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The Statistics of Residuals and The Detection of Outliers

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THE STATISTICS OF RESIDUALS AND THE DETECTION OF OUTLIERS*

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ABSTRACT. Insofar as possible it is desirable to base
the criteria for the detection of bad data on rigorous
statistical arguments. This report recapitulates the
statistics involved and describes the "tau" criterion
in detail. This criterion is especially suited for
use in simultaneous least-squares adjustments of tri-
angulation networks. Special note is taken of yet un-
solved problems involved in the rigorous derivation of
still more efficient and exact rejection criteria.

INTRODUCTION

The examination of least-squares residuals for the detection of
"bad data" is one of the most important and effective means for the
quality control of geodetic work. In order to provide some motiva-
tion for looking at residuals from joint least-squares adjustments at
an early stage, a general overview of the quality control problem
will be useful.

For this purpose, all large adjustment tasks can be broken down
into smaller components which are, in turn, decomposable...down to the
smallest redundant combinations of observations. It may or may not
be the case that the results of component adjustments at a given
level are in fact combined sequentially into an algebraic equivalent
of a component adjustment at the next higher level. This is always
possible in theory, though not always most practical or expedient.
More commonly, rather than sequentially built up, all higher level
adjustments are reinitiated from a common "data-base" level (for
example, the list of directions in triangulation) which is only one
step removed from the "raw" observations. For example, in triangu-
lation, one sequence of partial adjustments whose examination might
be undertaken for quality control purposes would be: station adjust-
ments, triangle adjustments, quadrilateral adjustments, project ad-
justments (several levels or sizes), block adjustments, and finally
datum adjustments.

However this sequence of adjustments is actually carried out,
the interest here is in the statistical evaluation of all stages.

The purpose of this statistical evaluation is quality control, which may be described as the search for the answers to the following questions:

1. What does the evidence of the data say about the accuracy of the observations? Does this evidence show that these observations meet the requirements associated with the specifications under which the work was done? If not, why, and what can be done about it?

2. What does the answer to 1 imply about the accuracy of the final products of the adjustment (e.g., positions)? Do these accuracies meet the project specifications, if any, or conform to standards associated with the specifications under which the work was done? If not, why, and what can be done about it?

3. Whatever the answers to 1 and 2, is there any additional evidence for the presence of large errors (which may be blunders) or for subsets of poor quality data? If so, can these anomalies be explained and can anything be done about them?

An ideal quality control procedure would also answer the additional questions:

4. What statistical measures of confidence can be associated with the assertions made in 1, 2, and 3? Do these measures of confidence meet conventional statistical standards? If not, are there alternative analysis procedures or survey designs which will enable these standards to be met? In 3, is the geometric and repetitive redundancy sufficient to insure (with a desired confidence) the detection of large errors when they occur?

A modern approach to survey design starts with preliminary answers to 1 in the form of accuracy figures of the component observations and proceeds by simulation to find the answers to 2 and 3. One may then attempt to perturb 1 to improve the answers to 2 and 3. This should be done in the light of a theory and proven methodology for joint optimization if it is not to have the character of a "groping in the dark." However, the finally arrived at accuracy figures still have to be proven to be operationally realizable and economic, and specifications furnished for an observational program which will reliably reproduce them.

The use of the word "accuracy" above needs some discussion. In the usual absence of true errors, direct estimates of accuracy are

impossible. It is likely that the total variance will have to be broken down into an "error budget" of component variances or error sources, each of which expresses a specific sort of internal precision. Instances are the within-nights component and between-nights component in astronomic work (Carroll 1975), and the station component and the work component (the notorious "hidden error variance" visible to the net adjustment but invisible in a station adjustment, due to horizontal refraction and errors of centering, targeting, systematic pointing errors). If an adequate components-of-variance model is used and the observational program and the physical-geometric constraints of the adjustment make possible the estimation of the various components (this is a generalization of the statistical model two, random effects, analysis of variance problem), then the sum of variance components in the error model provides a way of "creeping up on" an estimate of accuracy even when the total variance is itself not directly estimable from component adjustments. This assumes that all systematic, that is fixed, effects are either corrected for, canceled out by the design of the observational procedure, or modeled and estimated in the adjustment itself. Part of the value of the random effects model is that certain error sources that are difficult or impossible to model as fixed effects in ordinary triangulation, such as the errors mentioned above as being visible to the network adjustment but not the station adjustment, can be treated as random effects to achieve an error analysis that incorporates a statistical estimate of the influence of these errors on derived quantities as expressed in their variance. However, there does not yet seem to be any universally accepted solution for the general random-effects analysis of variance, in contrast with the fixed-effects analysis of variance, whose generalization is known to every deep student of adjustment theory. It is the same as the theory of the general linear hypothesis in the presence of singularities.

Obviously the answer to "What can be done about it?" depends on whether one is looking at a simulation for planning, "real time" reduction of new data, or old work from the files--leading in turn to the redesign of the survey, the acquisition of new data, and the acquisition of experience.

At this point one may envision a spectrum of approaches to quality control whose extremities fall on either side of the above mentioned division into components. A thoroughgoing approach would be to examine data in as many subsets and in as many different levels of size as is economically possible. Given the practical limitations on the thoroughness with which this can be done, one has the yet-unsolved problem of the selection of the sequence and coverage of the component adjustments that will insure quality control of a desired confidence. In fact the choice of components is typically an accident of the history of the growth of the triangulation network. Truly sequential techniques, ideally incorporating "back tracking"-, partial batching-, and localization-capabilities, are relevant here. The other extreme consists in proceeding immediately to the joint

adjustment of all data with as little preliminary evaluation as possible and relying upon the results of this adjustment (or repetitions of it) to point out any quality control problems.

A certain amount of "back tracking," in the general sense of moving from a larger adjustment to a smaller component, will prove useful as a diagnostic tool in the search for the answer to the "Why?" listed among the questions above. The basic statistical motivation for a thoroughgoing quality control procedure, as just described, is the belief that there are errors (or components of variance) that are only visible in larger net adjustments incorporating all redundancy, avoiding edge effects, and capturing a redundant sample of the random effects accounting for the "hidden" error variance, which varies with atmospheric conditions, terrain, observers, instruments, specifications of work, etc. On the other hand, there is also the conviction that the examination of the results of large joint adjustments, besides being cumbersome and expensive to repeat, cannot be relied upon to detect all errors.

Quality control, as described here, covers a great deal more than just the examination of residuals. It involves estimation of variances, various tests of significance on variances, and possibly other checks on closures of various types or on alternative measures of random variation other than the variance or its square root. This paper aims to describe one of the statistics involved in the examination of residuals, excluding other aspects of quality control.

Now it has to be confessed that there is still a fifth class of question involved in quality control. In any problem involving a sufficiently large mass of heterogeneous data and complex systems of programs for their reduction, the importance of this aspect grows even to overshadow the other four. That is:

5. Have any mispunches, operator's errors, programming blunders, etc., made nonsense of the results of the program just run? If the answer is "No," how are you sure? (Here one already knows the answers to "Why?" and "What can be done?" -- human error, and "go through your program again and again.")

Though not a statistical question, this too is part of the motivation for looking at residuals.

STATISTICS OF RESIDUALS, I

Unfortunately, residuals are not true errors. From the least-squares solution of full rank observation equations $AX + L = V$, one has the least squares residuals and their covariance matrix (using an estimate of the variance of an observation of unit weight, $\hat{\sigma}_0^2$):

$$V = \{I - A(A^tPA)^{-1} A^t P\} L \tag{1}$$

$$\hat{\Sigma}_V = \{P^{-1} - A(A^tPA)^{-1} A^t\} \hat{\sigma}_0^2 . \tag{2}$$

Introducing the true error $\varepsilon = L - E(L)$, with the assumption that the model of the observations is unbiased, $E(L) + AX = 0$, equation (1) becomes

$$V = M \varepsilon ,* \tag{3}$$

where M denotes the matrix in brackets in equation (1). By the substitution $\overline{V} = SV$, $\overline{\varepsilon} = S\varepsilon$, $\overline{A} = SA$, where $P = S^tS$, these equations take the form

$$\overline{V} = \overline{M} \; \overline{\varepsilon} \tag{4}$$

$$\hat{\Sigma}_{\overline{V}} = \overline{M} \; \hat{\sigma}_0^2 . \tag{5}$$

Note that $\overline{M} = I - \overline{A}(\overline{A}^t\overline{A})^{-1}\overline{A}^t$ is an idempotent matrix. That is, $\overline{M} \; \overline{M} = \overline{M}$. In the ordinary case of a diagonal weight matrix P, $\overline{V} = SV$ means $\overline{v}_i = \sqrt{p_i} \; v_i$. With $P = \Sigma_\varepsilon^{-1} \sigma_0^2$, $\overline{v}_i = v_i/\sigma_i$, σ_i being the a priori standard error of the error on the ith observation, ε_i. Also note that $\Sigma_{\overline{\varepsilon}} = I \sigma_0^2$, in contrast to $\Sigma_{\overline{V}} = \overline{M} \sigma_0^2$.

With these preliminaries, it is already possible to make several points about the distinction between V's and ε's.

Besides being idempotent, $\overline{M}$ is the projector onto the orthogonal complement of the model space (the column space of A). Thus for any $Y = \overline{A}X$, $\overline{V}^t Y = 0$. The situation is depicted in figure 1.

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*In a more precise notation, the least-squares residuals given by equation (1) should be distinguished from other values of V by writing, for example, V_{LS}. Here we follow common adjustment theory usage by omitting the LS. Alternate possibilities, $\hat{V}$ or $\hat{\varepsilon}$, are rejected in this discussion, the latter since we wish to emphasize the shortcomings of V_{LS} as an estimate of ε, and the former as imprecise.
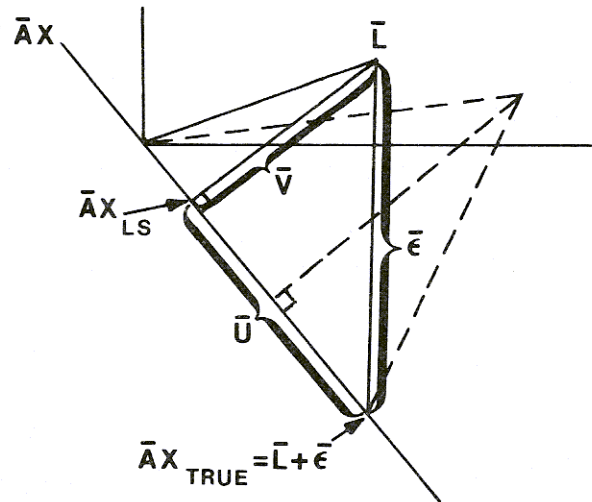
Figure 1.--Least-squares adjustment as an orthogonal projection in the space of the observables.

The projection of the true error vector onto the model space, $\bar{U}$, orthogonal to $\bar{V}$, is lost and irrecoverable. Now picture many similar configurations, such as the one indicated by dotted lines. $\bar{\varepsilon}$ varies randomly with a scatter described by $\Sigma_{\bar{\varepsilon}}$ but such that always $\bar{L} + \bar{\varepsilon} = \bar{A}X_{true}$. Averaging over all random occurrences of the true error, that is, taking expected values, one obtains $E(\bar{\varepsilon}^t\bar{\varepsilon}) = n\,\sigma_0^2$, $E(\bar{U}^t\bar{U}) = u\,\sigma_0^2$, and $E(\bar{V}^t\bar{V}) = (n-u)\sigma_0^2$, where n and u are the dimensions of L and X. Here we have used $E(\bar{\varepsilon}^t\bar{\varepsilon}) = \text{tr}\,\Sigma_{\bar{\varepsilon}}$ and a similar formula for $\bar{U}$ and $\bar{V}$, and the fact that $\text{tr}\,\bar{M} = \text{rank}\,\bar{M}$ for any idempotent matrix $\bar{M}$.

Thus $E(\bar{V}^t\bar{V}) = \dfrac{n-u}{n}\,E(\bar{\varepsilon}^t\bar{\varepsilon}) = (n-u)\sigma_0^2$, a familiar result that is the basis for the unbiased estimator of σ_0^2; $\hat{\sigma}_0^2 = \sqrt{\dfrac{V^t P V}{n-u}}$. (Note: $V^t P V = \bar{V}^t\bar{V}$.) The point is that we cannot know the "invisible" component $\bar{U}$ in any given instance, and it is only possible to circumvent this limitation in the average. The average square length of the invisible component is

$E(\overline{U}^t \overline{U}) = \frac{u}{n} E(\overline{\varepsilon}^t \overline{\varepsilon}) = u\,\sigma_0^2$. Obviously, for $n \gg u$; $\overline{V} \sim \overline{\varepsilon}$. This, when applicable, simplifies the statistical argument. Unfortunately it is a distinctive characteristic of geodetic networks that u/n does not become arbitrarily small, but remains remarkably constant over wide variations in the extent of the net. For triangulation (putting the residual in the net adjustment on the single mean direction to each remote station) the value of u/n is about 0.5, for leveling 0.33. In summary, residuals are but the visible components of true errors.

Another difference between $\overline{V}$ and $\overline{\varepsilon}$ is that they possess different covariance structures, as noted above. Returning to $\hat{\Sigma}_V$ in equation (2), we see that the first term $P^{-1}\sigma_0^2$ is just the covariance matrix of the true error (a priori or a posteriori, depending upon whether σ_0^2 or $\hat{\sigma}_0^2$ is used). The second term, which it is useful to call the "geometric" term because it reflects the geometry of the network through the design matrix A, happens to be in its own right the covariance matrix of the adjusted observables. The geometric term is generally full even if P is diagonal. A practical hurdle in computing Σ_V is the computation of this second term which entirely accounts for the inequality of Σ_V and Σ_ε. No theoretical or algorithmic difficulty is involved; it is solely a matter of time and expense for large triangulation adjustments (still a consideration even with today's computers). Even the computation of the diagonal terms alone is suspected to be already past the point of diminishing returns at which the small improvement in rejection procedures thus gained may not justify the expense. Hopefully, it will be possible to resolve this issue in the light of further investigation and experience.

The relative importance of the two terms can be roughly assessed by the measure $\text{tr}(\Sigma P)/n$, or what is the same thing, $(\text{tr } \Sigma)/n$ applied to the two terms of $\Sigma_{\overline{V}}$. This gives σ_0^2 and $(u/n)\sigma_0^2$, respectively, for the two terms.

The fact that $\overline{M}$ (and also the second term of $\overline{M}$) are idempotent and non-negative definite makes it possible to say quite a lot about the magnitude of their elements without actually computing any. The following equalities and bounds are easily proved.

(1) (average diagonal term of $\overline{M}$) $= (n - u)/n$

(2) $0 \leq$ (any diagonal term of $\overline{M}$) ≤ 1

(3) $d =$ (r.m.s. variation about their mean of the diagonal terms of $\overline{M}$) $\leq \sqrt{\left(\frac{n-u}{n}\right)\left(\frac{u}{n}\right)}$

(4) $r =$ (r.m.s. value of the off-diagonal terms of $\overline{M}$) $\leq \sqrt{\left(\frac{n-u}{n}\right)\left(\frac{u}{n}\right)\left(\frac{1}{n-1}\right)}$.

In fact $d^2 + (n-1)\, r^2 = \left(\frac{n-u}{n}\right)\left(\frac{u}{n}\right)$. Also note that if any diagonal term of $\overline{M}$ is either 0 or 1, then all the off-diagonal terms in that row and column must also be zero. The bound in (4) can be misleading. The number of off-diagonal terms increases with n^2, whereas the number of significantly nonzero off-diagonal terms probably increases linearly.

That $0 \leq \sigma_{v_i}^2 \leq \sigma_0^2/p_i$, a restatement of (2), is obvious from equation (2). This is somewhat paradoxical at first sight, since one might think that by manipulation of the weights and/or geometry the variances of residuals and adjusted observables could be varied arbitrarily.

Again note the important role played by the ratio u/n. For example, the bound in d is largest for (u/n) = 0.5, the triangulation value. The consequences of the large size and constancy of u/n hark back to the traditional objections to least-squares adjustments of triangulation; that they cannot be relied upon to localize the error and instead "spread it around," introduce spurious correlation, and the like.

STATISTICS OF RESIDUALS, II

The discussion thus far has been purely algebraic. Turning now to the distribution of the residuals, the standard assumption of normality of the true errors is made. That is, ε is distributed as multivariate normal, $N(0, \Sigma_\varepsilon)$. This gives $\bar{\varepsilon} \sim N(0, I\sigma_0^2)$, and $\bar{V} \sim N(0, \Sigma_{\bar{V}})$; therefore $n(0, \sigma_{v_i}^2)$ is the marginal distribution of the ith residual v_i, where (in the case of diagonal weights):

$$\sigma_{v_i}^2 = \frac{\bar{m}_{ii}}{p_i} \sigma_0^2 .$$

The story does not end here, however, for two reasons. First, this result still requires the assumption that the true value of σ_0^2 is known, whereas real data frequently give evidence that this is not the case by significant differences (as measured by χ^2) between the posterior estimate and the assumed prior value of σ_0^2. Second, this result applies to a single particular residual but there is as yet no provision for control of the significance level when examining groups of residuals. In this case one does not look at only one residual selected in advance, but instead examines the residuals in order of decreasing magnitude. Thus, complete statistical control of the test will require the distribution of the *largest* residual rather than of a particular residual.

The procedure which we have called the τ (tau) criterion for re-
jection of residuals incorporates these extensions, in the first case,
rigorously, in the second case, incorporating some approximations. To
discuss these features of tau it will be necessary to review briefly
some background on Studentization and tests of hypothesis. Before
this, however, a short digression on the operational meaning of sta-
tistical statements about residuals.

What does it mean to assert that $v_i \sim n(0, \sigma_{v_i}^2)$? One way to test
one's understanding of such an assertion is to construct a thought-
experiment in which its implied statements of probability can be real-
ized as the large sample limit of frequencies. Conceive of m = 100
(say) repetitions of a geodetic survey involving n observables, that
is, identical configuration, instrumentation, etc., differing only in
the errors affecting the observations. These errors are assumed to
come from a random normal population described by $N(0, \Sigma_\varepsilon)$. Each sur-
vey is then adjusted using $P = \Sigma_\varepsilon^{-1}$. These 100 adjustments produce

100 residuals on each of the n observables. If these 100 residuals on
observable i (say) are then used to plot a histogram, this histogram
will approximate $n(0, \sigma_{v_i}^2)$ and the approximation will improve as m (the
number of repetitions of the survey, *not* the number of observables
in the survey) increases. This assertion is true for i = 1, ..., n,
and in general this will involve n different distributions with n
different $\sigma_{v_i}^2$'s. This is because the geometric part of Σ_v is not, in
general, constant along the main diagonal even if P is. This in turn
is due to the variable geometry of the net. Whereas a uniform network
will produce relatively uniform $\sigma_{v_i}^2$'s, one fact of life in dealing
with the triangulation as it exists in North America is that the geom-
etry, instrumentation, and specifications of the component work are
often far from uniform, particularly in municipal surveys.

Of course, this thought experiment is never carried out in reality for we have only one survey with only one residual on each of the n observations. Pooling, then histogramming these residuals produces a mixture with no claim to normality, asymptotic or otherwise. It is

an interesting statistical exercise to derive the theoretical shape of the resulting probability density function, but this can be done only if the $\sigma_{v_i}^2$'s are known, or if some distribution of the $\sigma_{v_i}^2$ is assumed, in which case the mixture can be approximated by a compound distribution. One finds the characteristic departures from normality--more peaked, lower shoulders, higher tails. If the $\sigma_{v_i}^2$ are known, then the residuals can be *standardized* to $\tilde{v}_i = v_i/\sigma_{v_i}$. Then $\tilde{v}_i \sim n(0,1)$, and the $\tilde{v}_i$ can be pooled without producing a mixture since pooling of $n(0,1)$'s produces another $n(0,1)$. Any attempt to reason backward from residuals to deduce characteristics of the true errors, difficult in any case, must take account of the varying σ_{v_i}'s. In the absence of σ_{v_i}'s , which have to be computed from the relatively expensive formula (2), one frequently sees *partially standardized* residuals (v_i/σ_i).

Thus we see that histograms of residuals have to be interpreted with some care. Tau, the distribution of an internally Studentized residual, is impossible to realize as a histogram from one survey for the reason that there is only one value of the random variable $\hat{\sigma}_0^2$ per survey, and the tau distribution incorporates a random variation of $\hat{\sigma}_0^2$ that can be realized as a frequency only by the sort of thought experiment described above.

The term "Studentization" refers to the design of a statistic that is independent of the (unknown) true value of one or more population parameters. For example, if $y \sim n(\mu,\sigma^2)$, then $x_0 = (y-\mu)/\sigma \sim n(0,1)$. The distribution of x_0 is independent of the parameter values, but the statistic x_0 is not, since it requires knowledge of μ and σ. One way to

avoid this requirement is to "randomize" the parameter by replacing its unknown true value with a statistic, itself a random variable, which is in some sense an estimate of the parameter in question. (In the modern approach to Studentization expressed in the first sentence of this paragraph, the choice of alternative statistics is somewhat wider than this statement would imply.) The distribution of the new statistic must be known so that it can be used to make statements about probability.

In the example, the unknown parameter μ is easily eliminated (in fact, so easily that it is not usually thought of as an instance of Studentization) by use of

$$x_1 = (y - \bar{y})/\sigma \sim n\left(0, \frac{n-1}{n}\right)$$

where $\bar{y}$ is the sample mean. σ can be eliminated by use of

$$x_2 = (y - \mu)/\hat{\sigma} \sim t_{n-1}$$

where $\hat{\sigma} = \sqrt{\dfrac{\Sigma(y_i - \bar{y})^2}{n-1}}$ and t_{n-1} is Student's t distribution with n-1 degrees of freedom. (Alternately one could vary this by Studentizing the departure of the sample mean from the true mean or by using n instead of n-1 in the definition of $\hat{\sigma}$. These are standard cases considered in many statistics books.) For the elimination of both μ and σ, three alternatives present themselves: external, internal, or mixed Studentization of σ.

External Studentization of σ means that the estimates of σ and μ are formed from independent samples. This gives

$$x_3 = (y - \bar{y}_1)/\hat{\sigma}_2 \sim \sqrt{\frac{n-1}{n}} \; t_{n-1}$$

where the subscripts 1 and 2 on the sample mean and variance estimate indicate that they are to be computed using independent samples of y.

Internal Studentization means, then, the use of the same sample to compute the sample mean and variance estimate. This gives

$$x_4 = (y - \bar{y})/\hat{\sigma} \sim \sqrt{\frac{n-1}{n}} \, \tau_{n-1}$$

where the new random variable τ_ν is related to Student's t by

$$\tau_\nu = \frac{\sqrt{\nu} \; t_{\nu-1}}{\sqrt{\nu - 1 + t^2_{\nu-1}}} \tag{6}$$

This formula suffices to compute the distribution of τ. Because of the use of the same sample in computing $\bar{y}$ and $\hat{\sigma}$, the numerator and denominator in the statistic x_4 are not independent as is required for a t distribution.

By mixed (internal and external) Studentization it is meant that whereas $\bar{y}$ is computed from sample one (say), $\hat{\sigma}$ is arrived at by a pooling of the variance estimates from sample one and another independent sample two. In adjustment terminology, $\hat{\sigma}$ is an estimate of variance formed by pooling a priori and a posteriori estimates of variance. By "pooling" is meant the minimum variance combination of variance estimates of the form $\hat{\sigma}^2 = (\nu_1 \hat{\sigma}^2_1 + \nu_2 \hat{\sigma}^2_2)/(\nu_1 + \nu_2)$ with ν_1 and ν_2 the associated degree of freedom. This also leads to a tau distribution (Quesenberry and David 1961). This case is considered no further here since part of the motivation for using tau in triangulation is to provide a data-adaptive criterion that is uninfluenced by prior estimates. The pooling of variance estimates is justified only on the assumption that the variances of the populations from which the two samples are drawn are in fact the same.

The tau distribution was first published by W. R. Thompson (1935). The designation "tau" is not universal and the distribution has to be recognized by the occurrence of formula (6), or its inverse giving t in terms of τ, in which guise it is quite frequently encountered in obscure statistical references. τ_{n-1} is tabled in Rainsford (1957), following Logan (1955). The generalization to arbitrary degrees of freedom needed in applications to geodetic adjustments has begun to appear only quite recently (Ellenberg 1973). Because of its relative unfamiliarity, a brief sketch of a derivation of tau is now given.

$\overline{M}$ can be factored as $\overline{M} = U\,U^t$, where $U^t U = I$, and U is dimensioned n by ν. $\nu = \text{rank } \overline{M} = n - u = $ the degrees of freedom associated with $\hat{\sigma}_0^2$. Now denote $U = \{u_i^t\}$, u_i^t being the ith row of U, and $\kappa = U^t \overline{L}$. κ is a ν dimensional vector and $\kappa \sim N(0, I\sigma_0^2)$. Consider the quantity

$$a = \frac{(\nu-1)\ \kappa^t\ A\ \kappa/\sigma_0^2}{(1)\ \kappa^t\ B\ \kappa/\sigma_0^2}$$

with $A = \{u_i(u_i^t u_i)^{-1} u_i^t\}$ idempotent of rank 1, and

$B = \{I - A\}$, idempotent of rank $\nu - 1$. Note that $AB = 0$. Consulting Graybill's (1961) theorems 4.6, 4.15, and the definition of F, page 31, one concludes that $a \sim F_{1,\nu-1} = t_{\nu-1}^2$.

Therefore

$$b = \sqrt{\frac{\nu\,a}{\nu - 1 + a}} = \frac{\sqrt{\nu}\,(u_i^t\,\kappa)}{\sqrt{(\kappa^\tau \kappa)(u_i^t u_i)}} \sim \tau_\nu\ . \qquad (7)$$

But $\sqrt{p_i}\,v_i = \overline{v}_i = u_i^t\,\kappa$, $\kappa^t \kappa = \overline{V}^t\,\overline{V} = V^t\,PV$, and $u_i^t\,u_i = \overline{m}_{ii}$, giving

$$(v_i/\hat{\sigma}_{v_i}) \sim \tau_\nu , \tag{8}$$

where $\hat{\sigma}^2_{v_i} = \left(\dfrac{\overline{m}_{ii}}{pi}\right)\left(\dfrac{v^t p v}{\nu}\right)$ has been used.

Note that equation (7) implies that $|\tau| \le \sqrt{\nu}$ (using τ to denote both the statistic and the distribution, as commonly done), a surprising result on first sight. It can be shown that $\tau = \sqrt{\nu}\, r$, r being the sample correlation coefficient when the true value is zero.

The second distinctive feature of the tau criterion for detection of outliers is the control of the probability of type I error, the error of rejecting a true hypothesis. The rejection procedure is thought of as a test of the hypothesis that $v_i \sim n(0, \sigma_{v_i})$ for all i, where $\sigma_{v_i} = k(\hat{\sigma}_{v_i}/\hat{\sigma}_0) = k(\overline{m}_{ii}/p_i)$ for some unspecified k, by use of the test

accept H_0 if max $(v_i/\hat{\sigma}_{v_i}) < c$

reject H_0 if max $(v_i/\hat{\sigma}_{v_i}) \ge c$,

where c is a critical value, selected in advance so that the probability of rejecting a true hypothesis is α, a number selected in advance, say 0.05. The probability of accepting a true hypothesis is the significance of the test, $1 - \alpha$. The probabilities of accepting the hypothesis when false, β, and rejecting a false hypothesis, $1 - \beta$, are called the probability of type II error and the power of the test, respectively. The computation of c requires the distribution of max τ under the null hypothesis. This distribution is extremely difficult to compute exactly (Stefansky 1972), and various approximations have been suggested (Halperin et al. 1955), including Thompson's original one (eq. 9 below).

A simplified derivation that evades many of the subtleties involved in a more thorough approach goes as follows. Note that

$$\alpha = P\{\max \tau > c\} = P\{(\text{one or more of } \tau_i) > c\} = 1 - P\{\text{all } \tau_i \leq c\}$$

$$= 1 - P\{(\tau_1 \leq c) \text{ and } (\tau_2 \leq c) \text{ and } ...\} .$$

If we ignore the dependence of the τ's that is present because of the nonzero off-diagonal terms in Σ_v that arise from geometric part, this last probability can be written as $\prod_i P(\tau_i \leq c) = \{P(\tau \leq c)\}^n$, since all τ are identically distributed. Denote $a = P(\tau > c)$. Then

$$\alpha = 1 - (1 - a)^n$$

$$\text{or} \quad a = 1 - (1 - \alpha)^{\frac{1}{n}} \cong \frac{\alpha}{n} . \tag{9}$$

Equation (9) is referred to as the transformation for control of type I error. Here n is the total number of observations in the group for which control of type I error is desired and is conventionally, although not necessarily, taken to be the number of (nonspur) observations in the adjustment producing the residuals in question. By a "spur" observation (the term is suggested by leveling) is meant one for which σ_{v_i} and v_i are identically zero. This happens if there are some parameters that are only exactly (not redundantly) determined. A similar transformation was supposedly used by Logan (and quoted by Rainsford) but our programs do not check Logan's tables.

COMPUTATION OF THE TAU CRITERION

The tau rejection criterion is implemented by a subroutine TAURE which may be called from a FORTRAN program by:

CALL TAURE (NT, NU, ALPH, CRTAU)

where   NT is the number of (nonspur) observations

NU is the degrees of freedom

ALPH is the desired probability of type I error

and   CRTAU is the critical value produced by the subroutine (called c in the above discussion).

It is assumed that the variance of unit weight has been estimated from the same least-squares adjustment that produces the residuals to be tested. Then all residuals for which

$$\left| v_i / \hat{\sigma}_{v_i} \right| \geq c$$

are flagged for rejection. ("Blind" rejection without any effort at further diagnosis is never recommended, even though the statistical design of tau makes it possible if necessary.)

In leveling adjustments and station adjustments, $\hat{\sigma}_{v_i}$ is, in fact, computed for every v_i. For large triangulation network adjustments in which the computation of $\hat{\sigma}_{v_i}$ is still impractical, the following expedient compromise is recommended. Approximate σ_{v_i} by

$$\sigma_{v_i} = \sqrt{\frac{n - u}{n}} \; \frac{\hat{\sigma}_0}{\sqrt{p_i}}$$

and proceed as before. This approximation is based on the average value of $\bar{m}_{ii}$. It is particularly important to have good prior weights when computing either the exact or approximate σ_{v_i}.

The subroutine first computes "a" by the equality in (9). An approximate critical value c, such that $a \cong P(\tau \overset{>}{\leqslant} c)$, is computed with the aid of an approximate inverse t given in Abramowitz and Stegun (1965, p. 949). This is then refined by a Newton-Raphson iteration. Subroutine TAURE and a table of values of tau computed with it are included as appendices 1 and 2.

Limited experience thus far has shown tau to be a reasonable way of answering the old question, "How big is too big?" when looking at residuals from triangulation. The critical values of tau are quite different from those based on the normal law.

POSSIBLE EXTENSIONS AND REFINEMENTS OF TAU

The tau as described above represents a certain plateau in the search for a statistically rigorous rejection criterion for use in quality control. It is by no means the ultimate in this respect, however. A brief list of remaining problem areas in the search for statistical rigor follows.

1. A feasible implementation of Stefansky's methods for the computation of the exact distribution of max τ can perhaps be found and applied to simulations and special studies at least, if not routinely.

2. Computation and control of the probability of type II error, the error of retaining bad data, are particularly desirable in triangulation adjustments, which are subject to distortion from bad data remaining in. The control of type II error is somewhat more difficult than that of type I, requiring as it does formulation of definite alternative hypotheses, leading to non-central distributions and other complications.

3. The context here has been batch adjustments. Sequential adjustments have, from the statistical point of view, both advantages and disadvantages. The subject deserves more study.

4. The effect of rejection procedure on the re-estimation of the variance of unit weight is amenable to study.

5. Iterated rejection procedures have to be better understood. Tau at least is sensitive to changes in size and degrees of freedom, which a fixed rejection level is not.

6. The question of the optimum size adjustment for rejection purposes remains open, and

7. The rejection of bad data in satellite geodesy is quite a different problem, since u/n is small and the main problem is the unmodeled systematic errors, not the random part, which is typically a small part of the error budget. What, if anything, does tau have to offer in this situation, and are there statistically rigorous alternatives?

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A Note regarding the scan of NOS65 NGS1

Appendices II., III., and IV. contain tabulations of computations of tau, T, and X respectively. In light of modern computing capabilities, as compared with those of 1976, it was felt unnecessary to scan all pages of the appendices. Instead, the first page of each table was scanned and included for those that might wish to test their algorithms. These excerpts are pages 24, 61, and 98 of the original document.

APPENDIX I.   SUBROUTINE TAURE (PP. 20-22)

The purpose of subroutine TAURE is to compute the rejection level for normalized residuals for a given number of observations, degrees of freedom, and desired level of type I error. This subroutine may be called from a FORTRAN program by:

CALL TAURE (NT, NU, ALPH, CRTAU)

where NT is the number of (nonspur) observations (= n)
NU is the degrees of freedom (= ν)
ALPH is the desired probability of type I error (= α)
CRTAU is the critical value produced by the subroutine (= c).

The use of c as a rejection criterion assumes that the variance of unit weight σ_0^2 has been estimated from the residuals being tested.

All residuals for which the condition

$$\left| \frac{v_i}{\hat{\sigma}_{v_i}} \geq c \right|$$

holds true, are to be flagged for rejection.

If the estimates of the standard errors of the residuals, $\hat{\sigma}_{v_i}$, $i = 1, \ldots, n$, are not known, they can be approximated as:

$$\hat{\sigma}_{v_i} \simeq \sqrt{\frac{n-u}{n}} \; \frac{\hat{\sigma}_0}{\sqrt{p_i}}$$

where u is the number of unknowns in the adjustment and p_i is the weight of the observation. Thus the approximate rejection criterion can be written as

$$\left| v_i \sqrt{p_i} \right| \geq \left[\sqrt{\frac{n-u}{n}} \; \hat{\sigma}_0 \right] c.$$

For further information see pages 17 and 18 of this report.

```fortran
      SUBROUTINE TAURE( NT,NU, ALPH, CRTAU )
1     DATA PI/ 3.141592653589B /
      PD = 2. / PI
2     S = 1.
3     WNU = NU
4     U = WNU - 1.
5     IF( U.EQ.0. )    GO TO 72
6     IF( ALPH.EQ.0. )    GO TO 72
7     IF( ALPH.LT.1. )    GO TO 10
8     CRTAU = 0.
9     RETURN
10    Q = NT
11    IF( ALPH.GT..5 )    GO TO 19
12    AA = ALPH/ Q
13    DELT = AA
14    DO 18 I = 1, 100
15    XI = I
16    DELT = DELT * ALPH * (( XI*Q - 1. ) / (( XI+1.)*Q))
17    IF( DELT.LT.1.E-14)    GO TO 20
18    AA = AA + DELT
19    AA = 1. - (1. -ALPH)**(1./Q)
20    P = 1. - AA
21    IF( U.EQ.1. )    GO TO 71
22    F = 1.386294361199 - 2.*ALOG(AA)
23    G = -(2.515517 +.802853*G +.010328*F)
      X / (1. +1.432788*G +F*(.189269 +.001308*G))
24    Y = X ** X
25    A = X ** (1.+Y) / 4.
26    B = X ** (3. + Y *(16. +5. *Y)) / 96.
27    C = X ** (-15. +Y *(17. +3. *Y))) / 384.
28    E = X *(-945. +Y*(-1920. +Y*(1482. +Y*(776. +79. *Y)))) / 92160.
29    V = 1. / U
30    T = X + V *(A +V *(B +V*( C + E*V)))
31    S = T/ SQRT(U + T*T )
32    UM = U - 1.
      DELL = 1.
33    DO 70 M = 1,  50
34    H = 1. - S*S
36    R = 0.
38    IF( AMOD(U,2.) .EQ. 0. )    GO TO 49
39    DD = SQRT( H)
40    N = .5*UM
41    DO 45 I = 1, N
42    Z = 2 * I
43    R = R + DD
44    D = DD
45    DD = DD * H * (Z/(Z+1.))
46    R = PD*(R*S +ASIN(S))
47    D = PD * D * UM
48    GO TO 61
49    DD = 1.
50    N = .5 * U
51    DO 55 I = 1, N
52    Z = 2 * I
```

SUBROUTINE TAURE

CDC 6600

```
53      R = R + DD
54      D = DD
55      DD = DD * H *((Z-1.)/Z)
56      R = R*S
57      D = D*UM
61      CONTINUE
62      DEL = (P-R) / D
        IF( ABS( DEL/DELL ) .GT.  .5) GO TO 72
        DELL = DEL
63      S = S + DEL
64      IF( ABS(DEL) .LT. 1.E-8 )  GO TO 72
70      CONTINUE
        GO TO 72
71      S = SIN(P/PD)
72      CRTAU = S*SQRT(WNU)
73      RETURN
        END
```

APPENDIX II.   TABLE OF CRITICAL VALUES BASED ON TAU (PP. 23-59)

The tabulated value is the critical value, CRTAU, computed by sub-routine TAURE for corresponding values of NT, NU, and ALPH, denoted in the table by M, NU, and ALPHA, respectively.   The notations are connected by:

NU = n - u = ν, M = NT = n, ALPH = ALPHA = α, and CRTAU = c = τ_ν.

The critical values are tabulated for ALPH = 0.10, 0.05, and 0.01. For each value of ALPH NU is varied from 2 to 100 in increments of 1, 100 to 1,000 in increments of 10, and from 1,000 to 5,000 in increments of 100 with the addition of the two extreme values 10,000 and 20,000.   For each value of NU, M takes the value 1, M + 1, and M = integer nearest NU/(1-F) where F has the values given at the top of the page.   Thus F is approximately equal to (M - NU)/M = u/n. This sampling of M, based on (u/n) provides values of M likely to be representative and useful without a prohibitively lengthy listing for all M.

A precise interpolation can be obtained by linear interpolation on M exp (- 2 c^2/π), c being the tabulated value.   The dependence on M is due to the incorporation of the transformation for control of type I error (see p. 16).   M = 1 gives the value of CRTAU without any transformation for control of type I error.   M = NU + 1 gives the value of CRTAU for use with a simple mean (see p. 13, τ_{n-1} = CRTAU).

This table is not intended to replace the subroutine, but is to be used as a supplement for checking and anticipating values produced by TAURE.

ALPHA = .100

F =

.35 .30 .25 .20 .10 .01 .001

APPENDIX III. TABLE OF CRITICAL VALUES, T,
BASED ON STUDENT'S t (PP. 60-96)

This table is for use only with externally Studentized residuals; that is, the estimate of the variance of unit weight must not have been computed from the residuals being examined.

The format of the table is the same as that of the tau table.

ALPHA = .100

F =

.35 .30 .25 .20 .10 .01 .001

APPENDIX IV. TABLE OF CRITICAL VALUES, X, BASED ON THE NORMAL DISTRIBUTION (PP. 97-133)

This table is for use with a known variance of unit weight; that is, the variance of unit weight is considered to be a known constant, rather than a random variable. The transformation for control of type I error introduces dependence on NT. The format of the tables exhibits NT(= M) values dependent on NU, as described in Appendix I, thus introducing an apparent dependence of X on NU, even though the critical value for a given M is independent of NU, in fact representing the limit as NU grows large. This format is retained to facilitate comparison with the tau and t tables and to exhibit the normal critical values incorporating the transformation for control of type I error.

ALPHA = .100

Table of critical values.

Column group: .35

M	X
2	1.949
3	2.114
5	2.311
6	2.378
8	2.481
9	2.523
11	2.592
12	2.622
14	2.674
15	2.697
17	2.738
18	2.757
20	2.791
22	2.822
23	2.836
25	2.862
26	2.875
28	2.898
29	2.909
31	2.930
32	2.940
34	2.958
35	2.967
37	2.984
40	3.008
42	3.023
43	3.030
45	3.043
46	3.050
48	3.063
49	3.069
51	3.081
52	3.087
54	3.098
55	3.103
57	3.114
58	3.119
60	3.129
62	3.139
63	3.143
65	3.157
66	3.165
68	3.170
69	3.178
71	3.182
72	3.190
74	3.194
75	3.201
77	3.212
78	3.220
80	3.223
82	3.230
83	3.233
85	3.240
86	3.243
88	3.249
92	3.252

Column group: .30

M	X
1	1.645
3	1.949
4	2.114
6	2.226
7	2.378
9	2.434
10	2.523
11	2.560
13	2.592
14	2.649
16	2.674
17	2.718
19	2.738
20	2.774
21	2.791
23	2.807
24	2.836
26	2.849
27	2.875
29	2.887
30	2.909
33	2.920
34	2.930
36	2.949
37	2.958
39	2.976
40	2.984
43	3.000
44	3.008
46	3.015
47	3.030
49	3.037
50	3.050
51	3.057
53	3.069
54	3.075
56	3.081
57	3.092
59	3.098
60	3.109
61	3.114
63	3.124
64	3.129
66	3.134
67	3.143
69	3.148
70	3.157
71	3.161
73	3.170
74	3.174
76	3.178
77	3.186
79	3.190
80	3.198
81	3.209
83	3.216
84	3.223
86	3.233

Column group: .25

M	X
1	1.645
3	2.114
4	2.226
5	2.311
7	2.434
8	2.481
9	2.523
11	2.592
12	2.622
13	2.649
15	2.697
16	2.718
17	2.738
19	2.774
20	2.791
21	2.807
23	2.836
24	2.849
25	2.862
27	2.887
28	2.898
29	2.909
31	2.930
32	2.940
35	2.949
36	2.967
37	2.976
39	2.984
40	3.000
41	3.015
43	3.030
44	3.037
45	3.043
47	3.057
48	3.063
49	3.069
51	3.081
52	3.087
53	3.092
55	3.103
56	3.109
57	3.114
59	3.124
60	3.129
61	3.134
63	3.143
64	3.148
65	3.152
67	3.161
68	3.170
69	3.178
71	3.186
73	3.194
75	3.201
76	3.209
77	3.212
79	3.212
80	3.212

Column group: .20

M	X
1	1.645
3	2.114
4	2.226
5	2.311
6	2.378
8	2.481
9	2.523
10	2.560
11	2.592
13	2.674
14	2.697
15	2.718
16	2.757
18	2.774
20	2.791
21	2.807
23	2.836
24	2.849
25	2.862
26	2.875
28	2.898
29	2.909
30	2.920
31	2.930
33	2.949
34	2.958
35	2.967
36	2.976
38	2.992
39	3.000
40	3.008
41	3.015
43	3.030
44	3.037
45	3.043
46	3.050
48	3.063
49	3.069
50	3.075
51	3.081
53	3.092
54	3.098
55	3.103
56	3.109
58	3.119
59	3.124
60	3.129
61	3.134
63	3.143
65	3.152
66	3.157
68	3.165
69	3.170
70	3.178
71	3.178
73	3.186
75	3.194

Column group: .10

M	X
1	1.645
2	1.949
3	2.114
4	2.226
6	2.434
7	2.481
8	2.523
9	2.560
10	2.592
11	2.622
12	2.649
13	2.674
14	2.697
16	2.718
17	2.738
18	2.757
19	2.774
20	2.791
21	2.807
22	2.822
23	2.836
24	2.849
26	2.875
27	2.887
28	2.898
29	2.909
30	2.920
31	2.930
32	2.940
33	2.949
34	2.958
36	2.976
38	2.992
39	3.000
40	3.008
41	3.015
42	3.023
43	3.030
44	3.037
46	3.050
47	3.057
48	3.063
50	3.075
51	3.081
52	3.087
53	3.092
54	3.098
56	3.109
57	3.114
58	3.119
59	3.124
60	3.129
61	3.134
62	3.143
63	3.148
64	3.152
66	3.157
67	3.161

Column group: .01

M	X
1	1.645
2	1.949
3	2.114
4	2.226
5	2.311
6	2.378
7	2.434
8	2.481
9	2.523
10	2.560
11	2.592
12	2.622
13	2.649
14	2.674
15	2.697
16	2.718
17	2.738
18	2.757
19	2.774
20	2.791
21	2.807
22	2.822
23	2.836
24	2.849
25	2.862
26	2.875
27	2.887
28	2.898
29	2.909
30	2.920
31	2.930
32	2.940
33	2.949
34	2.958
35	2.967
36	2.976
37	2.984
38	2.992
39	3.000
40	3.008
41	3.015
42	3.023
43	3.030
44	3.037
45	3.043
46	3.050
47	3.057
48	3.063
49	3.069
50	3.075
51	3.081
52	3.087
53	3.092
54	3.098
55	3.103
56	3.109
57	3.114
58	3.119
59	3.124
60	3.129
61	3.134

F =

Column group: .001

M	X
1	1.645
2	1.949
3	2.114
4	2.226
5	2.311
6	2.378
7	2.434
8	2.481
9	2.523
10	2.560
11	2.592
12	2.622
13	2.649
14	2.674
15	2.697
16	2.718
17	2.738
18	2.757
19	2.774
20	2.791
21	2.807
22	2.822
23	2.836
24	2.849
25	2.862
26	2.875
27	2.887
28	2.898
29	2.909
30	2.920
31	2.930
32	2.940
33	2.949
34	2.958
35	2.967
36	2.976
37	2.984
38	2.992
39	3.000
40	3.008
41	3.015
42	3.023
43	3.030
44	3.037
45	3.043
46	3.050
47	3.057
48	3.063
49	3.069
50	3.075
51	3.081
52	3.087
53	3.092
54	3.098
55	3.103
56	3.109
57	3.114
58	3.119
59	3.124
60	3.129

Column group (X = .949 / 1.949 series)

M	X
2	1.949
3	2.114
4	2.226
5	2.311
6	2.378
7	2.434
8	2.481
9	2.523
10	2.560
11	2.592
12	2.622
13	2.649
14	2.674
15	2.697
16	2.718
17	2.738
18	2.757
19	2.774
20	2.791
21	2.807
22	2.822
23	2.836
24	2.849
25	2.862
26	2.875
27	2.887
28	2.898
29	2.909
30	2.920
31	2.930
32	2.940
33	2.949
34	2.958
35	2.967
36	2.976
37	2.984
38	2.992
39	3.000
40	3.008
41	3.015
42	3.023
43	3.030
44	3.037
45	3.043
46	3.050
47	3.057
48	3.063
49	3.069
50	3.075
51	3.081
52	3.087
53	3.092
54	3.098
55	3.103
56	3.109
57	3.114
58	3.119
59	3.124
60	3.129
61	3.134

Column group: .100 (X = 1.645 for all M)

M	X
1	1.645
1	1.645
1	1.645
...	1.645

(All X = 1.645 with M = 1 throughout.)

NU

NU = 1 through 60.