The objective function for determining the weight vectors for x and y is the covariance criterion $E\{(w^{\mathrm{T}}x)(v^{\mathrm{T}}y)\}$, where $E\{\cdot\}$ is the expectation operator. Denoting $t = w^{\mathrm{T}}x$ and $u = v^{\mathrm{T}}y$ as score variables, the covariance criterion between t and u becomes $E\{tu\}$, where the weight vectors are constraint to be of unit length [67]. Prior to the determination of subsequent pairs of weight vectors, the information that is encapsulated in t is subtracted, or deflated, from x and y. This yields the deflation procedure $x = xtp^{\mathrm{T}}$ and $y = ytq^{\mathrm{T}}$, where the loading vectors are $p = E\{xt\}/E\{t^2\}$ and $q = E\{yt\}/E\{t^2\}$. Stacking the weight and loading vectors as columns to form the matrices $W = \begin{bmatrix} w_1 & w_2 & \dots & w_n \end{bmatrix}$, $V = \begin{bmatrix} v_1 & v_2 & \dots & v_n \end{bmatrix}$, $P = \begin{bmatrix} p_1 & p_2 & \dots & p_n \end{bmatrix}$ and $Q = \begin{bmatrix} q_1 & q_2 & \dots & qn \end{bmatrix}$, the parametric regression matrix is given by $B = Q[W^{\mathrm{T}}P]^{-1}W^{\mathrm{T}}$. Note that $R^{\mathrm{T}} = [W^{\mathrm{T}}P]^{-1}W^{\mathrm{T}}$ can be directly determined from the PLS algorithm [66, 67] and hence $B = QR^{\mathrm{T}}$.

References

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