Partial Least squares regression and Optimal Control

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Abstract

The Partial Least Squares (PLS) algorithm is formulated as an optimal control problem.

1 PLS and optimal control

1.1 An optimal control problem

Given a dynamic system

$$x_{k+1} = Ax_k + Bu_k, \tag{1}$$
$$y_k = Dx_k, \tag{2}$$

where $k = 0, 1, \dots,$ is discrete time and with an initial state $x_0 = 0$. Consider a control objective criterion weighting only at the final time instant, say $k = a$.

$$J_0 = (r - y_a)^T (r - y_a). \tag{3}$$

The optimal controls minimizing the control objective is given by

$$x_k = A^k x_0 + C_k u_{0|k}, \tag{4}$$

where here C_k is the reversed controllability matrix of the pair (A, B). Putting this into the objective gives

$$J_0 = (r - DC_a u_{0|a})^T (r - DC_a u_{0|a}). \tag{5}$$

The optimal control is then

$$u^*_{0|a} = (C_a^T D^T D C_a)^{-1} C_a^T D^T r. \tag{6}$$

And the corresponding optimal state and output is given by

$$x^*_a = C_a u^*_{0|a} = C_a (C_a^T D^T D C_a)^{-1} C_a^T D^T r, \tag{7}$$
$$y^*_a = D x^*_a = D C_a (C_a^T D^T D C_a)^{-1} C_a^T D^T r. \tag{8}$$

1.2 PLS as an optimal control problem

Given a dynamic system

$$B_{k+1} = X^T X B_k + X^T X p_k, \quad (9)$$

$$y_k = X B_k, \quad (10)$$

where $k = 0, 1, \ldots, a$ is discrete time and with an initial state $B_0 = 0$. Consider a control objective criterion weighting only at the final time instant at $k = a$.

$$J_0 = (Y - y_a)^T (Y - y_a). \quad (11)$$

The optimal controls minimizing the control objective is given by

$$p^*_{0|a} = (K_a^T X^T X K_a)^{-1} K_a^T X^T Y. \quad (12)$$

And the corresponding optimal state and output is given by

$$B^*_a = K_a p^*_{0|a} = K_a (K_a^T X^T X K_a)^{-1} K_a^T X^T Y, \quad (13)$$

$$y^*_a = X B^*_a = X K_a (K_a^T X^T X K_a)^{-1} K_a^T X^T Y. \quad (14)$$