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A Restricted Least Squares Problem*

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In this note least squares problems with certain convex restraints are solved without the use of linear programming. The solution involves solving the normal equations for a number of unrestricted problems.

KEY WORDS
Least Squares
Regression Analysis

Let $X = (x_{ij})$ be a fixed $m \times n$ matrix of reals and $Y = (y_i)$ be a fixed n-dimensional column vector. The usual least squares problem is to minimize

$$(1) \qquad L(\lambda) = (Y - X^T\lambda)^T(Y - X^T\lambda),$$

where λ is a m-dimensional column vector and A^T denotes the transpose of the matrix A. In this note we consider minimizing $L(\lambda)$ where λ is subject to the restriction $\lambda_i \geq 0$ for $i = 1, 2, \cdots, m$. In the literature various types of inequality restrictions have been considered in least squares and regression problems [3], and the usual solution seems to involve linear programming. Below we solve our stated problem by considering 2^m unrestricted problems.

The real valued function $L(\lambda)$ can be considered defined on $([0, \infty))^m$. Now

$$(2) \qquad L(\lambda) = \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{m} x_{ij}\lambda_j\right)^2,$$

so that, with λ_j fixed for all $j \neq k$, we have either $\lim_{\lambda_k \to \infty} L(\lambda) = +\infty$ or $L(\lambda)$ constant. The latter situation occurs only when $x_{ik} = 0$ for all $i = 1, 2, \cdots, m$. Therefore, for the purpose of minimizing $L(\lambda)$, we could restrict λ to a closed and bounded subset of R^m and thus there is a $\lambda \in ([0, \infty))^m$ which minimizes $L(\lambda)$.

If we solve the system

$$(3) \qquad \frac{\partial L(\lambda)}{\partial \lambda_i} = 0, \qquad i = 1, 2, \cdots, m,$$

we find the solution to the unrestricted problem (by solving $XX^T\lambda = XY$, the usual normal equation). If this λ satisfies $\lambda_i \geq 0$, $i = 1, 2, \cdots, m$, then no further work need be done. Otherwise, as (3) is a necessary condition for a minimum to occur in the interior of a set, the solution of the restricted problem must be a boundary point of $([0, \infty))^m$ (see [1, p. 149]). Therefore, at least one $\lambda_i = 0$. Let the index set I range over all 2^m subsets of $\{1, 2, \cdots, m\}$. For each such set I, we consider

$$(4) \qquad L_I(\lambda_I) = \sum_{i=1}^{n} (y_i - \sum_{j \in I} x_{ij}\lambda_j)^2$$

and obtain the (unrestricted) solution. If all λ_k $(k \in I)$ satisfy $\lambda_k > 0$, we compute $L_I(\lambda_I)$. Finding a minimum $L_I(\lambda_I)$ solves the problem for we then set $\lambda_l = 0, l \notin I$.

What we have in fact done is perform unrestricted least squares calculations for the matrix obtained from X by deleting all lth rows where $l \notin I$. There are $\binom{m}{k}$ least squares calculations in which X has k rows deleted. This procedure is easy to program using existing regression programs. Some excellent treatments of the computation of all possible regressions can be found in [2] and [4].

For a simple example, we let $X = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 2 \\ 1 & 3 & 0 \end{bmatrix}$ and $Y = \begin{bmatrix} 2 \\ -3 \\ 6 \end{bmatrix}$. The table below exhibits those λ with all $\lambda_i \geq 0$ and the corresponding $L(\lambda)$.

λ^T	$L(\lambda)$
(11/3, 1/3, 0)	50/3
(4, 0, 0)	17
(0, 9/5, 0)	164/5
(0, 0, 0)	49

Therefore, the minimum value of $L(\lambda)$ is 50/3 and is assumed for $\lambda^T = (11/3, 1/3, 0)$.

The above procedure can be modified to yield

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solutions to problems where for each i we pick (exactly) one of the conditions (a) $\lambda_i \varepsilon R$, (b) $\lambda_i \geq a_i$, or (c) $\lambda_i \leq a_i$. The solution follows in the same manner.

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