ABSTRACT. It is shown that the homals package in R can be used for multiple regression, multi-group discriminant analysis, and canonical correlation analysis. The homals solutions are only different from the more conventional ones in the way the dimensions are scaled by the eigenvalues.

1. MORALS

Suppose we have $m + 1$ variables, with the first $m$ being predictors (or independent variables), and the last one the outcome (or dependent variable). In homals [De Leeuw and Mair 2009] we use ndim=1, sets=list(1:m,m+1), rank=1 which means the loss function looks like

$$\sigma(x,a,q) = (x-a_{m+1}q_{m+1})'(x-a_{m+1}q_{m+1}) + (x-\sum_{j=1}^{m}a_jq_j)'(x-\sum_{j=1}^{m}a_jq_j)$$

with $q_j$ the quantified or transformed variables. This must be minimized over $a,x,q$ under the conditions that $u'x = u'q_j = 0$ and $x'x = q'_jq_j = 1$, and of course that $q_j \in \mathcal{K}_j$, the appropriate set of admissible transformations.

Write

$$Q = \begin{bmatrix} q_1 & \cdots & q_m \end{bmatrix}$$

and $b = (a_1, \cdots, a_m)$. Also write $s = a_{m+1}$ and $y = q_{m+1}$. Then

$$\sigma(x,a,q) = (x-sy)'(x-sy) + (x-Qb)'(x-Qb).$$

It follows that

$$s = x'y,$$

$$b = (Q'Q)^{-1}Q'x,$$
as well as
\[ x = \frac{sy + Qb}{\|sy + Qb\|}. \]
Also \( x \) is the normalized eigenvector corresponding with the largest eigenvalue of 
\( K = yy' + P \), where \( P = Q(Q'Q)^{-1}Q' \). But the non-zero eigenvalues of \( K \) are the
squares of the non-zero singular values of 
\[ \begin{bmatrix} y & Q(Q'Q)^{-\frac{1}{2}} \end{bmatrix} \]
and these are the same as the non-zero eigenvalues of
\[ H = \begin{bmatrix} 1 & y'Q(Q'Q)^{-\frac{1}{2}} \\ (Q'Q)^{-\frac{1}{2}}Q'y & I \end{bmatrix} \]
Define the usual regression quantities \( \beta = (Q'Q)^{-1}Q'y \) and \( \rho^2 = y'Q(Q'Q)^{-1}Q'y \).
The eigenvalues of \( H \) are \( 1 + \rho, 1 - \rho \), and 1 with multiplicity \( m - 1 \). An eigenvector corresponding with the dominant eigenvalue is
\[ \begin{bmatrix} \rho \\ (Q'Q)^{-\frac{1}{2}}Q'y \end{bmatrix}. \]
It follows that an eigenvector corresponding with the dominant eigenvalue of \( K \) is
\( (Q'Q)^{-1}Q' + \rho I)y \), and
\[ x = \frac{1}{\rho \sqrt{2(1+\rho)}}(Q'Q)^{-1}Q' + \rho I)y. \]
Thus
\[ b = \frac{1}{\rho \sqrt{\frac{1+\rho}{2}}} \beta, \]
\[ s = \sqrt{\frac{1+\rho}{2}}. \]
The vector of regression coefficient \( \beta \) is thus proportional to \( b \), and the two are
identical if and only if \( \rho = 1 \). The minimum loss function value is \( 1 - \rho \). Thus,
ultimately, we find transformations \( q_j \) of the variables in such a way that the multiple
 correlation is maximized.
2. CRIMINALS

Again we have \( m + 1 \) variables, with the first \( m \) being predictors and the last one the outcome. But now the outcome is a categorical variable with \( k \) categories. In homals we use \( \text{ndim}=p, \text{sets} = \text{list}(1:m, m+1), \text{rank} = c(\text{rep}(1, m), p) \) where \( p < k \). The loss function is

\[
\sigma(X, A, Q, Y) = \text{tr} \left( X - GY \right)'(X - GY) + \text{tr} \left( X - QA \right)'(X - QA),
\]

where \( G \) is the indicator matrix of the outcome, and where we require \( u'X = u'Q = 0 \) and \( X'X = \text{diag}(Q'Q) = I \). Now we must have at the minimum

\[
Y = (G'G)^{-\frac{1}{2}}G'X, \\
A = (Q'Q)^{-\frac{1}{2}}Q'X.
\]

Thus \( X \) are the normalized eigenvectors corresponding with the \( p \) largest eigenvalues of \( K = G(G'G)^{-1}G' + Q(Q'Q)^{-1}Q' \). And \( X \) also are the normalized left singular vectors of

\[
\begin{bmatrix}
G(G'G)^{-\frac{1}{2}} & Q(Q'Q)^{-\frac{1}{2}}
\end{bmatrix}.
\]

We can find the right singular vectors as the eigenvectors of

\[
H = \begin{bmatrix}
I & (G'G)^{-\frac{1}{2}}G'Q(Q'Q)^{-\frac{1}{2}} \\
(Q'Q)^{-\frac{1}{2}}Q'G(G'G)^{-\frac{1}{2}} & I
\end{bmatrix}.
\]

Now let \( U\Psi V' \) be the singular value decomposition of \( (G'G)^{-\frac{1}{2}}G'Q(Q'Q)^{-\frac{1}{2}} \). Then \( \begin{bmatrix} U \\ V \end{bmatrix} \) are the eigenvectors of \( H \) corresponding with the largest eigenvalues \( I + \Psi \).

Take the eigenvectors \( \begin{bmatrix} U_p \\ V_p \end{bmatrix} \) corresponding with the \( p \) largest singular values \( \Psi_p \).

The corresponding left singular vectors are \( \tilde{X} = G(G'G)^{-\frac{1}{2}}U_p + Q(Q'Q)^{-\frac{1}{2}}V_p \). Because \( \tilde{X}'\tilde{X} = 2(I + \Psi_p) \) we find

\[
X = 2^{-\frac{1}{2}}(G(G'G)^{-\frac{1}{2}}U_p + Q(Q'Q)^{-\frac{1}{2}}V_p)(I + \Psi_p)^{-\frac{1}{2}}.
\]

Thus

\[
Y = 2^{-\frac{1}{2}}(G'G)^{-\frac{1}{2}}U_p(I + \Psi_p)^{\frac{1}{2}}, \\
A = 2^{-\frac{1}{2}}(Q'Q)^{-\frac{1}{2}}V_p(I + \Psi_p)^{\frac{1}{2}},
\]

and

\[
X = (GY + QA)(I + \Psi_p)^{-1}.
\]
Also note that \( Y'G'GY = A'QA = \frac{1}{2}(I + \Psi_p) \), while \( Y'G'QA = \frac{1}{2}\Psi_p(I + \Psi_p) \). The minimum value of the loss function is \( p - \text{tr} \Psi_p \).

Now let us compare these computations with the usual canonical discriminant analysis. There we compute the projector \( P = G(G'G)^{-1}G' \) and the between-groups dispersion matrix \( B = Q'PQ \) and we solve the generalized eigenvalue problem \( BZ = TZ\Lambda \), where \( T = Q'Q \) is the total dispersion. The problem is normalized by setting \( Z'TZ = I \). Thus, using the \( p \) largest eigenvalues, \( Q'(G'G)^{-1}G'QZ_p = Q'QZ_p\Lambda_p \). This immediately gives \( \Lambda_p = \Psi_p^2 \). Also \( (Q'Q)^{\frac{1}{2}}Z_p = V_p \) or \( Z_p = \sqrt{2}A(I + \Psi_p)^{-\frac{1}{2}} \). For the group means \( M_p = (G'G)^{-1}G'QZ_p \) we find \( M_p = \sqrt{2}Y(I + \Psi_p)^{-\frac{1}{2}} \).

Thus both \( Z_p \) and \( M_p \) are simple rescalings of \( A \) and \( Y \). homals find the transformations of the variables that maximizes the sum of the \( p \) largest singular values of \((G'G)^{-\frac{1}{2}}G'Q(Q'Q)^{-\frac{1}{2}} \).

### 3. CANALS

Canonical correlation analysis with homals has \( m_1 + m_2 \) variables, and we use \( \text{ndim=p, sets=\text{list}(1:m1,m1+(1:m2)), rank=\text{rep}(1,m1+m2)} \). The loss is

\[
\sigma(X,A,Q) = \text{tr} (X - Q_1A_1)'(X - Q_1A_1) + \text{tr} (X - Q_2A_2)'(X - Q_2A_2).
\]

Since our analysis of discriminant analysis in homals never actually used the fact that \( G \) was an indicator, the results are exactly the same as in the previous section (with the obvious substitutions).

In classical canonical correlation analysis the function \( \text{tr} R'Q_1Q_2S \) is maximized over \( R'Q_1Q_1R = I \) and \( S'Q_2Q_2S = I \). This means solving

\[
Q_1'Q_2S = Q_1'Q_1R\Phi, \\
Q_2'Q_1R = Q_2'Q_2S\Phi.
\]

From homals, as before,

\[
A_1 = 2^{-\frac{1}{2}}(Q_1'Q_1)^{-\frac{1}{2}}U_p(I + \Psi_p)^{\frac{1}{2}}, \\
A_2 = 2^{-\frac{1}{2}}(Q_2'Q_2)^{-\frac{1}{2}}V_p(I + \Psi_p)^{\frac{1}{2}}.
\]
In canonical analysis $\Phi = \Psi$ and

\[ R = (Q'_1Q_1)^{-\frac{1}{2}}U_p = \sqrt{2}A_1(I + \Psi_p)^{-\frac{1}{2}}, \]

\[ S = (Q'_2Q_2)^{-\frac{1}{2}}V_p = \sqrt{2}A_2(I + \Psi_p)^{-\frac{1}{2}}. \]

Again we see the same type of rescaling of the canonical weights.

Note that homals does not find the transformations that maximize the sum of the squared canonical correlations, which is the target function in the original CANALS approach [Young et al., 1976; Van Der Burg and De Leeuw, 1983]. Maximizing the square of the canonical correlations means maximizing a different aspect of the correlation matrix [De Leeuw, 1988, 1990].

REFERENCES


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