An Introduction to Partial Least Squares Regression

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Abstract

Partial least squares is a popular method for soft modelling in industrial applications. This paper introduces the basic concepts and illustrates them with a chemometric example. An appendix describes the experimental PLS procedure of SAS/STAT® software.

Introduction

Research in science and engineering often involves using controllable and/or easy-to-measure variables (*factors*) to explain, regulate, or predict the behavior of other variables (*responses*). When the factors are few in number, are not significantly redundant (collinear), and have a well-understood relationship to the responses, then multiple linear regression (MLR) can be a good way to turn data into information. However, if any of these three conditions breaks down, MLR can be inefficient or inappropriate. In such so-called *soft science* applications, the researcher is faced with many variables and ill-understood relationships, and the object is merely to construct a good predictive model. For example, spectrographs are often used to estimate the amount of different compounds in a chemical sample. (See Figure 2.) In this case, the factors are the measurements that comprise the spectrum; they can number in the hundreds but are likely to be highly collinear. The responses are component amounts that the researcher wants to predict in future samples.

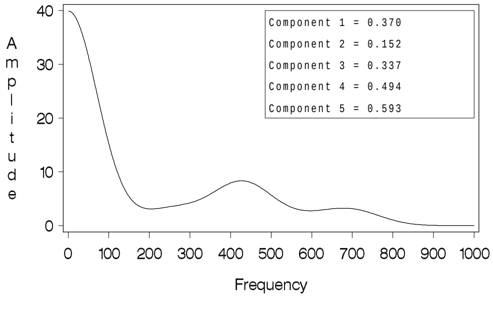

Figure 2: Spectrograph for a mixture

Partial least squares (PLS) is a method for constructing predictive models when the factors are many and highly collinear. Note that the emphasis is on predicting the responses and not necessarily on trying to understand the underlying relationship between the variables. For example, PLS is not usually appropriate for screening out factors that have a negligible effect on the response. However, when prediction is the goal and there is no practical need to limit the number of measured factors, PLS can be a useful tool.

PLS was developed in the 1960's by Herman Wold as an econometric technique, but some of its most avid proponents (including Wold's son Svante) are chemical engineers and chemometricians. In addition to spectrometric calibration as discussed above, PLS has been applied to monitoring and controlling industrial processes; a large process can easily have hundreds of controllable variables and dozens of outputs.

The next section gives a brief overview of how PLS works, relating it to other multivariate techniques such as principal components regression and maximum redundancy analysis. An extended chemometric example is presented that demonstrates how PLS models are evaluated and how their components are interpreted. A final section discusses alternatives and extensions of PLS. The appendices introduce the experimental PLS procedure for performing partial least squares and related modeling techniques.

How Does PLS Work?

In principle, MLR can be used with very many factors. However, if the number of factors gets too large (for example, greater than the number of observations), you are likely to get a model that fits the sampled data perfectly but that will fail to predict new data well. This phenomenon is called *over-fitting*. In such cases, although there are many manifest factors, there may be only a few underlying or latent factors that account for most of the variation in the response. The general idea of PLS is to try to extract these latent factors, accounting for as much of the manifest factor variation as possible while modeling the responses well. For this reason, the acronym PLS has also been taken to mean "projection to latent structure." It should be noted, however, that the term "latent" does not have the same technical meaning in the context of PLS as it does for other multivariate techniques. In particular, PLS does not yield consistent estimates of what are called "latent variables" in formal structural equation modelling (Dykstra 1983, 1985).

Figure 3 gives a schematic outline of the method. The overall goal (shown in the lower box) is to use the factors to predict the responses in the population. This is achieved indirectly by extracting latent variables T and U from sampled factors and responses, respectively. The extracted factors T (also referred to as *X-scores*) are used to predict the *Y-scores* U, and then the predicted Y-scores are used to construct predictions for the responses. This procedure actually covers various techniques, depending on which source of variation is considered most crucial.

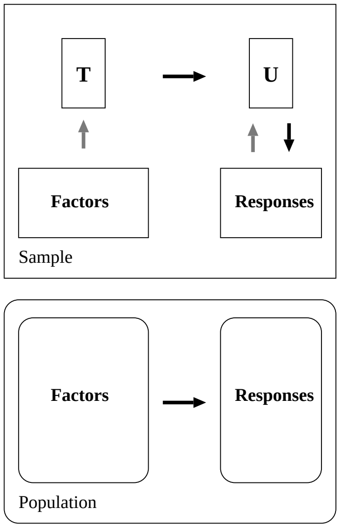

Figure 3: Indirect modeling

- **Principal Components Regression (PCR):** The X-scores are chosen to explain as much of the factor variation as possible. This approach yields informative directions in the factor space, but they may not be associated with the shape of the predicted surface.
- **Maximum Redundancy Analysis (MRA) (van den Wollenberg 1977):** The Y-scores are chosen to explain as much of the predicted Y variation as possible. This approach seeks directions in the factor space that are associated with the most variation in the responses, but the predictions may not be very accurate.
- **Partial Least Squares:** The X- and Y-scores are chosen so that the relationship between successive pairs of scores is as strong as possible. In principle, this is like a robust form of redundancy analysis, seeking directions in the factor space that are associated with high variation in the responses but biasing them toward directions that are accurately predicted.

Another way to relate the three techniques is to note that PCR is based on the spectral decomposition of $X'X$, where X is the matrix of factor values; MRA is based on the spectral decomposition of $\hat{Y}'\hat{Y}$, where $\hat{Y}$ is the matrix of (predicted) response values; and PLS is based on the singular value decomposition of $X'Y$. In SAS® software, both the REG procedure and SAS/INSIGHT® software implement forms of principal components regression; redundancy analysis can be performed using the TRANSREG procedure.

If the number of extracted factors is greater than or equal to the rank of the sample factor space, then PLS is equivalent to MLR. An important feature of the method is that usually a great deal fewer factors are required. The precise number of extracted factors is usually chosen by some heuristic technique based on the amount of residual variation. Another approach is to construct the PLS model for a given number of factors on one set of data and then to test it on another, choosing the number of extracted factors for which the total prediction error is minimized. Alternatively, van der Voet (1994) suggests choosing the least number of extracted factors whose residuals are not significantly greater than those of the model with minimum error. If no convenient test set is available, then each observation can be used in turn as a test set; this is known as *cross-validation*.

Example: Spectrometric Calibration

Suppose you have a chemical process whose yield has five different components. You use an instrument to predict the amounts of these components based on a spectrum. In order to calibrate the instrument, you run 20 different *known* combinations of the five components through it and observe the spectra. The results are twenty spectra with their associated component amounts, as in Figure 2.

PLS can be used to construct a linear predictive model for the component amounts based on the spectrum. Each spectrum is comprised of measurements at 1,000 different frequencies; these are the factor levels, and the responses are the five component amounts. The left-hand side of Table shows the individual and cumulative variation accounted for by

Table 2: PLS analysis of spectral calibration, with cross-validation

Number of PLS Factors	Percent Variation Accounted For				Cross-validation	
	Factors		Responses			Comparison
	Current	Total	Current	Total	PRESS	P
0					1.067	0
1	39.35	39.35	28.70	28.70	0.929	0
2	29.93	69.28	25.57	54.27	0.851	0
3	7.94	77.22	21.87	76.14	0.728	0
4	6.40	83.62	6.45	82.59	0.600	0.002
5	2.07	85.69	16.95	99.54	0.312	0.261
6	1.20	86.89	0.38	99.92	0.305	0.428
7	1.15	88.04	0.04	99.96	0.305	0.478
8	1.12	89.16	0.02	99.98	0.306	0.023
9	1.06	90.22	0.01	99.99	0.304	*
10	1.02	91.24	0.01	100.00	0.306	0.091

the first ten PLS factors, for both the factors and the responses. Notice that the first five PLS factors account for almost all of the variation in the responses, with the fifth factor accounting for a sizable proportion. This gives a strong indication that five PLS factors are appropriate for modeling the five component amounts. The cross-validation analysis confirms this: although the model with nine PLS factors achieves the absolute minimum predicted residual sum of squares (PRESS), it is insignificantly better than the model with only five factors.

The PLS factors are computed as certain linear combinations of the spectral amplitudes, and the responses are predicted linearly based on these extracted factors. Thus, the final predictive function for each response is also a linear combination of the spectral amplitudes. The trace for the resulting predictor of the first response is plotted in Figure 4. Notice that a PLS prediction is not associated with a single frequency or even just a few, as would be the case if we tried to choose optimal frequencies for predicting each response (stepwise regression). Instead, PLS prediction is a function of all of the input factors. In this case, the PLS predictions can be interpreted as contrasts between broad bands of frequencies.

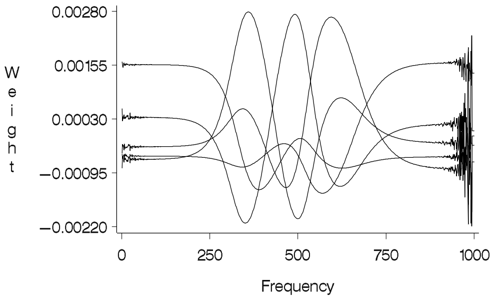

Figure 4: PLS predictor coefficients for one response

Discussion

As discussed in the introductory section, soft science applications involve so many variables that it is not practical to seek a ‘‘hard’’ model explicitly relating them all. Partial least squares is one solution for such problems, but there are others, including

- other factor extraction techniques, like principal components regression and maximum redundancy analysis
- ridge regression, a technique that originated within the field of statistics (Hoerl and Kennard 1970) as a method for handling collinearity in regression
- neural networks, which originated with attempts in computer science and biology to simulate the way animal brains recognize patterns (Haykin 1994, Sarle 1994)

Ridge regression and neural nets are probably the strongest competitors for PLS in terms of flexibility and robustness of the predictive models, but neither of them explicitly incorporates dimension reduction---that is, linearly extracting a relatively few latent factors that are most useful in modeling the response. For more discussion of the pros and cons of soft modeling alternatives, see Frank and Friedman (1993).

There are also modifications and extensions of partial least squares. The SIMPLS algorithm of de Jong

(1993) is a closely related technique. It is exactly the same as PLS when there is only one response and invariably gives very similar results, but it can be dramatically more efficient to compute when there are many factors. *Continuum regression* (Stone and Brooks 1990) adds a continuous parameter α, where $0 \leq \alpha \leq 1$, allowing the modeling method to vary continuously between MLR ($\alpha = 0$), PLS ($\alpha = 0.5$), and PCR ($\alpha = 1$). De Jong and Kiers (1992) describe a related technique called *principal covariates regression*.

In any case, PLS has become an established tool in chemometric modeling, primarily because it is often possible to interpret the extracted factors in terms of the underlying physical system---that is, to derive ‘‘hard’’ modeling information from the soft model. More work is needed on applying statistical methods to the selection of the model. The idea of van der Voet (1994) for randomization-based model comparison is a promising advance in this direction.

For Further Reading

PLS is still evolving as a statistical modeling technique, and thus there is no standard text yet that gives it in-depth coverage. Geladi and Kowalski (1986) is a standard reference introducing PLS in chemometric applications. For technical details, see Naes and Martens (1985) and de Jong (1993), as well as the references in the latter.

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Appendix 1: PROC PLS: An Experimental SAS Procedure for Partial Least Squares

An experimental SAS/STAT software procedure, PROC PLS, is available with Release 6.11 of the SAS System for performing various factor-extraction methods of modeling, including partial least squares. Other methods currently supported include alternative algorithms for PLS, such as the SIMPLS method of de Jong (1993) and the RLGW method of Rannar et al. (1994), as well as principal components regression. Maximum redundancy analysis will also be included in a future release. Factors can be specified using GLM-type modeling, allowing for polynomial, cross-product, and classification effects. The procedure offers a wide variety of methods for performing cross-validation on the number of factors, with an optional test for the appropriate number of factors. There are output data sets for cross-validation and model information as well as for predicted values and estimated factor scores.

You can specify the following statements with the PLS procedure. Items within the brackets <> are optional.

PROC PLS <*options*>**;**
CLASS *class-variables***;**
MODEL *responses* **=** *effects* < **/** *option* >**;**
OUTPUT OUT=*SAS-data-set* <*options*>**;**

PROC PLS Statement

PROC PLS <*options*>**;**

You use the PROC PLS statement to invoke the PLS procedure and optionally to indicate the analysis data and method. The following options are available:

DATA = *SAS-data-set*
specifies the input SAS data set that contains the factor and response values.

METHOD = *factor-extraction-method*
specifies the general factor extraction method to be used. You can specify any one of the following:

METHOD=PLS < **(***PLS-options***)** >
specifies partial least squares. This is the default factor extraction method.

METHOD=SIMPLS
specifies the SIMPLS method of de Jong (1993). This is a more efficient algorithm than standard PLS; it is equivalent to standard PLS when there is only one response, and it invariably gives very similar results.

METHOD=PCR
specifies principal components regression.

You can specify the following *PLS-options* in parentheses after **METHOD=PLS**:

ALGORITHM=*PLS-algorithm*
gives the specific algorithm used to compute PLS factors. Available algorithms are

ITER the usual iterative NIPALS algorithm

SVD singular value decomposition of $X'Y$, the most exact but least efficient approach

EIG eigenvalue decomposition of $Y'XX'Y$

RLGW an iterative approach that is efficient when there are many factors

MAXITER=*number*
gives the maximum number of iterations for the ITER and RLGW algorithms. The default is 200.

EPSILON=*number*
gives the convergence criterion for the ITER and RLGW algorithms. The default is 10^{-12}.

CV = *cross-validation-method*
specifies the cross-validation method to be used. If you do not specify a cross-validation method, the default action is not to perform cross-validation. You can specify any one of the following:

CV = ONE
specifies one-at-a-time cross- validation

CV = SPLIT < **(** *n* **)** >
specifies that every n^{th} observation be excluded. You may optionally specify n; the default is 1, which is the same as CV=ONE.

CV = BLOCK < **(** *n* **)** >
specifies that blocks of n^{th} observations be excluded. You may optionally specify n; the default is 1, which is the same as CV=ONE.

CV = RANDOM < **(** *cv-random-opts* **)** >

specifies that random observations be excluded.

CV = TESTSET(*SAS-data-set***)**

specifies a test set of observations to be used for cross-validation.

You also can specify the following *cv-random-opts* in parentheses after **CV = RANDOM**:

NITER = *number*

specifies the number of random subsets to exclude.

NTEST = *number*

specifies the number of observations in each random subset chosen for exclusion.

SEED = *number*

specifies the seed value for random number generation.

CVTEST < **(** *cv-test-options* **)** >

specifies that van der Voet's (1994) randomization-based model comparison test be performed on each cross-validated model. You also can specify the following *cv-test-options* in parentheses after **CVTEST**:

PVAL = *number*

specifies the cut-off probability for declaring a significant difference. The default is 0.10.

STAT = *test-statistic*

specifies the test statistic for the model comparison. You can specify either T2, for Hotelling's T^2 statistic, or PRESS, for the predicted residual sum of squares. T2 is the default.

NSAMP = *number*

specifies the number of randomizations to perform. The default is 1000.

LV = *number*

specifies the number of factors to extract. The default number of factors to extract is the number of input factors, in which case the analysis is equivalent to a regular least squares regression of the responses on the input factors.

OUTMODEL = *SAS-data-set*

specifies a name for a data set to contain information about the fit model.

OUTCV = *SAS-data-set*

specifies a name for a data set to contain information about the cross-validation.

CLASS Statement

CLASS *class-variables***;**

You use the CLASS statement to identify classification variables, which are factors that separate the observations into groups.

Class-variables can be either numeric or character. The PLS procedure uses the formatted values of *class-variables* in forming model effects. Any variable in the model that is not listed in the CLASS statement is assumed to be continuous. Continuous variables must be numeric.

MODEL Statement

MODEL *responses* **=** *effects* < **/ INTERCEPT** >**;**

You use the MODEL statement to specify the response variables and the independent effects used to model them. Usually you will just list the names of the independent variables as the model effects, but you can also use the effects notation of PROC GLM to specify polynomial effects and interactions. By default the factors are centered and thus no intercept is required in the model, but you can specify the INTERCEPT option to override this behavior.

OUTPUT Statement

OUTPUT OUT=*SAS-data-set keyword* **=** *names* < . . . *keyword* **=** *names* >**;**

You use the OUTPUT statement to specify a data set to receive quantities that can be computed for every input observation, such as extracted factors and predicted values. The following keywords are available:

PREDICTED	predicted values for responses
YRESIDUAL	residuals for responses
XRESIDUAL	residuals for factors
XSCORE	extracted factors (X-scores, latent vectors, T)
YSCORE	extracted responses (Y-scores, U)
STDY	standard error for Y predictions
STDX	standard error for X predictions
H	approximate measure of influence
PRESS	predicted residual sum of squares
T2	scaled sum of squares of scores

XQRES sum of squares of scaled residuals for factors

YQRES sum of squares of scaled residuals for responses

Appendix 2: Example Code

The data for the spectrometric calibration example is in the form of a SAS data set called SPECTRA with 20 observations, one for each test combination of the five components. The variables are

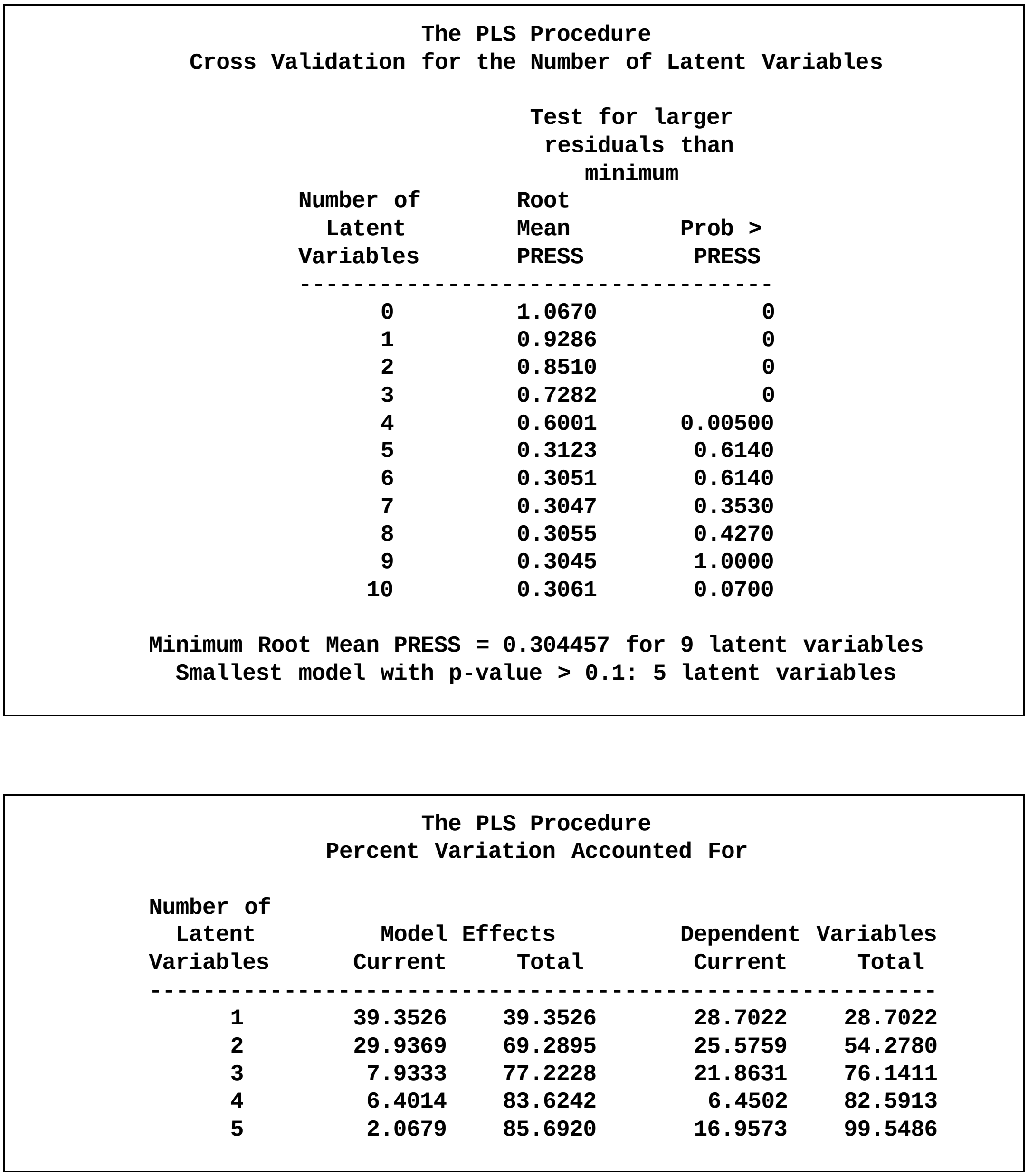
X1 . . . X1000 - the spectrum for this combination

Y1 . . . Y5 - the component amounts

There is also a test data set of 20 more observations available for cross-validation. The following statements use PROC PLS to analyze the data, using the SIMPLS algorithm and selecting the number of factors with cross-validation.

```
proc pls data   = spectra
         method = simpls
         lv     = 9
         cv     = testset(test5)
         cvtest(stat=press);
   model y1-y5 = x1-x1000;
run;
```

The listing has two parts (Figure 5), the first part summarizing the cross-validation and the second part showing how much variation is explained by each extracted factor for both the factors and the responses. Note that the extracted factors are labeled ‘‘latent variables’’ in the listing.



```
                      The PLS Procedure
          Cross Validation for the Number of Latent Variables

                              Test for larger
                               residuals than
                                  minimum
               Number of       Root
                 Latent        Mean        Prob >
               Variables       PRESS        PRESS
               ----------------------------------
                     0        1.0670            0
                     1        0.9286            0
                     2        0.8510            0
                     3        0.7282            0
                     4        0.6001      0.00500
                     5        0.3123       0.6140
                     6        0.3051       0.6140
                     7        0.3047       0.3530
                     8        0.3055       0.4270
                     9        0.3045       1.0000
                    10        0.3061       0.0700

     Minimum Root Mean PRESS = 0.304457 for 9 latent variables
       Smallest model with p-value > 0.1: 5 latent variables
```

```
                      The PLS Procedure
                 Percent Variation Accounted For

     Number of
       Latent        Model Effects        Dependent Variables
     Variables      Current     Total       Current     Total
     ----------------------------------------------------------
           1        39.3526   39.3526       28.7022   28.7022
           2        29.9369   69.2895       25.5759   54.2780
           3         7.9333   77.2228       21.8631   76.1411
           4         6.4014   83.6242        6.4502   82.5913
           5         2.0679   85.6920       16.9573   99.5486
```

Figure 5: PROC PLS output for spectrometric calibration example