THE LINEAR MODEL

Projections

Theorem: Let $a: n \times 1$ be a non-zero vector and let $d: n \times 1$ be any vector. Then d can be uniquely expressed as:

$$d = b_1 + b_2$$

where b_1 depends on a and b_2 is orthogonal to a. Furthermore, $b_1=ca$ with $c=\frac{d'a}{a'a}$ and $b_2=d-b_1$.

Proof:

Let $d = b_1 + b_2 = ca + b_2$ where $b_2 \perp a$. Then a'd = ca'a + 0 or $c = \frac{d'a}{a'a}$ since $a'a \neq 0$.

Conversely, if $c=rac{d'a}{a'a}$ and $m{b_2}=m{d}-m{b_1}$, then $m{b_2}=m{d}-cm{a}$. Therefore

 $\boldsymbol{b_2} \perp \boldsymbol{a}$ and since c is unique, $\boldsymbol{b_2}$ is also unique.

The vector b_1 is the projection of d on a and b_2 is the component of d orthogonal to a. The square of the length of the projection of d on a is

$$b_1'b_1=c^2a'a=\frac{(d'a)^2}{a'a}.$$

Theorem: Let V be a vector space and let d be any vector. Then d can be uniquely expressed as:

$$d = c + e$$

where $c \in V$ and $e \perp V$. If V is generated by the columns of $A: n \times m$, then

$$c = A(A'A)^*A'd$$
 and $e = (I - A(A'A)^*A')d$

Proof:

Let d=c+e where $c\in V$ and $e\perp V$. Then $d=Ac_1+e$ for some c_1 . In other words

$$A'Ac_1 = A'd$$
 since $A'e = 0$.

These equations to determine c_1 are consistent, because $\mathrm{rank}\,(A'A)=\mathrm{rank}\,(A'A,A'd)$. A solution of $A'Ac_1=A'd$ is

$$c_1 = (A'A)^*A'd$$

for any generalized inverse $(A'A)^*$ of A'A. Therefore

$$c = Ac_1 = A(A'A)^*A'd$$

and

$$e = d - c = (I - A(A'A)^*A')d.$$

Suppose now that a solution $oldsymbol{c_1}$ exists to

$$A'Ac_1 = A'd$$
.

Let $\boldsymbol{c} = \boldsymbol{A}\boldsymbol{c_1}$ and $\boldsymbol{e} = \boldsymbol{d} - \boldsymbol{c}$, then

$$d = c + e$$

where $c \in V$ and $e \perp V$, since

$$A'e = A'd - A'c = A'd - A'Ac_1 = 0.$$

To prove the uniqueness of the expression, let

$$d = Ac_0 + e_0$$

with $e_0 \perp V$. Then

$$A'd = A'Ac_0 = A'Ac_1.$$

Therefore $A'A(c_0-c_1)=0$ and $(c_0-c_1)'A'A(c_0-c_1)=0$. The last identity is the sum of squares of the elements of $A(c_0-c_1)$, which is zero. In other words, $A(c_0-c_1)=0$ and $Ac_0=Ac_1$. Furthermore,

$$e_0 = d - Ac_0 = d - Ac_1 = e$$

and the expression is unique.

The vector c is the projection of d on V and e is the component of d which is orthogonal to V. Thus, $c = Ac_1$ is the projection of d ($A'Ac_1 = A'd$)

Conclusion: The equations

$$A'Ax = A'y$$

imply that Ax is the projection of y on the vector space generated by the columns of A. Thus, $Ax = A(A'A)^*A'y$ is the projection of y. And $A(A'A)^*A'$ is the projection matrix.

Note: Let V^{\perp} represent the vector space orthogonal to V. Since V is generated by the columns of A: $n \times m$ the dim (V) + dim (V^{\perp}) = n.

Theorem: The projection matrix $P = A(A'A)^*A'$ is unique, symmetrical and idempotent. (Unique with respect to the choice of the generalized inverse and unique with respect to the specific A. The only condition is that the vector space V must be generated by the columns of A.)

Proof:

1. Uniqueness: Suppose that P_1 is such a projection matrix as well. Then

$$P_1d = Pd \quad \forall d \implies P_1 = P$$

2. Symmetry: It follows from (1) and the fact that $(A'A)^{*'}$ is also a generalized inverse of A'A. Therefore

$$(A(A'A)^*A')' = A(A'A)^{*'}A' = A(A'A)^*A'$$

3. Idempotent: $P^2d = P(Pd) = Pd$ since $Pd \in V \ \forall d$. Therefore $P^2 = P$.

Corollary:

1. If $A = (A_1, A_2)$ with $A_1'A_2 = \mathbf{0}$, it also follows that $P = A(A'A)^*A' = A_1(A_1'A_1)^*A_1' + A_2(A_2'A_2)^*A_2'.$

2. If the columns of \boldsymbol{A} are for instance mutually orthogonal, it follows that: (a)

$$P = A(A'A)^*A' = (a_1, a_2, \dots, a_m) \begin{pmatrix} (a'_1a_1)^{-1} & 0 & \cdots & 0 \\ 0 & (a'_2a_2)^{-1} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & (a'_ma_m)^{-1} \end{pmatrix} \begin{pmatrix} a'_1 \\ a'_2 \\ \cdots \\ a'_m \end{pmatrix}$$

$$= \sum_{i=1}^m a_i (a'_ia_i)^{-1} a'_i.$$

(b) The projection of the vector $oldsymbol{y}$ on V is:

$$Py = A(A'A)^*A'y = \sum_{i=1}^m a_i(a_i'a_i)^{-1}a_i'y = \sum_{i=1}^m \frac{a_i'y}{a_i'a_i}a_i$$

which is the sum of the projections on the individual mutually orthogonal vectors.

(c) The square of the length of the projection of \boldsymbol{y} on V is:

$$y'Py = \sum_{i=1}^m \frac{(a_i'y)^2}{a_i'a_i}.$$

The projection matrix P can be calculated easily by using a convenient basis for V. The following theorem can for instance be used.

Theorem: Suppose that V with rank (V) = r is generated by the columns of $A = (a_1, a_2, \dots, a_r)$. It is always possible to select a mutually orthogonal basis for V, say the columns of $B = (b_1, b_2, \dots, b_r)$, in such a way that b_s only depends on the first s columns of s.

Proof:

Assume the vector $oldsymbol{a_2}$. It can be expressed uniquely as

$$a_2 = b_1 + b_2$$

where b_1 is dependent on a_1 and b_2 is orthogonal to a_1 . The first two vectors a_1 and a_2 can be replaced by b_1 and b_2 in the basis, without changing V. If $b_1 = 0$, let $b_1 = a_1$ and $b_2 = a_2$. The vector a_3 can be uniquely expressed as

$$a_3 = b + b_3$$

where \boldsymbol{b} depends on $\boldsymbol{b_1}$ and $\boldsymbol{b_2}$ and where $\boldsymbol{b_3}$ is orthogonal to $\boldsymbol{b_1}$ and $\boldsymbol{b_2}$. It follows that

$$b = \frac{a_3'b_1}{b_1'b_1}b_1 + \frac{a_3'b_2}{b_2'b_2}b_2$$

and

$$b_3=a_3-b.$$

This process can be continued until all the a_i 's are replaced by b_i 's in the basis.

It follows that:

$$\begin{split} P &= A(A'A)^*A' = B(B'B)^*B' \\ &= (b_1,b_2,\cdots,b_r) \begin{pmatrix} (b_1'b_1)^{-1} & 0 & \cdots & 0 \\ 0 & (b_2'b_2)^{-1} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & (b_r'b_r)^{-1} \end{pmatrix} \begin{pmatrix} b_1' \\ b_2' \\ \cdots \\ b_r' \end{pmatrix} \\ &= \sum_{i=1}^r \ b_i (b_i'b_i)^{-1} b_i'. \end{split}$$

Examples:

1. Assume $\mathbf{A} = \begin{pmatrix} 2 & 0 \\ 1 & 1 \\ 3 & 1 \end{pmatrix}$. Then, it follows that:

$$b_1 = \frac{2}{7} {2 \choose 1}$$
 and $b_2 = a_2 - b_1 = \frac{1}{7} {-4 \choose 5}$

The projection matrix is:

$$\mathbf{P} = \frac{1}{14} \begin{pmatrix} 2\\1\\3 \end{pmatrix} (2 \quad 1 \quad 3) + \frac{1}{42} \begin{pmatrix} -4\\5\\1 \end{pmatrix} (-4 \quad 5 \quad 1)$$

$$= \frac{1}{14} \begin{pmatrix} 4 & 2 & 6\\2 & 1 & 3\\6 & 3 & 9 \end{pmatrix} + \frac{1}{42} \begin{pmatrix} 16 & -20 & -4\\-20 & 25 & 5\\-4 & 5 & 1 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 2 & -1 & 1\\-1 & 2 & 1\\1 & 1 & 2 \end{pmatrix}$$

A better choice for \mathbf{A} would be $\mathbf{A} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}$ since we can replace the first column with $\frac{1}{2}(\mathbf{a_1} - \mathbf{a_2})$

in $\mathbf{A} = \begin{pmatrix} 2 & 0 \\ 1 & 1 \\ 3 & 1 \end{pmatrix}$. Then, we have

$$\boldsymbol{b_1} = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$
$$\boldsymbol{b_2} = \boldsymbol{a_2} - \boldsymbol{b_1} = \frac{1}{2} \begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix}$$

The projection matrix is:

$$P = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} (1 \quad 0 \quad 1) + \frac{1}{6} \begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix} (-1 \quad 2 \quad 1)$$

$$= \frac{1}{2} \begin{pmatrix} 1 \quad 0 \quad 1 \\ 0 \quad 0 \quad 0 \\ 1 \quad 0 \quad 1 \end{pmatrix} + \frac{1}{6} \begin{pmatrix} 1 \quad -2 \quad -1 \\ -2 \quad 4 \quad 2 \\ -1 \quad 2 \quad 1 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 2 \quad -1 \quad 1 \\ -1 \quad 2 \quad 1 \\ 1 \quad 1 \quad 2 \end{pmatrix}$$

An alternative calculation of **P** follows from the fact that

rank $(V^{\perp}) = 1.V^{\perp}$ is for instance generated by

$$e = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$$

Therefore

$$I - P = e(e'e)^{-1}e'$$

$$= \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} (1 - 1) = \frac{1}{3} \begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}$$

and

$$\mathbf{P} = \frac{1}{3} \begin{pmatrix} 2 & -1 & 1 \\ -1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

2. For the previous Example 2 it follows that:

$$\mathbf{A} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 3 & 1 & 1 \end{pmatrix}$$

An orthogonal basis for V is the columns of

$$\mathbf{B} = \begin{pmatrix} 1 & -1 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}$$

The projection matrix is:

$$P = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} (1 \quad 0 \quad 1) + \frac{1}{3} \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix} (-1 \quad 1 \quad 1)$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} + \frac{1}{3} \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix} = \frac{1}{6} \begin{pmatrix} 5 & -2 & 1 \\ -2 & 2 & 2 \\ 1 & 2 & 5 \end{pmatrix}$$

Again it follows that $rank(V^{\perp}) = 1$ and V^{\perp} is generated by

$$e = \begin{pmatrix} 1 \\ 2 \\ -1 \end{pmatrix}$$

Therefore

$$I - P = e(e'e)^{-1}e'$$

$$= \frac{1}{6} \begin{pmatrix} 1\\2\\-1 \end{pmatrix} (1 \quad 2 \quad -1) = \frac{1}{6} \begin{pmatrix} 1 & 2 & -1\\2 & 4 & -2\\-1 & -2 & 1 \end{pmatrix}$$

and

$$\mathbf{P} = \frac{1}{6} \begin{pmatrix} 5 & -2 & 1 \\ -2 & 2 & 2 \\ 1 & 2 & 5 \end{pmatrix}$$

Sums of Squares of Linear Sets

Let $y: n \times 1 \sim (\mu, \sigma^2 I)$. The sum of squares of the linear function c'y is defined as the square of the length of the projection of y on c, namely:

$$s^{2} = \left(\frac{c'y}{c'c}c\right)'\left(\frac{c'y}{c'c}c\right)$$
$$= \frac{(c'y)^{2}}{c'c}.$$

Note that this sum of squares is the same as the sum of squares of the linear function dc'y, for any non-zero constant d. This sum of squares is therefore only dependent on the vector space generated by \mathbf{c} .

It follows that:

$$E(s^{2}) = E(c'y)^{2}/c'c$$

$$= \{ var(c'y) + [E(c'y)]^{2} \}/c'c$$

$$= \sigma^{2} + [c'E(y)]^{2}/c'c$$

The expected value of s^2 is therefore σ^2 plus a term which is obtained by replacing the random variables by their expected values in s^2 . Note that:

$$E(s^2) = \sigma^2 \iff E(c'v) = 0$$

The sum of squares of a linear set is defined similarly. Suppose that $C: n \times m = (c_1, c_2, \cdots, c_m)$ and rank C = r. Let C = r. Let C = r be the vector space generated by the columns of C = r. Let C = r be the linear set of all linear functions with coefficient vectors in C = r.

$$L_C = \{ \boldsymbol{c}' \boldsymbol{y} : \boldsymbol{c} \in V_C \}.$$

 L_C is generated by the linear functions $c_1'y, \cdots, c_m'y$ just as V_C is generated by c_1, \cdots, c_m . The linear functions are dependent or independent corresponding to dependence or independence of the coefficient vectors. Any r independent linear functions in L_C will therefore generate the linear set L_C . We say that L_C has r degrees of freedom.

The sum of squares of the linear set L_C is defined as the square of the length of the projection of y on V_C , namely:

$$S^2 = \{ C(C'C)^*C'y \}' \{ C(C'C)^*C'y \} = y'C(C'C)^*C'y \}$$

since $C(C'C)^*C'$ is unique, symmetrical and idempotent.

The expression for S^2 is independent of the specific functions Cy which generate L_C . Suppose that the columns of $B = (b_1, b_2, \dots, b_r)$ form a mutually orthogonal basis for V_C , so that $L_B = L_C$. It then follows that:

$$S^{2} = y'C(C'C)^{*}C'y = y'B(B'B)^{*}B'y$$

$$= y'(b_{1}, b_{2}, \dots, b_{r}) \begin{pmatrix} (b'_{1}b_{1})^{-1} & 0 & \cdots & 0 \\ 0 & (b'_{2}b_{2})^{-1} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & (b'_{r}b_{r})^{-1} \end{pmatrix} \begin{pmatrix} b'_{1} \\ b'_{2} \\ \cdots \\ b'_{r} \end{pmatrix} y$$

$$= \sum_{i=1}^{r} \frac{(b'_{i}y)^{2}}{b'_{i}b_{i}} = \sum_{i=1}^{r} s_{i}^{2}$$

where s_i^2 is the sum of squares of $b_i^\prime y$. Also,

$$E(S^{2}) = \sum_{i=1}^{r} E(s_{i}^{2}) = r\sigma^{2} + \sum_{i=1}^{r} (b_{i}'E(y))^{2}/b_{i}'b_{i}.$$

It follows that:

$$E(S^2) = r\sigma^2 + S_\mu^2$$

where S^2_μ is a term obtained by replacing the random variables in S^2 with their expected values.

Note that $E(S^2) = r\sigma^2 \Leftrightarrow \text{if and only if } E(B'y) = \mathbf{0}.$

But E(B'y) = 0 if and only if E(C'y) = 0, since $B = CD_1$ for some D_1 and $C = BD_2$ for some D_2 .

Suppose that V_{C_1} and V_{C_2} with ranks r_1 and r_2 respectively, are mutually orthogonal vector spaces with corresponding linear sets L_{C_1} and L_{C_2} . Therefore $C_1'C_2 = 0$. The linear sets L_{C_1} and L_{C_2} are orthogonal. Let

$$V_C = V_{C_1} \oplus V_{C_2}$$
 and $L_C = L_{C_1} \oplus L_{C_2}$.

The implication is that V_C is generated by the columns of $C = (C_1, C_2)$. If S_i^2 is the sum of squares of L_{C_i} and S^2 is the sum of squares of L_C , it then follows that:

$$S^{2} = y'C(C'C)^{*}C'y = y'C_{1}(C'_{1}C_{1})^{*}C'_{1}y + y'C_{2}(C'_{2}C_{2})^{*}C'_{2}y = S_{1}^{2} + S_{2}^{2}$$

The same line of reasoning can be used to show that if V_{C_i} , $i=1,\cdots,k$ are mutually orthogonal vector spaces with corresponding linear sets L_{C_i} , $i=1,\cdots,k$ and

$$V_C = \bigoplus V_{C_i}$$
 and $L_C = \bigoplus L_{C_i}$

in other words V_C is generated by the columns of ${\pmb C}=({\pmb C}_1,{\pmb C}_2,\cdots,{\pmb C}_k)$, then

$$S^{2} = y'C(C'C)^{*}C'y = \sum_{i=1}^{k} y'C_{i}(C'_{i}C_{i})^{*}C'_{i}y = \sum_{i=1}^{k} S_{i}^{2}$$

with S_i^2 the sum of squares of L_{C_i} .

Consider the linear set

$$L_C = \{ c' y : c \in V_C \}.$$

with $C: n \times m = (c_1, c_2, \dots, c_m)$, rank C = r and C the vector space generated by the columns of C. The mean square for C is

$$S^2/r$$

with expected value

$$\sigma^2 + S_u^2/r$$
.

Examples

1. Suppose that $y: 4 \times 1 \sim (\mu, \sigma^2 I)$ with

$$\boldsymbol{\mu} = \begin{pmatrix} \alpha \\ \alpha \\ \beta \\ \beta \end{pmatrix}$$

Let

$$m{c_1} = egin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix}, \ m{c_2} = egin{pmatrix} 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & -1 \end{pmatrix} \ \ \text{and} \ \ m{c} = (m{c_1}, m{c_2}).$$

The sums of squares of the linear sets $L_{\mathcal{C}_1}$ and $L_{\mathcal{C}_2}$ are

$$S_1^2 = \frac{1}{2}(y_1 + y_2)^2 + \frac{1}{2}(y_3 + y_4)^2$$

and

$$S_2^2 = \frac{1}{2}(y_1 - y_2)^2 + \frac{1}{2}(y_3 - y_4)^2.$$

respectively. The total sum of squares is

$$S^2 = y_1^2 + y_2^2 + y_3^2 + y_4^2 = S_1^2 + S_2^2$$

The expected values are:

$$E(S_1^2) = 2\sigma^2 + 2\alpha^2 + 2\beta^2$$

$$E(S_2^2) = 2\sigma^2$$

$$E(S^2) = 4\sigma^2 + 2\alpha^2 + 2\beta^2$$
.

2. Suppose that $y: n \times 1 \sim (\mu, \sigma^2 I)$. The set of all linear functions of y is generated by Iy, with sum of squares:

$$S^2 = y'I(I'I)^*I'y = y'y = \sum_{i=1}^n y_i^2.$$

Note also that the linear functions $y_1, y_2, \dots y_n$ form a mutually orthogonal basis for this linear set. The sum of squares, S^2 , is therefore the same as the total of the individual sums of squares of the y_i 's, and the sum of squares of

$$y_i = (0,0,\cdots,0,1,0,\cdots,0)y$$

is

$$s_i^2 = y_i^2$$
.

Let L_E be the set of linear functions orthogonal to \bar{y} . The sum of squares of L_E is

$$S_E^2 = y'y - n\bar{y}^2 = \sum_{i=1}^n (y_i - \bar{y})^2,$$

the mean square of L_E is

$$S_E^2/(n-1)$$

with expected value

$$\sigma^2 + \frac{1}{n-1} \sum_{i=1}^n (\mu_i - \bar{\mu})^2.$$

Also,

$$E(n\bar{y}^2) = \sigma^2 + n\bar{\mu}^2.$$