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ON EIGENVALUES, CASE DELETION AND EXTREMES IN REGRESSION

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Abstract

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Key words: Case deletion; Collinearity; Eigenvalues; Extreme cases; Gateaux differentiability; Multiple Linear Regression; Perturbation theory.

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ON EIGENVALUES, CASE DELETION AND EXTREMES IN REGRESSION

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1. Introduction

Consider the linear model

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

where Y is an n vector of observable responses, X is a known full rank n×m matrix, β is an m vector of unknown parameters, and ε is an n vector of unobservable errors with $E[\varepsilon]=0$ and $V[\varepsilon]=\sigma^2 I_n$. We assume that the model contains an intercept term and, therefore, $X=(1_n,X_1)$, where 1_n is an n vector of ones and X_1 is an n×p matrix. We have m=p+1. Sometimes, it is convenient to write the model (1.1) as

$$Y=1_n\alpha_o+Z\alpha+\varepsilon, \tag{1.2}$$

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where Z is the nxp matrix of centered and scaled predictors and $(\alpha_0,\alpha')'$ is an m vector of unknown parameters.

According to (1.2), Z'Z is the correlation matrix of the model (1.1). We write its spectral decomposition as

$$Z'Z=CDC', \tag{1.3}$$

where C, with columns γ_j, is a pxp orthogonal matrix of eigenvectors, and D is a pxp matrix of eigenvalues $0<\lambda_1\le \dots\le\lambda_p$. Closely related to (1.3) is the nxp matrix of principal components associated to (1.1), namely,

$$K=(k_{ij})=ZC, \tag{1.4}$$

with columns $k_j=Z\gamma_j$.

A linear least squares fit of (1.1) may be affected by collinearity among the columns of X. Collinearity refers to the near dependence of the regressor variates. Consequences of collinearity with regard to numerical and statistical instability of coefficient estimates are well documented (see Gunst (1983) for a detailed review). A useful indicator of the existence of a near linear dependence among the columns of X is the presence of small eigenvalues in D. Given that

$$\lambda_j=\gamma_j'Z'Z\gamma_j=k_j'k_j, \tag{1.5}$$

$\lambda_j\cong 0$ implies $Z\gamma_j\cong 0$. We define the jth condition index of the matrix Z, $\eta_j=(\lambda_p/\lambda_j)^{1/2}$. In particular, $\kappa=\eta_1=(\lambda_p/\lambda_1)^{1/2}$ is the condition number of Z. The set $\{\eta_j,\ 1\le j\le p\}$ of condition indexes is a diagnostic tool for detecting collinearity proposed by Belsley et al. (1980).

The nxn matrix $V=(v_{ij})=X(X'X)^{-1}X'$ is termed the hat matrix and its diagonal entries v_{ii} measure how far the associated cases are from the center of the data set. It is shown that $V=1_n1_n'/n+Z(Z'Z)^{-1}Z'$ and then, using (1.3) and (1.4),

$$v_{ii} = \frac{1}{n} + \sum_{j=1}^{p} \frac{k_{ij}^2}{\lambda_j} . \tag{1.6}$$

Cases with v_{ii}>2m/n are extremes or far from the bulk of the data.

It is well-known that a small group of cases might be distorting, either creating or masking, the perception of an approximate linear relationship among the columns of model (1.1). These points are dubbed collinearity-influential cases. For example, Mason and Gunst (1985) showed how a group of k outlying cases can induce k-1 near linear relationships among the regressor variates. Collinearity-influential cases were initially noted in Belsley et al. (1980) and Cook and Weisberg (1982).

Several authors have proposed different techniques for detecting collinearity-influential points, among others, Chaterjee and Hadi (1988), Walker (1989) and, recently, Wang and Nyquist (1991). For a recent review on diagnostic techniques for collinearity-influential points, see Belsley (1991, chap. 8).

Put $X_1=(x_1, \ldots, x_n)'$, where $x_i \in \mathbb{R}^p$. In what follows, the subscript (i) will mean that the corresponding quantity has been computed deleting the ith case $(1,x_i')$ of the analysis. Since collinearity measures are mainly constructed on the eigenvalues of the (centered ans scaled) cross products matrix, a method for diagnosing the presence of collinearity-influential points in a data set could be analyzing the relationship among the sets $\{\lambda_j\}$ and $\{\lambda_{j(i)}\}$. Unfortunately, with the exception of some special cases, there are no explicit expressions relating λ_j to $\lambda_{j(i)}$ and, therefore, some degree of approximation seems in order. The aim of this paper is to present a new technique of approximation for the differences $\lambda_j-\lambda_{j(i)}$. The accuracy of the approximation is reflected in a rate of convergence which depends on the sample size. Section 2 contains some preliminary background to the main results which are exposed in section 3. Section 4 is devoted to applications and examples. We will focus primarily on the effect of single deletion. Results concerning multiple cases and other possible extensions of the theory can be found in section 5.

2. Eigenvalues as functionals

Let $\mathcal{S}_m$ be the space of all real mxm symmetric matrices. For a given element $A=(a_{ij})$ in $\mathcal{S}_m$, we will take the norm $\|A\|=\|A\|_\infty=\max_{i,j}|a_{ij}|$. We write the spectral decomposition of A,

$$A=C(A)D(A)C(A)', \tag{2.1}$$

where C(A), with columns $q_j(A)$, is a mxm orthogonal matrix of eigenvectors, and D(A) is a mxm matrix of eigenvalues $\ell_1(A)\leq \ldots\leq\ell_m(A)$. Let F_n the distribution function in $\mathbb{R}^p$ of the *design measure* associated with the n rows x_1, ..., x_n of the matrix X_1. We have the integral representation

$$X'X/n=\int yy'F_n(dy)=T[F_n], \tag{2.2}$$

$y=(1,x')'\in\mathbb{R}^m$, where T[.] is an adequate functional defined in a space of measures. We can write $\ell_j(X'X)=n\ell_j(\int yy'F_n(dy))=n\ell_j(T[F_n])$ and, consequently,

$$\ell_j(X'X)-\ell_j(X'_{(i)}X_{(i)})=$$
$$\ell_j(T[F_n])+(n-1)\{\ell_j(T[F_n])-\ell_j(T[F_{n-1(i)}])\}, \tag{2.3}$$

where $F_{n-1(i)}$ is the distribution function of the design measure on the n-1 rows of $X_{1(i)}$, namely,

$$F_{n-1(i)}=F_n+\frac{1}{n-1}(F_n-\delta_{x_i}). \tag{2.4}$$

We can take advantage of (2.3) and (2.4) to develop an approximation for the difference $\ell_j(X'X)-\ell_j(X'_{(i)}X_{(i)})$ based on certain differentiabiliy properties of the functional $\ell_j(T[.])$. We make the following assumptions:

Assumption 1. The points x_1, ..., x_n are the first n elements of an infinite sequence $\{x_i\}$ of points contained in a compact set $C\subseteq\mathbb{R}^p$.

Assumption 2. Let $\mathcal{M}$ be the linear space of finite signed measures concentrated on C. The functional T[.] of (2.2) is defined in $\mathcal{M}$ in the form $T[\mu]=\int yy'\mu(dy)$. $\mathcal{M}$ is endowed with the norm $\|\cdot\|_V$ of the total variation (see Rudin (1974, chap. 6) for definition).

Observe:

a) Under assumption 1, both F_n and $F_{n-1(i)}$ are in $\mathcal{M}$ and $\|F_n\|_V=\|F_{n-1(i)}\|_V=1$;

b) The functional $T:(\mathcal{M},\|\cdot\|_V)\longrightarrow(\mathcal{S}_m,\|\cdot\|_\infty)$ is *linear* ($T[\alpha\mu+\beta\lambda]=\alpha T[\mu]+\beta T[\lambda]$, $\mu,\lambda\in\mathcal{M}$, $\alpha,\beta\in\mathbb{R}$); and *bounded* ($\|T[\mu]\|_\infty\leq M\|\mu\|_V$ for some fixed constant $M>0$ independent of μ);

c) For $\mu\in\mathcal{M}$, $\ell_j(T[\mu])$ means, in the ordering established above, the jth eigenvalue of $T[\mu]=\int_C yy'\mu(dy)=(t_{ik}[\mu])\in\mathcal{S}_m$. If $\ell_j(T[\mu])$ is simple, $h\in\mathcal{M}$ and $t\longrightarrow0$, we get, from standard results of perturbation theory for real symmetric matrices (see Kato (1982) for details),

$$\ell_j(T[\mu+th])=\ell_j(T[\mu]+tT[h])=\ell_j(T[\mu])+tq_j'(T[\mu])T[h]q_j(T[\mu])+o(|t|).$$

This entails,

$$\lim_{t\longrightarrow0}\frac{\ell_j(T[\mu+th])-\ell_j(T[\mu])}{t}=D\ell_j(T[\mu])(h), \qquad (2.5)$$

where $D\ell_j(T[\mu])(h)=q_j'(T[\mu])T[h]q_j(T[\mu])$. Since $D\ell_j(T[\mu])(h)$ is linear in h, (2.5) says that $\ell_j(T[\mu])$ is *Gâteaux* (weakly) differentiable at every $\mu\in\mathcal{M}$ such that the jth eigenvalue of $T[\mu]$ is simple.

We now proof the following theorem.

Theorem 1. Let $\mu,\lambda\in\mathcal{M}$ such that $\|\mu\|_V$, $\|\lambda\|_V\le 1$. If T[.] has all its eigenvalues simple at every point of the segment $(1-t)\mu+t\lambda$, $0\le t\le 1$, then,

$$\max_{1\le j\le m} |\ell_j(T[\lambda])-\ell_j(T[\mu])-D\ell_j(T[\mu])(\lambda-\mu)| \le Q(\lambda,\mu)\|\lambda-\mu\|_V, \tag{2.6}$$

where $Q(\lambda,\mu)\longrightarrow 0$, if $\|\lambda-\mu\|_V\longrightarrow 0$.

Proof. For each j=1, ...,m, the functional $\ell_j(T[.])$ is weakly differentiable in all the segment $[\mu,\lambda]$. We can then apply the mean value theorem (see Lang (1969, chap. 5)) to obtain

$$\max_{1\le j\le m} |\ell_j(T[\lambda])-\ell_j(T[\mu])-D\ell_j(T[\mu])(\lambda-\mu)| \le Q(\lambda,\mu)\|\lambda-\mu\|_V,$$

where $Q(\lambda,\mu)=\max_{1\le j\le m}\ \sup_{0\le t\le 1}\ \sup_{\|h\|_V\le 1} |\{D\ell_j(T[(1-t)\mu+t\lambda])-D\ell_j(T[\mu])\}(h)|$.

To proof that $Q(\lambda,\mu)\longrightarrow 0$, as $\|\lambda-\mu\|_V\longrightarrow 0$, we reason as follows. As remarked in Kato (1982, p. 136), the eigenvalues $\ell_j(A)$ and eigenvectors $\varphi_j(A)$ are uniformly continuous functions of matrix argument in any bounded region of $\mathcal{S}_m$ (i.e. in any region of $\mathcal{S}_m$ where $\|A\|_\infty$ is bounded). Since $\|T[\lambda]-T[\mu]\|_\infty\le M\|\lambda-\mu\|_V$, the eigenvalues $\ell_j(T[\nu])$ and eigenvectors $\varphi_j(T[\nu])$ are uniformly continuous functions of ν in the region $\|\nu\|_V\le 1$. On the other hand, we have, for $\|h\|_V\le 1$, the elementary inequality $|a'T[h]b|\le mM\|a\|_E\|b\|_E$, where $\|.\|_E$ denotes the euclidean norm in $\mathbb{R}^m$. It is easy to see that putting all these things together, we get the claim of the theorem. ■

As an example of possible applications of theorem 1, we establish the following corollary.

Corollary 1. Suppose that, for every n and $1\le i\le n$, the matrix $T[(1-t)F_n+tF_{n-1(i)}]$ has all its eigenvalues simple for $0\le t\le 1$. Then,

$$\max_{1\le j\le m}\ \max_{1\le i\le n} |\ell_j(X'X)-\ell_j(X'_{(i)}X_{(i)})-k^2_{ij}(X'X)| \le a_n, \tag{2.7}$$

where $k_{ij}(X'X)=(1,x'_i)\varphi_j(X'X)$ and $a_n\longrightarrow 0$ as $n\longrightarrow\infty$.

Proof. Put $\lambda=F_{n-1(l)}$ and $\mu=F_n$. By (2.4) and (2.5) above, $D\ell_j(T[F_n])(\lambda-\mu)$ equals,

$$[(\ell_j(X'X)/n)-k_{1j}^2(X'X)]/n-1.$$

Using (2.3), we get $\ell_j(X'X)-\ell_j(X'_{(l)}X_{(l)})-k_{1j}^2(X'X)=$

$$-(n-1)\{\ell_j(T[\lambda]-\ell_j(T[\mu])-D\ell_j(T[F_n])(\lambda-\mu)\}.$$

We have $\|\lambda-\mu\|_V=\|\frac{1}{n-1}(F_n-\delta_{X_l})\|_V=2/n$. From theorem 1 above, $\max_{1\le j\le m}\max_{1\le l\le n}|\ell_j(X'X)-\ell_j(X'_{(l)}X_{(l)})-k_{1j}^2(X'X)|\le(2/n)(n-1)b_n$, where the sequence $b_n=\max_{1\le l\le n}Q(F_{n-1(l)},F_n)$ tends to zero as n goes to ∞. The corollary follows with $a_n=(2/n)(n-1)b_n$. ■

Remark 1. For practical purposes, (2.7) yields the approximation

$$\ell_j(X'X)-\ell_j(X'_{(l)}X_{(l)})=k_{1j}^2(X'X)+O(1). \qquad (2.8)$$

(2.8) has been proposed previously by Critchley (1985), and, recently, by Wang and Nyquist (1991). They use empirical influence curve considerations. Chaterjee and Hadi (1988) also propose this approximation. Note that corollary 1 allows a direct formal statement for estimating the approximation error directly from the sample size n.

3. Approximations for the eigenvalues of Z'Z

The main task of this paper is to present the corresponding version of (2.8) for the eigenvalues $\{\lambda_j\}$ of the correlation matrix Z'Z. Let $\mu\in\mathcal{M}$ such that the functional $C:\mathcal{M}\longrightarrow\mathcal{S}_p$,

$$C[\mu]=\int_C[x-m][x-m]'\mu(dx),$$

where $m=\int_C x\mu(dx)$, yields a positive definite pxp matrix. Define the functionals $S[\mu]=I_p*C[\mu]$, where '*' is the Hadamard product of matrices (see Rao (1973), p. 30 for definition), and $CS[\mu]=S^{-1/2}[\mu]C[\mu]S^{-1/2}[\mu]$. It is easy to see that

$$Z'Z=CS[F_n], \tag{3.1}$$

and $\lambda_j=\ell_j(CS[F_n])$, $\gamma_j=\varphi_j(CS[F_n])$.

Let $h\in\mathcal{M}$. Define the pxp matrices

$$P(\mu,h)=\int_C xx'h(dx)-[\int_C x\mu(dx)][\int_C xh(dx)]'-[\int_C xh(dx)][\int_C x\mu(dx)]'$$

and

$$R(\mu,h)=S^{-1/2}[\mu]P(\mu,h)S^{-1/2}[\mu]-(1/2)(S^{-1/2}[\mu]C[\mu]Q+QC[\mu]S^{-1/2}[\mu]),$$

where $Q=I_p*P(\mu,h)*S^{-3/2}[\mu]$. We proof the following lemma.

Lemma 1. If $C[\mu]$ is p.d. and $\ell_j(CS[\mu])$ is simple, then, $\ell_j(CS[\mu])$ is weakly differentiable at μ and

$$D\ell_j(CS[\mu])(h)=\varphi_j'(CS[\mu])R(\mu,h)\varphi_j(CS[\mu]).$$

Proof. It is easy to see that $C[\mu+th]=C[\mu]+tP(\mu,h)+o(|t|)$. On the other hand, a standard first order Taylor expansion yields $S^{-1/2}[\mu+th]=S^{-1/2}[\mu]+tQ+o(|t|)$. Therefore,

$$CS[\mu+th]=CS[\mu]+tR(\mu,h)+o(|t|). \tag{3.2}$$

The rest follows from (3.2) and the perturbation series for $\ell_j(CS[\mu+th])$. ■

We now derive the approximation for $\lambda_j-\lambda_{j(1)}$.

Theorem 2. Suppose that, for every n and $1\le i\le n$, the matrix $CS[(1-t)F_n+tF_{n-1(1)}]$ is p.d. and has all its eigenvalues simple at every point of the segment $0\le t\le 1$. We have, uniformly in $1\le j\le p$ and $1\le i\le n$,

$$\lambda_j-\lambda_{j(1)}=\frac{n}{n-1}\,[k_{1j}^2-\lambda_j\sum_{k=1}^{p}\gamma_{kj}^2 z_{1k}^2]+o(1/n), \tag{3.3}$$

where $\gamma_j=(\gamma_{1j}, \ldots, \gamma_{pj})'$, and $z_i'=(z_{i1}, \ldots, z_{ip})'$ is the ith row of the matrix Z.

Proof. Let $\mu=F_n$, $\lambda=F_{n-1(i)}$ and $h=F_{n-1(i)}-F_n=(1/n-1)(F_n-\delta_{x_i})$, by (2.4). We need to determine the expression of $D\ell_j(CS[F_n])(h)$. We have $P(F_n,h)=[\mathcal{X}'\mathcal{X}/n-(x_i-\bar{x})((x_i-\bar{x})']/n-1$, where $\mathcal{X}$ is the nxp matrix of centered predictors. Therefore,

$$S^{-1/2}[F_n]P(F_n,h)S^{-1/2}[F_n]=[Z'Z-nz_iz_i']/n-1 \tag{3.4}$$

On the other hand, if $Q=I_p*P(F_n,h)*S^{-3/2}(F_n)$, we get

$$S^{-1/2}[F_n]C[F_n]Q=[Z'Z-nZ'Z\mathrm{diag}(z_iz_i')]/n-1,$$

and (3.5)

$$QC[F_n]S^{-1/2}[F_n]=[Z'Z-n\mathrm{diag}(z_iz_i')Z'Z]/n-1,$$

where $\mathrm{diag}(z_iz_i')$ is the pxp diagonal matrix of kth diagonal element equal to z_{ik}^2. According to lemma 1, (3.3), (3.4) and (3.5) lead to

$$D\ell_j(CS[F_n])(h)=[-nk_{ij}^2+n\lambda_j\sum_{k=1}^{p}\gamma_{kj}^2z_{ik}^2]/n-1. \tag{3.6}$$

We can now parallel the arguments in the proof of theorem 1 to obtain an analog of (2.6) which yields

$$\max_{1\le j\le m}\ \max_{1\le i\le n}|\lambda_{j(i)}-\lambda_j-D\ell_j(CS[F_n])(h)|\le c_n\left\|\frac{1}{n-1}(F_n-\delta_{x_i})\right\|_V,$$

where $c_n\longrightarrow 0$ as $n\longrightarrow\infty$. Since we have $\left\|\frac{1}{n-1}(F_n-\delta_{x_i})\right\|_V=2/n$, the theorem follows. ■

4. Applications

We now relate approximation (3.3) to the detection of collinearity-influential points.

4.1. Interpretation

From (3.3), we see that deletion of the ith case can produce different effects in λ_j. However, several particular cases are worth to observe:

a) If case i is extreme in the jth direction, i.e. k_{ij}^2/λ_j is large (recall decomposition (1.6) for v_{ii}) we have typically $k_{ij}^2/\lambda_j > \max_k z_{ik}^2 > \sum_{k=1}^{p} \gamma_{kj}^2 z_{ik}^2$ and, therefore, deletion of case i will tend to produce $\lambda_j - \lambda_{j(i)} > 0$. If λ_j is an eigenvalue of large or moderate size, we can deduce that case i might be shading the perception of a collinearity. However, if λ_j is small, deletion of case i will tend to strengthen the collinearity situation;

b) If case i is approximately orthogonal to γ_j, i.e. $k_{ij} = z_i'\gamma_j \cong 0$, we will expect that deletion of case i will produce $\lambda_j - \lambda_{j(i)} < 0$. Therefore, if λ_j is small, case i might be inducing a collinearity among the columns of X.

4.2. An example

We will use for illustration a data set presented by Gunst and Mason (1980, appendix A). The response variable is the GNP (Gross National Product) of 49 countries explained by six socioeconomic variables (see Gunst and Mason (1980) for details and meaning of the variables). These data set have been analyzed in Mason and Gunst (1985) and Belsley (1991, chap. 8).

For diagnostic purposes, approximation (3.3) can be supported with the use of a principal-component plot (k_j, k_l). The use of principal-component plots for both detecting extreme cases and collinearity is originally proposed by Hocking (1984). See also Velilla (1989).

For these data, we have $\lambda_1=0.0267$ which is an indicator of a slight degree of collinearity. Figure 1 shows a principal-component plot (k_1,k_5). The two starred points are Hong Kong and Singapore which outlie in the k_5 direction. Since, $k_5'k_5=\lambda_5$ these two points are suspicious of inflating artificially the eigenvalue λ_5 and this might be provoking, according to the restriction $\sum_{j=1}^{6}\lambda_j=6$, the small value of λ_1 above.

Figure 1

Table 1 shows the coordinates of γ_1 and the centered and scaled coordinates of the cases Hong Kong and Singapore. It can be seen that both Hong Kong and Singapore are, approximately, orthogonal to γ_1. The first summand in the right hand side of (3.3) is dominated by a negative quantity and, therefore, if I=(Hong Kong, Singapore) it can be anticipated that $\lambda_1-\lambda_{1(I)}<0$. In fact, $\lambda_{1(I)}=0.1800$ and hence cases Hong Kong and Singapore are creating artificially a collinearity among the six socioeconomic variables.

Table 1

5. Final coments

A natural companion of the approximation (3.3) is the extension to multiple cases deletion and the associated masking problems. For (3.3), for example, the aproximation for deletion of the group of cases $I=\{i_1, \ldots, i_k\}$ adopts the form

$$\lambda_j-\lambda_{j(I)}= \frac{nk}{n-k} [\sum_{l\in I} k_{lj}^2-(\lambda_j/k) \sum_{l=1}^{p} \gamma_{lj}^2 (\sum_{l\in I} z_{1l}^2)] + o(1/n). \qquad (5.1)$$

Other possible application of the techniques in section 2 refers to the set of condition indexes $\{\eta_j\}$. It can be shown that, under conditions similar to those appearing in the statement of theorem 2, we have, uniformly in $1\le j\le p$ and $1\le i\le n$,

$$\eta_{j(i)}-\eta_j=\frac{n}{2(n-1)} \eta_j[(k_{ij}^2/\lambda_j)-(k_{ip}^2/\lambda_p)+ \sum_{k=1}^{p} (\gamma_{kp}^2-\gamma_{kj}^2)z_{ik}^2]+o(1/n). \qquad (5.2)$$

Chaterjee and Hadi (1988) have proposed the measure $H_1=|\kappa_{(1)}-\kappa|/\kappa$ as a diagnostic tool for collinearity-influential points. Approximation (5.2), in the particular case of j=1, might be used to obtain a natural approximation $\tilde{H}_1$ for H_1. See also Chaterjee and Hadi (1988) for an approach to H_1 based on a power method for approximating the maximal and minimal eigenvalues of a matrix.

The theory presented in this paper is an extension of the results obtained in Velilla (1988). The functional-based technique presented here can be suitably modified to treat problems in which the design matrix differs from Z, whenever the modified cross products matrix can be expressed in terms of a functional depending on the empirical F_n. For example, Belsley (1991) strongly recommends not centering the data and scaling the columns of X to unit length to form the matrix $\tilde{\tilde{X}}$, say. It is straightforward to express $\tilde{\tilde{X}}'\tilde{\tilde{X}}$ as a functional depending on F_n and, as a consequence, analyze, via the techniques exposed in section 2, the importance of the rows of X in the collinearity measures related to $\tilde{\tilde{X}}$.

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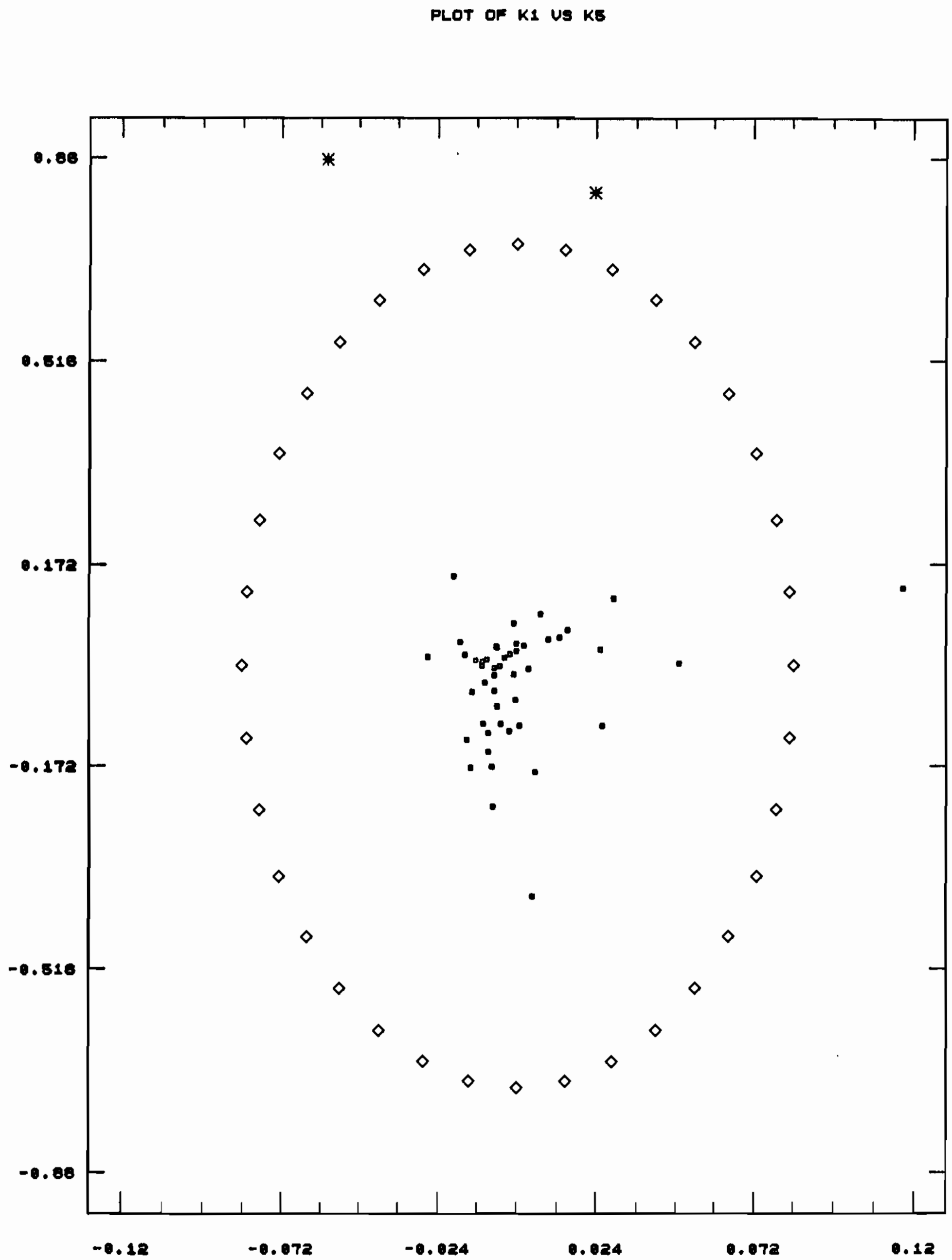
PLOT OF K1 VS K5
0.86
0.516
0.172
-0.172
-0.516
-0.86
-0.12
-0.072
-0.024
0.024
0.072
0.12

Figure 1

Variable	1	2	3	4	5	6
γ_1	.0066	.0340	.7090	-.7034	.0275	.0252
Hong Kong	.0361	.1301	.6763	.6449	-.1395	-.0976
Singapore	-.0730	.0481	.6338	.7158	-.1869	.0108

Table 1. Loadings for the eigenvector γ_1 and values of the standardized coordinates of the design matrix for Hong Kong and Sinagapore.