FURTHER STUDY OF ROBUSTIFICATION VIA A BAYESIAN APPROACH

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ABSTRACT

The Bayesian outlier procedure discussed by Box and Tiao (1968) which uses the contaminated normal model is further explored in this report. For a simple location estimate suggested by their method, the weight given each observation is expressed explicitly in terms of standardized residuals so allowing comparison with M-estimators.

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SIGNIFICANCE AND EXPLANATION

A Bayesian model has been proposed which describes the generation of an observation by a process whereby with prior probability \(1-\alpha\) the usually assumed statistical structure is correct but with small probability \(\alpha\) it is incorrect (for example, the observation has a very large variance). For a simple location estimate the nature of the down weighting of outlying observations produced by this model is studied and is compared with that of the presently popular M-estimators.
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1. Introduction

Statistics is a science which helps extract meaningful information from data which are subject to errors. Two important aspects of statistical analysis are

(i) The building of probabilistic models, defining the functional form of a relationship between variables as well as the distribution of the errors.

(ii) The development of techniques of analysis which are efficient supposing the data to be derived from the specified model.

Model building begins with preliminary and graphic analysis of the data. This information is combined with theoretical knowledge about the system to produce a tentative model. One desirable criterion for choosing a model is simplicity. Such a model is easy to interpret and can give greater precision than less parsimonious models (Box, 1978). An iterative model building procedure is needed which can move from a perhaps initially faulty model to one which is adequate for the purpose at hand.

Two techniques are of value in this process.

(i) Robustification: By employing robust methods (or models) we are unlikely to be misled by those model inadequacies guarded against.

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(ii) Iterative fixing: Conditional inference can be made assuming that the tentative model is true, and one can then make diagnostic checks to reveal possible inadequacies. If there are indications of inadequacy, the model can be modified appropriately.

Both techniques have their advantages and limitations. It is impossible to make a procedure robust against every possible contingency. On the other hand, situations can arise where tests may fail to show up inadequacies that could, nevertheless, cause serious problems. Looking for inadequacies after the event may not always be successful.

A practical policy is to robustify for one or more contingencies that seem likely in the context of a particular application and then to study the residuals to seek for the unexpected.

The Standard Statistical Models

Consider the standard statistical model

\[ y_i = \eta(x_i, \theta) + \epsilon_i \quad i = 1, \ldots, n \quad (1.1) \]

where \( \epsilon_i \)'s are independently, identically and normally distributed. In this model, it is assumed that
(i) The observation \( y_i \) is a function of dependent variables \( x_i \) and parameter \( \theta \) plus an error \( \epsilon_i \).

(ii) The errors \( \epsilon_1, \epsilon_2, \ldots, \epsilon_n \) are independently distributed.

(iii) All the errors \( \epsilon_i \)'s have the same normal distribution with a fixed variance.

Violations of any of these assumptions can cause problems. However, this thesis is concerned only with departures from the third assumption.

It is well known that real data can be affected with discordant values produced by a mistake or a sudden change of some unknown factor. It is usually, therefore, unrealistic to assume that every observation is from the same normal distribution. A more sensible possibility suggested by Dixon (1953) and by Tukey (1960) is to allow errors to be from two different distributions. The standard distribution \( f(c) \) occurs with probability \( 1-\alpha \) and an alternative distribution \( g(c) \) generates discordant values with probability \( \alpha \). We will call this the contaminated model. From, for example, the study made in Chapter 3 of this thesis, it is clear that this is not the only possibility. As we saw there, a model which could be realistic in some cases would have errors generated from one distribution up to a certain point and then randomly switching to a different distribution having either a different mean or a different variance or both for a certain period of time and then switching again. A model which
has this property for switches in means was proposed by George Barnard (1959) in his justification of the cumulative sum chart. We will only consider the contaminated model.

2. A Bayesian Analysis of the Contaminated Model

In those situations where a contaminated distribution is appropriate, a point estimate may be obtained by taking the mean of the posterior distribution of the appropriate parameter and Bayesian intervals can be calculated. The posterior mean takes the form of a weighted average in which the weights are posterior probabilities. The use of the Bayesian posterior mean as an estimator may be justified on the grounds that it minimizes the mean square error loss.

The formulation of Box and Tiao (1968) can be readily generalized to include nonlinear models as follows.

Consider a model \( Y = \eta(X, \theta) + \epsilon \), where \( Y \) is an \( n \times 1 \) vector of observations, \( X \) is an \( n \times p \) matrix of fixed elements with rank \( p \), \( \theta \) is a \( q \times 1 \) vector of parameters, \( \eta(X, \theta) \) is an \( n \times 1 \) vector for each given \( X \) and \( \theta \), and \( \epsilon \) is an \( n \times 1 \) vector of random errors. Suppose now that each of the errors independently comes from either one of the two distributions — a standard distribution \( f(\epsilon|\xi_1) \) and an alternative distribution \( g(\epsilon|\xi_2) \), where \( \xi_1 \) and \( \xi_2 \) are nuisance parameters and \( \theta \) is the parameter of interest.
Let \( a(r) \) be the event that a particular set of \( r \) of the \( n \) \( \epsilon \)'s are from \( g(\epsilon|\xi_2) \) and the remaining \( s = n-r \) from \( f(\epsilon|\xi_1) \). Corresponding to \( a(r) \), vector \( \epsilon \) was partitioned into \( \epsilon(r), \epsilon(s) \); vector \( Y \) into \( Y(r), Y(s) \) and matrix \( X \) into \( X(r), X(s) \). Let \( p(r) \) be the prior probability of event \( a(r) \), \( P(\theta, \xi_1, \xi_2) \) be the prior distribution of the parameters. The posterior distribution is then given by

\[
P(\theta|Y) = \sum_{(r)} P(a(r)|Y)P(\theta|a(r), Y)
\]

where \( P(\theta|a(r), Y) = \)

\[
\frac{\int P(\theta, \xi_1, \xi_2) \hat{f}(Y(r) - n(X(r), \theta)/\xi_1) \hat{g}(Y(r) - n(X(r), \theta)/\xi_2) d\xi_1 d\xi_2}{\int P(\theta, \xi_1, \xi_2) \hat{f}(Y(r) - n(X(r), \theta)/\xi_1) \hat{g}(Y(r) - n(X(r), \theta)/\xi_2) d\xi_1 d\xi_2 d\theta}
\]

where \( \hat{f} \) denotes the product of densities of the elements of \( Y(s) - n(X(s), \theta) \) and \( \hat{g} \) that of \( Y(r) - n(X(r), \theta) \). The denominator is the probability of the event that the \( \epsilon(r) \) are drawn from \( g(\epsilon|\xi_2) \) and the \( \epsilon(s) \) from \( f(\epsilon|\xi_1) \). If we denote it by \( h(Y(r) - g, Y(s) - f) \) then

\[
P(a(r)|Y) = \frac{p(r)h(X(r) - g; Y(s) - f)}{\sum_{(r)} p(r)h(Y(r) - g; Y(s) - f)} = c \frac{p(r)h(Y(r) - g; Y(s) - f)}{p(o)h(Y(r) - f; Y(s) - f)}
\]

\[
= c \frac{p(r)h(Y(s) - f)h(Y(r) - g; Y(s) - f)}{p(o)h(Y(s) - f)h(Y(r) - f; Y(s) - f)} = c \frac{p(r)h(Y(r) - g|Y(s) - f)}{p(o)h(Y(r) - f|Y(s) - f)}
\]
where \( h(Y(s) - f) \) is the marginal probability that \( \varepsilon(s) \) is from \( f(\varepsilon|\xi_1) \), \( h(Y(r) - g|Y(s) - f) \) is the conditional probability that \( \varepsilon(r) \) is from \( g(\varepsilon|\xi_2) \) given that \( \varepsilon(s) \) is from \( f(\varepsilon|\xi_1) \).

3. The Contaminated Normal Distribution

Since all experimental data are subject to unpredictable mistakes, a probability model which would be more realistic than the standard normal model would often be one where with probability \( 1-\alpha \), the error is normally distributed with mean 0 and variance \( \sigma^2 \) and with small probability \( \alpha \) the error has a mean 0 but an inflated variance \( k^2\sigma^2 \).

One argument in favor of this model is as follows. The trimmed mean has been recommended as a sensible estimator for location parameters by Tukey and McLaughlin (1963), Huber (1972) and Stigler (1977). More recently M-estimators have been recommended by Huber, Hampel and Andrews (Andrews et al (1972)). From the study in TSR# 1997 we have seen that the contaminated normal distributions would produce via the Bayesian route estimators which are very similar to those recommended by these authors.

Furthermore, results of TSR# 2002 suggest that heavy-tailed distributions are sometimes caused by inhomogeneity in mean and variance such as might be encountered early in an experiment because of start-up difficulties. After such inhomogeneity has been allowed for, the observations seem to be adequately repre-
presented by a contaminated normal distribution. Thus, for a carefully planned experiment, a contaminated normal distribution is likely to be appropriate.

4. Bayesian Inference with Contaminated Normal Model

Consider that the error distribution is a contaminated normal distribution \((1-\alpha)N(0, \sigma^2) + \alpha N(0, k^2 \sigma^2)\). This is the special case where

\[
f(\varepsilon | \xi_1) = \frac{1}{\sqrt{2\pi \sigma}} e^{-\frac{\varepsilon^2}{2\sigma^2}}, \quad g(\varepsilon | \xi_2) = \frac{1}{\sqrt{2\pi k\sigma}} e^{-\frac{\varepsilon^2}{2k^2 \sigma^2}}
\]

and \(p(r) = \alpha^r (1-\alpha)^{n-r}\). Assume, a priori that the information about \(\theta\) and about \(\sigma\) are independent and, as in Box and Tiao (1968) approximate the locally noninformative prior by

\[
P(\theta, \sigma) \propto P(\theta) \cdot \frac{1}{\sigma}.
\]

Then

\[
P(\theta, \xi_1, \xi_2) = P(\theta, \sigma) \propto P(\theta) \frac{1}{\sigma}.
\]

and if we let \(w(r) = P(a(r)|Y)\) and \(P(r|\theta) = P(\theta|a(r), Y)\) we have

\[
P(\theta|Y) = \sum_{(r)} w(r) P(r|\theta|Y)
\]

with

\[
P(r|\theta|Y) = \int_{0}^{\infty} \frac{\sigma^{-(n+1)} p(\sigma) \exp\left[-\frac{1}{2\sigma^2} S(r)(\theta)\right]}{\sigma} d\sigma
\]

\[
= P(\theta)[S(r)(\theta)]^{-\frac{n}{2}}
\]

where

\[
S(r)(\theta) = (Y(s)-\eta(X(s), \theta))' (Y(s)-\eta(X(s), \theta)) + \frac{1}{k^2} (Y(r)-\eta(X(r), \theta))' (Y(r)-\eta(X(r), \theta))
\]
and
\[ w(r) = c \frac{p(r)h(Y(r) \sim g; Y(s) \sim f)}{p(o)h(Y(r) \sim f; Y(s) \sim f)} \]
\[ = c(\frac{\alpha}{1-\alpha}) r^{-\sigma} (n+1)^{-\frac{1}{2}} \frac{r_{e}^{-\sigma}}{P(o)} \frac{1}{\frac{1}{2}[(Y-n(X, \theta))'(Y-n(X, \theta))]^{-2}} \]
\[ = c(\frac{\alpha}{1-\alpha}) r^{-\sigma} \frac{f(P(o)[S(r)(\theta)]^2 \frac{n}{2} d\theta}{f(P(o)[(Y-n(X, \theta))'(Y-n(X, \theta))]^{-n/2} d\theta} \]

where \( c \) is some constant.

When \( n \) is approximately linear in \( \theta \) over the range considered, it would also be reasonable to take \( P(o) \) as approximately constant. In such case the above formula becomes

\[ P(r)(\theta|Y) \propto \{S(r)(\theta)\}^{-\frac{1}{2}n} \]

\[ w(r) = c(\frac{\alpha}{1-\alpha}) r^{-\sigma} \frac{f(S(r)(\theta))^{-\frac{n}{2}} d\theta}{f((Y-n(X, \theta))'(Y-n(X, \theta)))^{-n/2} d\theta} \]

A robust point estimate for \( \theta \) is then given by the posterior mean

\[ \int \theta P(\theta|Y) d\theta = \sum_{(r)} w(r) \int \theta P(\theta|Y) d\theta. \]

Furthermore, probabilities can be calculated which are useful in spotting possible bad values. (Observations generated by \( g \) are referred to as bad values.) If we let \( w(r) \) be the posterior probability of event \( a(r) \) given the sample \( Y \):
\(a_i\) be the event that the observation \(y_i\) is from \(g\) and all the others are from \(f\).

\(a_{ij}\) be the event that the observations \(y_i\) and \(y_j\) are from \(g\) and all the others are from \(f\).

Then \(w_i, w_{ij}\) are the posterior probabilities associated with \(a_i\) and \(a_{ij}\).

Using these individual probabilities, one can calculate

\[q_1, \text{ the posterior probability that only one observation is from } g \text{ is } \sum_{i=1}^{n} w_i\]

\[q_2, \text{ the posterior probability that only two observations are from } g \text{ is } \sum_{i,j=1, i<j}^{n} w_{ij}\]

and similarly \(q_3, q_4, \ldots, \text{etc.}\)

Also, the posterior conditional probabilities can be calculated as follows:

\[q_{i/1} = P(\text{the } i\text{-th observation is from } g/ \text{there is only one bad value}) = w_i/q_1\]

\[q_{ij/2} = P(\text{the } i\text{-th and } j\text{-th observations are from } g/ \text{there are only two bad values}) = w_{ij}/q_2\]

\[\vdots\]

\[\vdots\]

etc.
The distribution \( g \) is regarded as the source of "bad values," and these probabilities can be interpreted as the posterior probabilities that there is one bad value, two bad values, ..., etc., and the conditional probabilities as the posterior probabilities that the \( i_1 \)th, \( i_2 \)th, ..., \( i_k \)th observations are bad values given that there are \( k \) bad values.

Although the posterior probabilities \( q_i \)'s depend on the choices of \( \alpha \) and \( k \), the conditional probabilities are independent of \( \alpha \) and rather insensitive to \( k \). It seems that, in practice by comparing these conditional probabilities one can readily identify questionable observations.

5. Some Further Study of the Linear Model

When \( n(X, \theta) = X\theta \), We have the general linear model and the posterior distribution of \( \theta \) can be written as in Box and Tiao in the following way

\[
P(\theta | Y) = \sum_{(r)} W(r) P(r) \theta | Y) \]

with

\[
W(r) = c(\frac{a}{n-\alpha} k-r) ^{1/a} \frac{|X'X| ^{1/2}}{|X'X-\phi X(r)'X'(r)| ^{1/2}} \left\{ \frac{s^2_{(r)}}{s^2} \right\} ^{-\frac{1}{2}v} \]

\[
P(r)(\theta | Y) = \frac{\Gamma(\frac{1}{2}n)|X'X-\phi X(r)'X'(r)| ^{1/2}}{\Gamma(\frac{1}{2}v)(\pi s^2_{(r)})^{1/2}} \]

\[
\times \left\{ 1 + (\theta-\hat{\theta}(r))(X'X-\phi X(r)'X'(r))(\theta-\hat{\theta}(r)) \right\} ^{-\frac{1}{2}n} \]

\[
(5.1)
\]

\[
(5.2)
\]
where

\[
\hat{\theta}(r) = (X'(n-r)X(n-r) + \frac{1}{k^2} X'(r)X(r))^{-1}(X'(n-r)y(n-r) + \frac{1}{k^2} X'(r)y(r))
\]  

(5.3)

\[
s^2(r) = \frac{1}{v}S(r)^2(\hat{\theta}(r)) = \frac{1}{v} \left\{(y(n-r) - X(n-r)\hat{\theta}(r))' \times (y(n-r) - X(n-r)\hat{\theta}(r))
\right. 
\left. + \frac{1}{k^2} (y(r) - X(r)\hat{\theta}(r))' (y(r) - X(r)\hat{\theta}(r)) \right\}
\]  

(5.4)

\[\nu = n-p \quad \text{and} \quad s^2 = s^2_0.\]

The posterior distribution \(P_r(\theta|y)\) is a \(p\)-dimensional multivariate t-distribution with mean \(\hat{\theta}(r)\), dispersion matrix \(s^2(r)(X'X-\phi X'(r)X(r))^{-1}\) and \(\nu = n-p\) degrees of freedom. It is then easy to see that the robust point estimate - the posterior mean - is equal to \(\sum_r W(r)\hat{\theta}(r)\). As mentioned before, the posterior mean is justified because it minimizes the mean square error loss.

The Weighting Structure of this Bayesian Posterior Mean

A most important feature of a robust estimator is the weighting pattern it puts on the observations. As expected, for an estimator to be insensitive to outlying observations, the weights given to extreme observations must be small. Different criteria can be used. In L-estimators, the weight given to an observation depends on the
percentage point it takes in the ordered sample, while in M-
estimators, the weights are determined by the relative distances of
the observations. It is, therefore, informative to study the
weighting structure of the Bayesian posterior mean. Two things of
special interest would be the variables through which the weight
for each observation is determined and the roles \( \alpha \) and \( k \) play
in this estimator.

As stated previously, the posterior mean is

\[ \sum_{r} w(r) \hat{\theta}(r) \]

with formula for \( w(r) \) and \( \hat{\theta}(r) \) given by (5.1) and (5.3).

Box and Tiao (1968) give the following two equations

\[ \begin{align*}
vs^2(r) &= \text{var}(Y(r) - X(r)\hat{\theta})
\end{align*} \]

(5.5)

\[ \hat{\theta}(r) = \hat{\theta} - \phi(X'X)^{-1}X'(r)(X'X)^{-1}X(r)\hat{\theta}.
\]

(5.6)

Using equation (5.6)

\[ \begin{align*}
Y(r) - X(r)\hat{\theta}(r) &= Y(r) - X(r)\hat{\theta} + \phi X(r)(X'X)^{-1}X'(r)(I - \phi X(r)(X'X)^{-1}X(r))^{-1}X(r)\hat{\theta} \\
&\quad \times (Y(r) - X(r)\hat{\theta}) \\
&= \{I + \phi X(r)(X'X)^{-1}X'(r)(I - \phi X(r)(X'X)^{-1}X(r))^{-1}\}
\end{align*} \]

(5.7)
Since
\[ \{I+\phi X(r)(X'X)^{-1}X'_r\} \{I-\phi X(r)(X'X)^{-1}X'_r\}^{-1} \]
\[ \cdot \{I-\phi X(r)(X'X)^{-1}X'_r\} \]
\[ = I-\phi X(r)(X'X)^{-1}X'_r + \phi X(r)(X'X)^{-1}X'_r \]
\[ = I \]

it follows that
\[ \{I+\phi X(r)(X'X)^{-1}X'_r\} \{I-\phi X(r)(X'X)^{-1}X'_r\}^{-1} \]
\[ = \{I-\phi X(r)(X'X)^{-1}X'_r\}^{-1} \]

Equation (5.7) becomes
\[ Y(r)-X(r)^\hat{\theta}(r) = \{I-\phi X(r)(X'X)^{-1}X'_r\}^{-1}(Y(r)-X(r)^\hat{\theta}(r)) \]
so
\[ Y(r)-X(r)^\hat{\theta}(r) = \{I-\phi X(r)(X'X)^{-1}X'_r\}(Y(r)-X(r)^\hat{\theta}(r)). \tag{5.8} \]

Dividing both sides of equation (5.5) by \( vs^2(r) \) and using equation (5.8), we have

\[ \frac{s^2}{s^2(r)} = 1+ \frac{\phi}{vs^2(r)}(Y(r)-X(r)^\hat{\theta}(r))' \{I-\phi X(r)(X'X)^{-1}X'_r\}^{-1}(Y(r)-X(r)^\hat{\theta}(r)) \]
\[ = 1+ \frac{\phi}{vs^2(r)}(Y(r)-X(r)^\hat{\theta}(r))' \{I-\phi X(r)(X'X)^{-1}X'_r\}' \{I-\phi X(r)(X'X)^{-1}X'_r\} \]
\[ \cdot \{I-\phi X(r)(X'X)^{-1}X'_r\}^{-1}(Y(r)-X(r)^\hat{\theta}(r)) \]
\[ = 1+ \frac{\phi}{s(r)} \frac{(Y(r)-X(r)^\hat{\theta}(r))' \{I-\phi X(r)(X'X)^{-1}X'_r\} \left( Y(r)-X(r)^\hat{\theta}(r) \right)}{s^2(r)} \] \tag{5.9}
Note that $\hat{\theta}_\alpha(r)$ and $s^2(r)$ are the estimates obtained by downweighting the observations which under the assumption that $a(r)$ occurs, come from a distribution with the larger variance. Also

$$r(r) = \frac{Y(r) - X(r)\hat{\theta}_\alpha(r)}{s(r)}$$

is the residual vector for the observations which are downweighted under such an assumption.

From (5.1), we can write

$$w(r) = c(\frac{\alpha}{1-\alpha}) k^{-r} \frac{1}{|x'x|^{1/2}} \left\{ \frac{s^2}{s^2(r)} \right\}^{1/2}$$

$$= c(\frac{\alpha}{1-\alpha}) k^{-r} \frac{1}{|x'x-\phi x'_i(r)x_i(r)|^{1/2} \left\{ 1 + \frac{\phi}{\nu} r_i(r) \right\}^{1/2}}$$

$$\cdot \{I-\phi x'_i(r)(x'x)^{-1}x'_i(r)r_i(r)\}^{1/2}.$$

If we let $\Sigma = \phi(I-\phi x'_i(r)(x'x)^{-1}x'_i(r))\frac{\nu-r}{\nu}$, then

$$|x'x|^{-1}|\Sigma| = |x'x|^{-1}|I-\phi x'_i(r)(x'x)^{-1}x'_i(r)|\left(\frac{\nu-r}{\nu}\right)^r$$

$$= \left| x'_i(r) \begin{pmatrix} x'_i(r) \end{pmatrix} \left(\frac{\nu-r}{\nu}\phi \right)^r \right| \left| \begin{array}{ccc} I & \phi x'_i(r) \\ \phi x'_i(r) & x'x \end{array} \right| \left(\frac{\nu-r}{\nu}\phi \right)^r$$

$$= |I||x'x-x'_i(r)\phi x'_i(r)|\left(\frac{\nu-r}{\nu}\phi \right)^r = |x'x-\phi x'_i(r)x'_i(r)|\left(\frac{\nu-r}{\nu}\phi \right)^r.$$
Thus

\[ |\Sigma| = |X'X||X'X - xx'\Sigma xx'| \left( \frac{\nu - r}{\nu} \phi \right)^r \]

and

\[ w(r) = c |X'X| \left( \frac{\alpha}{1 - \alpha} \right) k^{-r} \left( \frac{\nu - r}{\nu} \phi \right)^{\frac{r}{2}} \frac{1}{|\Sigma|^{1/2}(1 + \frac{1}{\nu - r} r(r)\Sigma r(r))^2} \frac{1}{\nu}. \]  

(5.11)

This \( w(r) \) is proportional to the inverse of a multivariate-t ordinate at \( r(r) \) with precision matrix \( \Sigma \) and \( \nu - r \) degrees of freedom. It is seen then that \( r(r) \) is an important factor which determines the weighting structure. If the components of \( r(r) \), which are the standardized residuals for the observations down-weighted in the process of estimation, are very large, then \( w(r) \) will be large and \( \hat{\theta}(r) \) will be a more influential constituent of the posterior mean. This is; in some sense, similar to an M-estimator where the weighting pattern is determined through the standardized residuals. However, the estimates must be calculated iteratively in that case.

6. A Method of Comparing the Weights with Those of the M-estimators

Recall that an M-estimate is the solution to the following equation

\[ \sum_{i=1}^{n} x_i \left( \frac{y_i - x_i \hat{\theta}}{s} \right) w\left( \frac{y_i - x_i \hat{\theta}}{s} \right) = 0. \]  

(6.1)
If we write $v_i = 1/w \left( \frac{y_i - x_i \theta}{s} \right)$, then (6.1) can be written as

$$\sum_{i=1}^{n} x_i'y_iw_i^{-1} - \sum_{i=1}^{n} x_i'x_iw_i^{-1} = 0$$

or equivalently,

$$X'V^{-1}Y - X'V^{-1}X\theta = 0$$

where

$$X = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \quad V = \begin{pmatrix} v_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & v_n \end{pmatrix}.$$

The solution $\hat{\theta}$ is then given by $(X'V^{-1}X)^{-1}X'V^{-1}Y$. This is the same solution as the weighted least square estimates in a linear model when $\text{Var}(Y) = \sigma^2 V_\theta = \sigma^2 \begin{bmatrix} v_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & v_n \end{bmatrix}$ and the weighting function $w$ corresponds to the weights $v_i^{-1}$ used in the weighted least square method. In order to compare the weighting pattern for the Bayesian posterior mean with the $w$ function in an M-estimator, one needs to write the posterior mean approximately in the form of

$$(X'V^{-1}X)^{-1}X'V^{-1}Y$$

and the matrix $V$ will then provide the information about the weighting structure. It is not always possible to obtain such a matrix $V$ for the general linear model, and even when possible, its form is often complicated. However, in the special case
of a location parameter, simple results can be obtained and much insight gained.

The Location Case

Consider the model \( y_i = \theta + \epsilon_i \)

\[ \epsilon_i \text{ i.i.d. from } (1-\alpha)N(0,\sigma^2) + \alpha N(0,k^2\sigma^2), \quad i=1,...,n. \]

Then \( X'X = n, \ X'_iX(r) = 1, \ I-\phi X(r)(X'X)^{-1}X'_i = I - \frac{\phi}{n} X(r)X'_i \)

and following (4.5.11) \( w(r) \) reduces to

\[
\frac{1}{r} \sum c\left(\frac{r}{1-r}\right)^k r^{r} \left(\frac{n}{r\phi}\right) \left\{1+ \frac{\phi}{n-1} r(r)\left[I- \frac{\phi}{n} X(r)X'_i(r)r(r)\right]\right\}^{\frac{1}{2}(n-1)}.
\] (6.2)

Also from (5.6)

\[
\hat{\theta}(r) = \bar{y} - \frac{r\phi}{n-r\phi} (\bar{y}(r)-\bar{y}),
\]

where \( \bar{y} \) is the sample average and \( \bar{y}(r) \) is the average of elements of \( Y(r) \).

The posterior mean is then

\[
\sum c\left(\frac{r}{1-r}\right)^k r^{r} \left(\frac{n}{r\phi}\right) \left\{1+ \frac{\phi}{n-1} r(r)\left[I- \frac{\phi}{n} X(r)X'_i(r)r(r)\right]\right\}^{\frac{1}{2}(n-1)}
\]

\[
\times (\bar{y} - \frac{r\phi}{n-r\phi} (\bar{y}(r)-\bar{y})).
\] (6.3)

We shall now discuss this formula in the following cases:

(i) when there is at most one discordant observation in the sample,

(ii) when there are at most two discordant observations in the sample.
Only One Discordant Observation Present

In this circumstance, the \( w_i \) associated with two or more observations coming from the distribution with the larger variance will be negligible. The terms left in (6.3) would then be associated with no bad values and with one bad value.

\[
c + \sum_{i=1}^{n} c(\frac{\alpha}{1-\alpha})k^{-1}(\frac{n}{n-\phi})^2 \left(1 + \frac{\phi}{n-1} \frac{1}{r_i^2} \right) \left(\frac{1}{r_i^2} \right) \left(\frac{1}{n-1} \right) \left(y_i - \frac{\phi}{n-\phi}(y_i - \bar{y})\right) = c + \sum_{i=1}^{n} c(\frac{\alpha}{1-\alpha})k^{-1}(\frac{n}{n-\phi})^2 \left(1 + \frac{\phi}{n-1} \frac{1}{r_i^2} \right) \left(\frac{1}{r_i^2} \right) \left(\frac{1}{n-1} \right) \left(y_i - \frac{\phi}{n-\phi}(y_i - \bar{y})\right) \tag{6.4}
\]

where \( c \) is a constant such that the weights would sum up to unity.

Let \( R_i = \left(1 + \frac{\phi}{n-1} \frac{1}{r_i^2} \right) \left(\frac{1}{r_i^2} \right) \left(\frac{1}{n-1} \right) \left(y_i - \frac{\phi}{n-\phi}(y_i - \bar{y})\right) \) and \( R = \sum_{i=1}^{n} R_i \).

then \( c + \sum_{i=1}^{n} c(\frac{\alpha}{1-\alpha})k^{-1}(\frac{n}{n-\phi})^2 R_i = 1 \)

or equivalently \( c + c(\frac{\alpha}{1-\alpha})k^{-1}(\frac{n}{n-\phi})^2 R = 1 \)

which implies \( c = 1/(1 + \frac{\alpha}{1-\alpha} k^{-1}(\frac{n}{n-\phi})^2 R) \).

Substituting \( c \), \( R_i \) and \( R \), (6.4) becomes

\[ -18 - \]
\[
\sum_{i=1}^{n} \left[ \frac{c(\frac{\alpha}{1-\alpha})k^{-1}(\frac{n}{n-\phi}) R_i}{n}\frac{\bar{y}}{1}\frac{c(\frac{\alpha}{1-\alpha})k^{-1}(\frac{n}{n-\phi}) R_i}{n}\frac{\phi}{n-\phi} y_i \right] \\
= \sum_{i=1}^{n} \left[ \frac{c(\frac{\alpha}{1-\alpha})k^{-1}(\frac{n}{n-\phi}) \frac{1}{1} \frac{1}{n-\phi} R_i}{1} \frac{c(\frac{\alpha}{1-\alpha})k^{-1}(\frac{n}{n-\phi}) \frac{1}{1} \frac{1}{n-\phi} \phi R_i y_i}{1} \right] \\
= \frac{\alpha}{1-\alpha} k^{-1}(\frac{n}{n-\phi}) \frac{1}{1} \frac{1}{n-\phi} \sum_{i=1}^{n} (R-\phi R_i) y_i \\
1+ \frac{\alpha}{1-\alpha} k^{-1}(\frac{n}{n-\phi}) R \\
\text{We, therefore, have} \\
\text{posterior mean} = \frac{1}{1+ \frac{\alpha}{1-\alpha} k^{-1}(\frac{n}{n-\phi}) R} \bar{y} + \frac{\alpha}{1-\alpha} k^{-1}(\frac{n}{n-\phi}) R \frac{1}{1+ \frac{\alpha}{1-\alpha} k^{-1}(\frac{n}{n-\phi}) R} \sum_{i=1}^{n} \frac{R-\phi R_i}{(n-\phi) R} y_i \\
(6.5) \\
\text{Let } \bar{Y}_o = \bar{y} = \text{ordinary mean}, \quad \bar{Y}_1 = \sum_{i=1}^{n} \frac{R-\phi R_i}{(n-\phi) R} y_i, \\
\text{and} \quad Q = \frac{1}{1+ \frac{\alpha}{1-\alpha} k^{-1}(\frac{n}{n-\phi}) R} \\
\text{the posterior mean} = Q \bar{Y}_o + (1-Q) \bar{Y}_1. \\
\text{It is clear now that the posterior mean can be written as a convex combination of two location estimates, } \bar{Y}_0 - \text{ which is the conditional posterior mean given that there is no outlier} - \text{ and}
\( \tilde{Y}_1 \) — which is the conditional posterior mean given there is exactly one outlier. The quantity \( Q \) is the posterior probability that there are no outliers, and \( 1-Q \) is the posterior probability that there is exactly one outlier. The crucial quantities here are \( R_i \)'s, which are the inverse of the t-ordinates of \( r_i \)'s. If a particular observation \( y_i \) is abberant, the corresponding residual \( r_i \) will be large. By taking \( R_i \) as the inverse of the corresponding t-ordinate, contrasts with other \( R_j \)'s will be exaggerated. Thus \[
\frac{R-\phi R_i}{(n-\phi)R}
\] will be made relatively small. The quantity \( \tilde{Y}_1 \) will then put little weight on \( y_1 \). Also if there is a discrepant observation, \( R \) will be large which will make \( Q \) small and the posterior mean close to \( \tilde{Y}_1 \). Conversely, if there are no discrepant observations, the posterior mean will lie close to \( \bar{Y} \).

The value of \( Q \) depends not only on the sample through \( R \), but also on values of \( \alpha \) and \( k \). If one assumes a larger prior probability \( \alpha \) of outliers, then the posterior probability of no outlier could be smaller. Notice too that the posterior mean depends on \( \alpha \) only through \( Q \) so that the role that \( \alpha \) plays is only to adjust the overall weight associated with fixed numbers of outliers.

When \( k \) is fairly large, \( \phi = 1 - \frac{1}{k^2} \) would be close to 1 (\( \phi = .96 \) when \( k = 5 \)). From the formula of \( R_i \) and (6.5), it
seems that $\tilde{y}_1$ would be rather insensitive to $k$ since it involves only $\phi$ and so is $R$. If we let $G = \frac{\alpha}{1-\alpha} k^{-1}$ and approximate $\phi$ by 1, then the posterior mean involves only one constant $G$. One interpretation associated with $G$ is the following.

Assume $y_1$ is an observation from $(1-\alpha)N(\theta, \sigma^2) + \alpha N(0, k^2 \sigma^2)$ then $G$ is the ratio of the posterior probability that $y_1$ is from $N(\theta, k^2 \sigma^2)$ to the posterior probability that $y_1$ is from $N(\theta, \sigma^2)$ given that $y_1 = \theta$.

$$\frac{P(y_1 = \theta / y_1 = N(\theta, k^2 \sigma^2))}{P(y_1 = \theta / y_1 = N(\theta, \sigma^2))} = \frac{P(y_1 = \theta / y_1 = N(\theta, k^2 \sigma^2))}{P(y_1 = \theta / y_1 = N(\theta, \sigma^2))} = \frac{1}{\sqrt{2\pi \sigma}} \cdot \frac{\alpha}{\sqrt{2\pi \sigma}} (1-\alpha) = \frac{\alpha}{1-\alpha} k = G. $$

$G$ can also be viewed as

- expected value of $\sqrt{\text{information from } N(0, k^2 \sigma^2)}$
- expected value of $\sqrt{\text{information from } N(0, \sigma^2)}$
- probability of an observation being from $N(0, k^2 \sigma^2)$
- probability of an observation being from $N(0, \sigma^2)$
- $\sqrt{\text{information in } N(0, k^2 \sigma^2)}$
- $\sqrt{\text{information in } N(0, \sigma^2)}$

$$= \frac{\alpha \sqrt{\sigma^2}}{1-\alpha \sqrt{\sigma^2}} = \frac{\alpha}{1-\alpha} k. $$

-21-
So for \( k \) large, we need to determine only one parameter in the model, namely \( G \).

**The Weighting Pattern**

In the case of a single location parameter,

\[
(X'V^{-1}X)^{-1}X'V^{-1}Y = \sum_{i=1}^{n} \frac{v_i^{-1}}{\sum_{i=1}^{n} v_i^{-1}} y_i. 
\]

Thus the weighting function \( V^{-1} = \left( \begin{array}{ccc} v_1^{-1} \\ \vdots \\ v_n^{-1} \end{array} \right) \) used in obtaining the weighted least square estimate is proportional to the weight given to each observation. It is, therefore, possible to write the posterior mean in the form of \( (X'V^{-1}X)^{-1}X'V^{-1}Y \) and compare \( V^{-1} \) with the weighting patterns used in the M-estimators.

If we assume at most one outlier, the posterior mean is

\[
Q\tilde{Y}_o + (1-Q)\tilde{Y}_1 \text{ as shown above. It can also be written as }
\]

\[
\sum_{i=1}^{n} \left( \frac{Q}{n} + (1-Q) \frac{R-\phi R_i}{(n-\phi)R} \right) y_i. 
\]

Therefore,

\[
v_i^{-1} = \frac{Q}{n} + (1-Q) \frac{R-\phi R_i}{(n-\phi)R}.
\]

The right-hand side is a function of \( r_i \); we can thus obtain the weighting pattern of this Bayesian posterior mean in terms of the standardized residuals. This weighting pattern is sample dependent. We illustrate with a random sample of size 10 from \( N(0,1) \).
Ten observations generated from a computer random sampling routine and the corresponding residuals $r_i$'s and weights $(v_i^{-1})$'s with $\alpha = .05$ and $k = 5.0$ are listed in Table 1. It is seen that the weight given to each observation is approximately constant and close to .1. The weights change when a discrepant observation is present. We have added in turn 1, 2, 3, 4, 5, to the seventh observation and again calculated the $r_i$ and $v_i^{-1}$; the results are also shown in Table 1.

If we plot $v_7^{-1}$ versus $r_7$, with 0, 1, 2, 3, 4, 5 added to $y_7$, we found that they lie on a smooth curve and such a curve is comparable with the weighting function of the M-estimators since they both determine the weights given to observations as a function of properly standardized residuals. Figure 1 gives plots of $v_7^{-1}$ versus $r_7$ for $\alpha = .01, .05$ and .10 and $k = 5.0$. In terms of $G$, they are weighting curves for $G = .002, .011$ and .022.

The weighting curves for M-estimators are shown in Figure 2.

Examination of Figure 1 shows that the weights are roughly equal for residuals between zero and one and start to descend as they go farther and farther away from the center. The larger $\alpha$ is (or the larger $G$ is) the sooner and faster the weights decrease.

Comparing with Figure 2 this weighting pattern has the desired property (Beaton and Tukey, 1974) that it is almost as constant in
Figure 1 Weighting curves for different $\alpha(G)$ values with $k = 5.0$. 

-24-
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**add 1 to 7-th observation**

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**add 4 to 7-th observation**

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**add 5 to 7-th observation**

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Table 1: The correspondences among $y_i$, $r_i$ and $v_i^{-1}$ with $\alpha = 0.05$, $k = 5.0$
Figure 2  \( w \)-functions for various \( M \)-estimators.

(i) Normal

\[
\frac{1}{\sqrt{2\pi}} e^{-x^2/2}
\]

(ii) Huber's

\[
\begin{cases} 
1 & |x| \leq k \\
\frac{k}{c} & |x| > k
\end{cases}
\]

(iii) Andrews'

\[
|x|^c
\]

(iv) Hampel's

\[
a = 1.42 \\
b = 2.70 \\
c = 5.54
\]

(v) Tukey's

\[
c = 5.4
\]

(vi) Tukey's

\[
c = 4.05
\]
the center (normal-like) as Huber's and Hampel's and reduces to small values as smoothly as Andrews' and Tukey's. Smoothness may be another desired property since a sudden change in the slope is rather artificial and one does not have reason to expect such a change.

Figure 1 depends on a particular sample. However, in all, totally five samples were drawn. All of the weighting patterns are similar and those in Figure 1 are typical.

As discussed before, when $k$ is large, $G$ seems to be the only relevant parameter to be determined. Figure 1 has shown the weighting patterns for $G = .002, .011$ and $0.022$ where systematic changes have been observed. With this same sample, one can also fix $G$ and calculate the weights for different $\alpha$ and $k$ values. Figure 3 exhibits five weighting patterns all with $G = .011$ and the following pairs of $\alpha$ and $k$ values.

\[
\begin{array}{cccccc}
\alpha & .050 & .095 & .136 & .174 & .208 \\
k & 5.0 & 10.0 & 15.0 & 20.0 & 25.0 \\
\end{array}
\]

All five curves look very much alike with the greatest discrepancy being that for the values $(\alpha, k) = (.05, 5.0)$. This confirms our conjecture that $G$ is the only critical parameter when $k \geq 5$.

At Most Two Discordant Observations Present

As we have seen, the terms in (6.3) corresponding to no bad values and one bad value can be written as $c\gamma$ and
Figure 3: Weighting patterns for fixed $G$ and different $\alpha, k$ values.
The term corresponding to two bad values is

\[
\sum_{i=1}^{n} \sum_{j=1, i<j}^{\infty} c_i \left( \frac{\alpha}{1-\alpha} \right)^2 \left( \frac{n}{n-2\phi} \right)^2 \left( 1 + \frac{\phi}{n-1} r_{ij}^i \left( I - \frac{\phi}{n} X_{ij} \right) r_{ij}^j \right)^2 \frac{1}{\sigma_i^2} \frac{1}{\sigma_j^2} \frac{1}{\sigma_{ij}^2} \frac{1}{\sigma_{ij}^2}
\]

where \( c_i \) is the weight of the \( i \)-th observation, \( \phi \) is the degree of freedom, \( X_{ij} \) is the \( (i,j) \)-th element of the matrix \( X \), and \( \sigma_i^2, \sigma_j^2, \sigma_{ij}^2 \) are the variances of the \( i \)-th, \( j \)-th, and \( (i,j) \)-th elements, respectively.

The weighted least squares estimates are obtained by minimizing the following function:

\[
\sum_{i=1}^{n} \sum_{j=1, i<j}^{\infty} c_i \left( \frac{\alpha}{1-\alpha} \right)^2 \left( \frac{n}{n-2\phi} \right)^2 \left( 1 + \frac{\phi}{n-1} r_{ij}^i \left( I - \frac{\phi}{n} X_{ij} \right) r_{ij}^j \right)^2 \frac{1}{\sigma_i^2} \frac{1}{\sigma_j^2} \frac{1}{\sigma_{ij}^2} \frac{1}{\sigma_{ij}^2}
\]

subject to \( y_{ij} = \sum_{i=1}^{n} \sum_{j=1, i<j}^{\infty} c_i \left( \frac{\alpha}{1-\alpha} \right)^2 \left( \frac{n}{n-2\phi} \right)^2 \left( 1 + \frac{\phi}{n-1} r_{ij}^i \left( I - \frac{\phi}{n} X_{ij} \right) r_{ij}^j \right)^2 \frac{1}{\sigma_i^2} \frac{1}{\sigma_j^2} \frac{1}{\sigma_{ij}^2} \frac{1}{\sigma_{ij}^2} \)

and

\[
\sum_{i=1}^{n} \sum_{j=1, i<j}^{\infty} c_i \left( \frac{\alpha}{1-\alpha} \right)^2 \left( \frac{n}{n-2\phi} \right)^2 \left( 1 + \frac{\phi}{n-1} r_{ij}^i \left( I - \frac{\phi}{n} X_{ij} \right) r_{ij}^j \right)^2 \frac{1}{\sigma_i^2} \frac{1}{\sigma_j^2} \frac{1}{\sigma_{ij}^2} \frac{1}{\sigma_{ij}^2} \]

subject to \( \sum_{i=1}^{n} \sum_{j=1, i<j}^{\infty} c_i \left( \frac{\alpha}{1-\alpha} \right)^2 \left( \frac{n}{n-2\phi} \right)^2 \left( 1 + \frac{\phi}{n-1} r_{ij}^i \left( I - \frac{\phi}{n} X_{ij} \right) r_{ij}^j \right)^2 \frac{1}{\sigma_i^2} \frac{1}{\sigma_j^2} \frac{1}{\sigma_{ij}^2} \frac{1}{\sigma_{ij}^2} \)
(6.7) reduces to
\[
\sum_{i,j=1}^{n} c\left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij}\left(\frac{n}{n-2\phi}\right) y_i - c \sum_{i,j=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i + y_j
\]
\[
= c \sum_{i=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i - c \sum_{i,j=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i + y_j
\]
\[
= c \sum_{i,j=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i - c \sum_{i,j=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i + y_j
\]
\[
= c \sum_{i,j=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i
\]
\[
= c \sum_{i,j=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i
\]

It is easy to see that \( T_{ij} = T_{ji} \) so
\[
\sum_{i,j=1}^{n} T_{ij} y_i = \sum_{i,j=1}^{n} T_{ij} y_i + \sum_{i,j=1}^{n} T_{ij} y_j
\]
\[
= \sum_{i,j=1}^{n} T_{ij} y_i + \sum_{i,j=1}^{n} T_{ij} y_j = n \left( \sum_{j=1}^{n} T_{ij} \right) y_i
\]

The above formula can now be written as
\[
c \sum_{i=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i - c \sum_{i,j=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i + y_j
\]
\[
= c \sum_{i=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i
\]
\[
= c \sum_{i=1}^{n} \left(\frac{\alpha}{1-\alpha}\right)^2 k^{-2}\left(\frac{n}{n-2\phi}\right)^{1/2} T_{ij} y_i
\]
Thus the posterior mean will be

\[
c\tilde{y} + c \frac{\alpha}{1-\alpha} k^{-1} \left( \frac{n}{n-\varphi} \right) R + \frac{1}{2} \left( \frac{n}{n-2\varphi} \right) \begin{pmatrix} \frac{n}{2} \sum_{j=1}^{n} T_{i,j} \\ \frac{n}{2} \sum_{j \neq i}^{n} T_{i,j} \end{pmatrix} y_i.
\]

We have

\[
c + c \frac{\alpha}{1-\alpha} k^{-1} \left( \frac{n}{n-\varphi} \right) R + c \left( \frac{\alpha}{1-\alpha} \right)^2 k^{-2} \left( \frac{n}{n-2\varphi} \right)^T = 1
\]

which implies

\[
c = 1/ \left( 1 + \frac{\alpha}{1-\alpha} k^{-1} \left( \frac{n}{n-\varphi} \right) R + \left( \frac{\alpha}{1-\alpha} \right)^2 k^{-2} \left( \frac{n}{n-2\varphi} \right)^T \right).
\]

If now

\[
\tilde{y}_0 = \tilde{y}
\]

\[
\tilde{y}_1 = \sum_{i=1}^{n} \left( \frac{R - R_i}{(n-\varphi)R} \right) y_i
\]

\[
\tilde{y}_2 = \frac{1}{\sum_{i=1}^{n} \left( \frac{T - \sum_{j=1}^{n} T_{i,j}}{(n-2\varphi)T} \right) y_i}
\]

we can write the posterior mean as

\[
\frac{1}{1 + \frac{\alpha}{1-\alpha} k^{-1} \left( \frac{n}{n-\varphi} \right) R + \left( \frac{\alpha}{1-\alpha} \right)^2 k^{-2} \left( \frac{n}{n-2\varphi} \right)^T} \tilde{y}_0 + \frac{\frac{\alpha}{1-\alpha} k^{-1} \left( \frac{n}{n-2\varphi} \right) R}{1 + \frac{\alpha}{1-\alpha} k^{-1} \left( \frac{n}{n-\varphi} \right) R + \left( \frac{\alpha}{1-\alpha} \right)^2 k^{-2} \left( \frac{n}{n-2\varphi} \right)^T} \tilde{y}_1
\]
Again, let 
\[ G = \frac{\alpha}{1-\alpha} \frac{1}{k} \]
and
\[ Q_0 = \frac{1}{1 + G\left(\frac{n}{n-\phi}\right) + G^2\left(\frac{n}{n-2\phi}\right)} \]
\[ Q_1 = \frac{G\left(\frac{n}{n-2\phi}\right)}{1 + G\left(\frac{n}{n-\phi}\right) + G^2\left(\frac{n}{n-2\phi}\right)} \]
\[ Q_2 = 1 - Q_0 - Q_1 \]
the posterior mean is then a weighted average of three estimators,
\[ Q_0\tilde{Y}_0 + Q_1\tilde{Y}_1 + Q_2\tilde{Y}_2 \]
where \( \tilde{Y}_i \) is the conditional posterior mean given that there are exactly \( i \) bad values and \( Q_i \) is the posterior probability that there are \( i \) bad values.

Generalization to the case of \( \lambda \)-bad values is not difficult but is tedious. In general, however,

1. The posterior mean for \( \lambda \)-outliers is a weighted average
\[ Q_0\tilde{Y}_0 + \ldots + Q_\lambda\tilde{Y}_\lambda \]
of \( \lambda+1 \) estimators where \( \tilde{Y}_i \) is the conditional posterior mean given that there are exactly \( i \) bad values and \( Q_i \) is the posterior probability of \( i \) bad values.

-32-
(2) If \( k \) is large then \( \phi \) can be taken to be 1 and \( G \) is the only parameter to be determined in advance in the model.

(3) Each \( \tilde{Y}_i \) itself is a weighted average with the weight for the \( j \)-th observation heavily dependent on the series of quantity

\[
\left\{ 1 + \frac{\phi}{n-1} r_{j_{j_1} \ldots j_{i-1}} \left( \begin{array}{ccc} \frac{n-\phi}{n} & \cdots & \frac{-\phi}{n} \\ \vdots & \ddots & \vdots \\ \frac{\phi}{n} & \cdots & \frac{n-\phi}{n} \end{array} \right) \right\}^{\frac{1}{2}(n-1)}
\]

\[
= \left\{ 1 + \frac{\phi}{n-1} \left( r_{j_{j_1} \ldots j_{i-1}}^j + r_{j_{j_1} \ldots j_{i-1}}^{j_1} + \ldots + r_{j_{j_1} \ldots j_{i-1}}^{j_{i-1}} \right) \right\}^{\frac{1}{2}(n-1)}
\]

for all possible combinations of \( j_1, j_2, \ldots, j_{i-1} \).

In this expression, \( r_{j{j_1} \ldots j_{i-1}} \) is the residual vector for observations \( y_j, y_{j_1}, \ldots, y_{j_{i-1}} \) calculated from the estimate where these observations are down weighted. If the \( j \)-th observation itself is a bad value, then (6.8) will always be large since \( r_{j{j_1} \ldots j_{i-1}}^j \) will be large. When \{\( y_j, y_{j_1}, \ldots, y_{j_{i-1}} \)\} are exactly the \( i \) bad values in the sample, the above quantity reaches its maximum. This will result in a small weight for the \( j \)-th observation. If the \( j \)-th
observation is not a bad value then no matter how we choose $i_1, \ldots, i_{i-1}$, the expression (6.8) will never reach its maximum and so the weight given to the $j$-th observation will not be very small.

(4) Equation (6.8) is a direct extension of (6.7). From the form of (6.7), it is seen that, if the absolute values of $r_{ij}^1$ and $r_{ij}^2$ were fixed, the value of (6.7) would be larger when they were both positive or both negative and smaller when they had opposite signs. This implies that if there are two bad values in a sample, these bad values will have less weight if they fall on different sides of the mean and more weight if they fall on the same side. For the case of 2 bad values, similarly, equation (6.8) indicates that the bad values will have less weight if they are equally spread on both sides of the mean and more weight if more of them are concentrated on the same side.

**Example: Darwin's Data**

We illustrate how observations are weighted in such a Bayesian analysis using Darwin's data concerning fifteen differences of the heights of cross- and self-fertilized plants quoted by Fisher (1960, p 37). Our interest here will be to examine more closely the weighting structure of the Bayesian posterior mean, and to further develop the analysis of Box and Tiao (1965).
The data consist of measurements on 15 pairs of plants, each pair contained a self-fertilized and a cross-fertilized plant grown in the same pot. The 15 differences $y_i$ were recorded in Table 2 in ascending order.

<table>
<thead>
<tr>
<th>$y_1$</th>
<th>$y_2$</th>
<th>$y_3$</th>
<th>$y_4$</th>
<th>$y_5$</th>
<th>$y_6$</th>
<th>$y_7$</th>
<th>$y_8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-67</td>
<td>-48</td>
<td>6</td>
<td>8</td>
<td>14</td>
<td>16</td>
<td>23</td>
<td>24</td>
</tr>
<tr>
<td>$y_9$</td>
<td>$y_{10}$</td>
<td>$y_{11}$</td>
<td>$y_{12}$</td>
<td>$y_{13}$</td>
<td>$y_{14}$</td>
<td>$y_{15}$</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>29</td>
<td>41</td>
<td>49</td>
<td>56</td>
<td>60</td>
<td>75</td>
<td></td>
</tr>
</tbody>
</table>

**Table 2 Darwin's Data**

Inspection of the data indicates that two observations -67 and -48 are remote from the rest. We shall assume there are at most two bad values in the sample and $k = 5$. Then the posterior mean 

$$\hat{\theta} = Q_0 \tilde{Y}_0 + Q_1 \tilde{Y}_1 + Q_2 \tilde{Y}_2.$$  

Applying these results to Darwin's data we find that $\tilde{Y}_0 = 20.97$.

To calculate $\tilde{Y}_1$, we need $r_i$ - the standardized residual, $R_i$, R and $\frac{R_0 - \Phi R_i}{(n - \Phi)R}$ - the weight $\tilde{Y}_1$ puts on the i-th observation. These values are given in Table 4.3 resulting in the value 

$$\tilde{Y}_1 = 24.65.$$
Table 3 Necessary information for calculating $\bar{y}_1$

Note that $R_1$ is very insensitive to $r_i$ when $|r_i|$ is between zero and one and dramatically increases when $|r_i|$ becomes larger. For this sample $R_1$ is much larger than the others and results in a small weight for $y_1$.

The calculation of $\bar{y}_2$ is more complicated; we need $r_{ij}$, $r_{ij}$, $T_{ij}$, $T_i$, and $\sum_{j=1}^{n} T_{ij}$. Table 4 gives all the relevant quantities. Since, by symmetry $T_{ij} = T_{ji}$, we use the upper
right half of the table to record \( r_{ij}^i, r_{ij}^j, T_{ij} \) and \( \hat{\theta}_{ij} \),

and the lower left half to record \((r_{ij}^i)^2, (r_{ij}^j)^2, (r_{ij}^i + r_{ij}^j)^2\)

and \( A_{ij} = 1 - \frac{\phi}{n-1} ((r_{ij}^i)^2 + (r_{ij}^j)^2 - \frac{\phi}{n} (r_{ij}^i + r_{ij}^j)^2) \). Their corresponding positions are explained at the bottom of Table 4.

For each \( i \), \( \sum_{j=1}^{n} T_{ij} \) is given in the last row and \( T \) is shown at the lower right corner. From these quantities, one can then calculate \( T - \frac{\phi}{n-1} \sum_{j \neq i} T_{ij} \)

\[
\frac{T - \phi \sum_{j=1}^{n} T_{ij}}{(n-2\phi)^{\frac{1}{2}}}, \quad \text{the weight applied to the } i\text{-th observation (Table 5) and } \tilde{Y}_2 = 30.74.
\]

<table>
<thead>
<tr>
<th>( i )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y_i )</td>
<td>-67</td>
<td>-48</td>
<td>6</td>
<td>8</td>
<td>14</td>
<td>16</td>
<td>23</td>
<td>24</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( i )</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y_i )</td>
<td>28</td>
<td>29</td>
<td>41</td>
<td>49</td>
<td>56</td>
<td>60</td>
<td>75</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( i )</th>
<th>0.007</th>
<th>0.017</th>
<th>0.075</th>
<th>0.075</th>
<th>0.075</th>
<th>0.075</th>
<th>0.075</th>
<th>0.075</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y_i )</td>
<td>0.075</td>
<td>0.075</td>
<td>0.075</td>
<td>0.075</td>
<td>0.075</td>
<td>0.075</td>
<td>0.073</td>
<td></td>
</tr>
</tbody>
</table>

Table 5: The weight applied to each observation in \( \tilde{Y}_2 \)
We again noticed that \( T_{ij} \) which is proportional to the inverse of a ordinate at \( (r_{ij}^1, r_{ij}^j) \) is not sensitive to \( r_{ij}^1 \) and \( r_{ij}^j \) when they are both between zero and one. But they increase at a very fast rate if either one gets large (over 1.5, say), and even faster if both are large. In Table 4 \( T_{15j} \) is larger than average for all \( j \) since the standardized residuals \( (r_{15j})'s \) are all larger than 1.5. \( T_{2j} 's \) are even larger but still not as dramatically large as \( T_{1j} \) for all \( j \). And the dominating term is really \( T_{12} \) where both \( r_{12}^1 \) and \( r_{12}^2 \) are large. Under such circumstances, \( \sum_{j=1}^{n} T_{1j} \) and \( \sum_{j=1}^{n} T_{2j} \) are much larger than all other \( \sum_{j=1}^{n} T_{ij} \) since they are the only two which include \( T_{12} \) in the summation. This results in the small weights for \( y_1 \) and \( y_2 \) in Table 5.

So far we have \( \bar{Y}_0 = 20.93, \bar{Y}_1 = 24.65, \bar{Y}_2 = 30.74 \) and furthermore we can calculate:

\[
Q_0 = \frac{1}{1 + G \cdot 61.04 + G^2 \cdot 4720.35} \quad G = \frac{\alpha}{1-\alpha} \frac{1}{k}
\]

\[
Q_1 = \frac{G \cdot 61.04}{1 + G \cdot 61.04 + G^2 \cdot 4720.35}
\]

\[
Q_2 = \frac{G^2 \cdot 4720.35}{1 + G \cdot 61.04 + G^2 \cdot 4720.35}
\]
The values taken by $Q_0$, $Q_1$, $Q_2$ depend on $R$, $T$ and $G$. The larger $G$ and $T$ are, the larger $Q_2$ will be, the larger $R$ is, the larger $Q_1$ will be. Since $R$ and $T$ are fixed once observations are obtained, and $k$ is fixed at 5 for this example, the only thing we can change now is $\alpha$ (or $G$). Table 6 gives $Q_0$, $Q_1$, $Q_2$ and posterior mean $Q_0 \bar{y}_0 + Q_1 \bar{y}_1 + Q_2 \bar{y}_2$ for different $\alpha$ (or $G$) values.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>.01</th>
<th>.05</th>
<th>.10</th>
<th>.20</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G$</td>
<td>.002</td>
<td>.011</td>
<td>.022</td>
<td>.050</td>
</tr>
<tr>
<td>$Q_0$</td>
<td>.875</td>
<td>.462</td>
<td>.213</td>
<td>.063</td>
</tr>
<tr>
<td>$Q_1$</td>
<td>.108</td>
<td>.297</td>
<td>.289</td>
<td>.193</td>
</tr>
<tr>
<td>$Q_2$</td>
<td>.017</td>
<td>.242</td>
<td>.497</td>
<td>.744</td>
</tr>
</tbody>
</table>

$Q_0 \bar{y}_0 + Q_1 \bar{y}_1 + Q_2 \bar{y}_2 \quad 21.50 \quad 24.41 \quad 26.89 \quad 28.95$

Table 6 $Q_0$, $Q_1$, $Q_2$ and posterior means for different $\alpha$ (or $G$) values.

It is seen that different choices of $\alpha$, and hence of $G$, greatly influence the value of $Q_1$ and hence change the emphasis on $\bar{y}_0$, $\bar{y}_1$, and $\bar{y}_2$, leading in this example to different results.

When there are no bad values or very obvious bad values, the results are not particularly sensitive to the choice of $\alpha$. In practice, it may be worthwhile to actually run the analysis on the computer and change the value of $\alpha$ (or $G$). Estimates which are
very sensitive to different choices of $\alpha$ (or $C$) indicate strongly, as in this example, the presence of bad values.

**Empirical Study of the Dependency of the Posterior Mean on $G$**

Recall we concluded that $G$ is the only important parameter the results depend on when $k$ is large. In the case of one bad value, we have shown that this is generally true for $k \geq 5$. For the general case of $\lambda$ bad values, we believe this is still true but we probably will need a larger $k$.

Box and Tiao listed posterior means for Darwin's data with different choices of $\alpha$ and $k$; from these we can calculate $G$ corresponding to each posterior mean, as shown in Table 7.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$k$</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
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</thead>
<tbody>
<tr>
<td>0.01</td>
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<td>21.50</td>
<td>21.45</td>
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<td>21.35</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>(.0020)</td>
<td>(.0017)</td>
<td>(.0014)</td>
<td>(.0013)</td>
<td>(.0011)</td>
<td>(.0010)</td>
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<tr>
<td>0.02</td>
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<td>21.79</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>(.0041)</td>
<td>(.0034)</td>
<td>(.0029)</td>
<td>(.0026)</td>
<td>(.0023)</td>
<td>(.0020)</td>
</tr>
<tr>
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<td></td>
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<td>(.0039)</td>
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<td>(.0071)</td>
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<td>(.0125)</td>
<td>(.0108)</td>
<td>(.0094)</td>
<td>(.0084)</td>
<td>(.0075)</td>
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<td>(.0165)</td>
<td>(.0141)</td>
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<td>(.0110)</td>
<td>(.0099)</td>
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<td>(.0185)</td>
<td>(.0159)</td>
<td>(.0139)</td>
<td>(.0123)</td>
<td>(.0111)</td>
</tr>
</tbody>
</table>

Table 7 The posterior mean for Darwin's data with different $\alpha$ and $k$ and the corresponding $G$ given in the bracket under the posterior mean.
It is clear from the table that for fixed $G$, the posterior means are in general not too different, for example,

<table>
<thead>
<tr>
<th>$G$</th>
<th>$(\alpha, k)$</th>
<th>Mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>.0111</td>
<td>($0.10, 10.0$)</td>
<td>25.85</td>
</tr>
<tr>
<td>.0110</td>
<td>($0.09, 9.0$)</td>
<td>25.69</td>
</tr>
<tr>
<td>.0109</td>
<td>($0.08, 8.0$)</td>
<td>25.49</td>
</tr>
<tr>
<td>.0108</td>
<td>($0.07, 7.0$)</td>
<td>25.24</td>
</tr>
<tr>
<td>.0106</td>
<td>($0.06, 6.0$)</td>
<td>24.90</td>
</tr>
<tr>
<td>.0105</td>
<td>($0.05, 5.0$)</td>
<td>24.41</td>
</tr>
</tbody>
</table>

But there is a systematic change as $k$ decreases indicating the dependency on $k$. It is also seen that such a change is smaller when $k$ is larger. For this example, it seems that we need to have $k$ at least as large as 7 for the results to be essentially dependent on $G$.

In general, this property would depend on the ratio

\[
\frac{\text{number of bad values}}{\text{number of observations}}.
\]

The larger this ratio is, the larger $k$ must be for $G$ to be the dominant parameter.

**The $2^2$ Factorial Design**

It is much more difficult to obtain results in terms of weighting as soon as we deal with more complicated designs. As a simple example, consider the $2^2$ factorial design with the linear model

\[
Y = X\theta + \varepsilon
\]

where
If we assume there is at most one bad value, we can obtain the posterior mean as follows:

Let \( p = \frac{1}{k^2} \)

\( \hat{\theta}(0) = \) posterior mean given there are no bad values

\[
\begin{bmatrix}
 y_1 + y_2 + y_3 + y_4 \\
 -y_1 + y_2 + y_3 + y_4 \\
 -y_1 - y_2 + y_3 + y_4
\end{bmatrix}
\]

\( \hat{\theta}(1) = \) the conditional posterior mean given that \( y_1 \) is a bad value

\[
\begin{bmatrix}
 \frac{2}{6p+2} \left[ 2py_1 + (p+1)y_2 + (p+1)y_3 + 2py_4 \right] \\
 -2py_1 + 2py_2 - (p+1)y_3 + (p+1)y_4 \\
 -2py_1 - (p+1)y_2 + 2py_3 + (p+1)y_4
\end{bmatrix}
\]

\( \hat{\theta}(2) = \) the conditional posterior mean given that \( y_2 \) is a bad value

\[
\begin{bmatrix}
 \frac{1}{6p+2} \left[ (p+1)y_1 + 2py_2 + 2py_3 + (p+1)y_4 \right] \\
 -2py_1 + 2py_2 - (p+1)y_3 + (p+1)y_4 \\
 -(p+1)y_1 - 2py_2 + (p+1)y_3 + 2py_4
\end{bmatrix}
\]
\( \hat{\theta}(3) = \) the conditional posterior mean given that \( y_3 \) is a bad value
\[
\frac{1}{6p+2} \left[ (p+1)y_1 + 2py_2 + 2py_3 + (p+1)y_4 \\
- (p+1)y_1 + (p+1)y_2 + 2py_3 + 2py_4 \\
- 2py_1 -(p+1)y_2 + 2py_3 + (p+1)y_4 \right]
\]

\( \hat{\theta}(4) = \) the conditional posterior mean given that \( y_4 \) is a bad value
\[
\frac{1}{6p+2} \left[ 2py_1 + (p+1)y_2 + (p+1)y_3 + 2py_4 \\
- (p+1)y_1 + (p+1)y_2 - 2py_3 + 2py_4 \\
- (p+1)y_1 - 2py_2 + (p+1)y_3 + 2py_4 \right]
\]

and from (5.10) we have

\( w_i = \) the posterior probability that the \( i \)-th observation is a bad value
\[
= c \frac{\alpha}{1-\alpha} \frac{1}{k} \frac{8}{(4-\phi)^3-3(4-\phi)-2} \{1 + \phi r_1 (1 - \frac{3}{4} \phi) r_1^{1/2} \}
\]

\( = c \frac{\alpha}{1-\alpha} \frac{1}{k} \frac{8}{(4-\phi)^3-3(4-\phi)-2} \{1 + \phi (1 - \frac{3}{4} \phi) r_1^{1/2} \} \).

The quantity \( w_0 \) is the posterior probability that there are no bad values and is equal to \( c \). Then,

the posterior mean = \( \frac{1}{4} \sum_{i=0}^{4} w_i \hat{\theta}(i) \).

To see how this posterior mean weights each observation, we write the posterior mean as
\[
\begin{pmatrix}
1 & 1 & 1 \\
-1 & +1 & -1 +1 \\
-1 & -1 & +1 \\
\end{pmatrix}
\begin{pmatrix}
v_1^{-1} & 0 & 0 \\
v_2^{-1} & 0 & 0 \\
v_3^{-1} & 0 \\
\end{pmatrix}
\begin{pmatrix}
1 & -1 & -1 \\
1 & +1 & -1 +1 \\
1 & -1 & +1 \\
\end{pmatrix}
\begin{pmatrix}
v_1^{-1} & 0 & 0 \\
v_2^{-1} & 0 & 0 \\
v_3^{-1} & 0 \\
\end{pmatrix}
\begin{pmatrix}
y_1 \\
y_2 \\
y_3 \\
\end{pmatrix}
\]

then \(v_i^{-1}\) is the weight applied to the \(i\)-th observation in this Bayesian procedure.

By equating the above formula with the posterior mean, we can solve for \(v_i^{-1}\) and we have

\[v_1^{-1} = \frac{1}{(4-4w_1-w_0)p+4w_1+w_0}\]
\[v_2^{-1} = \frac{1}{(4-4w_2-w_0)p+4w_2+w_0}\]
\[v_3^{-1} = \frac{1}{(4-4w_3-w_0)p+4w_3+w_0}\]
\[v_4^{-1} = \frac{1}{(4-4w_4-w_0)p+4w_4+w_0}\]

Since \(p = \frac{1}{k^2}\) which is usually small, we can approximate \(p\) by zero and have approximately

\[v_1^{-1} \approx \frac{1}{4w_1+w_0}\]
\[v_3^{-1} \approx \frac{1}{4w_3+w_0}\]
\[v_2^{-1} \approx \frac{1}{4w_2+w_0}\]
\[v_4^{-1} \approx \frac{1}{4w_4+w_0}\]

The results are not surprising because we would expect that the weight given to the \(i\)-th observation would be small, if the posterior probability indicates that the \(i\)-th observation is bad.
For the general linear model where we do not have orthogonality, no general interpretative results of the kind possible for simple cases occur. However, of course, the Bayesian procedure described by Box and Tiao (1968) can still be carried through.

8. Summary

The Bayesian procedure proposed by Box and Tiao (1968) has been studied in further detail. We conclude that

(i) The posterior probability that a particular set of observations is discordant depends on the inverse of the multivariate-t ordinate of the standardized residuals corresponding to those observations.

(ii) In the location case, the posterior mean can be written as \( Q_0 \bar{Y}_0 + Q_1 \bar{Y}_1 + \ldots + Q_2 \bar{Y}_2 \) if we assume at most 2 bad values present. The quantity \( \bar{Y}_i \) is the posterior mean given that there are \( i \) bad values and does not involve \( \alpha \). The quantity \( Q_i \) is the posterior probability of \( i \) bad values which involves both \( \alpha \) and \( k \).

(iii) If \( k \) is large enough so that \( \phi \) is approximately one, \( \bar{Y}_i \) does not depend heavily on \( k \), and \( Q_i \) depends almost exclusively on \( G = \frac{\alpha}{1-\alpha} \frac{1}{k} \). Thus, as an approximation, one can talk about this procedure in terms of one parameter \( G \) only. For this to be true in the location
case where there is only one bad value in a sample of size 10, simulation shows that $k$ must be larger than five. As the number of bad values becomes larger relative to the sample size, a larger $k$ value seems to be needed.

(iv) Bad values are given less weight if they are more evenly spread on both sides of the location parameter and more weight if they are more concentrated on either one side.

(v) For a $2^2$ factorial design, it is shown one can also write the posterior mean in a weighted least square form. In this case, the weight for the $i$-th observation is approximately proportional to $\frac{1}{4w_i + w_0}$. 
References


FURTHER STUDY OF ROBUSTIFICATION VIA A BAYESIAN APPROACH

The Bayesian outlier procedure discussed by Box and Tiao (1968) which uses the contaminated normal model is further explored in this report. For a simple location estimate suggested by their method, the weight given each observation is expressed explicitly in terms of standardized residuals so allowing comparison with M-estimators.