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Estimation under Multicollinearity : Application of Restricted Liu and Maximum Entropy Estimators to the Portland Cement Dataset

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1. Introduction: A high degree of multicollinearity among the explanatory variables, X , of a linear regression model, $y = X\beta + u$, has a disastrous effect on estimation of the coefficients, β , by the Ordinary Least Squares (OLS). Several methods have been suggested to ameliorate the deleterious effects of multicollinearity.

2. Various Methods of Estimation under Severe Multicollinearity Conditions: In what follows, we give a brief account of some important methods of estimation under severe multicollinearity conditions:

(i). *The Restricted Least Squares (RLS) Estimator of β* : If we can put some restriction on the linear combination of regression coefficients such that $R\beta = r$, then the RLS estimator of β denoted by β^* is given by $\beta^* = \hat{\beta} + S^{-1}R'(RS^{-1}R')^{-1}(r - R\hat{\beta})$: $\hat{\beta} = S^{-1}X'y$; $S = X'X$.

(ii). *The Ordinary Ridge Regression (ORR) Estimator of β* : As suggested by Hoerl and Kennard (1970) it is possible to mitigate the multicollinearity problem by perturbation of S matrix such that its principal diagonal elements are inflated. The Ordinary Ridge Regression estimator is given by $\hat{\beta}(\kappa) = (S + \kappa I)^{-1}X'y$. As stated by Kaçiranlar et al., writing $W_\kappa = (I + \kappa S^{-1})^{-1}$ we may describe the ORR estimator as $\hat{\beta}(\kappa) = W_\kappa \hat{\beta} = (I + \kappa S^{-1})^{-1}S^{-1}X'y$.

(iii). *The Restricted Ridge Regression (RRR) Estimator of β* : Sarkar (1992) grafted the ORR estimator into the RLS estimation procedure and obtained his RRR estimator given as $\beta^*(\kappa) = W_\kappa \beta^*$ where $\beta^* = \hat{\beta} + S^{-1}R'(RS^{-1}R')^{-1}(r - R\hat{\beta})$: $\hat{\beta} = S^{-1}X'y$; $S = X'X$ as stated earlier. Since the expectation of $\beta^*(\kappa) = E[\beta^*(\kappa)] = W_\kappa \beta + W_\kappa S^{-1}R'(RS^{-1}R')^{-1}\delta$, the RRR estimator is always biased unless $\kappa = 0$ and $\delta = (r - R\beta) = 0$.

(iv). *The Liu Estimator of β* : Liu (1993) introduced a family of estimators for any parameter $d \in (-\infty, +\infty)$ given by $\hat{\beta}_d = (S + I)^{-1}(X'y + d\hat{\beta})$: $\hat{\beta} = S^{-1}X'y$. The Liu estimator can be described as $\hat{\beta}_d = F_d \hat{\beta}$ for $F_d = (S + I)^{-1}(S + dI)$. For $d = 1$ the Liu estimator is identical to the OLS estimator $\hat{\beta}$.

(v). *The Restricted Liu (RL) Estimator of β* : Kaçiranlar et al. (1999) grafted the Liu estimator into the restricted Least Squares estimation procedure and obtained a new family of estimators given by $\hat{\beta}_{rd} = F_d \beta^*$: $d \in (-\infty, +\infty)$. For $d = 1$ the Restricted Liu estimator is identical to the RLS estimator β^* . The authors suggested how to choose the appropriate value of d when restrictions hold or when they do not hold. Since the optimal value of d is a function of β and σ^2 (error variance) in the population, one has to estimate it. The authors provided methods to obtain the estimated value of near-optimal d . The authors also proved the superiority of the RL estimator to the Liu estimator.

Of the five methods of estimation enumerated above, the last three methods, namely, those of Sarkar (1992), Liu (1993) and Kaçiranlar et al. (1999) are improvements on the ORR estimator of Hoerl & Kennard and therefore, they inherit from ORR the property of being dependent on the population β and σ^2 .

(vi). *The Generalized Maximum Entropy (GME) estimator of β* : Golan et al. (1996) introduced the *Generalized Maximum Entropy (GME)* estimator to resolve the multicollinearity problem. This estimator requires a number of support values supplied subjectively and exogenously by the researcher. The estimates as well as their standard errors depend on those support values. In a real life situation it is too demanding on the researcher to supply appropriate support values, which limits the application of GME.

(vii). *The Maximum Entropy Leuven (MEL) estimators of β* : Paris (2001-a, 2001-b) introduced the *Maximum Entropy Leuven (MEL)* estimators. The MEL estimators exploit the information available in the sample data more efficiently than the OLS does; unlike the RLS or GME estimator they do not require any constraints or additional information to be supplied by the researcher, and unlike the RRR, the Liu or the Restricted Liu estimators, they do not need the estimated surrogate parameters (representing the population parameters) in the estimation procedure. The MEL₁ estimator of Paris maximizing entropy in the regression coefficients $\hat{\beta}$ is formulated as $\min H_1 = p'_\beta \log(p_\beta) + L_\beta \log(L_\beta) + u'u$, subject to three equality restrictions given as follows: (1) $y = X\beta + u$; (2) $L_\beta = \beta'\beta$; and (3) $p_\beta = \beta\Theta\beta / L_\beta$; $0 \leq p_\beta \leq 1$. The symbol Θ indicates the element-by-element Hadamard product. The product $p_i \log(p_i) = 0$ if $p_i = 0$.

Analogously, the MEL₂ estimator of Paris maximizes entropy in the regression coefficients as well as the regression residuals. It is formulated so as to minimize $H_2 = p'_\beta \log(p_\beta) + L_\beta \log(L_\beta) + p'_u \log(p_u) + L_u \log(L_u)$ subject to five restrictions given as: (1) $y = X\beta + u$; (2) $L_\beta = \beta'\beta$; (3) $p_\beta = \beta\Theta\beta / L_\beta$; $0 \leq p_\beta \leq 1$; (4) $L_u = u'u$; (5) $p_u = u\Theta u / L_u$; $0 \leq p_u \leq 1$. Additionally, the product $p_i \log(p_i) = 0$ if $p_i = 0$.

(viii). *An Extended Family of Maximum Entropy Leuven (MEL) estimators of β* : It is possible to extend the family of MEL estimators by making the choice of the norm flexible in defining the probabilities, p_β and p_u . Paris used the Euclidean norm to obtain the probabilities, since $\text{prob}(\beta_j) = \beta_j^2 / \beta'\beta = \{\beta_j / (\beta'\beta)^{1/2}\}^2$; $j = 1, 2, \dots, m$. The same is true of the $\text{prob}(u_i)$; $i = 1, 2, \dots, n$. Mishra (2004) used the absolute norm to obtain the $\text{prob}(\beta)$ such that

$\text{prob}(\beta_j) = |\beta_j| / \sum_{j=1}^m |\beta_j|$. Thus, by using the absolute norm (instead of the Euclidean norm) in

defining the $\text{prob}(\beta_j)$, the author modified MEL₁ estimator of Paris to obtain a new estimator – the MMEL (or call it MMEL₁) estimator. Monte Carlo experiments carried out by the author showed that the MMEL estimator outperforms the MEL (that is MEL₁) estimator. The idea of using the absolute norm in defining the probabilities may be extended to $\text{prob}(u_i)$ also.

The members of the extended MEL family of estimators may be described in terms of three parameters, $k_1 = (1 \text{ or } 2)$, $k_2 = (1 \text{ or } 2)$ and $k_3 = (0 \text{ or } 1)$ in the following manner:

$$\text{Min } H(k_1, k_2, k_3) = p'_\beta \log(p_\beta) + L_\beta \log(L_\beta) + k_3 \{ p'_u \log(p_u) + L_u \log(L_u) \} + |k_3 - 1| \left\{ \sum_{i=1}^n |u_i|^{k_1} \right\}$$

subject to the following restrictions chosen on the k_3 -criterion:

if $k_3 = 0$ or 1 then [(1) $y = X\beta + u$; (2) $L_\beta = \sum_{j=1}^m |\beta_j|^{k_2}$; (3) $p_\beta = |\beta_j|^{k_2} / L_\beta : 0 \leq p_\beta \leq 1$]

if $k_3 = 1$ then [(4) $L_u = \sum_{i=1}^n |u_i|^{k_2}$; (5) $p_u = |u_i|^{k_2} / L_u : 0 \leq p_u \leq 1$].

if $p_i = 0$ then $p_i \log(p_i) = 0$ for p_β as well as p_u .

In the equations above, $k_1 = (1 \text{ or } 2)$ indicates the absolute or the Euclidean norm used for determining the length of the error term, u . In the Least Squares formulation $k_1=2$ is chosen such

that $u'u = \sum_{i=1}^n |u_i|^2$ (\Rightarrow the Euclidean norm). In the LAD (Least Absolute Deviation estimation;

Dasgupta & Mishra, 2004) one chooses $k_1=1$ such that $u'u$ is replaced by $\sum_{i=1}^n |u_i|$ (\Rightarrow the absolute

norm). The parameter $k_2 = (1 \text{ or } 2)$ is the norm to be used in order to define $prob(\beta)$ or $prob(u)$. In the MEL₁ and the MEL₂ of Paris (2001-b), $k_2 = 2$ is used. However, the MMEL (Mishra, 2004) uses $k_2 = 1$. The parameter $k_3 = (0 \text{ or } 1)$ indicates whether the entropy of β alone is minimized ($k_3 = 0$) or the entropy of β conjointly with the entropy of u is minimized ($k_3 = 1$). It is to be noted that LAD estimators have their own utility, especially when the error term is infested with large outliers.

3. The objectives of the Present Investigation: The present work aims at comparing the results of Kaçiranlar et al. with those obtained by us applying the MEL family of estimators on the widely analyzed dataset on Portland cement. This dataset (see table 1) has been obtained from an experimental investigation of the heat evolved during the setting and hardening of Portland cements of varied composition and the dependence of this heat on the percentage of four compounds ($x_j; j=1,2,3,4$) in the clinkers from which the cement was produced. The relevance of the relationship between the heat evolved and the chemical processes undergone while setting takes place is best stated in the words of Woods et al. (p. 1207) : “This property is of interest in the construction of massive works as dams, in which the great thickness severely hinder the outflow of the heat. The consequent rise in temperature while the cement is hardening may result in contractions and cracking when the eventual cooling to the surrounding temperature takes place.”

4. Estimation of Regression Coefficients of Homogenous Model by the OLS: Wood et al. set up the linear regression model (without intercept term) as follows:

$$y = X\beta + u = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + u$$

The Ordinary Least Squares (OLS) estimates of β presented by them (Woods et al. p.1212) are as $\hat{\beta}'_{OLS} = (2.18 \ 1.206 \ 0.73 \ 0.526)$.

Kaçiranlar et al. re-estimated $\hat{\beta}'_{OLS} = (2.1930 \ 1.1533 \ 0.7585 \ 0.4863)$ by OLS. They used the JMP statistical package for computations. The difference between OLS estimates of β obtained by Woods et al. and Kaçiranlar et al. has been explained by Kaçiranlar et al. in the following words: “while the computational algorithms available today are surely more accurate than 65 years ago, we note that Woods, Steinour and Starke ... present the values of the four

compounds ... as integers – percentages rounded to the nearest integer – and it is possible that the values of these percentages which these authors used to compute their OLS estimates ... were not so rounded.”

We obtain $\hat{\beta}'_{OLS} = (2.171 \ 1.158 \ 0.728 \ 0.499)$ by SPSS (SPSS Inc., 1996) and $\hat{\beta}'_{OLS} = (2.170685 \ 1.158001 \ 0.728356 \ 0.499202)$ by STATISTICA (StatSoft, Inc., 1993) under extended precision computations. We also obtain $\hat{\beta}'_{OLS} = VD^{-1}V'X'y$, where V and D are eigenvectors and eigenvalues (respectively) of $X'X$ such that $X'X = VDV'$. The resulting $\hat{\beta}'_{OLS} = (2.17068539 \ 1.15800117 \ 0.72835584 \ 0.49920151)$ is computed by the computer program (in FORTRAN 77) written by us. All computations are carried out with the double precision arithmetic. The results obtained by SPSS, STATISTICA and ours own program agree. It appears that Kaçiranlar et al. have not gone in for high precision in their computations.

5. Estimation of the Nonhomogenous Model by Different Estimators: Following Hald (1952, pp. 648-649), Gorman & Toman (1966, pp. 35-36) and Daniel & Wood (1980, p. 89) Kaçiranlar et al. augment X matrix by adding a column of ones to it such that $x'_5 = (1 \ 1 \ \dots \ 1)$ and fit a non-homogenous linear regression model with intercept to the data. They obtain $\hat{\beta}'_{OLS} = (1.5511 \ 0.5102 \ 0.1019 \ -0.1441 \ 62.4054)$. Running our own program we have obtained $\hat{\beta}'_{OLS} = (1.55923438 \ 0.53028708 \ 0.10683607 \ -0.12048488 \ 60.30287081)$. We observe that the estimated coefficients of the non-homogenous regression model are at a great disagreement with those of the homogenous regression equation. This is due to the fact that the augmented $X(13,5)$ is suffering from the multicollinearity problem. According to our computation, $\lambda_1 / \lambda_5 = 6414.38$, where λ_1 and λ_5 are the largest and the smallest eigenvalues of $X'X$ matrix. Kaçiranlar et al. obtain the said ratio = 6056.3744. Balesley's (Belsley, et al., 1980, Ch. 3) condition number is obtained as $C_n = 1449.60$. All these measures suggest a very high degree of multicollinearity in the columns of X matrix.

Kaçiranlar et al. estimated the nonhomogenous model described above by their Restricted Liu estimator, while the restrictions on β are correct and while they are not so. The present study adopts them as they have been reported in their paper. However, the MEL estimators of various types – including the MEL₁ and the MEL₂ of Paris (2001-b) and MMEL estimator of Mishra (2004) – have been applied to the model. Computations have been done on a Pentium-3 Personal Computer by running the programs written by us in Fortran 77. Double precision arithmetic has been used to obtain the results. The findings are presented in Table 2.

6. Formulation and Estimation of an Extended Homogenous Model : In the dataset that we are dealing with, x_j ; $j = 1, 2, 3, 4$ are measured in percentage, but they do not sum up to 100. The

residual may be designated as $x_5 = 100 - \sum_{j=1}^4 x_j$. Now, if we specify our model as $y = \sum_{j=1}^5 \beta_j x_j + u$,

we obtain a homogenous regression model with *perfect multicollinearity*. The $x_5 = (1 \ 1 \ \dots \ 1)'$ of the nonhomogenous model considered earlier may be interpreted as a dummy of

$x_5 = 100 - \sum_{j=1}^4 x_j$. Thus, assuming of $x_5 = (1 \ 1 \ \dots \ 1)'$ or otherwise has its own implications to its correlation with other explanatory variables as well as the errors in y . The coefficients of correlation between the estimated error (\hat{u}) obtained by different estimation methods and $x_5 = (100 - \text{sum}(x_1, x_2, x_3, x_4))$ are between 0.25 and 0.28, although statistically insignificant at 5% level of significance and 11 degrees of freedom. In particular, $r(x_5, \hat{u}_{OLS}) = 0.2704$, $r(x_5, \hat{u}_{RL}) = 0.2535$ and $r(x_5, \hat{u}_{MEL(2,1,0)}) = 0.2686$. It is not unlikely that the residual chemicals (x_5) is the percentage of other (relevant!) chemicals in the composition of the Portland cement. It may or may not have any role in evolvment of heat in the process of setting and hardening of cement; it is for the chemist to investigate.

If we make an attempt to estimate the coefficients of the extended model described above, OLS cannot be used since the $X'X$ matrix is deficient in rank. However, we may obtain the Moore-Penrose inverse (Theil, 1971, pp. 268-270) of $X'X$ given by $(X'X)^+ = VD^+V'$, where V and D are the eigenvectors and the eigenvalues of $X'X$ matrix. To obtain D^+ we define $d_{ii}^+ = d_{ii}^{-1}$ if $d_{ii} \neq 0$ else $d_{ii}^+ = 0$. Thus we obtain $\hat{\beta}_{OLS^+} = VD^+V'X'y$. Estimation of β by the MEL estimators does not pose any problem. The results of this exercise are presented in table 3.

7. A Summary of the Relative Performance of Various Estimators: Using the OLS-estimates of the original model (4-variable homogenous regression equation) coefficients as reference, that is $\hat{\beta}'_{OLS} = (2.1707 \ 1.1580 \ 0.7284 \ 0.4992)$, we obtain the Euclidean norm of the alternative estimates obtained by various estimators (such as OLS^+ , RL, MEL), presented in table 4. Overall, the norm of RL estimates (incorrect restriction) is the largest (2.9911) followed by the norm of OLS (nonhomogenous model) estimates, which is 1.2403 (not shown in table 4). On the other end, the norm of MEL(2,1,0) is the smallest (0.0221). The MEL(2,1,0) is the MMEL estimator (Mishra, 2004). The MEL(2,2,1) and the MEL(1,2,1) have norm = 0.0233. The MEL(2,2,1) is the MEL₂ of Paris. In the sequel come the estimates obtained by MEL(2,2,0), which is the MEL₁ of Paris, MEL(2,1,1) and MEL(2,1,0) applied on the extended homogenous model. Now come the RL (correct restriction) estimates which has norm = 0.0364. Further, note that the OLS^+ (which is a minimum norm LS estimator) and MEL(2,2,0) \equiv MEL₁ of Paris are identical for the extended homogenous model.

Obviously, the RL estimator (even when it uses the correct restriction) is dominated by a number of members of the MEL family estimators. Moreover, MEL estimators withstand perfect multicollinearity without its destabilizing effects on the estimates of the regression coefficients.

8. Conclusion: Our findings suggest that several members of the MEL family of estimators outperform the OLS and the Restricted Liu estimators. The MEL estimators perform well even when perfect multicollinearity is there. A few of them outperform the OLS^+ estimator. Since the MEL estimators do not seek extra information from the analyst, they are easy to apply. Therefore, one may rely on the MEL estimators for obtaining the coefficients of a linear regression model under the conditions of severe multicollinearity among the explanatory variables.

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y'	78.5	74.3	104.3	87.6	95.9	109.2	102.7	72.5	93.1	115.9	83.8	113.3	109.4
x'_1	7	1	11	11	7	11	3	1	2	21	1	11	10
x'_2	25	29	56	31	52	55	71	31	54	47	40	66	68
x'_3	6	15	8	8	6	9	17	22	18	4	23	9	8
x'_4	60	52	20	47	33	22	6	44	22	26	34	12	12
$\sum_{j=1}^4 x'_j$	98	97	95	97	98	97	97	98	96	98	98	98	98

$x_1=3\text{CaO}.\text{Al}_2\text{O}_3$; $x_2=3\text{CaO}.\text{SiO}_2$; $x_3=4\text{CaO}.\text{Al}_2\text{O}_3.\text{Fe}_2\text{O}_3$; $x_4=2\text{CaO}.\text{SiO}_2$; y = heat (calories per gram of cement) evolved after 180 days of curing. The matrices X and y are transposed for tabular presentation here.

Estimators	Specification of parameters	Estimated Regression Coefficients				
		β_1	β_2	β_3	β_4	β_5
Restricted Liu estimator	$\hat{d}_{RLS} = 0.7892$	2.1901	1.1539	0.7563	0.4867	0.0099
	$\hat{d}_{RLS} = 0.9527$	0.6207	-0.2819	-0.8298	-0.9301	142.0379
Maximum Entropy Leuven Family of Estimators	$(k_1, k_2, k_3) = (2, 2, 0)$	2.1357	1.1643	0.7038	0.5029	0.1295
	$(k_1, k_2, k_3) = (2, 2, 1)$	2.1528	1.1594	0.7136	0.4993	0.2369
	$(k_1, k_2, k_3) = (2, 1, 0)$	2.1541	1.1628	0.7151	0.5025	-0.0518
	$(k_1, k_2, k_3) = (2, 1, 1)$	2.2028	1.1392	0.8407	0.4947	-0.1288
	$(k_1, k_2, k_3) = (1, 1, 0)$	2.1926	1.1388	0.8368	0.4943	0.0021
	$(k_1, k_2, k_3) = (1, 1, 1)$	2.2029	1.1392	0.8407	0.4947	-0.1288
	$(k_1, k_2, k_3) = (1, 2, 0)$	1.9536	1.1910	0.7302	0.5099	0.0739
	$(k_1, k_2, k_3) = (1, 2, 1)$	2.1528	1.1593	0.7136	0.4993	0.2369
OLS Estimator	Non-homogenous	1.5592	0.5303	0.1068	-0.1205	60.6514
	Homogenous	2.1707	1.1580	0.7284	0.4992	-

Table 3. Estimated Coefficients of Portland Cement Dataset by RL, MEL and OLS⁺ (Extended Homogenous Model $y = \sum_{j=1}^5 \beta_j x_j + u : x_5 = 100 - \sum_{j=1}^4 x_j$)						
Estimator	Specifications	Estimated Regression Coefficients				
		β_1	β_2	β_3	β_4	β_5
Maximum Entropy Leuven Family of Estimators	k-Parameters					
	$(k_1, k_2, k_3) = (2, 2, 0)$	2.1657	1.1368	0.7133	0.4860	0.6065
	$(k_1, k_2, k_3) = (2, 2, 1)$	2.1267	1.1503	0.6879	0.4948	0.4825
	$(k_1, k_2, k_3) = (2, 1, 0)$	2.1584	1.1385	0.7080	0.4870	0.6071
	$(k_1, k_2, k_3) = (2, 1, 1)$	2.1562	1.1432	0.7075	0.4900	0.4981
	$(k_1, k_2, k_3) = (1, 1, 0)$	2.1956	1.1423	0.8258	0.4959	-0.0692
	$(k_1, k_2, k_3) = (1, 1, 1)$	2.2030	1.1393	0.8409	0.4949	-0.0701
	$(k_1, k_2, k_3) = (1, 2, 0)$	2.1956	1.1423	0.8258	0.4959	-0.0692
	$(k_1, k_2, k_3) = (1, 2, 1)$	2.0389	1.1501	0.7886	0.5054	0.2103
OLS ⁺ Estimator	Homogenous	2.1657	1.1368	0.7133	0.4860	0.6065

Note : The OLS⁺ and MEL(2,2,0) \equiv MEL₁ of Paris are identical for the extended homogenous model.

Table 4. Euclidean Norm of Estimated Regression Coefficients by Various Estimators (with Reference to the OLS-estimated Homogenous 4-variable Model of Portland Cement Dataset)					
Nonhomogenous Model			Extended Homogenous Model		
Estimator	Specification	Norm	Estimator	Specification	Norm
R L Estimator Correct Restriction	$\hat{d}_{RLS} = 0.7892$	0.0364	OLS ⁺ Estimator Obtained by Moore-Penrose Inverse of XX'	Extended Homogenous $x_5 = 100 - \sum_{j=1}^4 x_j$	<u>0.0296</u>
R L Estimator Incorrect Restriction	$\hat{d}_{RLS} = 0.9527$	2.9911			
MEL Estimators	$(k_1, k_2, k_3) = (2, 2, 0)$	0.0434	MEL Estimators	$(k_1, k_2, k_3) = (2, 2, 0)$	<u>0.0296</u>
	$(k_1, k_2, k_3) = (2, 2, 1)$	0.0233		$(k_1, k_2, k_3) = (2, 2, 1)$	0.0605
Model: Nonhomogenous	$(k_1, k_2, k_3) = (2, 1, 0)$	<u>0.0221</u>	Model: Extended Homogenous	$(k_1, k_2, k_3) = (2, 1, 0)$	0.0331
	$(k_1, k_2, k_3) = (2, 1, 1)$	0.1184		$(k_1, k_2, k_3) = (2, 1, 1)$	0.0308
Definition: $x_{i5} = 1 \forall i$	$(k_1, k_2, k_3) = (1, 1, 0)$	0.1124	Definition: $x_5 = 100 - \sum_{j=1}^4 x_j$	$(k_1, k_2, k_3) = (1, 1, 0)$	0.1018
	$(k_1, k_2, k_3) = (1, 1, 1)$	0.1184		$(k_1, k_2, k_3) = (1, 1, 1)$	0.1186
	$(k_1, k_2, k_3) = (1, 2, 0)$	0.2199		$(k_1, k_2, k_3) = (1, 2, 0)$	0.1018
	$(k_1, k_2, k_3) = (1, 2, 1)$	0.0233		$(k_1, k_2, k_3) = (1, 2, 1)$	0.1452

Note: The best estimator(s) under a particular model specification is (are) underlined.