GENERALISED NATURAL CONJUGATE PRIOR DENSITIES : SINGULAR MULTIVARIATE LINEAR MODEL

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Comunicación Técnica No I-03-11/05-06-2003
(PE/CIMAT)

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KEY WORD AND PHRASES: Generalised natural conjugate prior, Generalised Inverse Wishart and Pseudo-Wishart distributions, Hausdorff measure, Moore-Penrose inverse, Matrix-variate Singular Normal distribution, Multivariate linear model.

AMS 2000 Subject Classification: Primary 62F15
Secondary 62H12

ABSTRACT

We consider the problem of finding a generalised natural conjugate prior density for the parameters (β, Σ) in the context of the singular multivariate linear model, $Y = X\beta + \epsilon$, $Y \in I\!R^{N\times p}$, $X \in I\!R^{N\times q}$, $r(X) = q$ (full rank), $\beta \in I\!R^{q\times p}$ and $\epsilon \sim \mathcal{N}^{N,r}_{N\times p}(0, \Sigma, I_N)$, matrix-variate singular normal distribution, that is $r(\Sigma) = r < p$ (singular model). We also provide the posterior distribution of

*This article was written while the first author was a Visiting Professor at the Centro de Investigación en Matemáticas, Guanajuato, Gto., México.

(β, Σ), as well as the corresponding marginal posterior distributions for β and Σ.

1. INTRODUCTION

In the classical approach of statistics, the multivariate linear model under different kinds of singularities, has been studied by a number of authors, see for example, Khatri (1968) and Srivastava and Khatri [pp. 174-175] (1979). In the area of Bayesian inference, the nonsingular multivariate linear model has been considered using both noninformative and informative priors, by, among others, Box and Tiao [Chapter 8] (1979) and Press[Section 8.6] (1982). However, due to the inherent difficulties when dealing with probability distributions of singular random matrices, the multivariate linear model had not been studied from a bayesian point of view when there are singularities in its parameters. Recently, Díaz-García *et al* (2003a) have approached the subject of Bayesian inference for the singular multivariate linear model using noninformative priors, also they have treated informative priors for inference on covariance matrices, see Díaz-García *et al* (2003b).

Following the ideas presented in Press (1982), we extend in this paper the study of generalised natural conjugate prior distributions to the singular multivariate linear model with errors distributed as matrix-variate singular normal distribution. Conjugate prior distributions is a class of prior distributions with the property that the posterior falls within the same family as the prior, this property is particularly useful in the singular case to avoid computational difficulties. The structure of the paper is as follows. In section 2 we introduce necessary notation and give explicit expressions for the densities of the matrix-variate singular normal and generalised inverse Wishart distributions. The generalised natural conjugate prior for the parameters (β, Σ) in the singular multivariate linear model is obtained in Section 3. We summarize this result in Theorem 1 together with the expressions for the joint posterior and the corresponding marginal distributions. We point out in passing, that the marginal posterior distribution for Σ, as obtained by Press (1982) is incorrect, the corrected version can be obtained from Theorem 1 (*iii*) as a particular case.

2. NOTATION AND PRELIMINARY RESULTS

Let $\mathcal{L}^{+}_{p,N}(s)$ be the linear space of all $N \times p$ real matrices of rank $s \leq \min(N,p)$ with s distinct singular values. The set of matrices $H_1 \in \mathcal{L}_{p,N}$ such that $H_1'H_1 = I_p$ is a manifold denoted $\mathcal{V}_{p,N}$, called Stiefel manifold. In particular, $\mathcal{V}_{p,p}$ is the group of orthogonal matrices $\mathcal{O}(p)$. Denote by $\mathcal{S}_p$, the homogeneous space of $p \times p$ positive definite symmetric matrices; $\mathcal{S}^{+}_{p}(s)$, the $(ps - s(s-1)/2)$-dimensional manifold of rank s positive semidefinite $p \times p$ symmetric matrices with s distinct positive eigenvalues. Finally, A^{-} and A^{+} denote the generalised and Moore-Penrose inverse of matrix A, respectively.

Definition 1. [Matrix-variate Singular Normal Distribution] *Let* $X \in \mathcal{L}^{+}_{p,N}(s)$*, such that* $X \sim \mathcal{N}_{N\times p}(\mu, \Sigma, \Xi)$*, with* Σ $p \times p$*,* $r(\Sigma) = r < p$ *or* Ξ $N \times N$*,* $r(\Xi) = k < N$ *and* $s = \min(r, k)$*. This distribution will be called a matrix-variate singular normal distribution and will be denoted as*

$$X \sim \mathcal{N}^{k,r}_{N\times p}(\mu, \Sigma, \Xi)$$

omitting the supra-index when $r = p$ *and* $k = N$*. In addition, its density function is given by*

$$\frac{1}{(2\pi)^{rk/2} \left(\prod_{i=1}^{r} \lambda_i^{k/2}\right) \left(\prod_{j=1}^{k} \delta_j^{r/2}\right)} \operatorname{etr}\left(-\tfrac{1}{2}\Sigma^{-}(X-\mu)'\Xi^{-}(X-\mu)\right) \tag{1}$$

$$\left.\begin{array}{rcl} H_2'XP_1' & = & H_2'\mu P_1' \\ H_1'XP_2' & = & H_1'\mu P_2' \\ H_2'XP_2' & = & H_2'\mu P_2' \end{array}\right\} \quad a.\ s. \tag{2}$$

where A^{-} *is a symmetric generalised inverse,* λ_i *and* δ_j *are the nonzero eigenvalues of* Σ *and* Ξ *respectively, and* $H = (H_1|H_2) \in \mathcal{O}(N)$ *and* $P = (P_1'|P_2') \in \mathcal{O}(p)$ *are the matrices associated with the spectral decomposition of matrices* Σ *and* Ξ *respectively with* $H_1 \in V_{k,N}$*,* $H_2 \in V_{N-k,N}$*,* $P_1' \in V_{r,p}$ *and* $P_2' \in V_{p-r,p}$*, see Díaz-García et al (1997).*
Alternatively, this density can be written as

$$dF_X(X) = \frac{1}{(2\pi)^{rk/2} \left(\prod_{i=1}^{r} \lambda_i^{k/2}\right) \left(\prod_{j=1}^{k} \delta_j^{r/2}\right)} \operatorname{etr}\left(-\tfrac{1}{2}\Sigma^{-}(X-\mu)'\Xi^{-}(X-\mu)\right)(dX), \tag{3}$$

where (dX) is the Hausdorff measure, which coincides with that of Lebesgue when it is defined on the subspace $\mathcal{M}$ given by the hyperplane (2), see Díaz-García *et al* (1997), Cramér [p. 297, 1999] and Billingsley [p. 247, 1979]. An explicit form of (dX) would be given by

$$(dX) = 2^{-s} \prod_{i=1}^{s} \nu_i^{N+p-2s} \prod_{i<j}^{s} (\nu_i^2 - \nu_j^2) \left(\bigwedge_{i=1}^{s} d\nu_i\right) (R_1' dR_1)(Q_1' dQ_1)$$

where $X = R_1 D_\nu Q_1'$ is the nonsingular part of the singular value decomposition, with $R_1 \in \mathcal{V}_{s,N}$, $Q_1 \in \mathcal{V}_{s,p}$ and $D_\nu = \operatorname{diag}(\nu_1, \dots, \nu_s)$, $\nu_1 > \cdots > \nu_s > 0$, see Díaz-García *et al* (1997).

Definition 1. [Generalised Inverse Wishart and Pseudo-Wishart Distributions] *Let* $U \in \mathcal{S}^{+}_{p}(s)$ *be a random matrix.* U *is said to have a central generalised inverse Wishart or Pseudo-Wishart distribution of rank* s*, with* n *degrees of freedom and scale matrix* G*, this fact being denoted by* $U \sim \mathcal{W}^{+}_{p}(s, n, G)$ *and by* $U \sim \mathcal{P}W^{+}_{p}(s, n, G)$ *respectively, if the density function is given by*

$$dF_U(U) = \frac{\pi^{(n-p-1)(s-r)/2} \left(\prod_{i=1}^{r} \delta_i^{(n-p-1)/2}\right)}{2^{(n-p-1)r/2} \Gamma_s\left[\frac{1}{2}(n-p-1)\right] \prod_{i=1}^{s} \alpha_i^{(n+2p-2s)/2}} \operatorname{etr}\left(-\tfrac{1}{2}GU^{+}\right)(dU) \tag{4}$$

where $U = H_1 D_\alpha H_1$ is the nonsingular part of the spectral decomposition of U, with $D_\alpha = \operatorname{diag}(\alpha_1, \dots, \alpha_s)$, $\alpha_1 > \cdots > \alpha_s > 0$, $H_1 \in \mathcal{V}_{s,p}$; $G = R_1 D_\delta R_1'$ is the nonsingular part of the spectral decomposition of G, with $D_\delta = \operatorname{diag}(\delta_1, \dots, \delta_r)$ $\delta_1 > \cdots > \delta_r > 0$, $R_1 \in \mathcal{V}_{r,p}$, and where the measure (dU) is explicitly given by

$$(dU) = 2^{-p} \prod_{i=1}^{s} \alpha_i^{p-s} \prod_{i<j} (\alpha_i - \alpha_j)(H_1' dH_1) \wedge \bigwedge_{i=1}^{s} d\alpha_i,$$

see Uhlig (1994), Díaz-García and Gutiérrez (1997) and Díaz-García et al (2003a).

3. GENERALISED NATURAL CONJUGATE PRIOR DISTRIBUTION

In this section, we consider Bayesian inference for the parameters β and Σ in the linear model of the singular multivariate full rank model defined by:

$$\underset{N\times p}{Y} = \underset{N\times q}{X} \underset{q\times p}{\beta} + \underset{N\times p}{\epsilon}, \tag{5}$$

where $p(\epsilon|\beta, \Sigma) \equiv \mathcal{N}_{N\times p}^{N,r}(0, \Sigma, I_N)$ with $\Sigma \geq 0$, $r(\Sigma) = r < p < N$ and $r(X) = q$.

Let $S(\beta)$ be the symmetric matrix

$$\begin{aligned} S(\beta) &= (Y - X\beta)'(Y - X\beta) \\ &= (Y - \hat{\beta})'(Y - \hat{\beta}) + (\beta - \hat{\beta})' X' X (\beta - \hat{\beta}) \\ &= V + (\beta - \hat{\beta})' X' X (\beta - \hat{\beta}) \end{aligned}$$

with $V = (Y - \hat{\beta})'(Y - \hat{\beta})$ y $\hat{\beta} = X^+ Y = (X'X)^{-1} X' Y$ is the least squares estimator of β. From these observations, and from expression (3), the likelihood function can be written as

$$\begin{aligned} \mathcal{L}(\beta, \Sigma|Y) &\propto dP(\epsilon|\beta, \Sigma)(d\beta)(d\Sigma) \\ &\propto \textstyle\prod_{i=1}^{r} \lambda_i^{-N/2} \operatorname{etr}\left(-\frac{1}{2}\Sigma^+ S(\beta)\right)(d\beta)(d\Sigma) \\ &\propto \frac{\operatorname{etr}\left(-\frac{1}{2} V \Sigma^+\right)}{\prod_{i=1}^{r} \lambda_i^{N/2}} \exp\left(-\frac{1}{2} \operatorname{vec}'(\beta - \hat{\beta})[\Sigma^+ \otimes (X'X)] \operatorname{vec}(\beta - \hat{\beta})\right) \end{aligned} \tag{6}$$

where λ_i, $i = 1, 2, \dots, r$, are the non-null eigenvalues of Σ. Thus, it can be seen, following Press [p.252-253] (1982), that the natural enriched parametric prior densities are given by

$$p(\Sigma) = \mathcal{W}_p^+(r, m, G) \quad \text{and} \quad p(\beta|\Sigma) = \mathcal{N}_{q\times p}^{q,r}(\phi.\Sigma, B) \tag{7}$$

where ϕ,B, G and m are arbitrary parameters that potentially would give flexibility for choosing the appropiate priors. However, as pointed out in Press (1982), even under arbitrary parameters, the resulting priors turn out to be constrained so that we can not freely choose the prior that better reflects our prior beliefs. Therefore, we opt for constructing a generlised natural prior distribution following the procedure outlined in Press [p. 253-254] (1982).

Assuming a fixed Σ we have that

$$dP(\beta) \propto \operatorname{etr}\left(-\tfrac{1}{2}\Sigma^{+}(\beta-\hat{\beta})'X'X(\beta-\hat{\beta})\right)(d\beta). \tag{8}$$

or, alternatively, considering the vectorization of β, we have

$$dP(\operatorname{vec}\beta) \propto \exp\left(-\tfrac{1}{2}\operatorname{vec}'(\beta-\hat{\beta})(\Sigma\otimes(X'X)^{-1})^{+}\operatorname{vec}(\beta-\hat{\beta})\right)(d\operatorname{vec}\beta). \tag{9}$$

from here, with an appopiate normalizing constant and leaving ϕ and $F \in \mathcal{S}_{+}^{qp}(qr)$ as arbitrary parameters, we have

$$p(\operatorname{vec}\beta) = \mathcal{N}_{qp}^{qr}(\operatorname{vec}\phi, F) \tag{10}$$

Similarly, assuming a fixed β, we see that the density for Σ is of the form

$$dP(\Sigma) \propto \prod_{i=1}^{r}\lambda_i^{-m/2}\operatorname{etr}\left(-\tfrac{1}{2}\Sigma^{+}G\right)(d\Sigma) \tag{11}$$

where m and G are arbitrary. Now, considering the appropiate normalizing constant and letting m be a positive integer and $G \in \mathcal{S}_p^{+}(r)$, we have

$$p(\Sigma) = \mathcal{W}_p^{+}(r, m, G). \tag{12}$$

Finally, we arrive at the joint generalised natural conjugate prior by taking the product of (10) and (12)

$$\begin{aligned} dP(\beta,\Sigma) &= \mathcal{N}_{qp}^{qr}(\operatorname{vec}\phi, F)\mathcal{W}_p^{+}(r,m,G)(d\beta)(d\Sigma) \\ &\propto \frac{\exp\left[-\frac{1}{2}\left(\operatorname{tr}\Sigma^{+}G + \operatorname{vec}'(\beta-\phi)F^{-}\operatorname{vec}(\beta-\phi)\right)\right]}{\prod_{i=1}^{r}\lambda_i^{m/2}}(d\beta)(d\Sigma). \end{aligned} \tag{13}$$

By analogy with the nonsingular case, distribution (13) will be called Singular Normal-Generalised inverse Wishart. This distribution, used as prior, no longer has the constraints associated with the ordinary natural conjugate prior distribution.
Now, if we multiply (6) by (13) we obtain, except for a normalizing constant, the joint posterior distribution for (β, Σ)

$$dP(\beta,\Sigma|Y) \propto \frac{\exp\left(-\frac{1}{2}\operatorname{tr}\Sigma^{+}\left(G+S(\beta)\right) - \frac{1}{2}\operatorname{vec}'(\beta-\phi)F^{-}\operatorname{vec}(\beta-\phi)\right)}{\prod_{i=1}^{r}\lambda_i^{(N+m)/2}}(d\beta)(d\Sigma), \tag{14}$$

which is seen to be again Normal-Generalised inverse Wishart distribution (see equation (18)).
All Bayesian inferences will be drawn from the marginal posteriors for β and Σ; we now proceed to their computation. The marginal posterior for β is

obtained by integrating (14) with respect to Σ. Using the fact that (4) is a density, we get

$$\begin{aligned} dP(\beta|Y) &= \int_{\Sigma\in\mathcal{S}_p^+(r)} p(\beta,\Sigma|Y)(d\Sigma)(d\beta) \\ &\propto \frac{\exp\left(-\frac{1}{2}\operatorname{vec}'(\beta-\phi)F^{-}\operatorname{vec}(\beta-\phi)\right)}{\prod_{i=1}^{r}\alpha_i^{(N+m-3p+2r-1)/2}}(d\beta), \end{aligned} \tag{15}$$

where α_i, $i=1,\dots,r$ are the non-null eigenvalues of the matrix

$$(G+V+(\beta-\hat{\beta})'X'X(\beta-\hat{\beta})). \tag{16}$$

If (16) is positive definite, we see that (15) can be written as

$$dP(\beta|Y) \propto \frac{\exp\left(-\frac{1}{2}\operatorname{vec}'(\beta-\phi)F^{-}\operatorname{vec}(\beta-\phi)\right)}{|G+V+(\beta-\hat{\beta})'X'X(\beta-\hat{\beta})|^{(N+m-3p+2r-1)/2}}(d\beta) \tag{17}$$

Now, to determine the marginal posterior distribution for Σ, we rewrite (14) as

$$\begin{aligned} dP(\beta,\Sigma|Y) \propto \frac{\exp\left(-\frac{1}{2}\operatorname{tr}\Sigma^{+}(G+V)\right)}{\prod_{i=1}^{r}\lambda_i^{(N+m)/2}} \\ \exp\left(-\frac{1}{2}\operatorname{vec}'(\beta-\hat{\beta})(\Sigma\otimes(X'X)^{-1})^{+}\operatorname{vec}(\beta-\hat{\beta})\right) \\ \exp\left(-\frac{1}{2}\operatorname{vec}'(\beta-\phi)F^{-}\operatorname{vec}(\beta-\phi)\right)(d\beta)(d\Sigma). \end{aligned}$$

Now, using algebra to expand terms in the second exponential and assuming that $(F^{-}\operatorname{vec}\phi+(\Sigma^{+}\otimes X'X)\operatorname{vec}\hat{\beta})\in\mathcal{R}(F^{-}+(\Sigma^{+}\otimes X'X)^{+}$ (where $\mathcal{R}(A)$ is the image or range of A) we have that

$$\begin{aligned} &\operatorname{vec}'(\beta-\hat{\beta})(\Sigma\otimes(X'X)^{-1})^{+}\operatorname{vec}(\beta-\hat{\beta})+\operatorname{vec}'(\beta-\phi)F^{-}\operatorname{vec}(\beta-\phi) \\ &\quad=\operatorname{vec}'(\beta-\bar{\beta})M\operatorname{vec}(\beta-\bar{\beta})-\operatorname{vec}'\bar{\beta}M\operatorname{vec}\bar{\beta}+\operatorname{vec}'\hat{\beta}(\Sigma\otimes(X'X)^{-1})^{+}\operatorname{vec}\hat{\beta} \\ &\qquad+\operatorname{vec}'\phi F^{-}\operatorname{vec}\phi. \end{aligned}$$

Where $M=F^{-}+(\Sigma^{+}\otimes X'X)$ and $\bar{\beta}=M^{+}[F^{-}\operatorname{vec}\phi+(\Sigma^{+}\otimes X'X)\operatorname{vec}\hat{\beta}]$. Now, by observing that $\operatorname{vec}'\hat{\beta}(\Sigma\otimes(X'X)^{-1})^{+}\operatorname{vec}\hat{\beta}=\operatorname{tr}\Sigma^{+}\hat{\beta}'X'X\hat{\beta}$ and that $\operatorname{vec}'\phi F^{-}\operatorname{vec}\phi$ is constant with respect to β and that it does not depend on Σ,

$$\begin{aligned} dP(\beta,\Sigma|Y) \propto \frac{\exp\left[-\frac{1}{2}\operatorname{tr}\Sigma^{+}\left(G+V+\hat{\beta}'X'X\hat{\beta}\right)-\frac{1}{2}\operatorname{vec}'\bar{\beta}M\operatorname{vec}\bar{\beta}\right]}{\prod_{i=1}^{r}\lambda_i^{(N+m)/2}} \\ \exp\left(-\frac{1}{2}\operatorname{vec}'(\beta-\bar{\beta})M\operatorname{vec}(\beta-\bar{\beta})\right)(d\beta)(d\Sigma). \end{aligned} \tag{18}$$

From here, using (3), we integrate with respect to β to get the marginal posterior distribution for Σ,

$$\begin{aligned} dP(\Sigma|Y) &= \int_{\beta\in\mathcal{L}_{p,q}^+(r)} p(\beta,\Sigma|Y)(d\beta)(d\Sigma) \\ &\propto \frac{\exp\left[-\frac{1}{2}\operatorname{tr}\Sigma^{+}\left(G+V+\hat{\beta}'X'X\hat{\beta}\right)-\frac{1}{2}\operatorname{vec}'\bar{\beta}M\operatorname{vec}\bar{\beta}\right]}{\prod_{i=1}^{r}\lambda_i^{(N+m)/2}\prod_{j=1}^{rq}\tau_j^{1/2}}(d\Sigma) \end{aligned} \tag{19}$$

where τ_j, $j = 1, \dots, r$ are the non-null eigenvalues of $F + \Sigma \otimes (X'X)^{-1}$.

Remark 1. The equivalent result on the marginal posterior for Σ obtained by Press [eq.8.6.23 p. 256](1982) for the non-singular case is incorrect, because after completing the square with respect to β, there are two omitted terms in the exponent, which, indeed are constant with respect to β but depend on Σ and therefore can not be left out. As a consequence, the asymptotic result on Theorem 8.6.5 in Press [p.256](1982) is also incorrect. The correct results for the marginal posterior for Σ can be obtained from the following Theorem as a particular case.

In summary, we have the following result.

Theorem 1. *Given the general multivariate linear model (5), and assuming an informative prior joint distribution for the parameters (β, Σ), the joint generalised natural conjugate prior density is*

$$dP(\beta, \Sigma) \propto \prod_{i=1}^{r} \lambda_i^{-m/2} \exp\left[-\tfrac{1}{2}\left(\operatorname{tr} \Sigma^{+} G + \operatorname{vec}'(\beta - \phi) F^{-} \operatorname{vec}(\beta - \phi)\right)\right] (d\beta)(d\Sigma),$$

where F^{-} is a symmetric generalised inverse. $F \in \mathcal{S}_{qp}^{+}(qr)$, $G \in \mathcal{S}_{p}^{+}(r)$, $\phi \in \mathcal{L}_{q,p}^{+}(r)$, m positive integer are arbitrary parameters and λ_j, $j = 1, 2, \dots, r$, are the non-null eigenvalues of Σ. Also we have.
(i) The joint posterior density function of (β, Σ) is given by

$$dP(\beta, \Sigma | Y) \propto \frac{\exp\left(-\frac{1}{2} \operatorname{tr} \Sigma^{+} \left(G + S(\beta)\right) - \frac{1}{2} \operatorname{vec}'(\beta - \phi) F^{-} \operatorname{vec}(\beta - \phi)\right)}{\prod_{i=1}^{r} \lambda_i^{-(N+m)/2}} (d\beta)(d\Sigma),$$

(ii) The marginal posterior density of β is

$$dP(\beta | Y) \propto \frac{\exp\left(-\frac{1}{2} \operatorname{vec}'(\beta - \phi) F^{-} \operatorname{vec}(\beta - \phi)\right)}{\prod_{i=1}^{r} \alpha_i^{(N+m-3p+2r-1)/2}} (d\beta)$$

where α_i, $i = 1, \dots, r$ are the no-null eigenvalues of $(G + V + (\beta - \hat{\beta})' X' X (\beta - \hat{\beta}))$. Or by

$$dP(\beta | Y) \propto \frac{\exp\left(-\frac{1}{2} \operatorname{vec}'(\beta - \phi) F^{-} \operatorname{vec}(\beta - \phi)\right)}{|V + G + (\beta - \hat{\beta})' X' X (\beta - \hat{\beta})|^{(N+m-3p+2r-1)/2}} (d\beta),$$

when $(V + G + (\beta - \hat{\beta})' X' X (\beta - \hat{\beta}) \in \mathcal{S}_m$.
(iii) And the marginal posterior density of Σ is

$$dP(\Sigma | Y) \propto \frac{\exp\left(-\frac{1}{2} \operatorname{tr} \Sigma^{+} \left(V + G + \hat{\beta}' X' X \hat{\beta}\right) - \frac{1}{2} \operatorname{vec}' \bar{\beta} M \operatorname{vec} \bar{\beta}\right)}{\prod_{i=1}^{r} \lambda_i^{-(N+m)/2} \prod_{j=1}^{rq} \tau_j^{1/2}} (d\Sigma)$$

where τ_j are the nonzero eigenvalues of $(F + (\Sigma \otimes (X'X)^{-1}))$, $M = (F^{-} + (\Sigma^{+} \otimes (X'X))$ and $\bar{\beta} = M^{+}(F^{-} \operatorname{vec} \phi + \operatorname{vec} X' X \hat{\beta} \Sigma^{+})$.

Remark 2. Except for the case of the marginal posterior for Σ which we commented in Remark 1, if we make $r = p$ in Theorem 1, we obtain the same results as Press [Section 8.6.2](1982), for the nonsingular multivariate linear model.

4. ACKNOWLEDGMENT

This work was supported partially by the research project 39017E of CONA-CYT-México.

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