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Lecture 14. 16.11.2015

2. Quadratic forms in normal variates

In deriving the normal equations, we minimised the *total sum of squares*

$$SS := (y - A\beta)^T (y - A\beta)$$

w.r.t. β. The minimum value is called the *sum of squares for error*,

$$SSE := (y - A\hat{\beta})^T (y - A\hat{\beta}).$$

From the normal equations (NE) and the definition of the projection matrix P,

$$A\hat{\beta} = Py.$$

So

$$SSE = (y - Py)^T (y - Py) = y^T y - y^T Py - y^T Py + y^T P^T Py = y^T (I - P)y,$$

using $P^T = P$ and $P^2 = P$, and a little matrix algebra (see e.g. [BF], 3.4) gives also

$$SSE = (y - A\beta)^T (I - P)(y - A\beta).$$

The *sum of squares for regression* is

$$SSR := (\hat{b} - \beta)^T C(\hat{\beta} - \beta).$$

Again, a little matrix algebra (see e.g. [BF], 3.4) gives

$$SSR = (y - A\beta)^T P(y - A\beta).$$

So

$$SS = SSR + SSE :$$

$$(y - A\beta)^T (y - A\beta) = (y - A\beta)^T P(y - A\beta) + (y - A\beta)^T (I - P)(y - A\beta); \quad (SSD)$$

either of both of these are called the *sum-of-squares decomposition.* Now from the model equations (ME), $y - A\beta = \epsilon$ is a random n-vector whose components are iid $N(0, \sigma^2)$. So (SSD) decomposes a quadratic form in normal variates $\epsilon = (\epsilon_1, \ldots, \epsilon_n)^T$ with matrix I into the sum of two quadratic forms with matrices P and $I - P$. Now by *Craig's theorem* ([KS1], (15.55)) such quadratic forms with matrices A, B are independent iff $AB = 0$. But since

$$P(I - P) = P - P^2 = P - P = 0,$$

this shows that SSR and SSE are independent. Thus (SSD) decomposes the total sum of squares into a sum of *independent* sums of squares – the main tool used in regression.

We recall some results from Linear Algebra (see e.g. [BF] Ch. 3 and the references cited there). We need the *trace* $trace(A)$ of a square matrix $A = (a_{ij})$, defined as the sum of its diagonal elements:

$$trace(A) = \sum a_{ii}.$$

(i) A real symmetric matrix A can be diagonalised by an orthogonal transformation O to a diagonal matrix D:

$$O^T AO = D.$$

(ii) For A idempotent (a projection), its eigenvalues are 0 or 1.
(iii) For A idempotent, its trace is its rank.
So if we have a quadratic form $x^T Px$ with P a projection of rank r and x an n-vector $(x_1, \ldots, x_n)^T$ with x_i iid $N(0, \sigma^2)$, we can diagonalise by an orthogonal transformation $y = Ox$ to a sum of squares of r normals (wlog the first r):

$$x^T Px = y_1^2 + \ldots + y_r^2, \qquad y_i \text{ iid } N(0, \sigma^2).$$

So by definition of the chi-square distribution,

$$x^T Px \sim \sigma^2 \chi^2(r).$$

Sums of Projections

Suppose that $P_1, \ldots, P_k$ are symmetric projection matrices with sum the identity:

$$I = P_1 + \ldots + P_k.$$

Take the trace of both sides: the $n \times n$ identity matrix I has trace n. Each P_i has trace its rank n_i, so as trace is additive

$$n = n_1 + \ldots + n_k.$$

Then squaring,

$$I = I^2 = \sum\nolimits_i P_i^2 + \sum\nolimits_{i<j} P_i P_j = \sum\nolimits_i P_i + \sum\nolimits_{i<j} P_i P_j.$$

Taking the trace,

$$n = \sum n_i + \sum_{i<j} trace(P_i P_j) = n + \sum_{i<j} trace(P_i P_j) :$$

$$\sum_{i<j} trace(P_i P_j) = 0.$$

Now

$$\begin{aligned} trace(P_i P_j) &= trace(P_i^2 P_j^2) \qquad (P_i,\, P_j \text{ projections}) \\ &= trace((P_j P_i).(P_i P_j)) \qquad (trace(AB) = trace(BA)) \\ &= trace((P_i P_j)^T.(P_i P_j)) \quad ((AB)^T = B^T A^T;\ P_i,\, P_j \text{ symmetric}) \\ &\geq 0, \end{aligned}$$

since for a matrix M

$$\begin{aligned} trace(M^T M) &= \sum_i (M^T M)_{ii} \\ &= \sum_i \sum_j (M^T)_{ij} (M)_{ji} \\ &= \sum_i \sum_j m_{ij}^2 \\ &\geq 0. \end{aligned}$$

So we have a sum of non-negative terms being zero. So each term must be zero. That is, the square of each element of $P_i P_j$ must be zero. So each element of $P_i P_j$ is zero, so matrix $P_i P_j$ is zero:

$$P_i P_j = 0 \qquad (i \neq j).$$

This is the condition that the *linear forms* $P_1 x, \ldots, P_k x$ be independent (below). Since the $P_i x$ are independent, so are the $(P_i x)^T (P_i x) = x^T P_i^T P_i x$, i.e. $x^T P_i x$ as P_i is symmetric and idempotent. That is, the *quadratic forms* $x^T P_1 x, \ldots, x^T P_k \vec{x}$ are also independent.

We now have

$$x^T x = x^T P_1 x + \ldots + x^T P_k x.$$

The left is $\sigma^2 \chi^2(n)$; the ith term on the right is $\sigma^2 \chi^2(n_i)$.

We summarise our conclusions.

Theorem (Chi-Square Decomposition Theorem). If

$$I = P_1 + \ldots + P_k,$$

with each P_i a symmetric projection matrix with rank n_i, then
(i) the ranks sum:

$$n = n_1 + \ldots + n_k;$$

(ii) each quadratic form $Q_i := x^T P_i x$ is chi-squared:

$$Q_i \sim \sigma^2 \chi^2(n_i);$$

(iii) the Q_i are mutually independent.

This fundamental result gives all the distribution theory commonly needed for the Linear Model (for which see e.g. [BF]). In particular, since F-distributions are defined in terms of distributions of independent chi-squares, it explains why we constantly encounter F-statistics, and why all the tests of hypotheses that we encounter will be F-tests. This is so throughout the Linear Model – Multiple Regression, as here, Analysis of Variance, Analysis of Covariance and more advanced topics.
Note. The result above generalises beyond our context of projections. With the projections P_i replaced by symmetric matrices A_i of rank n_i with sum I, the corresponding result (Cochran's Theorem, 1934, also known as the Fisher-Cochran theorem) is that (i), (ii) and (iii) are *equivalent*. The proof is harder (one needs to work with *quadratic* forms, where we were able to work with *linear* forms). For monograph treatments, see e.g. Rao [R], sections 1c.1 and 3b.4 and Kendall & Stuart [KS1], sections 15.16 - 15.21.

3. The multivariate normal (Gaussian) distribution

In n dimensions, for a random n-vector $\mathbf{X} = (X_1, \cdots, X_n)^T$, one needs
(i) a *mean vector* $\mu = (\mu_1, \cdots, \mu_n)^T$ with $\mu_i = EX_i$, $\mu = E[X]$;
(ii) a *covariance matrix* $\Sigma = (\sigma_{ij})$, with $\sigma_{ij} = cov(X_i, X_j)$: $\Sigma = cov(X)$.

First, note how mean vectors and covariance matrices transform under linear changes of variable:

Proposition. If $Y = AX + b$, with Y, b m-vectors, A an $m \times n$ matrix and X an n-vector, (i) the mean vectors are related by $E[Y] = AE[X] + b = A\mu + b$; (ii) the covariance matrices are related by $\Sigma_Y = A\Sigma_X A^T$.