

1 PLS algorithm (canonical mode)

1. $X_0 = X, Y_0 = Y$
2. For $h = 1 \dots H$:
 - (a) Initialize
 $\xi_h = \text{first column of } X_{h-1} \quad \omega_h = \text{first column of } Y_{h-1}$
 - (b) Until convergence of a_h :
 - i. $a_h = X'_{h-1}\xi_h/\xi'_h\xi_h$, norm a_h
 - ii. $\xi_h = X_{h-1}a_h$, norm ξ_h
 - iii. $b_h = Y'_{h-1}\xi_h/\xi'_h\xi_h$, norm b_h
 - iv. $\omega_h = Y_{h-1}b_h$, norm ω_h
 - (c) $c_h = X'_{h-1}\xi_h \quad e_h = Y'_{h-1}\omega_h$
 - (d) $X_h = X_{h-1} - \xi_h c'_h \quad Y_h = Y_{h-1} - \omega_h e'_h$

Step (c) computes the regression coefficients of the matrices X_{h-1} and Y_{h-1} on the latent variables ξ_h and ω_h .

Step (d) computes the deflated (residual) matrices.

2 sparse PLS algorithm (canonical mode)

Sparse PLS initializes step (a) in PLS by extracting the first pair of singular vectors (a_h, b_h) of the crossproduct $X'_{h-1}Y_{h-1}$, which includes variation in both X and Y and the correlation between the two sets.

The two loading vectors (a_h, b_h) are then computed with penalizations λ_a and λ_b in step (b), and the latent vectors (ξ_h, ω_h) are then computed, where $g_\lambda(y) = \text{sign}(y)(|y| - \lambda)_+$ is the soft-thresholding penalty function.

1. $X_0 = X \quad Y_0 = Y$
2. For $h = 1 \dots H$:
 - (a) Set $\tilde{M}_{h-1} = X'_{h-1}Y_{h-1}$, decompose \tilde{M}_{h-1} and extract the first pair of singular vectors $a_{old} = a_h$ and $b_{old} = b_h$
 - (b) Until convergence of a_{new} and b_{new} :
 - i. $a_{new} = g_{\lambda_a}(\tilde{M}_{h-1}b_{old})$, norm a_{new}
 - ii. $b_{new} = g_{\lambda_b}(\tilde{M}'_{h-1}a_{old})$, norm b_{new}
 - iii. $a_{old} = a_{new}, b_{old} = b_{new}$
 - (c) $\xi_h = X_{h-1}a_{new}$
 $\omega_h = Y_{h-1}b_{new}$
 - (d) $c_h = X'_{h-1}\xi_h \quad e_h = Y'_{h-1}\omega_h$
 - (e) $X_h = X_{h-1} - \xi_h c'_h \quad Y_h = Y_{h-1} - \omega_h e'_h$

3 Canonical Correlation Analysis with Elastic Net penalization

CCA-EN initializes step (a) in PLS by setting $\xi_h = X_{h-1}^j$ and $\omega_h = Y_{h-1}^k$ such that $\text{cor}(X_{h-1}^j, Y_{h-1}^k)$ is maximized, for $j = 1 \dots p$ and $k = 1 \dots q$. Hence, this algorithm aims at maximizing the correlation (rather than the covariance for PLS and sPLS).

The approximation on Elastic Net penalization finally consists in introducing soft-thresholding penalizations, as in sparse PLS, which makes both algorithms similar, except for the initialization step.

1. $X_0 = X \quad Y_0 = Y$
2. For $h = 1 \dots H$:
 - (a) Set $\xi_h = X_{h-1}^j$ and $\omega_h = Y_{h-1}^k$ such that $\text{cor}(X_{h-1}^j, Y_{h-1}^k)$ is maximized
 $a_{new} = X_{h-1}' \xi_h / \xi_h' \xi_h \quad b_{new} = Y_{h-1}' \omega_h / \omega_h' \omega_h$, norm a_{new} and b_{new}
 - (b) Until convergence of a_{new} and b_{new} :
 - i. $a_{new} = g_{\lambda_a}(Y_{h-1} b_{old})$, norm a_{new}
 - ii. $b_{new} = g_{\lambda_b}(X_{h-1} a_{old})$, norm b_{new}
 - iii. $a_{old} = a_{new}, b_{old} = b_{new}$
 - (c) $\xi_h = X_{h-1} a_{new}$, norm ξ_h
 $\omega_h = Y_{h-1} b_{new}$ norm ω_h
 - (d) $c_h = X_{h-1}' \xi_h \quad e_h = Y_{h-1}' \omega_h$
 - (e) $X_h = X_{h-1} - \xi_h c_h' \quad Y_h = Y_{h-1} - \omega_h e_h'$