A GENERALIZATION OF VERHELST'S SOLUTION
FOR A CONSTRAINED REGRESSION PROBLEM IN
ALSCAL AND RELATED MDS-ALGORITHMS

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Verhelst derived a solution for a constrained regression problem which occurs in the interval measurement application of ALSCAL and related MDS-algorithms. In the present paper it is shown that Verhelst's solution is based on an implicit nonsingularity assumption. A general solution, which contains Verhelst's solution as a special case, is derived by a simple completing-the-squares type approach instead of partial differentiation with a Lagrange multiplier. In addition, this approach permits the identification of a small interval which uniquely contains the optimal value of a parameter needed to solve the special case where Verhelst's solution is valid.

Takane, Young and De Leeuw [1977] considered a constrained regression problem which occurs in the interval measurement case of ALSCAL. Verhelst [1981] pointed out that their solution is erroneous and offered an alternative solution. However, it can be shown that Verhelst's solution is only valid if a certain assumption is met. In the present paper a generalized solution, which contains Verhelst's solution as a special case, will be derived. First, however, we shall explain the problem and outline Verhelst's solution.

The problem at hand is that of minimizing the function

$$\phi^2(\chi) = (d - 0\chi)(d - 0\chi)$$

subject to the constraint $$\beta^2 = 4\alpha\gamma$$, where $$\chi' = (\alpha, \beta, \gamma)$$, $$d$$ is a given $$n$$-vector of squared distances, and $$0$$ is a given $$n \times 3$$ matrix of rank 3 of the Vandermonde type. Let $$0'0$$ have the lower-triangular decomposition

$$0'0 = (F')^{-1}F^{-1}.$$  

Let $$B$$ be a $$3 \times 3$$ matrix with $$b_{31} = b_{13} = -\frac{1}{2}, b_{22} = 1$$ and zeroes elsewhere. Then

$$\chi = Bg$$

where $$g' = (-2\gamma, \beta, -2\alpha)$$. Let $$G$$ be defined as

$$G = F^{-1}B(F')^{-1}$$

with eigendecomposition

$$G = P\Delta P',$$

$$\delta_1 < \delta < \delta_2 \leq \delta_3$$, $$P'P = PP' = I_3$$. With these definitions, Verhelst [1981] arrives at the following necessary condition for a minimum of $$\phi^2$$:

$$(B - \lambda FF')g = 0,$$

where $$\lambda = (0'0)^{-1}0'd$$ and $$\lambda$$ is a Lagrange multiplier. When $$(B - \lambda FF')$$ is nonsingular then

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(6) implies that \( \lambda \) must be a root of
\[
y'(\Lambda - \lambda I)^{-1}\Lambda(\Lambda - \lambda I)^{-1}y = \sum_{i=1}^{3} \frac{y_i^2\delta_i}{(\delta_i - \lambda)^2} = 0
\] (7)
where \( y = P'F^{-1}v = P'F0'd. \) Verhelst implicitly assumes that \( (B - \lambda FF') \) is nonsingular at the solution points and suggests finding the roots of (7). Solutions corresponding to the different roots of (7) are then compared in terms of the associated value of \( \phi^2 \) and the best-fitting solution is retained.

We shall now derive a general solution for the problem at hand which is free from implicit assumptions. The solution derived by Verhelst will appear to be a special case of our solution. In addition it will be shown that in the case where Verhelst’s solution is valid the value of \( \lambda \) which corresponds to the global constrained minimum of \( \phi^2 \) is the unique root of (7) in the interval \( (\delta_1, \delta_2) \).

A General Solution

Consider the transformation \( h = F^{-1}x \) and \( z = F^{-1}v. \) Then the problem of minimizing \( \phi^2(x) \) subject to the constraint \( \beta^2 = 4\alpha y \) is equivalent to that of minimizing
\[
f(h) = d'd - 2z'h + h'h
\] (8)
subject to the constraint
\[
h'G^{-1}h = 0. \] (9)
Define the interval \( L(y, \Delta) \) as follows:
\[
L(y, \Delta) = [\delta_1, \delta_2) \quad \text{if} \quad y_1 = 0 \quad \text{(Case 1)}; \]
\[
L(y, \Delta) = (\delta_1, \delta_2] \quad \text{if} \quad y_1 \neq 0, \quad \delta_2 < \delta_3 \quad \text{and} \]
\[
\frac{y_1^2\delta_1}{(\delta_1 - \delta_2)^2} + \frac{y_2^2\delta_3}{(\delta_3 - \delta_2)^2} \leq 0
\] (10)
\[
or \quad y_1 \neq 0, \quad y_2 = 0, \quad \delta_2 < \delta_3 \quad \text{and} \quad y_3 = 0 \quad \text{Case 2}; \]
and
\[
L(y, \Delta) = (\delta_1, \delta_2) \quad \text{otherwise (Case 3).} \]
(11)
Consider the matrix \( (I - 2\Delta^{-1}) \). In each Case this matrix is positive semidefinite for \( \lambda \in L(y, \Delta). \) Define its generalized inverse as \( (I - 2\Delta^{-1})^{-}. \) For every \( \lambda \in L(y, \Delta) \) we have
\[
\{(I - \lambda\Delta^{-1})^{1/2}P'h - ((I - \lambda\Delta^{-1})^{-1/2}y)^{1/2}\} (I - \lambda\Delta^{-1})^{1/2}P'h - ((I - \lambda\Delta^{-1})^{-1/2}y) \geq 0.
\] (12)
Writing (9) as \( h'P\Delta^{-1}P'h = 0 \) and expanding (13) yields
\[
h'h - 2h'P(I - \lambda\Delta^{-1})^{1/2}((I - \lambda\Delta^{-1})^{-1/2}y)^{1/2} \geq -y'(I - \lambda\Delta^{-1})^{-}y. \]
(14)
In each Case \( (I - \lambda\Delta^{-1})^{1/2}((I - \lambda\Delta^{-1})^{-1/2}y = y. \) Hence (14) can be simplified to
\[
h'h - 2h'Py \geq -y'(I - \lambda\Delta^{-1})^{-}y. \]
(15)
Combining (8) and (15) yields
\[
f(h) \geq d'd - y'(I - \lambda\Delta^{-1})^{-}y, \quad \lambda \in L(y, \Delta). \]
(16)
Defining \( g(\lambda) = y'(I - \lambda\Delta^{-1})^{-}y \) we have
\[
f(h) \geq d'd - g(\lambda), \quad \lambda \in L(y, \Delta). \]
(17)