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Influence Assessment in Robust Regression

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Abstract

Robust regression based on M-estimator reduces and/or bounds the influence of outliers in the y-direction only. Therefore, when several influential observations exist, diagnostics in the robust regression is required in order to detect them. In this paper, we propose influence diagnostics in the robust regression based on M-estimator and its one-step version. Noting that M-estimator can be obtained through iterative weighted least squares regression by using internal weights, we apply the weighted least squares (WLS) regression diagnostics to robust regression.

1. Introduction

Robust regression is designed to reduce or bound the influence of outlying responses that often occur when sampling from symmetric long-tailed distributions. This approach tries to set up a regression procedure that is not so strongly affected by outliers and therefore is more stable than ordinary least squares (OLS) regression. Regression diagnostics and robust regression really have the same goal, only are in the opposite order: When using regression diagnostic tools, one first tries to delete the outliers and then to fit a regression model to the good data by OLS, whereas a robust analysis first tries to fit a regression model to the majority of the data and then to discover the outliers as those observations which possess large residuals from the fit. For a review of robust regression estimators and the related literatures, see Rousseeuw and Leroy (1987, Chapter 1).

The weighted least square (WLS) model is given by

$$Y = X\beta + \varepsilon, \tag{1.1}$$

where Y is an $n\times 1$ vector of dependent observations, X is an $n\times p'$ full column rank matrix of known explanatory variables possibly including a constant predictor, β is a $p'\times 1$ vector of unknown parameters to be estimated, and error term ε is an $n\times 1$ vector of independent random errors with zero mean and unknown variance $\mathrm{Var}(\varepsilon) = \sigma^2 D_w^{-1}$ and D_w

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is a known $n \times n$ diagonal matrix with $w_{ii} > 0$. The w_{ii} are often called case weights.

In fitting the multiple linear regression model (1.1) by the method of WLS, the WLS estimato r $\widehat{\beta}_w$ is obtained by minimizing $\sum w_i(y_i - x_i^T\beta)^2$. We have

$$\widehat{\beta}_w = (X^TD_wX)^{-1}X^TD_wY.$$

Let $\widehat{\beta}_{w(i)}$ denote the *WLS* estimator computed without the ith observation. Then

$$\widehat{\beta}_{w(i)} = \widehat{\beta}_w - \frac{w_i(X^TD_wX)^{-1}x_ie_{w,i}}{1 - w_ih_{w,ii}}, \tag{1.2}$$

where $h_{w,ii} = x_i^T(X^TDX)^{-1}x_i$. The scalar form of weighted fitted value $\hat{Y}_w$, is

$$\hat{y}_{w,i} = x_i^T(X^TD_wX)^{-1}X^TD_wY = \sum_{j=1}^n w_jh_{w,ij}y_j \tag{1.3}$$

The elements of H_w, especially the diagonals element $h_{w,ii}$, play an important role in the technique of *WLS* regression diagonostics, which aim at discovering whether individual observations have unusually great influence on the weighted regression model. To illustrate the interpretation of $h_{w,ii}$, we examine how the weighted fitted value $\hat{y}_{w,i}$ changes when y_i varies. If we add an increment Δy_i to y_i, then y_i becomes, from equation (1.3),

$$\hat{y}_{w,i} + \Delta\hat{y}_{w,i} = \sum_{j=1}^n w_jh_{w,ij}y_j + w_ih_{w,ii}\Delta y_i. \tag{1.4}$$

Thus

$$\Delta\hat{y}_{w,i} = w_ih_{w,ii}\Delta y_i.$$

We see that the impact on $\hat{y}_{w,i}$ by the change in y_i is that change multiplied by w_i and $h_{w,ii}$. And we can interpret $w_ih_{w,ii}$ as the amount of leverage of the response value y_i on the corresponding value $\hat{y}_{w,i}$ by y_i. Therefore, we call them the high leverage points (Cook and Weisberg, 1982).

Also, we derive weighted version of Cook's distance

$$WC_i = \frac{(\widehat{\beta}_{w(i)} - \widehat{\beta}_w)^T(X^TD_wX)(\widehat{\beta}_{w(i)} - \widehat{\beta}_w)}{p'\widehat{\sigma}^2}, \tag{1.5}$$

and WC_i can also be written as

$$WC_i = \frac{(\hat{Y}_{(i)} - \hat{Y})^TD_w(\hat{Y}_{(i)} - \hat{Y})}{p'\widehat{\sigma}^2} = \frac{1}{p'}t_i^2\frac{w_ih_{w,ii}}{1 - w_ih_{w,ii}}, \tag{1.6}$$

where $\hat{Y}_{w(i)} = X\widehat{\beta}_{w(i)}$ is the vector of predicted values when $Y_{(i)}$ is regressed on $X_{(i)}$ in weighted least squares regression. Thus, WC_i can be interpreted as the weighted Euclidean distance between the two vectors of fitted values when the fitting is done by including or excluding the ith observation.

2. Case Deletion Scheme for M-estimator

The various influence diagnostics that rely on case-deletion are regarded as global influence measure since they are designed to measure total change at various corners of $\Omega = (0, 1)^n$, where n is the sample size. In this section, we discuss the global influence measure for robust regression.

In multiple linear regression model, M-estimator $\hat{\beta}$ is obtained by minimizing

$$\sum_i \rho\, [\, (y_i - x_i^T \beta\,) \,/\, \tilde{\sigma}\,]\,, \tag{2.1}$$

where $1 \times p'$ vector x_i^T is the explanatory vector of the ith observation, $\tilde{\sigma}$ is the robust estimate of scale parameter σ, and $\rho(\cdot)$ is a differentiable convex function. To minimize (2.1), taking the derivative of (2.1) with respect to β yields

$$\sum_i \psi\, [\, (y_i - x_i^T \beta\,) \,/\, \tilde{\sigma}\,] x_i \;=\; 0\,, \tag{2.2}$$

where $\psi(t) = \rho'(t)$. The M-estimator $\hat{\beta}_M$ is a solution of the equation (2.2). This solution can be obtained by using the Newton-Raphson method or Huber's method (Huber 1977). Also, setting $w(t) = \psi(t)\,/\,t$, the equation (2.2) yields

$$\sum_i w[\, (y_i - x_i^T \beta\,) \,/\, \tilde{\sigma}\,] x_i (y_i - x_i^T \beta\,) \;=\; 0\,, \tag{2.3}$$

and, letting $w[\, (y_i - x_i^T \beta\,) \,/\, \tilde{\sigma}\,] = w_i$, the equation (2.3) is written as

$$\Big(\sum_i w_i x_i x_i^T \Big) \beta \;=\; \sum_i w_i x_i y_i\,. \tag{2.4}$$

That is, $\hat{\beta}_M$ is obtained by iterating weighted least squares regression based on the internally occurred weights w_i. So it is called the reweighted least-squares method (Li 1985, Chapter 8).

Unfortunately, when the ith observation is omitted, the M-estimator $\hat{\beta}_M$ cannot be expressed by the already available quantities as in OLS regression. Thus, the M-estimator with the ith observation omitted, $\hat{\beta}_{M(i)}$, should be obtained by directly solving equations (2.2) or (2.4) with full iteration. Then the change is

$$\Delta \hat{\beta}_{M,i} \;=\; \hat{\beta}_M - \hat{\beta}_{M(i)}\,. \tag{2.5}$$

Because this change is a $p' \times 1$ vector, it must be normalized so that observations can be ordered in a meaningful way. That is,

$$RC_i \;=\; \frac{(\Delta \hat{\beta}_{M,i})^T (X^T D X)(\Delta \hat{\beta}_{M,i})}{p'\, \tilde{\sigma}^2}\,, \tag{2.6}$$

where $D = diag(w_1, \ldots, w_n)$, and

$$w_i = \psi'[\, (y_i - x_i^T \hat{\beta}_M) \,/\, \tilde{\sigma}\,] \,/\, [\, (y_i - x_i^T \hat{\beta}_M) \,/\, \tilde{\sigma}\,]\;.$$

3. Case Deletion Scheme using WLS Regression

As seen in (2.4), we can obtain the M-estimator $\hat{\beta}_M$ by using internal weights, like WLS estimator $\hat{\beta}_w$. The fully iterative estimator $\hat{\beta}_M$ in (2.4) is written as

$$\hat{\beta}_M = \hat{\beta}_w = (X^T D_w X)^{-1} X^T D_w Y. \tag{3.1}$$

Although the $\hat{\beta}_{w(i)}$ in (1.2) is not equivalent to $\hat{\beta}_{M(i)}$, we hope the difference in these estimators is insignificant. If so, we can substitute $\hat{\beta}_{w(i)}$ for $\hat{\beta}_{M(i)}$ for practical reasons. Therefore, using the updating formula, the $\hat{\beta}_{w(i)}$ yields

$$\hat{\beta}_{w(i)} = \frac{\hat{\beta}_w - w_i (X^T D_w X) x_i e_{w,i}}{1 - w_i h_{w,ii}}, \tag{3.2}$$

where $D_w = diag(w_1, \dots, w_n)$ and

$$w_i = \psi'[(y_i - x_i^T \hat{\beta}_M)/\tilde{\sigma}]/[(y_i - x_i^T \hat{\beta}_M)/\tilde{\sigma}].$$

Then the change is evaluated by

$$\Delta \hat{\beta}_{M,i} = \hat{\beta}_w - \hat{\beta}_{w(i)},$$

where $\hat{\beta}_w = \hat{\beta}_M$. The normalized change as the influence measure is

$$MC_i = \frac{(\Delta \beta_{M,i})^t (X^t D_w X)(\Delta \hat{\beta}_{M,i})}{p' \tilde{\sigma}^2}. \tag{3.3}$$

As a simple version of regresson M-estimator, the one-step Newton-Raphson approximation was introduced by Bickel (1975). He showed that under mild regularity conditions, this one-step estimator has the same asymptotic properties (consistency and normality) as the corresponding fully iterated M-estimator, provided that reasonably good preliminary estimates are used. Now we will derive the influence measure on the one-step estimator.

The weighted version of (2.1) is expressed by

$$\sum \omega_i \rho [(y_i - x_i^T \beta)/\tilde{\sigma}], \tag{3.4}$$

where ω_i are given external weights. Hence setting $\omega_1 = \cdots = \omega_n = 1$, the solution that minimizes (2.2) becomes $\hat{\beta}_M$, and it is used as the preliminary estimator for case deletion scheme.

Theorem 1. Let $\hat{\beta}^{(1)}_{M(i)}$ be the one-step estimator from the preliminary estimator $\hat{\beta}_M$ when the ith observation is omitted. That is, $\omega_i = 0$ and remaining external weights $\omega_j = 1 (j \neq i)$, then the Newton-Raphson one-step estimator is

$$\hat{\beta}^{(1)}_{M(i)} = \hat{\beta}_M - \frac{\tilde{\sigma}(X^T D_{\psi'} X)^{-1} x_i \psi_i}{(1 - \psi'_i k_{ii})}, \tag{3.5}$$

where $D_{\psi'} = diag(\psi'_1, \ldots, \psi'_n)$, ψ'_i is the first derivative of ψ_i,

$$\psi'_i = \psi'[(y_i - x_i^T\hat{\beta}_M)/\tilde{\sigma}], \quad \text{and} \quad k_{ii} = x_i^T(X^TD_{\psi'}X)x_i. \qquad \blacksquare$$

The proof is omitted to save the space. Readers may refer to the first author's doctoral thesis (Sohn 1994, pp. 49-50).

The change in these estimate and influence measure are, respectively,

$$\Delta\hat{\beta}^{(1)}_{M,i} = \hat{\beta}^{(1)}_{M} - \hat{\beta}^{(1)}_{M(i)} \tag{3.6}$$

$$OC_i = \frac{(\Delta\hat{\beta}^{(1)}_{M,i})^T(X^TD_{\psi'}X)^{-1}(\Delta\hat{\beta}^{(1)}_{M,i})}{p'\tilde{\sigma}^2}. \tag{3.7}$$

4. Case-Weight Perturbation Scheme

The influence graph provides a pictorial tool for the detection of influential observations. We will derive the local measure of influence on M-estimator and $\hat{\beta}^{(1)}_{M(\omega)}$ in (3.5) with respect to a selected external weight ω. The local influence is the rate of change around given external weight. We observe the change of $\hat{\beta}_M$ in (3.1) when the ith observation is perturbed by ω.

Theorem 2. Suppose that $\hat{\beta}_{M(\omega)}$ is the M-estimator when the ith observations are perturbed by ω. Setting $\omega_1 = \cdots = \omega_{i-1} = \omega_{i+1} = \cdots = \omega_n = 1$, setting $\omega_i = \omega$, then this estimator is

$$\hat{\beta}_{M(\omega)} = \hat{\beta}_M - \frac{(w_i - \omega)(X^TD_wX)^{-1}x_i\tilde{e}_i}{1-(w_i-\omega)\tilde{h}_{ii}}, \tag{4.1}$$

where $\tilde{e}_i = y_i - x_i^T\hat{\beta}_M$, $\tilde{h}_{ii} = x_i^T(XD_wX)^{-1}x_i$, $D_w = diag(w_1, \ldots, w_n)$, and

$$w_i = \psi_i[(y_i - x_i^T\hat{\beta}_M)/\tilde{\sigma}]/[(y_i - x_i^T\hat{\beta}_M)/\tilde{\sigma}]. \qquad \blacksquare$$

Readers may refer to Sohn (1994, pp. 52-53) for the proof.

Then the change between $\hat{\beta}_M$ and $\hat{\beta}_{M(\omega)}$ is

$$\Delta\hat{\beta}_{M(\omega),i} = \hat{\beta}_M - \hat{\beta}_{M(\omega)}, \tag{4.2}$$

and the influence measure is defined by

$$MC_{(\omega),i} = \frac{(\Delta\hat{\beta}_{M(\omega),i})^T(X^TD_wX)(\Delta\hat{\beta}_{M(\omega),i})}{p'\tilde{\sigma}^2} \tag{4.3}$$

For $\omega = 0$, $\hat{\beta}_{M(0)}$ is equivalent to $\hat{\beta}_{w(i)}$ in (3.2). To derive the change at the external weight ω or the local influence measure, we must obtain the derivative of $\widehat{\beta}_{M(\omega)}$ in (4.1) with respect to ω. That is,

$$\frac{\partial \widehat{\beta}_{M(\omega)}}{\partial \omega} = \frac{(X^T D_w X)^{-1} x_i \tilde{e}_i}{[1-(w_i - \omega)\tilde{h}_{ii}]^2} \tag{4.4}$$

$$\Delta LM_i = \left[\frac{\partial \widehat{\beta}_{M(\omega)}}{\partial \omega} \right]_{\omega = w_i} = (X^T D_w X)^{-1} x_i \tilde{e}_i \tag{4.5}$$

Because the (4.5) is a $p' \times 1$ vector, the normalization of the rate of this change is given by

$$LMC_i = \frac{(\Delta LM_i)^T (X^t D_w X)(\Delta LM_i)}{p' \tilde{\sigma}^2} = \frac{\tilde{h}_{ii} \tilde{e}_i^2}{p' \tilde{\sigma}^2}. \tag{4.6}$$

Let $\widehat{\beta}^{(1)}_{M(\omega)}$ be the one-step M-estimator when the ith observations are perturbed by ω. In Theorem 1, Setting $\omega_i = \omega$, we can derive the estimator $\widehat{\beta}^{(1)}_{M(\omega)}$ and influence measure for $\widehat{\beta}^{(1)}_{M(\omega)}$. That is,

$$\widehat{\beta}^{(1)}_{M(\omega)} = \widehat{\beta}_M - \tilde{\sigma} \frac{(1-\omega)(X^T D_{\psi'} X)^{-1} x_i \psi_i}{1-(1-\omega)\psi'_i k_{ii}} \tag{4.7}$$

$$OC_{(\omega),i} = \frac{(\Delta \widehat{\beta}^{(1)}_{M(\omega),i})^T (X^T D_w X)(\Delta \widehat{\beta}^{(1)}_{M(\omega),i})}{p' \tilde{\sigma}^2} \tag{4.8}$$

To derive local influence measure of $\widehat{\beta}^{(1)}_{M(\omega)}$, we need to differentiate $\widehat{\beta}^{(1)}_{M(\omega)}$ with respect to ω. That is

$$\frac{\partial \beta^{(1)}_{M(\omega)}}{\partial \omega} = \tilde{\sigma} \frac{(X^T D_{\psi'} X)^{-1} x \psi_i}{[1-(1-\omega)\psi'_i h_{ii}]^2} \tag{4.9}$$

Then the rate of the change around $\omega=1$ is

$$\Delta LO_i = \left[\frac{\partial \beta^{(1)}_{M(\omega)}}{\partial \omega} \right]_{\omega=1} = \tilde{\sigma} (X^T D_{\psi'} X)^{-1} x \psi_i \tag{4.10}$$

and the normalized rate of this change or the local influence measure is

$$LOC_i = \frac{(\Delta LO_i)^T (X^T D_{\psi'} X)(\Delta LO_i)}{p' \tilde{\sigma}^2}. \tag{4.11}$$

5. Influence Graph

In this section, we discuss the influence graph for each observation. The influence statistic C_i proposed by Cook (1977) can be expressed as the scaled Euclidean distance, that is,

$$C_i = \frac{\| \widehat{Y} - \widehat{Y}_{(i)} \|^2}{p' \widehat{\sigma}^2}. \tag{5.1}$$

Let $\hat{Y}_{\omega}$ be the vector of fitted values obtained when the ith observation has external weight ω. Then the more general version of C_i is

$$C_{(\omega),i} = \frac{\| \hat{Y} - \hat{Y}_{\omega} \|^2}{p' \hat{\sigma}^2}. \tag{5.2}$$

Cook (1986) proposed the influence graph that plot $p' C_{(\omega),i}$ versus external weight ω for each observation.

From the influence graph we can see that the influences of each observation are compared each other. In particular, even when $C_{(\omega),i} = C_{(\omega),j}$ for the ith and the jth observation in single case deletion scheme, we have a more complete understanding of the influence of single cases by investigating the behaviour of $C_{(\omega),i}$ at values other than ω=0. We may construct the influence graphs which plot LMC_i in (4.6) and LOC_i in (4.11) versus the external weight ω.

6. Numerical Example: Stack Loss Data

We will give a numerical example with Brownlee's stack loss data (Li 1985, Atkinson 1986) listed in Table 1, using various diagnostic methods in Sections 2, 3 and 4 in robust regression via Huber's ψ-function.

The stack loss data is obtained from 21 days of operation of a chemical plant that oxidizes ammonia(NH_3) to nitric acid(HNO_3). This data consists of three explanatory variables; X_1 =air flow, X_2 = temperature of the cooling water in the coils of the absorbing tower, X_3 = concentration of nitric acid in the absorbing liquid, and the response observation Y =percent of the ingoing ammonia that is lost by escaping in the absorbed nitric oxides.

We will try to diagnose robust regression when M-estimate is computed by Huber's ψ-function (with tunning constants k=2.0),

$$\psi(t) = \begin{cases} t, & \text{for } |t| \le k, \\ k\,sign(t), & \text{for } |t| > k. \end{cases} \tag{6.1}$$

The robust regression equation is

$$Y = -39.9898 + 0.8286 X_1 + 0.7638 X_2 - 0.1089 X_3. \tag{6.2}$$

With global influence measures in Table 2, we observe that observations 1, 3, 4 and 21 which are influential in OLS regression still remains strong and observation 2 ($w_{22}\, h_{22}$ = 0.4656) is a high leverage design point (see, Figure 1) and is also influential observation (see, Figure 2). Influence graphs (the plot of $MC_{(\omega),i}$ versus ω) in Figure 4 and Figure 5 show that observations 1, 3, 4, and 21 have larger influence than the others when observations are perturbed by a given external weight ω.

Huh and Park (1990) proposed the principal compontents plot of case influence derivatives and observed a fact that observations 1, 3 and 4 are jointly influential. That is, these observations are masking each other. To avoid the masking effect, we may use local influence LMC_i and LMC_i given in Table 2 and can assess the joint influence of masked observations.

From Figure 3, Figure 6 and Figure 7, observations 1, 2, 3, and 21 are identified as potentially influential. Table 3 shows that MC_i is closely correlated with $RC_i(\hat{\beta})$ and OC_i.

7. Conclusion

Robust regression by M-estimation can reduce or bound the influence of outliers only in the y-direction. Thus we proposed the assessment of case influences in robust regression using a robust regression version of Cook distance, RC_i. But RC_i may need too much computing time to be used in practice. In order to tackle this problem, we proposed severval alternative global influence measures and local influences based on M-estimator and one-step estimator. Also, we applied weighted least squares regression diagnostics to the robust regression problem. We conclude that our diagnostic tools are practical and effective in identifying influential observations in robust regression.

Table 1. Stack Loss Data

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
X_1	42	37	37	28	18	18	19	20	15	14	14	13	11	12	8	7	8	8	9	15	15
X_2	80	80	75	62	62	62	62	62	58	58	58	58	58	58	50	50	50	50	50	56	70
X_3	27	27	25	24	22	23	24	24	23	18	18	17	18	19	18	18	19	19	20	20	20
Y	89	88	90	87	87	87	93	93	87	80	89	88	82	93	89	86	72	79	80	82	91

Table 2. Influence Measures in Robust Regression by Huber's ψ-Function

Observation Number	Global				Local	
	$RC_i(\hat{\beta})$	$w_i h_{w,ii}$	MC_i	OC_i	LMC_i	LOC_i
1	0.8569	0.2074	0.7110	0.7186	2.0713	0.7186
2	3.1063	0.4654	0.3752	2.6327	0.1072	0.1716
3	0.5943	0.1056	0.3371	0.4414	1.7611	0.4414
4	0.2192	0.0422	0.1698	0.1984	2.1249	0.1984
5	0.0713	0.0654	0.0340	0.0512	0.0297	0.0421
6	0.1742	0.0881	0.1132	0.1252	0.1072	0.1252
7	0.2260	0.2416	0.1557	0.2020	0.0895	0.1043
8	0.0043	0.2416	0.0037	0.0047	0.0021	0.0024
9	0.2404	0.1634	0.1914	0.2424	0.1340	0.1580
10	0.0141	0.2298	0.0093	0.0139	0.0055	0.0070
11	0.1837	0.1884	0.1246	0.1597	0.0821	0.0967
12	0.1775	0.2735	0.1205	0.1748	0.0636	0.0776
13	0.2706	0.1463	0.2569	0.2409	0.3065	0.2409
14	0.0995	0.2261	0.1101	0.1203	0.0659	0.0697
15	0.3172	0.2029	0.3091	0.3514	0.1964	0.2135
16	0.0286	0.1403	0.0171	0.0195	0.0126	0.0139
17	0.1179	0.4285	0.1742	0.1964	0.0569	0.0596
18	0.0002	0.1718	0.0002	0.0002	0.0001	0.0002
19	0.0138	0.1976	0.0131	0.0151	0.0084	0.0093
20	0.0908	0.0838	0.0720	0.0837	0.0604	0.0685
21	0.7711	0.0901	0.5031	0.5799	8.9089	0.5799

Table 3. Correlations between Global Influence Measures

	$RC_i(\hat{\beta})$	OC_i	MC_i
$RC_i(\hat{\beta})$	1.00000	0.99781	0.56177
OC_i	0.99781	1.00000	0.55343
MC_i	0.56177	0.55343	1.00000

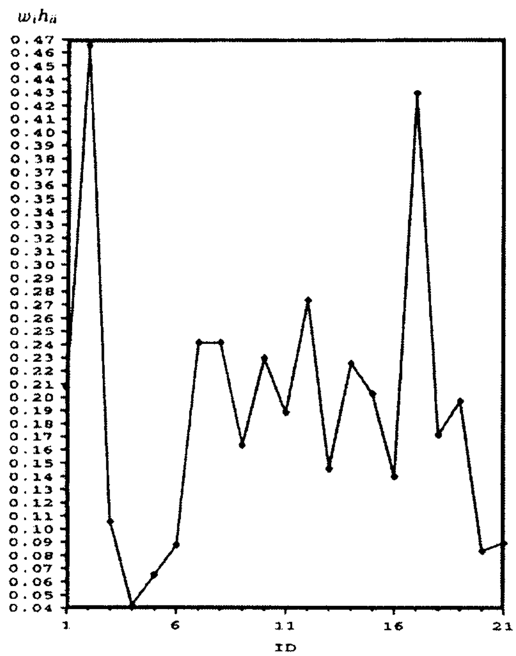

Figure 1. Index Plot of $w_i h_{ii}$

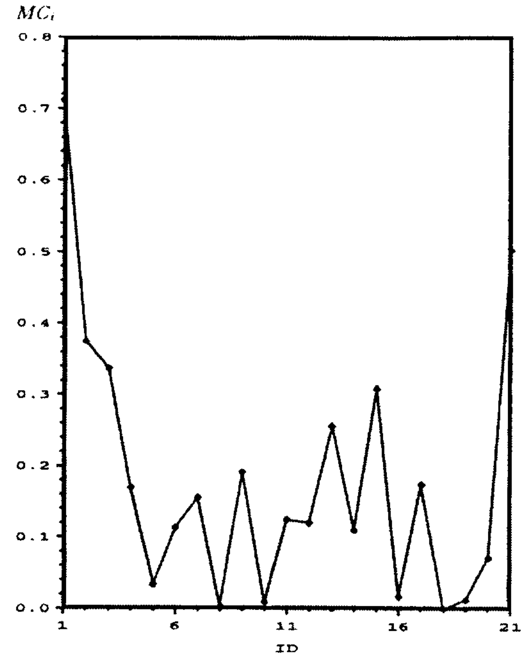

Figure 2. Index Plot of MC_i

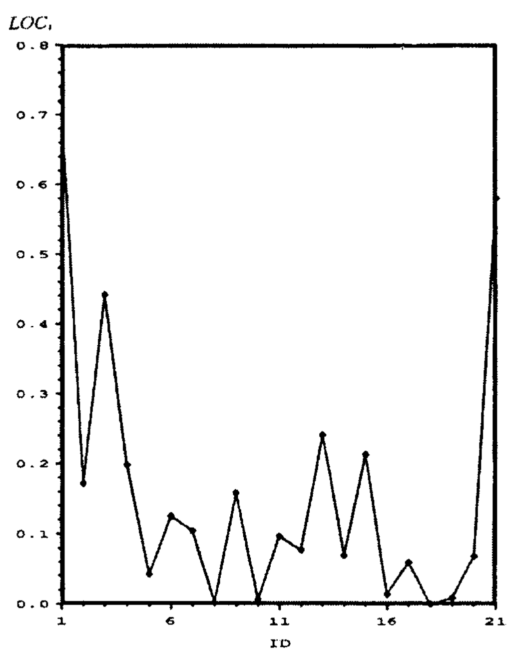

Figure 3. Index Plot of LOC_i

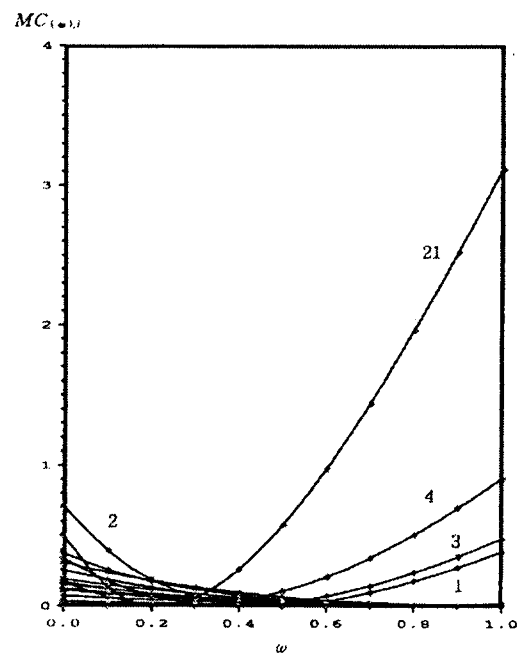

Figure 4. $MC_{(w),i}$ versus ω

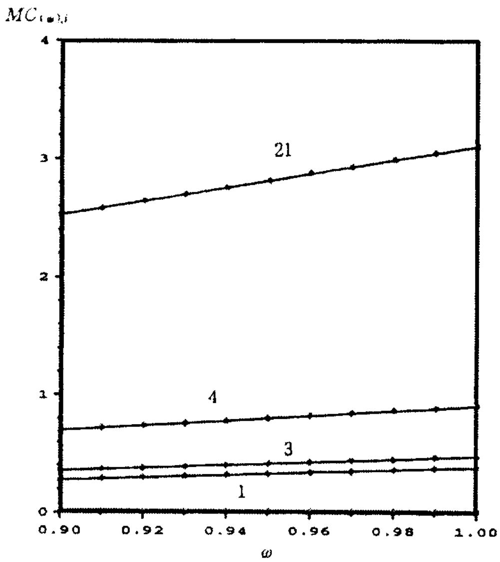

Figure 5. $MC_{(w),i}$ versus ω

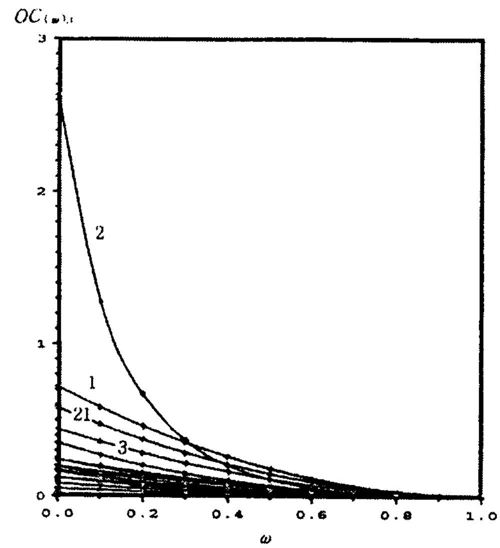

Figure 6. $OC_{(w),i}$ versus ω

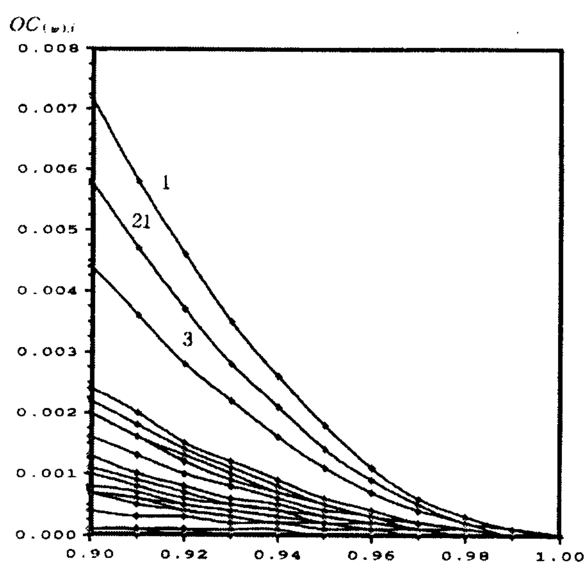

Figure 7. $OC_{(w),i}$ versus ω

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