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Comparison of MINQUE and LMVQUIE by Simulation *

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Abstract

The analytical expression for a density function of the minimum norm quadratic unbiased estimator (MINQUE) or of the locally minimum variance quadratic unbiased invariant estimator (LMVQUIE) of the variance components in the mixed linear model is unknown even if the observation vector is normally distributed. In comparison with the LMVQUIE which requires the knowledge of the third and fourth moments of the observation vector, the MINQUE not requiring it seems to be more suitable for practical purposes. Density functions induced by MINQUE and LMVQUIE from several basic distributions and differences between them are analyzed by the simulations. The theoretical variances of the LMVQUIE and the MINQUE are compared as well.

Key words: MINQUE, LMVQUIE, simulation.

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Introduction

Consider a general linear model in commonly used form $Y = X\beta + \varepsilon$, where Y is an *n*-dimensional random vector, X is a known $n \times k$ matrix with the rank r(X) = k < n, β is an unknown parameter, $\beta \in \mathbb{R}^k$ (k-dimensional Euclidean space) [3], [8]. The error vector ε has the mean value $E(\varepsilon) = 0$ and the covariance matrix $Var(\varepsilon) = \sum_{i=1}^{p} \vartheta_i V_i$. The symmetric $n \times n$ matrices V_i , $i = 1, \ldots, p$, are known and the *p*-dimensional vector $\vartheta = (\vartheta_1, \ldots, \vartheta_p)'$ of the variance components is unknown, $\vartheta \in \underline{\vartheta}$ (open set) $\subset \mathbb{R}^p$. The MINQUE of a linear function $g(\vartheta) = g'\vartheta, \vartheta \in \underline{\vartheta}, g = (g_1, \ldots, g_p)'$ being known, coincides with the LMVQUIE provided Y is normally distributed (cf. [10]).

The aim of the paper is to compare these two types of estimators under different distributions of the observation vector Y, characterized by their third and fourth moments.

1 Preliminaries

We shall use the results stated in [3] and [5].

Denote $\Sigma = \Sigma(\vartheta) = \sum_{i=1}^{p} \vartheta_i V_i$, $M = I - X(X'X)^{-1}X'$ (*I* being identical matrix), and consider an estimator of the function $g(\vartheta) = g'\vartheta$, $\vartheta \in \underline{\vartheta}$, in the form Y'AY, where A is a symmetric matrix.

The estimator Y'AY is unbiased iff X'AX = 0, $Tr(AV_i) = g_i$, i = 1, ..., p, (cf. [10]) and is regression invariant, i.e.

$$\forall \{\delta \in \mathbb{R}^k\} (Y + X\delta)' A (Y + X\delta) = Y' A Y$$

iff AX = 0 (cf. [10]).

As unbiasedness and invariance are preferable from the practical point of view, the class of estimators for the function $g(\vartheta) = g'\vartheta$, $\vartheta \in \underline{\vartheta}$, is considered in the form

$$\mathcal{A}_{g} = \{ Y'AY : A = A', \ AX = 0, \ Tr(AV_{i}) = g_{i}, \ i = 1, \dots, p \}.$$

The class \mathcal{A}_g is not empty if $g \in \mathcal{M}(C^{(I)})$ (the column space of the matrix $C^{(I)}$), where

$$\{C^{(1)}\}_{i,j} = Tr(MV_iMV_j), \quad i, j = 1, \dots, p.$$

If $C^{(I)}$ is regular, then there exists an unbiased invariant quadratic estimator for given $g \in \mathbb{R}^p$, i.e., for each variance component. In this case the matrix $S_{(M\Sigma M)^+}$ defined by

$$\{S_{(M\Sigma M)^+}\}_{i,j} = Tr[(M\Sigma M)^+ V_i(M\Sigma M)^+ V_j], \quad i,j = 1, \dots, p,$$

is regular and the ϑ_0 -MINQUE of the vector ϑ is

$$\hat{\vartheta} = S_{(M\Sigma_0 M)^+}^{-1} \kappa. \tag{1}$$

Here

$$\kappa = (\kappa_1, \dots, \kappa_p)', \kappa_i = Y'A_{i,M}Y = [vec(A_{i,M})]'Y^{2\otimes n}$$

where $vec(A_{i,M}) = (a'_1, \ldots, a'_n)'$, a_j is the *j*th column of the matrix $A_{i,M}$, $i = 1, \ldots, n, Y^{2\otimes}$ means $Y \otimes Y$, \otimes denotes the Kronecker multiplication (e.g. $(1, 2)' \otimes (a, b)' = (a, b, 2a, 2b)'$),

$$A_{i,M} = (M\Sigma_0 M)^+ V_i (M\Sigma_0 M)^+, \quad i = 1, \dots, p_i$$

 $(M\Sigma_0 M)^+$ is the Moore-Penrose g-inverse (a matrix A^+ is the Moore-Penrose g-inverse of a matrix A iff $AA^+A = A$, $A^+AA^+ = A^+$, $(AA^+)' = AA^+$, $(A^+A)' = A^+A$; cf. [9]) of the matrix $M\Sigma_0 M$. (The following relationship

$$(M\Sigma_0 M)^+ = \Sigma_0^{-1} - \Sigma_0^{-1} X (X'\Sigma_0^{-1} X)^{-1} X'\Sigma_0^{-1}$$

can be proved.)

Further

$$\Sigma_0 = \sum_{i=1}^p \vartheta_{0,i} V_i$$

 ϑ_0 is an a priori chosen parameter (as near to the actual value of ϑ as possible).

If Y is normally distributed, then ϑ_0 -MINQUE coincides with ϑ_0 -LMVQUIE of ϑ , i.e. with the quadratic unbiased and invariant estimator which possesses the smallest variance at ϑ_0 in the class of all unbiased and invariant quadratic estimators.

To find an efficient procedure of numerical evaluation of the LMVQUIE when the assumption of normality is not fulfilled, the following operations are introduced.

Let T be a symmetric $n \times n$ matrix whose (i, j)th element is $t_{i,j}$. Then

 $vech(T) = (t_{1,1}, \dots, t_{1,n}; t_{2,2}, \dots, t_{2,n}; \dots; t_{n-1,n-1}, t_{n-1,n}; t_{n,n})'$

is an n(n+1)/2-dimensional vector formed by the parts of the columns beginning at the main diagonal of the matrix T (i.e. the first element of the column is the diagonal element of the matrix T) and continued under the main diagonal of the matrix T.

Let A be a $p \times m^2$ matrix divided into m blocks. The first block is created by the first m columns, the second block by the following m columns, etc. The *j*th column in the *i*th block is denoted as $a_{i,j}$, i.e.

$$A = (a_{1,1}, \ldots, a_{1,m}; a_{2,1}, \ldots, a_{2,m}; \ldots; a_{m,1}, \ldots, a_{m,m}).$$

Then $p \times [m(m+1)/2]$ matrix (cC)(A) is defined as follows:

$$(cC)(A) = (a_{1,1}, a_{1,2} + a_{2,1}, \dots, a_{1,m} + a_{m,1}; a_{2,2}, a_{2,3} + a_{3,2}, \dots, a_{2,m} + a_{m,2}; \dots; a_{m-1,m-1}, a_{m-1,m} + a_{m,m-1}; a_{m,m})$$

and analogously for an $m^2 \times p$ matrix B the operation (cR)(.) is defined as (cR)(B) = [(cC)(B')]'.

Let Ψ denote the matrix of the fourth moments (cf. [3])

$$\Psi = E[(arepsilonarepsilon') \otimes (arepsilonarepsilon')] ext{ and } ilde V = [vec(V_1), \dots, vec(V_p)].$$

The following statement is valid [4], [5]:

If $C^{(I)}$ is regular, then the ϑ_0 -LMVQUIE of the vector ϑ is given by

$$\hat{\vartheta}^{(I)} = \left\{ [(cR)(X \otimes I)(cC)(X' \otimes I) + (cR)(\tilde{V})(cC)(\tilde{V}')]^{-}_{m[(cC)(cR)D^{(I)}_{2,2}]} \times (cR)(\tilde{V}) \right\}' (cR)(Y^{2\otimes}) \\
= \begin{pmatrix} Y'A_{1,L}Y \\ \vdots \\ Y'A_{p,L}Y \end{pmatrix} = \begin{pmatrix} (vech(A_{1,L}))' \\ \vdots \\ (vech(A_{p,L}))' \end{pmatrix} (cR)(Y^{2\otimes})$$
(2)

where

$$D_{2,2}^{(I)} = \Psi - vec[\Sigma(artheta_0)]\{vec[\Sigma(artheta_0)]\}' = \Psi - ilde{V}artheta_0artheta_0artheta'.$$

The symbol $B_{m(N)}^{-}$ denotes the minimum N-seminorm g-inverse of the matrix B; cf. [9].

In the following two symbols for an $n \times n$ matrix A will be used, i.e. diag(A) and Diag(A). The first one means the vector created by the diagonal of the matrix A and the other one means the matrix with the same diagonal as the diagonal of A and with other elements equals to zero. The notation $Diag(a_{1,1}, \ldots, a_{n,n})$ means the diagonal matrix with the diagonal given by the elements $a_{1,1}, \ldots, a_{n,n}$.

Let p = 1 and $V_1 = I$, i.e. $\Sigma = \sigma^2 I$. Then the following statement is due to Hsu [2]:

Proposition 1 Let $Y_i = \{Y\}_{i,1}$, i = 1, ..., n, be independent components of the observation vector Y, $\gamma_{2,i} = [E(\varepsilon_i^4)/\sigma^4] - 3$ and $\Gamma_2 = Diag(\gamma_{2,1}, ..., \gamma_{2,n})$.

(i) The estimator Y'MY/Tr(M) is Γ_2 -LMVQUIE of the parameter σ^2 iff

$$(M * M)diag(M) = \{[diag(M)]'\Gamma_2 diag(M)/Tr(M)\}diag(M),$$

where C * D denotes the Hadamard product of the matrices C and D, i.e. $\{C * D\}_{i,j} = \{C\}_{i,j} \{D\}_{i,j}$.

(ii) If Y_1, \ldots, Y_n are i.i.d. random variables, i.e. $\Gamma_2 = \gamma_2 I$, then Y'MY/Tr(M) is uniformly minimum variance quadratic unbiased invariant estimator of σ^2 iff

$$(M * M)diag(M) = \{[diag(M)]'diag(M)/Tr(M)\}diag(M).$$

In the following the quantity

$$\delta^2 = [(M * M)diag(M) - \lambda diag(M)]'[(M * M)diag(M) - \lambda diag(M)], \quad (3)$$

(where $\lambda = [diag(M)]'[diag(M)]/Tr(M)$) is used as a measure of a nonfulfilling the Hsu condition in the case (ii).

For several 5×1 design matrices X the corresponding values of δ^2 are given in Table 1.1.

Table 1.1Values of δ^2 (measure of nonfulfilling the Hsu condition)for different design matrices X

		X'			δ^2
(1,	5,	30,	90,	100)	 0.095613
(1,	2,	3,	4,	5)	 0.044313
(10,	20,	30,	40,	50)	 0.044313
(2,	4,	8,	16,	32)	 0.040692
(1,	1,	1,	1,	1)	 0.000000

2 Solution

Let the approximate density function of a random variable ε be given by the formula (Edgeworth series [1]):

$$f(x;\gamma_1,\gamma_2) = \phi(x;0,1)[1-(\gamma_1/6)(x^3-3x)+(\gamma/24)(x^4-6x^2+3)+ (\gamma_1^2/72)(x^6-15x^4+45x^2-15)]$$
(4)

where $\phi(x; 0, 1) = (1/\sqrt{2\pi})exp(-x^2/2)$, $x \in \mathbb{R}^1$ and $\gamma_1 = E(\varepsilon^3)/\sigma^3$, $\sigma^2 = Var(\varepsilon) = 1$, $\gamma_2 = [E(\varepsilon^4)/\sigma^4] - 3$.

This density is chosen from the following reason. The aim of the paper is to study the statistical behaviour of the mentioned quadratic estimators for different distributions. The most important among them is the normal distribution. The class of distributons given by (4) and parametrized by γ_1 and γ_2 contains the normal distributon (for $\gamma_1 = 0$ and $\gamma_2 = 0$) and thus it seems to be the most suitable for the first investigation.

Other distributions considered bellow (which differ essentially from the normal distribution) are:

the uniform distribution on the interval $\left[-\sqrt{3},\sqrt{3}\right]$ with density

$$r(x) = \begin{cases} 1/(2\sqrt{3}), & x \in [-\sqrt{3}, \sqrt{3}] \\ 0 & x \notin [-\sqrt{3}, \sqrt{3}], \end{cases}$$
(5)

i.e. $\sigma^2 = 1$, $\gamma_1 = 0$, $\gamma_2 = -1.2$; and the U-distribution with density

$$u(x) = \begin{cases} \frac{9\sqrt{3}x^2}{2.5\sqrt{2.5}}, & x \in [-\sqrt{5/3}, \sqrt{5/3}], \\ 0, & x \notin [-\sqrt{5/3}, \sqrt{5/3}], \end{cases}$$
(6)

i.e. $\sigma^2 = 1$, $\gamma_1 = 0$, $\gamma_2 = -1.80952$.

2.1 Case 1

Let $\varepsilon_1, \ldots, \varepsilon_5$ be i.i.d. random variables with $E(\varepsilon_i) = 0$, $Var(\varepsilon_i) = 1$, $i = 1, \ldots, 5$ and $Y = X\beta + \varepsilon$. In this case the MINQUE from (1) is given by Y'MY/Tr(M) (i.e. MINQUE is uniform with respect to γ_2) and

$$Var(\hat{\sigma}_{\text{MINQUE}}^{2}|\sigma^{2},\gamma_{2}) = [2\sigma^{4}/Tr(M)] + \gamma_{2}\sigma^{4}\sum_{i=1}^{5}[\{M/Tr(M)\}_{i,i}]^{2}.$$
 (7)

The $\gamma_2^{(0)}$ -LMVQUIE is $Y'A_{1,L}Y$, where $A_{1,L}$ from (2) is (cf. [7])

$$A_{1,L} = kM - (\gamma_2^{(0)}/2) M Diag(A_{1,L}) M,$$
(8)

$$k = 1/\{\mathbf{1}'[I + (\gamma_2^{(0)}/2)(M * M)]^{-1}diag(M), \\ diag(A_{1,L}) = k[I + (\gamma_2^{(0)}/2)(M * M)]^{-1}diag(M)$$

and 1 = diag(I). The variance of the $\gamma_2^{(0)}$ -LMVQUIE is

$$Var(\hat{\sigma}_{\text{LMVQUIE}}^{2}|\sigma^{2},\gamma_{2}) = 2\sigma^{4}Tr(A_{1,L}^{2}) + \gamma_{2}\sigma^{4}\sum_{i=1}^{5}[\{A_{1,L}\}_{i,i}]^{2}.$$
 (9)

For the greatest value $\delta^2 = 0.095613$ from Table 1.1. the variances (7), for different values $\gamma_2 \in [-2, 3]$ and the variances (9) of the $\gamma_2^{(0)}$ -LMVQUIEs with matrices $A_{1,L}$ from (8) for the same different values γ_2 are compared in Table 2.1.

Table 2.1

Variances of $\gamma_2^{(0)}$ -LMVQUIE and MINQUE in Case 1

LMVQUIE		a anti-t		~		
$\gamma_2^{(0)}$ γ_2	-2.00	-1.00	0.00	1.00	2.00	3.00
-2	0.000	0.923	1.845	2.768	3.690	4.613
-1.80952	0.012	0.314	0.617	0.919	1.221	1.524
-1.2	0.037	0.278	0.518	0.759	0.999	1.240
0	0.068	0.284	0.500	0.716	0.932	1.149
1	0.083	0.293	0.503	0.713	0.922	1.132
2	0.094	0.301	0.507	0.714	0.921	1.127
3	0.102	0.307	0.512	0.717	0.921	1.126
4	0.108	0.312	0.515	0.719	0.923	1.127
5	0.113	0.316	0.519	0.722	0.925	1.128
6	0.116	0.319	0.522	0.724	0.927	1.129
7	0.120	0.322	0.524	0.726	0.928	1.131
8	0.122	0.324	0.526	0.728	0.930	1.132
9	0.125	0.326	0.528	0.730	0.931	1.133
10	0.127	0.328	0.530	0.731	0.933	1.134
100	0.164	0.364	0.564	0.765	0.965	1.165
MINQUE	0.068	0.284	0.500	0.716	0.932	1.149

It is of some interest

(i) to compare the strong dependence of variances of $\gamma_2^{(0)}$ -LMVQUIE on γ_2 with a relatively weak dependence of variances of MINQUE on γ_2 and (ii) a striking increase of the variance of $\gamma_2^{(0)}$ -LMVQUIE at large values of γ_2 ($\gamma_2 > 0$) is caused by a choice of $\gamma_2^{(0)}$ different significantly from γ_2 ($\gamma_2^{(0)} < 0$).

The values $\gamma_2^{(0)}$ are chosen from interval [-2;100]. The value of σ^2 is 1 for both estimators and for all cases.

Fig. 2.1 illustrates the dependence of variances on the choice of $\gamma_2^{(0)}$ and on the actual values of γ_2 as given in Table 2.1.

Fig. 2.1 The dependence of variances of $\gamma_2^{(0)}$ -LMVQUIE on γ_2



If X' = (1, 1, 1, 1, 1), (classical location model) and $\delta^2 = 0$, i.e. if the Hsu condition is fulfilled [2], then $\hat{\sigma}^2 = Y'MY/Tr(M)$ is uniformly minimum variance quadratic unbiased and invariant estimator of σ^2 and its variance is

$$Var(\hat{\sigma}^2|\sigma^2,\gamma_2)=rac{2\sigma^4}{5-1}+rac{\gamma_2\sigma^4}{5}.$$

For $\sigma^2 = 1$ and $\gamma_2 = -1.80952; -1.2; 0; 1$, the values of variances are

A comparison of empirical densities of MINQUE and LMVQUIE obtained by simulation for X = (1, 2, 3, 4, 5)', (simple linear regression model passing through origin) $\gamma_1 = 0$ and for different γ_2 is given in Figs. 2.2b)-2.5b).

Data were simulated as follows. From 500 independently generated values ε from considered distributions ((6), (5), normal and (4) each with $\sigma^2 = 1$) hundred 5-dimensional vectors were created as a basis for the calculation of 100 estimates of both types. Due to the invariance of the considered estimators it was sufficient to simulate the data from the centered distributions.



Fig. 2.3
a) --- density function of Y according to (5); normal density
b) --- empirical density of \(\gamma_2^{(0)}\)-LMVQUIE; empirical density of MINQUE





Fig. 2.4

In the last case the reader can conclude that differences between distributions of MINQUE and LMVQUIE are (practically) negligible. It may be caused by the fact that the parameter γ_1 is equal to 0 in each of considered distributions.

2.2Case 2

Let $Y = X\beta + \varepsilon$, $Var(\varepsilon) = \vartheta_1 V_1 + \vartheta_2 V_2$. The variance of a random variable $Y'A_iY$, where $A_i = A'_i$, $A_iX = 0$, $E(Y'A_iY|\vartheta) = \vartheta_i$, i = 1, 2, is

$$Var(Y'A_iY|\vartheta,\Psi) = Tr[(A_i \otimes A_i)\Psi] - \vartheta_i^2.$$
⁽¹⁰⁾

a)

¹It is the same as MINQUE in this case

Let X = (1, 2, 3, 4, 5)', $V_1 = \begin{pmatrix} I_{3,3}, 0_{3,2} \\ 0_{2,3}, 0_{2,2} \end{pmatrix}$, $V_2 = \begin{pmatrix} 0_{3,3}, 0_{3,2} \\ 0_{2,3}, I_{2,2} \end{pmatrix}$ and $\vartheta_1 = 1$, $\vartheta_2 = 4$. The dependence of the variances (10) on the parameter γ_2 is illustrated in Table 2.2.

Table 2.2 Variances of LMVQUIE and MINQUE for ϑ_1 and ϑ_2 in Case 2

		$\gamma_2^{(0)}$ -1.2 0 1						MINQUE	
γ	2	ϑ_1	ϑ_2	ϑ_1	ϑ_2	ϑ_1	ϑ_2	ϑ_1	ϑ_2
-1	.2	0.408	23.577	0.504	23.683	0.521	23.788	0.504	23.683
0		0.964	24.677	0.937	24.503	0.942	24.531	0.937	24.503
1		1.361	25.593	1.298	25.196	1.292	25.180	1.298	25.196

 $A_{i,M}, A_{i,L}, i = 1, 2$, according to (1) and (2) were calculated for $\vartheta_1^{(0)} = 1$, $\vartheta_{2}^{(0)} = 4.$

As the matrix $A_{i,L}$ according to (2) depends on $\gamma_2^{(0)}$, three different values of $\gamma_2^{(0)}$ (i.e. -1.2, 0, 1) are considered.

In the following a comparison of empirical densities of LMVQUIE and MIN-QUE is made. Even if the distribution of Y is not normal, the distribution of considered estimators seems to differ unsubstiantially as illustrated in Fig. 2.6 and Fig. 2.7 (it is obvious that a shape of the empirical densities in c) differ from that in b) according to $\vartheta_2 \gg \vartheta_1$ (cf. (10)). The number of simulated data was the same as in Case 1.

Fig. 2.6 a) — density function of Y according to (4) with $\gamma_1 = 1, \gamma_2 = -1.2;$ normal density b) — empirical density of LMVQUIE for $\vartheta_1;$ empirical density of MINQUE for ϑ_1 c) — empirical density of LMVQUIE for ϑ_2 ; empirical density of MINQUE for ϑ_2 0.4 40 0.220 0 0 -3 0 3 0 1 2 3 4 5 a) b)









2.3Case 3

The two-stage regression model [6], [11], [12] (occurring frequently in metrology, geodesy etc.) is considered in the following. Let

$$X = \begin{pmatrix} 1, 0, 0 \\ 0, 2, 0 \\ -1, 1, 0 \\ 0, 2, 2 \end{pmatrix}$$
(11)

The matrices V_1, V_2 are the same as in Case 2. The parameters ϑ_1, ϑ_2 chosen for simulation are $\vartheta_1 = 1, \vartheta_2 = 4$. A comparison of $\gamma_2^{(0)}$ -LMVQUIE and MINQUE is given in Table 2.3.

Table 2.3 Comparison of $\gamma_2^{(0)}$ -LMVQUIE and MINQUE in Case 3

	$\gamma_2^{(0)} -1.2 \qquad 0 \qquad 1$						MINQUE	
γ_2	ϑ_1	ϑ_2	ϑ_1	ϑ_2	ϑ_1	ϑ_2	ϑ_1	ϑ_2
-1.2	1.508	49.554	1.511	49.560	1.516	49.572	1.511	49.560
0	2.002	50.685	2.000	50.679	2.002	50.682	2.000	50.679
1	2.414	51.627	2.407	51.611	2.406	51.608	2.407	51.611

An analogy of Figures 2.2–2.5 for Case 3 is Fig. 2.8.

Fig. 2.8² a) — density function of Y according to (4) with $\gamma_1 = -1$, $\gamma_2 = 1$; normal density b) — empirical density of LMVQUIE for ϑ_1 ; empirical density of MINQUE for ϑ_1 --- empirical density of LMVQUIE for ϑ_2 ; empirical density of MINQUE for ϑ_2 c)





3 General conclusions

It is to be said that MINQUE approach is preferred by many statisticians at least from two reasons. This approach need not use the higher statistical moments and the procedure is relatively simple. Nevertheless, it is of general interest to know something about the statistical behaviour of MINQUE in a situation when the distribution of errors is known. Thus a comparison with a locally or uniformly best estimator must be made. Linear models, where the conditons for the existence of the uniformly best estimators are fulfilled, occur rarely in a practice; thus the comparison with the locally best estimators seems to be reasonable and sufficient. The simplest way how to do such a comparison is via simulations. Despite the fact that the experience attained in this way cannot be generalized on other situations and models, at least the following is obvious.

The MINQUE procedure is much less sensitive on the a priori information on ϑ than LMVQUIE. Thus, if we know nothing on the values of the variance components in advance, then it is quite reasonable to use MINQUE.

On the other hand, if we know the distribution of errors (i.e. we have some a priori information on the third and fourth statistical moments) and we know an approximate value of the vector ϑ , then it is necessary to use LMVQUIE.

Final remark MINQUE and LMVQUIE are the same in the case of normally distributed errors. MINQUE is less sensitive on the a priori information about ϑ than LMVQUIE. Thus the MINQUE is to be preferred to LMVQUIE also in the case the non-normality of errors when the deviations from normality are not too significant.

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