Kernel PLS path modelling
Arthur Tenenhaus

To cite this version:

Arthur Tenenhaus. Kernel PLS path modelling. 6th International Conference on Partial Least Squares and Related (PLS’09), Sep 2009, Beijing, China. pp.13-16. hal-00441038

HAL Id: hal-00441038
https://centralesupelec.hal.science/hal-00441038
Submitted on 14 Dec 2009

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Kernel PLS path modelling

Arthur Tenenhaus
Supélec, Department of signal processing and electronics systems
Gif-sur-Yvette, 91192, France.
E-mail: arthur.tenenhaus@supelec.fr

Abstract: This paper deals with a kernel extension of a companion paper entitled “new criterion based PLS path modeling approach to structural equation modeling” [Tenenhaus, 2009] which will be presented during the PLS’09 conference.

Keywords: Multi-block data analysis, Structural Equation Modelling, PLS path modelling, Kernel methods.

1. Introduction

Throughout this paper $X_1, X_2, ..., X_J$ are matrices with columns defined by centered variables observed on the same set of $n$ individuals and $K_1, K_2, ..., K_J$ the associated kernel matrices. Let us note $p_j$ the number of variables for the block $X_j$. We are interested in studying the relation between $J$ blocks of variables $X_1, X_2, ..., X_J$ even though those data sets live in different spaces. We achieve this by projecting the $J$ blocks onto $J$ separate directions specified by vector $a_1, a_2, ..., a_J$ to obtain $J$ univariate variables on which “link” (such as covariance) can be computed easily. In this paper is presented a kernel version of a companion paper entitled “A criterion based PLS approach to structural equation modelling” [Tenenhaus and Tenenhaus, 2009] which will be presented during the PLS’09 conference. The paper is organized as follows: the first part briefly introduces the primal formulation of the proposed method and the second part is devoted to its dual formulation.

2. The general optimization problem (primal form)

In this paper, the following general problem is considered:

$$\{a_1, a_2, ..., a_J\} = \arg\max_{a_1, a_2, ..., a_J} \sum_{i=1}^{J} \sum_{j=1}^{J} c_{ij} g(\text{cov}(X_i a_i, X_j a_j))$$

subject to the constraints: $(1 - \tau_j) \text{var}(X_j a_j) + \tau_j \|a_j\|^2 = 1$, $j = 1, ..., J$

where $g(x) = x$ (Horst Scheme), $g(x) = x^2$ (factorial scheme) or $g(x) = |x|$ (centroid scheme).

The regularisation parameters $\tau_j \in [0, 1]$, $j = 1, ..., J$ control the stability of the solution (specifically useful in a high dimensional block context) and interpolate smoothly between the maximisation of the covariance (all $\tau_j s' = 1$) and the maximisation of the correlation (all $\tau_j s' = 0$). The $J \times J$ design matrix $(C)_{ij} = c_{ij}$ equals to 1 if the blocks $X_i$ and $X_j$ are connected and to 0 otherwise allows to immediately extend the multiblock data analysis framework to the structural equation modelling one by limiting the summation to connected blocks. For sake of simplicity, in this part of the paper, we
focus our presentation on the Horst scheme. Applying the Lagrangian multiplier technique to the optimization of (1) gives us $J$ stationary equations:

$$a_i = \frac{1}{\sqrt{Z_i'X_iM_i^{-1}X_i'Z_i}} \left( 1 - \tau_i \right) \frac{1}{n} X_i'X_i + \tau_i I_p$$

subject to the constraints:

$$\left( 1 - \tau_j \right) \text{var}(X_j'X_j'\alpha_j) + \tau_j \|X_j'\alpha_j\|^2 = 1,$$

$$j = 1, ..., J$$

To simplify the presentation, we focus on the Horst Scheme $(g(x) = x)$

$$\Rightarrow$$

subject to the constraints:

$$\alpha_j' \left( 1 - \tau_j \right) \frac{1}{n} K^2_j + \tau_j K_j \alpha_j = 1,$$

$$j = I, ..., J$$

We note that this maximization problem is expressed only in terms of kernel matrices. The regularisation parameters not only makes this optimisation problem well posed numerically but also provide control over the capacity of the function space where the solution is sought. The larger the
values of $\tau_j$ are, the less sensitive the method to the input data is and the more stable (less prone to finding spurious relations) the solution becomes.

$$\Leftrightarrow \left\{ \alpha_1, \alpha_2, ..., \alpha_J \right\} = \arg\max_{\alpha_1, \alpha_2, ..., \alpha_J} \frac{1}{n} \sum_{i=1}^{J} \sum_{j=1}^{J} \alpha_i^j R_i^j R_j^j \alpha_j$$

subject to the constraints: $\alpha_j^j \left( (1 - \tau_j) \frac{1}{n} R_j^j R_j^j + \tau_j R_j^j R_j \right) \alpha_j = 1, \quad j = 1, ..., J$

Let us note $w_j = R_j \alpha_j$ and $n_j = \text{rank}(X_j)$

$$\Leftrightarrow \left\{ w_1, w_2, ..., w_J \right\} = \arg\max_{w_1, w_2, ..., w_J} \frac{1}{n} \sum_{i=1}^{J} \sum_{j=1}^{J} w_i^j R_i^j w_j$$

subject to the constraints: $w_j^j \left( (1 - \tau_j) \frac{1}{n} R_j^j + \tau_j I_{n_j} \right) w_j = 1, \quad j = 1, ..., J$

A 3-step procedure is proposed to maximize (2) subject to (3):

1. Construct the Lagrangian function related to the maximization problem.

$$L = \sum_{i=1}^{J} \sum_{j=1}^{J} c_{ij}^j \frac{1}{n} R_i^j R_j^j w_j - \sum_{i=1}^{J} \lambda_i \left( (1 - \tau_i) \frac{1}{n} R_i^j R_i^j w_i + \tau_i w_i^j w_i - 1 \right)$$

where $\lambda_i, i = 1, ..., J$ are the Lagrangian multiplier.

2. Define stationary equations by cancelling and simplifying the derivatives of the Lagrangian function.

$$w_i = \frac{1}{\sqrt{Z_i^j R_i^j N_i^{-1} R_i Z_i}} \left( (1 - \tau_i) \frac{1}{n} R_i^j + \tau_i I_{n_i} \right) R_i^j \left( j = 1, ..., J \right)$$

3. Find a solution of the $J$ stationary equations by using a PLS style iterative procedure (derived to the Wold procedure which guaranty the monotonic convergence).

It is worth pointing out that for specific values of the regularization parameters, the proposed method provides as particular cases (and among others):

- For the 2 blocks cases: Kernel PLS [Rosipal et al., 2001] ($\tau_1 = \tau_2 = 1$), Kernel Redundancy Analysis [Takane and Hwang, 2007] which is equivalent to Kernel PLS for discrimination [Rosipal et al., 2003] ($\tau_1 = 1$ and $\tau_2 = \tau$), Kernel Canonical Correlation Analysis [e.g. Bach and Jordan, 2002] ($\tau_1 = \tau_1$ and $\tau_2 = \tau_2$).

- For the $J$ blocks cases: a “Horst” Generalized Kernel CCA with the flavour of the one proposed by [Bach and Jordan, 2002; Shawe-Taylor and Cristianini, 2004] (all $\tau_j s' = \tau_j$ ; Horst scheme).
Moreover, our general optimisation problem provides a “regularized” kernel extension of the Kettenring’s generalized CCA (all $\tau_j s' = \tau_j$ and Factorial scheme).

4. Conclusion

In this paper we present a very general optimization problem covering a large spectrum of methods. This paper provides a criterion point of view of the PLS path modelling framework. To the best of our knowledge, all the Kernel CCA version proposed by the machine learning community does not consider other scheme than the Horst one. In this paper, we explore the factorial and the centroid scheme which sound more reasonable when the number of block is greater than 2. Moreover, the introduction of the design matrix allows analysing data where all blocks are not necessarily connected.

To conclude this paper, we note that by using non linear kernel such as Gaussian or polynomial kernel, we can assess non linear relation between blocks.

5. References


