

Partial Least Squares (PLS) Regression.

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INTRODUCTION

PLS regression is a recent technique that generalizes and combines features from principal component analysis and multiple regression. It is particularly useful when we need to predict a set of dependent variables from a (very) large set of independent variables (i.e., predictors). It originated in the social sciences (specifically economy, Herman Wold 1966) but became popular first in chemometrics (i.e., computational chemistry) due in part to Herman's son Svante, (see, e.g., Geladi & Kowalski, 1986) and in sensory evaluation (Martens & Naes, 1989). But PLS regression is also becoming a tool of choice in the social sciences as a multivariate technique for non-experimental and experimental data alike (e.g., neuroimaging, see McIntosh, Bookstein, Haxby, & Grady, 1996). It was first presented as an algorithm akin to the power method (used for computing eigenvectors) but was rapidly interpreted in a statistical framework. (Frank, & Friedman, 1993; Helland, 1990; Höskuldsson, 1988; Tenenhaus, 1998).

PREREQUISITE NOTIONS AND NOTATIONS

The I observations described by K dependent variables are stored in a $I \times K$ matrix denoted \mathbf{Y} , the values of J predictors collected on these I observations are collected in the $I \times J$ matrix \mathbf{X} .

GOAL

The goal of PLS regression is to predict \mathbf{Y} from \mathbf{X} and to describe their common structure. When \mathbf{Y} is a vector and \mathbf{X} is full rank, this goal could be accomplished using ORDINARY MULTIPLE REGRESSION. When the number of predictors is large compared to the number of observations, \mathbf{X} is likely to be singular and the regression approach is no longer feasible (i.e., because of MULTICOLLINEARITY). Several approaches have been developed to cope with this problem. One approach is to eliminate some predictors (e.g., using step-wise methods) another one, called principal component regression, is to perform

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a PRINCIPAL COMPONENT ANALYSIS (PCA) of the \mathbf{X} matrix and then use the principal components of \mathbf{X} as regressors on \mathbf{Y} . The orthogonality of the principal components eliminates the multicollinearity problem. But, the problem of choosing an *optimum* subset of predictors remains. A possible strategy is to keep only a few of the first components. But they are chosen to explain \mathbf{X} rather than \mathbf{Y} , and so, nothing guarantees that the principal components, which “explain” \mathbf{X} , are relevant for \mathbf{Y} .

By contrast, PLS regression finds components from \mathbf{X} that are also relevant for \mathbf{Y} . Specifically, PLS regression searches for a set of components (called *latent vectors*) that performs a simultaneous decomposition of \mathbf{X} and \mathbf{Y} with the constraint that these components explain as much as possible of the *covariance* between \mathbf{X} and \mathbf{Y} . This step generalizes PCA. It is followed by a regression step where the decomposition of \mathbf{X} is used to predict \mathbf{Y} .

SIMULTANEOUS DECOMPOSITION OF PREDICTORS AND DEPENDENT VARIABLES

PLS regression decomposes both \mathbf{X} and \mathbf{Y} as a product of a common set of orthogonal factors and a set of specific loadings. So, the independent variables are *decomposed* as $\mathbf{X} = \mathbf{TP}^T$ with $\mathbf{T}^T\mathbf{T} = \mathbf{I}$ with \mathbf{I} being the identity matrix (some variations of the technique do not require \mathbf{T} to have unit norms). By analogy with PCA \mathbf{T} is called the *score* matrix, and \mathbf{P} the *loading* matrix (in PLS regression the loadings are not orthogonal). Likewise, \mathbf{Y} is *estimated* as $\hat{\mathbf{Y}} = \mathbf{TBC}^T$ where \mathbf{B} is a diagonal matrix with the “regression weights” as diagonal elements (see below for more details on these weights). The columns of \mathbf{T} are the *latent vectors*. When their number is equal to the rank of \mathbf{X} , they perform an exact decomposition of \mathbf{X} . Note, however, that they only *estimate* \mathbf{Y} . (i.e., in general $\hat{\mathbf{Y}}$ is not equal to \mathbf{Y}).

PLS REGRESSION AND COVARIANCE

The latent vectors could be chosen in a lot of different ways. In fact in the previous formulation, any set of orthogonal vectors spanning the column space of \mathbf{X} could be used to play the rôle of \mathbf{T} . In order to specify \mathbf{T} , additional conditions are required. For PLS regression this amounts to finding two sets of weights \mathbf{w} and \mathbf{c} in order to create (respectively) a linear combination of the columns of \mathbf{X} and \mathbf{Y} such that their covariance is maximum. Specifically, the goal is to obtain a first pair of vectors $\mathbf{t} = \mathbf{Xw}$ and $\mathbf{u} = \mathbf{Yc}$ with the constraints that $\mathbf{w}^T\mathbf{w} = 1$, $\mathbf{t}^T\mathbf{t} = 1$ and $\mathbf{t}^T\mathbf{u}$ be maximal. When the first latent vector is found, it is *subtracted* from both \mathbf{X} and \mathbf{Y} and the procedure is re-iterated until \mathbf{X} becomes a null matrix (see the algorithm section for more).

A PLS REGRESSION ALGORITHM

The properties of PLS regression can be analyzed from a sketch of the original algorithm. The first step is to create two matrices: $\mathbf{E} = \mathbf{X}$ and $\mathbf{F} = \mathbf{Y}$. These matrices are then column centered and normalized (i.e., transformed into Z -scores). The sum of squares of these matrices are denoted SS_X and SS_Y . Before starting the iteration process, the vector \mathbf{u} is initialized with random

values. (in what follows the symbol \propto means “to normalize the result of the operation”).

Step 1. $\mathbf{w} \propto \mathbf{E}^T \mathbf{u}$ (estimate \mathbf{X} weights).

Step 2. $\mathbf{t} \propto \mathbf{E} \mathbf{w}$ (estimate \mathbf{X} factor scores).

Step 3. $\mathbf{c} \propto \mathbf{F}^T \mathbf{t}$ (estimate \mathbf{Y} weights).

Step 4. $\mathbf{u} = \mathbf{F} \mathbf{c}$ (estimate \mathbf{Y} scores).

If \mathbf{t} has not converged, then go to Step 1, if \mathbf{t} has converged, then compute the value of b which is used to predict \mathbf{Y} from \mathbf{t} as $b = \mathbf{t}^T \mathbf{u}$, and compute the factor loadings for \mathbf{X} as $\mathbf{p} = \mathbf{E}^T \mathbf{t}$. Now subtract (i.e., partial out) the effect of \mathbf{t} from both \mathbf{E} and \mathbf{F} as follows $\mathbf{E} = \mathbf{E} - \mathbf{t} \mathbf{p}^T$ and $\mathbf{F} = \mathbf{F} - b \mathbf{t} \mathbf{c}^T$. The vectors \mathbf{t} , \mathbf{u} , \mathbf{w} , \mathbf{c} , and \mathbf{p} are then stored in the corresponding matrices, and the scalar b is stored as a diagonal element of \mathbf{B} . The sum of squares of \mathbf{X} (respectively \mathbf{Y}) explained by the latent vector is computed as $\mathbf{p}^T \mathbf{p}$ (respectively b^2), and the proportion of variance explained is obtained by dividing the explained sum of squares by the corresponding total sum of squares (i.e., SS_X and SS_Y).

If \mathbf{E} is a null matrix, then the whole set of latent vectors has been found, otherwise the procedure can be re-iterated from Step 1 on.

Table 1: The \mathbf{Y} matrix of dependent variables.

Wine	Hedonic	Goes with meat	Goes with dessert
1	14	7	8
2	10	7	6
3	8	5	5
4	2	4	7
5	6	2	4

Table 2: The \mathbf{X} matrix of predictors.

Wine	Price	Sugar	Alcohol	Acidity
1	7	7	13	7
2	4	3	14	7
3	10	5	12	5
4	16	7	11	3
5	13	3	10	3

PLS REGRESSION AND THE SINGULAR VALUE DECOMPOSITION

The iterative algorithm presented above is similar to the power method which finds eigenvectors. So PLS regression is likely to be closely related to the eigen

and singular value decompositions, and this is indeed the case. For example, if we start from Step 1 which computes: $\mathbf{w} \propto \mathbf{E}^T \mathbf{u}$, and substitute the rightmost term iteratively, we find the following series of equations: $\mathbf{w} \propto \mathbf{E}^T \mathbf{u} \propto \mathbf{E}^T \mathbf{F} \mathbf{c} \propto \mathbf{E}^T \mathbf{F} \mathbf{F}^T \mathbf{t} \propto \mathbf{E}^T \mathbf{F} \mathbf{F}^T \mathbf{E} \mathbf{w}$. This shows that the first weight vector \mathbf{w} is the first right singular vector of the matrix $\mathbf{X}^T \mathbf{Y}$. Similarly, the first weight vector \mathbf{c} is the left singular vector of $\mathbf{X}^T \mathbf{Y}$. The same argument shows that the first vectors \mathbf{t} and \mathbf{u} are the first eigenvectors of $\mathbf{X} \mathbf{X}^T \mathbf{Y} \mathbf{Y}^T$ and $\mathbf{Y} \mathbf{Y}^T \mathbf{X} \mathbf{X}^T$.

Table 3: The matrix \mathbf{T} .

Wine	\mathbf{t}_1	\mathbf{t}_2	\mathbf{t}_3
1	0.4538	-0.4662	0.5716
2	0.5399	0.4940	-0.4631
3	0	0	0
4	-0.4304	-0.5327	-0.5301
5	-0.5633	0.5049	0.4217

Table 4: The matrix \mathbf{U} .

Wine	\mathbf{u}_1	\mathbf{u}_2	\mathbf{u}_3
1	1.9451	-0.7611	0.6191
2	0.9347	0.5305	-0.5388
3	-0.2327	0.6084	0.0823
4	-0.9158	-1.1575	-0.6139
5	-1.7313	0.7797	0.4513

Table 5: The matrix \mathbf{P} .

	\mathbf{p}_1	\mathbf{p}_2	\mathbf{p}_3
Price	-1.8706	-0.6845	-0.1796
Sugar	0.0468	-1.9977	0.0829
Alcohol	1.9547	0.0283	-0.4224
Acidity	1.9874	0.0556	0.2170

Table 6: The matrix \mathbf{W} .

	\mathbf{w}_1	\mathbf{w}_2	\mathbf{w}_3
Price	-0.5137	-0.3379	-0.3492
Sugar	0.2010	-0.9400	0.1612
Alcohol	0.5705	-0.0188	-0.8211
Acidity	0.6085	0.0429	0.4218

Table 7: The matrix \mathbf{B}_{PLS} when 3 latent vectors are used.

	Hedonic	Goes with meat	Goes with dessert
Price	-1.0607	-0.0745	0.1250
Sugar	0.3354	0.2593	0.7510
Alcohol	-1.4142	0.7454	0.5000
Acidity	1.2298	0.1650	0.1186

Table 8: The matrix \mathbf{B}_{PLS} when 2 latent vectors are used.

	Hedonic	Goes with meat	Goes with dessert
Price	-0.2662	-0.2498	0.0121
Sugar	0.0616	0.3197	0.7900
Alcohol	0.2969	0.3679	0.2568
Acidity	0.3011	0.3699	0.2506

Table 9: The matrix \mathbf{C} .

	\mathbf{c}_1	\mathbf{c}_2	\mathbf{c}_3
Hedonic	0.6093	0.0518	0.9672
Goes with meat	0.7024	-0.2684	-0.2181
Goes with dessert	0.3680	-0.9619	-0.1301

Table 10: The \mathbf{b} vector.

	b_1	b_2	b_3
	2.7568	1.6272	1.1191

Table 11: Variance of \mathbf{X} and \mathbf{Y} explained by the latent vectors.

Latent Vector	Percentage of Explained Variance for \mathbf{X}	Cumulative Percentage of Explained Variance for \mathbf{X}	Percentage of Explained Variance for \mathbf{Y}	Cumulative Percentage of Explained Variance for \mathbf{Y}
1	70	70	63	63
2	28	98	22	85
3	2	100	10	95

PREDICTION OF THE DEPENDENT VARIABLES

The dependent variables are predicted using the multivariate regression formula as $\hat{\mathbf{Y}} = \mathbf{T}\mathbf{B}\mathbf{C}^T = \mathbf{X}\mathbf{B}_{\text{PLS}}$ with $\mathbf{B}_{\text{PLS}} = (\mathbf{P}^{T+})\mathbf{B}\mathbf{C}^T$ (where \mathbf{P}^{T+} is the Moore-Penrose pseudo-inverse of \mathbf{P}^T). If all the latent variables of \mathbf{X} are used, this regression is equivalent to principal component regression. When only a subset of the latent variables is used, the prediction of \mathbf{Y} is optimal for this number of predictors.

An obvious question is to find the number of latent variables needed to obtain the best generalization for the prediction of *new* observations. This is, in general, achieved by cross-validation techniques such as bootstrapping.

The interpretation of the latent variables is often helped by examining graphs akin to PCA graphs (e.g., by plotting observations in a $\mathbf{t}_1 \times \mathbf{t}_2$ space).

A SMALL EXAMPLE

We want to predict the subjective evaluation of a set of 5 wines. The dependent variables that we want to predict for each wine are its likeability, and how well it goes with meat, or dessert (as rated by a panel of experts) (see Table 1). The predictors are the price, the sugar, alcohol, and acidity content of each wine (see Table 2).

The different matrices created by PLS regression are given in Tables 3 to 11. From Table 11 one can find that 2 latent vectors explain 98% of the variance of \mathbf{X} and 85% of \mathbf{Y} . This suggests to keep these 2 dimensions for the final solution. The examination of the 2-dimensional regression coefficients (i.e., \mathbf{B}_{PLS} , see Table 8) shows that sugar is mainly responsible for choosing a dessert wine, and that price is negatively correlated with the perceived quality of the wine whereas alcohol is positively correlated with it (at least in this example ...). Looking at the latent vectors shows that \mathbf{t}_1 expresses price and \mathbf{t}_2 reflects sugar content.

RELATIONSHIP WITH OTHER TECHNIQUES

PLS regression is obviously related to canonical correlation and to multiple factor analysis (Escofier, & Pagès, 1988). These relationships are explored in details by Tenenhaus (1998) and Pagès and Tenenhaus (2001). The main originality of PLS regression is to preserve the asymmetry of the relationship between predictors and dependent variables, whereas these other techniques treat them symmetrically.

SOFTWARE

PLS regression necessitates sophisticated computations and therefore its application depends on the availability of software. For chemistry, two main programs are used: the first one called SIMCA-P was developed originally by Wold, the second one called the UNSCRAMBLER was first developed by Martens who was another pioneer in the field. For brain imaging, SPM, which is one of the most widely used programs in this field, has recently (2002) integrated a PLS regression module. Outside these domains, SAS PROC PLS is probably the most

easily available program. In addition, interested readers can download a set of MATLAB programs from the author's home page (www.utdallas.edu/~herve). Also, a public domain set of MATLAB programs is available from the home page of the *N-Way* project (www.models.kvl.dk/source/nwaytoolbox/) along with tutorials and examples. And finally, a commercial MATLAB toolbox has also been developed by EIGENRESEARCH.

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