residuals $u_1, u_2, \cdots, u_N$ depends only upon the assumption that the values $y_i (i \geq 1)$ are independently distributed with a $N(\alpha+\beta x_i, \sigma^2)$ distribution. Thus if the cases are permuted into a new ordered set say $(x_1^*, y_1^*), (x_2^*, y_2^*), \cdots, (x_N^*, y_N^*)$, so that these satisfy the normal regression model assumptions of (1), then new uniform residuals $u_1^*, u_2^*, \cdots, u_N^*$ can be computed from this permutation, and these will be iid U(0, 1) random variables. However, the vector $(u_1^*, \cdots, u_N^*)$ is not independent of the vector $(u_1, \cdots, u_N)$. Note, particularly, that the reordering of $(x_1, y_1), \cdots, (x_n, y_n)$ to $(x_1^*, y_1^*), \cdots, (x_n^*, y_n^*)$ can be done in any manner, so long as the values $y_1^*, \cdots, y_n^*$ are independent and y_i^* is a $N(\alpha+\beta x_i^*, \sigma^2)$ random variable for $i \in \{1, 2, \cdots, n\}$. Thus the values of the x_i's can be used to reorder the cases and the distribution theory is still valid. However, if the values of the y_i's are used in any way to define the new ordering $y_1^*, \cdots, y_N^*$; the distribution theory is vitiated and the values $u_1^*, \cdots, u_N^*$ are not, in general, iid U(0, 1) random variables. The set $u_1^*, u_2^*, \cdots, u_N^*$ may be screened for outliers in the same manner as $u_1, \cdots, u_N$ with, say, the same rejection rate α. While the rejection rate α is correct for each procedure separately, the overall rejection rate under the normal

model, that is, the probability that a particular observation will be declared an outlier in both orderings, is, in general, less than α.

The analysis proposed in this section for a sample of past data assumes no knowledge of the number of outliers present in the data. As was mentioned earlier, in some of the outliers literature authors assume that the number k of outliers in a sample is either known or can be estimated, and sometimes that suspect cases can be identified in advance. If information of this type is available, then one can proceed as follows. Suppose that in a sample of n observations a subset of m can be identified that contains all suspected outliers, in addition to other observations. In other words, from the original sample of n cases a subset of n − m can be identified that are not outliers. Then the m deleted uniform residuals are computed for only these m observations, using all n − m of the others as the basis. The number R of these observations declared outliers is a random variable with binomial probability function given by (6), with N replaced by m under the iid normal model assumptions for the entire sample. Note that this procedure does not depend upon the order of the n − m 'clean' observations in the basis set

The Multiple Regression Model

In this section we consider the univariate multiple linear regression model with independent normal errors. The formulas used here are given in Quesenberry (1986b), Q86b. Notation is defined in display (7).

$$
\begin{aligned}
&\underset{\sim}{y}_n = (y_1, \cdots, y_n)', \text{ a vector of independent random variables} \\
&\underset{\sim}{X}_n = [X_{ij}], \text{ an nxp matrix of independent variables of full rank } (n > p) \\
&\underset{\sim}{\beta} = (\beta_1, \cdots, \beta_p)', \text{ a vector of p coefficient parameters} \\
&\underset{\sim}{x}_i' = (x_{i1}, \cdots, x_{ip}), \text{ the } i^{th} \text{ row of } \underset{\sim}{X}_n \\
&\underset{\sim}{X}_i, \text{ the matrix consisting of the first i rows of } \underset{\sim}{X}_n
\end{aligned}
\tag{7}
$$

If

$$y_i = \underset{\sim}{x}_i' \underset{\sim}{\beta} = \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i \; ; \; i = 1, \cdots, n \tag{8}$$

and the ϵ_i's are iid $N(0, \sigma^2)$, then y is said to satisfy a univariate multiple linear regression model with independent variables $(x_1, \cdots, x_p)$. When this model is correct the uniform

residuals $\underset{\sim}{u}' = (u_1, \cdots, u_N)$ of the conditional probability integral transformation can be computed from the formulas given in display (9).

$$\underset{\sim}{b}_i = (\underset{\sim}{X}_i' \underset{\sim}{X}_i)^{-1} \underset{\sim}{X}_i' \underset{\sim}{y}_i, \text{ the least squares estimate of } \underset{\sim}{\beta} \text{ from the first i cases}$$

$$S_i^2 = \underset{\sim}{y}_i' \left[I - \underset{\sim}{X}_i (\underset{\sim}{X}_i' \underset{\sim}{X}_i)^{-1} \underset{\sim}{X}_i' \right] \underset{\sim}{y}_i, \text{ the sum of squares for residuals from the first i cases}$$

$$B_i = \frac{\sqrt{i-p-1}(y_i - \underset{\sim}{x}_i' \underset{\sim}{b}_i)}{\sqrt{[1 - \underset{\sim}{x}_i' (\underset{\sim}{X}_i' \underset{\sim}{X}_i)^{-1} \underset{\sim}{x}_i] S_i^2 - (y_i - \underset{\sim}{x}_i' \underset{\sim}{b}_i)^2}} \tag{9}$$

$$u_{i-p-1} = G_{i-p-1}(B_i), \; i = p+2, \cdots, n$$

For this model there are $N = n-p-1$ uniform residuals. The computation of u_{i-p-1} requires $\underset{\sim}{X}_{i-1}$ to be of full rank p. In practice it will be necessary to assure that this condition is met, it can be a problem especially for the earlier cases for some data. An example where colinearity among the rows of $\underset{\sim}{X}_{i-1}$ is a factor that must be recognized in the analysis is seen in Example 2 below.

The following updating formulas [Plackett (1950), Bartlett (1954)] are particularly convenient for carrying out the computations. To screen the cases $(y_i, \underset{\sim}{x}_i')$ for outliers from the model (8), we use the screening rule given above in (4). These methods will be illustrated below. The formulas of (9) and (10) are readily evaluated using a computer language with matrix algebra capability.

$$(\underset{\sim}{X}_i' \underset{\sim}{X}_i)^{-1} = (\underset{\sim}{X}_{i-1}' \underset{\sim}{X}_{i-1})^{-1} - \frac{(\underset{\sim}{X}_{i-1}' \underset{\sim}{X}_{i-1})^{-1} \underset{\sim}{x}_i \underset{\sim}{x}_i' (\underset{\sim}{X}_{i-1}' \underset{\sim}{X}_{i-1})^{-1}}{1 + \underset{\sim}{x}_i' (\underset{\sim}{X}_{i-1}' \underset{\sim}{X}_{i-1})^{-1} \underset{\sim}{x}_i}$$

$$\underset{\sim}{b}_i = \underset{\sim}{b}_{i-1} + (\underset{\sim}{X}_i' \underset{\sim}{X}_i)^{-1} \underset{\sim}{x}_i (y_i - \underset{\sim}{x}_i' \underset{\sim}{b}_{i-1}) \qquad (10)$$

$$S_i^2 = S_{i-1}^2 + \frac{(y_i - \underset{\sim}{x}_i' \underset{\sim}{b}_{i-1})^2}{1 + \underset{\sim}{x}_i' (\underset{\sim}{X}_{i-1}' \underset{\sim}{X}_{i-1})^{-1} \underset{\sim}{x}_i}$$

$$B_i = \frac{\sqrt{i - p - 1}\,(y_i - \underset{\sim}{x}_i' \underset{\sim}{b}_{i-1})}{S_{i-1} \sqrt{1 + \underset{\sim}{x}_i' (\underset{\sim}{X}_{i-1}' \underset{\sim}{X}_{i-1})^{-1} \underset{\sim}{x}_i}}$$

Examples

Example 1. For this example we consider diameter measurements made on 45 consecutively produced automatic transmission parts. Due to tool wear in the process a linear regression model relating diameters to part numbers is known to be a reasonable model for this process. However, as is often the case with tool-wear processes, this process is prone to produce outlying measurements. These parts were made immediately after an adjustment to the tool, and in this situation it is necessary to re-estimate the process regression model parameters after each tool adjustment. A sequential rule is required for screening individual measurements. Table 1 gives the part number in the order of production in column 1 and the measurements in column 2. The uniform residuals without deletion of outliers are given in column 3. The uniform residuals with deletion of outliers using a deletion rate of 0.001 on each end are shown in column 4. Observation 19 has a uniform residual of 0.000259 and the measurement 27.176 is a left outlier at this level. Observation 43 has a uniform residual of 0.999050 when the preceding observation 19 is not deleted. When observation 19 is deleted, measurement number 43 has a uniform residual of 0.999942. Note the difference in these values due to the masking effect of leaving measurement 19 in the analysis!

TABLE 1

Number	Observation	Uniform Residual Not Deleted	Uniform Residual Deleted
1	27.187	0	0
2	27.200	0	0
3	27.196	0	0
4	27.192	.267720	.267720
5	27.191	.325022	.325022
6	27.194	.535285	.535285
7	27.194	.514700	.514700
8	27.192	.372761	.372761
9	27.191	.347668	.347668
10	27.189	.264093	.264093
11	27.192	.607050	.607050
12	27.190	.421665	.421665
13	27.192	.663498	.663498
14	27.190	.448106	.448106
15	27.190	.489122	.489122
16	27.195	.925912	.925912
17	27.191	.519500	.519500
18	27.189	.310192	.310192
19	27.176	.000259	.000259*
20	27.191	.799023	.598480
21	27.192	.835452	.715955
22	27.189	.592503	.333387
23	27.193	.871119	.838375
24	27.190	.634851	.455745
25	27.191	.715676	.613171
26	27.189	.530351	.343818
27	27.190	.635319	.521246
28	27.184	.137743	.022682
29	27.191	.782302	.777563
30	27.188	.500957	.378277
31	27.193	.898225	.935185
32	27.187	.374847	.243069
33	27.194	.930521	.965682
34	27.185	.192433	.085514
35	27.189	.596597	.563020
36	27.194	.931585	.966110
37	27.190	.643509	.636198
38	27.191	.729105	.751802
39	27.192	.796426	.835819
40	27.189	.504934	.466147
41	27.188	.410802	.349951
42	27.188	.426783	.374316
43	27.201	.999050	.999942*
44	27.191	.628609	.782127
45	27.193	.786099	.923256

Example 2: To illustrate the use of the screening rule for outliers in samples of past data using the formulas for p-values given in (5), we consider the stack loss data from Brownlee (1965, section 13.12). The data are given in Table 2 and are from 21 successive days of operations of a plant oxidizing ammonia to nitric acid. The variable x_1 is the air flow to the plant. The variable x_2 is the temperature of cooling water and x_3 is concentration of nitric acid in the absorbing liquid. The response variable y is a measure of the ingoing amonia lost as unabsorbed nitric acids.

Here $p = 4$ and the $N = n - p - 1 = 16$ uniform residuals are given in column 6 of Table 1. We use a nominal level 0.05 to check for outliers. The smallest uniform residual is 0.002119 for observation 21 and this gives $P_S(21) = 1 - (1 - 0.002119)^{16} = 0.033370$, and observation 21 is a left outlier at the 0.05 level. No other observation is significantly small at this level. The largest uniform residual of column 3 is 0.809920 for observation 15 with a p-value of $P_L = 1 - (0.809920)^{15} = 957672$, which is not significant. Note that it could be called a significant inlier at the 0.05 level, however.

Next, we delete the 21^{st} case and compute the residuals in reverse order as given as column 7 in Table 2. The values in column 7 require careful study. First, note that case 15 which was not nearly significant in the forward pass now has a p-value of $P_L = 1 - (0.999999)^{15} = 0.000015$, which appears highly significant. However, for reasons to be explained below, we do not delete this case and call it an outlier. However,

$P_L(4) = 1 - 0.99999^{15} = 0.00015$, $P_L(3) = 1 - 0.998970^{15} = 0.015$ and, $P_L(1) = 0.003$ are all significantly large. Thus the cases 1, 3, 4 and 21 are identified as outlying cases.

Now let us consider the value of the uniform residual for observation 15 in the reverse pass mentioned above. Examination of the cases in the basis for computing this value shows that the determinant of the basis is way small and colinearity in the basis is the real problem. Even a slight change of the value of one of the independent variables for a case in the basis will cause a dramatic reduction in the residual for case 15. Thus we do not identify observation 15 as a outlier. As noted above in the discussion of the first pass, it can be considered an inlier in the first pass.

These data were analyzed also by Daniel and Wood (1974, Chap. 5), who also concluded that cases 1, 3, 4 and 21 are outliers.

TABLE 2

i	Y	X_1	X_2	X_3	Forward Pass	Reverse Pass
1	42	80	27	89	.000000	.999781*
2	37	80	27	88	.000000	.952327
3	37	75	25	90	.000000	.998970*
4	28	62	24	87	.000000	.999990*
5	18	62	22	87	.000000	.489672
6	18	62	23	87	.078305	.294584
7	19	62	24	93	.063449	.411257
8	20	62	24	93	.456826	.753536
9	15	58	23	87	.282464	.253759
10	14	58	18	80	.613737	.744091
11	14	58	18	89	.675124	.795409
12	13	58	17	88	.537633	.920923
13	11	58	18	82	.226155	.375449
14	12	58	19	93	.362358	.018563
15	8	50	18	89	.809920	.999999
16	7	50	18	86	.640881	.000000
17	8	50	19	72	.514957	.000000
18	8	50	19	79	.577734	.000000
19	9	50	20	80	.601348	.000000
20	15	56	20	82	.702272	.000000
21	15	70	20	91	.002119	---------*

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