QR-decomposition from the statistical point of view

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Abstract

1. Orthogonalization procedure due to Erhard Schmidt (Gram-Schmidt orthogonalization)

Let $x_1, \ldots, x_k$ be elements of a vector-space and $q_1, \ldots, q_k$ be orthogonal vectors spanning the same subspace. If also $span\,\{x_1, \ldots, x_i\}$ and $span\,\{q_1, \ldots, q_i\}$ coincide, then $x_1 = q_1$ and

$$x_i = \sum_{j=1}^{i} \chi_j q_j; \qquad \text{where} \qquad \chi_j = \frac{(x_i, q_j)}{(q_j, q_j)}, \text{ if } q_j \neq 0$$

From this it follows that

$$q_i = \left(x_i - P_{span\{q_1,\ldots,q_i\}} x_i\right) \frac{(q_i, q_i)}{(x_i, q_i)},$$

if $(x_i, q_i) \neq 0$. Thus $q_i = \mu_i \left(x_i - P_{span\{q_1,\ldots,q_i\}} x_i\right)$ with some constant μ_i. From this it follows that $\mu_i = 1$ is a possible choice for the μ_i and the q_i. Moreover, $(q_j, x_i) = 0$ if $j > i$ and $(x_i, q_i) = (q_i, q_i)$.

2. Linear model and QR-decomposition

$Ey = \beta_1 x_1 + \ldots + \beta_k x_k = X\beta$, where $X = (x_1 \ldots, x_k)$ and $\beta = (\beta_1, \ldots, \beta_k)'$, $Cov(y) = \sigma^2 I$.
$\hat{y} = P_{span\{x_1,\ldots,x_k\}} y = P_{im(X)} y$ is BLUE of $E(y)$.
Let $q_1, \ldots, q_r, 0, \ldots, 0$ $(r = Rank(X))$ be the vectors obtained by orthogonalizing $x_1, \ldots, x_k$. Then $\hat{y} = \sum_{i=1}^{r} \hat{\alpha}_i q_i$, $\hat{\alpha}_i = (q_i, y)/(q_i, q_i)$.
From $\sum_{j=1}^{k} \hat{\beta}_j x_j = \sum_{i=1}^{r} \hat{\alpha}_j q_j$ we get by forming the inner product with q_i, that $\sum_{j=1}^{k} r_{ij} \hat{\beta}_j = \alpha_i$, $i = r, r-1, \ldots, 1$, where $r_{ij} = (q_i, x_j)/(q_i, q_i)$. This is a triangular system of equations and can easily be solved. Let $R = (r_{ij}) = ((q_i, x_j)/(q_i, q_i))$.Than $R\hat{\beta} = \hat{\alpha}$ and $X = QR$.

<u>Theorem:</u> Let $\hat{\beta}$ be any solution of $R\hat{\beta} = \hat{\alpha}$. Than $(\hat{\beta}, l)$ is BLUE of (β, l) whenever (β, l) is estimable.

3. Estimable functions

Theorem: Let the model $E(y) = X\beta$, $Cov(y) = \sigma^2 I$ be given.

(i) (β, l) is estimable iff $Xl \notin X(l)^\perp$.

(ii) The BLUE of (β, l) is given by $(\beta, l) = \|l\|^2 (q, y)/(q, q)$ where $q = (I - P_{X(l)^\perp})Xl$

(iii) $var(l, \hat{\beta}) = \sigma^2 \|l\|^4 \|q\|^2$.

The computation of the BLUE can proceed as follows: Let $l_1, \ldots, l_{k-1}$ be a basis of $(l)^\perp$. Then orthogonalize $Xl_1, \ldots, Xl_{k-1}, Xl$ and obtain $q_1, \ldots, q_k$. Then $\|l\|^2 (q_k, y)/(q_k, q_k)$ is the BLUE of (β, l).

4. Linear sufficiency

Let $q_1, \ldots, q_r, 0, \ldots, 0$ be the vectors obtained from $x_1, \ldots, x_k$ by applying the Gram-Schmidt orthogonalization procedure. Then $Q'y$ and $Q_1'y$ are both linearly sufficient statistics, where

$$Q_1 = (q_1, \ldots, q_r), \qquad Q = (q_1, \ldots, q_r, 0, \ldots, 0).$$

The BLUE of $X\beta$ is given by

$$Q(Q'Q)^- Q'y \qquad \text{or} \qquad Q_1(Q_1'Q_1)^- Q_1'y.$$

5. Application

The results will be applied to some real data.