Chapter 51
The PLS Procedure

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Overview

The PLS procedure fits models using any one of a number of linear predictive methods, including *partial least squares* (PLS). Ordinary least squares regression, as implemented in SAS/STAT procedures such as PROC GLM and PROC REG, has the single goal of minimizing sample response prediction error, seeking linear functions of the predictors that explain as much variation in each response as possible. The techniques implemented in the PLS procedure have the additional goal of accounting for variation in the predictors, under the assumption that directions in the predictor space that are well sampled should provide better prediction for *new* observations when the predictors are highly correlated. All of the techniques implemented in the PLS procedure work by extracting successive linear combinations of the predictors, called *factors* (also called *components* or *latent vectors*), which optimally address one or both of these two goals—explaining response variation and explaining predictor variation. In particular, the method of partial least squares balances the two objectives, seeking for factors that explain both response and predictor variation.

Note that the name "partial least squares" also applies to a more general statistical method that is *not* implemented in this procedure. The partial least squares method was originally developed in the 1960s by the econometrician Herman Wold (1966) for modeling "paths" of causal relation between any number of "blocks" of variables. However, the PLS procedure fits only *predictive* partial least squares models, with one "block" of predictors and one "block" of responses. If you are interested in fitting more general path models, you should consider using the CALIS procedure.

Basic Features

The techniques implemented by the PLS procedure are

- principal components regression, which extracts factors to explain as much predictor sample variation as possible.
- reduced rank regression, which extracts factors to explain as much response variation as possible. This technique, also known as (maximum) redundancy analysis, differs from multivariate linear regression only when there are multiple responses.
- partial least squares regression, which balances the two objectives of explaining response variation and explaining predictor variation. Two different formulations for partial least squares are available: the original method of Wold (1966) and the SIMPLS method of de Jong (1993).

The number of factors to extract depends on the data. Basing the model on more extracted factors improves the model fit to the observed data, but extracting too many factors can cause *over-fitting*, that is, tailoring the model too much to the current data, to the detriment of future predictions. The PLS procedure enables you to choose the number of extracted factors by *cross validation*, that is, fitting the model to part of the data and minimizing the prediction error for the unfitted part. Various methods of cross validation are available, including one-at-a-time validation, splitting the data into blocks, and test set validation.

You can use the general linear modeling approach of the GLM procedure to specify a model for your design, allowing for general polynomial effects as well as classification or ANOVA effects. You can save the model fit by the PLS procedure in a data set and apply it to new data by using the SCORE procedure.

Getting Started

Predicting Biological Activity

The example in this section illustrates basic features of the PLS procedure. The data are reported in Umetrics (1995); the original source is Lindberg, Persson, and Wold (1983). Suppose that you are researching pollution in the Baltic Sea, and you would like to use the spectra of samples of sea water to determine the amounts of three compounds present in samples from the Baltic Sea: lignin sulfonate (ls: pulp industry pollution), humic acids (ha: natural forest products), and optical whitener from detergent (dt). Spectrometric calibration is a type of problem in which partial least squares can be very effective. The predictors are the spectra emission intensities at different frequencies in sample spectrum, and the responses are the amounts of various chemicals in the sample.

For the purposes of calibrating the model, samples with known compositions are used. The calibration data consist of 16 samples of known concentrations of ls, ha, and dt, with spectra based on 27 frequencies (or, equivalently, wavelengths). The following statements create a SAS data set named Sample for these data.

```
data Sample;
   input obsnam $ v1-v27 ls ha dt @@;
   datalines;
EM1   2766 2610 3306 3630 3600 3438 3213 3051 2907 2844 2796
      2787 2760 2754 2670 2520 2310 2100 1917 1755 1602 1467
      1353 1260 1167 1101 1017         3.0110  0.0000   0.00
EM2   1492 1419 1369 1158  958  887  905  929  920  887  800
       710  617  535  451  368  296  241  190  157  128  106
        89   70   65   56   50         0.0000  0.4005   0.00
EM3   2450 2379 2400 2055 1689 1355 1109  908  750  673  644
       640  630  618  571  512  440  368  305  247  196  156
       120   98   80   61   50         0.0000  0.0000  90.63
EM4   2751 2883 3492 3570 3282 2937 2634 2370 2187 2070 2007
      1974 1950 1890 1824 1680 1527 1350 1206 1080  984  888
       810  732  669  630  582         1.4820  0.1580  40.00
EM5   2652 2691 3225 3285 3033 2784 2520 2340 2235 2148 2094
```

```
      2049 2007 1917 1800 1650 1464 1299 1140 1020  909  810
       726  657  594  549  507         1.1160  0.4104  30.45
EM6   3993 4722 6147 6720 6531 5970 5382 4842 4470 4200 4077
      4008 3948 3864 3663 3390 3090 2787 2481 2241 2028 1830
      1680 1533 1440 1314 1227         3.3970  0.3032  50.82
EM7   4032 4350 5430 5763 5490 4974 4452 3990 3690 3474 3357
      3300 3213 3147 3000 2772 2490 2220 1980 1779 1599 1440
      1320 1200 1119 1032  957         2.4280  0.2981  70.59
EM8   4530 5190 6910 7580 7510 6930 6150 5490 4990 4670 4490
      4370 4300 4210 4000 3770 3420 3060 2760 2490 2230 2060
      1860 1700 1590 1490 1380         4.0240  0.1153  89.39
EM9   4077 4410 5460 5857 5607 5097 4605 4170 3864 3708 3588
      3537 3480 3330 3192 2910 2610 2325 2064 1830 1638 1476
      1350 1236 1122 1044  963         2.2750  0.5040  81.75
EM10  3450 3432 3969 4020 3678 3237 2814 2487 2205 2061 2001
      1965 1947 1890 1776 1635 1452 1278 1128  981  867  753
       663  600  552  507  468         0.9588  0.1450 101.10
EM11  4989 5301 6807 7425 7155 6525 5784 5166 4695 4380 4197
      4131 4077 3972 3777 3531 3168 2835 2517 2244 2004 1809
      1620 1470 1359 1266 1167         3.1900  0.2530 120.00
EM12  5340 5790 7590 8390 8310 7670 6890 6190 5700 5380 5200
      5110 5040 4900 4700 4390 3970 3540 3170 2810 2490 2240
      2060 1870 1700 1590 1470         4.1320  0.5691 117.70
EM13  3162 3477 4365 4650 4470 4107 3717 3432 3228 3093 3009
      2964 2916 2838 2694 2490 2253 2013 1788 1599 1431 1305
      1194 1077  990  927  855         2.1600  0.4360  27.59
EM14  4380 4695 6018 6510 6342 5760 5151 4596 4200 3948 3807
      3720 3672 3567 3438 3171 2880 2571 2280 2046 1857 1680
      1548 1413 1314 1200 1119         3.0940  0.2471  61.71
EM15  4587 4200 5040 5289 4965 4449 3939 3507 3174 2970 2850
      2814 2748 2670 2529 2328 2088 1851 1641 1431 1284 1134
      1020  918  840  756  714         1.6040  0.2856 108.80
EM16  4017 4725 6090 6570 6354 5895 5346 4911 4611 4422 4314
      4287 4224 4110 3915 3600 3240 2913 2598 2325 2088 1917
      1734 1587 1452 1356 1257         3.1620  0.7012  60.00
;
```

Fitting a PLS Model

To isolate a few underlying spectral factors that provide a good predictive model, you can fit a PLS model to the 16 samples using the following SAS statements:

```
proc pls data=sample;
   model ls ha dt = v1-v27;
run;
```

By default, the PLS procedure extracts at most 15 factors. The procedure lists the amount of variation accounted for by each of these factors, both individual and cumulative; this listing is shown in Figure 51.1.

```
                             The PLS Procedure

                    Percent Variation Accounted for
                    by Partial Least Squares Factors

       Number of
       Extracted       Model Effects        Dependent Variables
         Factors     Current       Total     Current       Total

               1     97.4607     97.4607     41.9155     41.9155
               2      2.1830     99.6436     24.2435     66.1590
               3      0.1781     99.8217     24.5339     90.6929
               4      0.1197     99.9414      3.7898     94.4827
               5      0.0415     99.9829      1.0045     95.4873
               6      0.0106     99.9935      2.2808     97.7681
               7      0.0017     99.9952      1.1693     98.9374
               8      0.0010     99.9961      0.5041     99.4415
               9      0.0014     99.9975      0.1229     99.5645
              10      0.0010     99.9985      0.1103     99.6747
              11      0.0003     99.9988      0.1523     99.8270
              12      0.0003     99.9991      0.1291     99.9561
              13      0.0002     99.9994      0.0312     99.9873
              14      0.0004     99.9998      0.0065     99.9938
              15      0.0002    100.0000      0.0062    100.0000
```

Figure 51.1. PLS Variation Summary

Note that all of the variation in both the predictors and the responses is accounted for by only 15 factors; this is because there are only 16 sample observations. More importantly, almost all of the variation is accounted for with even fewer factors—one or two for the predictors and three to eight for the responses.

Selecting the Number of Factors by Cross Validation

A PLS model is not complete until you choose the number of factors. You can choose the number of factors by using cross validation, in which the data set is divided into two or more groups. You fit the model to all groups except one, then you check the capability of the model to predict responses for the group omitted. Repeating this for each group, you then can measure the overall capability of a given form of the model. The Predicted REsidual Sum of Squares (PRESS) statistic is based on the residuals generated by this process.

To select the number of extracted factors by cross validation, you specify the CV= option with an argument that says which cross validation method to use. For example, a common method is split-sample validation, in which the different groups are comprised of every nth observation beginning with the first, every nth observation beginning with the second, and so on. You can use the CV=SPLIT option to specify split-sample validation with $n = 7$ by default, as in the following SAS statements:

```
proc pls data=sample cv=split;
   model ls ha dt = v1-v27;
run;
```

The resulting output is shown in Figure 51.2 and Figure 51.3.

```
                               The PLS Procedure

          Split-sample Validation for the Number of Extracted Factors

                             Number of        Root
                             Extracted        Mean
                               Factors       PRESS

                                     0    1.107747
                                     1    0.957983
                                     2    0.931314
                                     3    0.520222
                                     4    0.530501
                                     5    0.586786
                                     6    0.475047
                                     7    0.477595
                                     8    0.483138
                                     9    0.485739
                                    10     0.48946
                                    11    0.521445
                                    12    0.525653
                                    13    0.531049
                                    14    0.531049
                                    15    0.531049


                    Minimum root mean PRESS           0.4750
                    Minimizing number of factors           6
```

Figure 51.2. Split-Sample Validated PRESS Statistics for Number of Factors

```
                               The PLS Procedure

                        Percent Variation Accounted for
                        by Partial Least Squares Factors

           Number of
           Extracted       Model Effects        Dependent Variables
             Factors     Current       Total     Current       Total

                   1     97.4607     97.4607     41.9155     41.9155
                   2      2.1830     99.6436     24.2435     66.1590
                   3      0.1781     99.8217     24.5339     90.6929
                   4      0.1197     99.9414      3.7898     94.4827
                   5      0.0415     99.9829      1.0045     95.4873
                   6      0.0106     99.9935      2.2808     97.7681
```

Figure 51.3. PLS Variation Summary for Split-Sample Validated Model

The absolute minimum PRESS is achieved with six extracted factors. Notice, however, that this is not much smaller than the PRESS for three factors. By using the CVTEST option, you can perform a statistical model comparison suggested by van der Voet (1994) to test whether this difference is significant, as shown in the following SAS statements:

```
proc pls data=sample cv=split cvtest(seed=12345);
   model ls ha dt = v1-v27;
run;
```

The model comparison test is based on a rerandomization of the data. By default, the seed for this randomization is based on the system clock, but it is specified here. The resulting output is shown in Figure 51.4 and Figure 51.5.

```
                         The PLS Procedure

        Split-sample Validation for the Number of Extracted Factors

               Number of        Root
               Extracted        Mean                  Prob >
                 Factors       PRESS        T**2        T**2

                       0    1.107747    9.272858    0.0010
                       1    0.957983    10.62305    <.0001
                       2    0.931314    8.950878    <.0001
                       3    0.520222    5.133259    0.1430
                       4    0.530501    5.168427    0.1330
                       5    0.586786    6.437266    0.0150
                       6    0.475047           0    1.0000
                       7    0.477595    2.809763    0.4750
                       8    0.483138    7.189526    0.0110
                       9    0.485739    7.931726    0.0060
                      10     0.48946    6.612597    0.0140
                      11    0.521445    6.666235    0.0130
                      12    0.525653    7.092861    0.0070
                      13    0.531049    7.538298    0.0020
                      14    0.531049    7.538298    0.0020
                      15    0.531049    7.538298    0.0020


           Minimum root mean PRESS                     0.4750
           Minimizing number of factors                     6
           Smallest number of factors with p > 0.1          3
```

Figure 51.4. Testing Split-Sample Validation for Number of Factors

```
                         The PLS Procedure

                      Percent Variation Accounted for
                      by Partial Least Squares Factors

        Number of
        Extracted       Model Effects        Dependent Variables
          Factors     Current       Total     Current       Total

                1     97.4607     97.4607     41.9155     41.9155
                2      2.1830     99.6436     24.2435     66.1590
                3      0.1781     99.8217     24.5339     90.6929
```

Figure 51.5. PLS Variation Summary for Tested Split-Sample Validated Model

The p-value of 0.1430 in comparing the cross-validated residuals from models with 6 and 3 factors indicates that the difference between the two models is insignificant; therefore, the model with fewer factors is preferred. The variation summary shows that over 99% of the predictor variation and over 90% of the response variation are accounted for by the three factors.

Predicting New Observations

Now that you have chosen a three-factor PLS model for predicting pollutant concentrations based on sample spectra, suppose that you have two new samples. The following SAS statements create a data set containing the spectra for the new samples:

```
data newobs;
   input obsnam $ v1-v27 @@;
   datalines;
EM17  3933 4518 5637 6006 5721 5187 4641 4149 3789
      3579 3447 3381 3327 3234 3078 2832 2571 2274
      2040 1818 1629 1470 1350 1245 1134 1050  987
EM25  2904 2997 3255 3150 2922 2778 2700 2646 2571
      2487 2370 2250 2127 2052 1713 1419 1200  984
       795  648  525  426  351  291  240  204  162
;
```

You can apply the PLS model to these samples to estimate pollutant concentration. To do so, append the new samples to the original 16, and specify that the predicted values for all 18 be output to a data set, as shown in the following statements:

```
data all; set sample newobs;
proc pls data=all nfac=3;
   model ls ha dt = v1-v27;
   output out=pred p=p_ls p_ha p_dt;
proc print data=pred;
   where (obsnam in ('EM17','EM25'));
   var obsnam p_ls p_ha p_dt;
run;
```

The new observations are not used in calculating the PLS model, since they have no response values. Their predicted concentrations are shown in Figure 51.6.

```
Obs    obsnam      p_ls        p_ha       p_dt

 17     EM17      2.54261    0.31877    81.4174
 18     EM25     -0.24716    1.37892    46.3212
```

Figure 51.6. Predicted Concentrations for New Observations

Syntax

The following statements are available in PROC PLS. Items within the brackets < > are optional.

PROC PLS < *options* > **;**
BY *variables* **;**
CLASS *variables* **;**
MODEL *dependent-variables = effects* < */ options* > **;**
OUTPUT OUT= *SAS-data-set* < *options* > **;**

To analyze a data set, you must use the PROC PLS and MODEL statements. You can use the other statements as needed.

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*
names the SAS data set to be used by PROC PLS. The default is the most recently created data set.

METHOD=PLS < **(** *PLS-options* **)** >
METHOD=SIMPLS
METHOD=PCR
METHOD=RRR
specifies the general factor extraction method to be used. The value PLS requests partial least squares, SIMPLS requests the SIMPLS method of de Jong (1993), PCR requests principal components regression, and RRR requests reduced rank regression. The default is METHOD=PLS. You can also specify the following optional *PLS-options* in parentheses after METHOD=PLS:

ALGORITHM=NIPALS | SVD | EIG | RLGW names the specific algorithm used to compute extracted PLS factors. NIPALS requests the usual iterative NIPALS algorithm, SVD bases the extraction on the singular value decomposition of $X'Y$, EIG bases the extraction on the eigenvalue decomposition of $Y'XX'Y$, and RLGW is an iterative approach that is efficient when there are many predictors (Ränner et al. 1994). ALGORITHM=SVD is the most accurate but least efficient approach; the default is ALGORITHM=NIPALS.

MAXITER=*n* specifies the maximum number of iterations for the NIPALS and RLGW algorithms. The default value is 200.

EPSILON=*n* specifies the convergence criterion for the NIPALS and RLGW algorithms. The default value is 10^{-12}.

CV=ONE
CV=SPLIT $<$ **(***n***)** $>$
CV=BLOCK $<$ **(***n***)** $>$
CV=RANDOM $<$ **(***cv-random-opts***)** $>$
CV=TESTSET(*SAS-data-set***)**

specifies the cross validation method to be used. By default, no cross validation is performed. The method CV=ONE requests one-at-a-time cross validation, CV=SPLIT requests that every nth observation be excluded, CV=BLOCK requests that blocks of n observations be excluded, CV=RANDOM requests that observations be excluded at random, and CV=TESTSET(*SAS-data-set*) specifies a test set of observations to be used for validation (formally, this is called "test set validation" rather than "cross validation"). You can, optionally, specify n for CV=SPLIT and CV=BLOCK; the default is $n = 7$. You can also specify the following optional *cv-random-options* in parentheses after the CV=RANDOM option:

NITER=*n* specifies the number of random subsets to exclude. The default value is 10.

NTEST=*n* specifies the number of observations in each random subset chosen for exclusion. The default value is one-tenth of the total number of observations.

SEED=*n* specifies the seed value for random number generation (the clock time is used by default).

CVTEST $<$ **(***cvtest-options***)** $>$

specifies that van der Voet's (1994) randomization-based model comparison test be performed to test models with different numbers of extracted factors against the model that minimizes the predicted residual sum of squares; see the "Cross Validation" section on page 2709 for more information. You can also specify the following *cv-test-options* in parentheses after the CVTEST option:

PVAL=*n* specifies the cut-off probability for declaring an insignificant difference. The default value 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. The default value is T2.

NSAMP=*n* specifies the number of randomizations to perform. The default value is 1000.

SEED=*n* specifies the seed value for randomization generation (the clock time is used by default).

NFAC=*n*

specifies the number of factors to extract. The default is $\min\{15, p, N\}$, where p is the number of predictors (the number of dependent variables for METHOD=RRR) and N is the number of runs. This is probably more than you need for most applications. Extracting too many factors can lead to an over-fit model, one that matches the training data too well, sacrificing predictive ability. Thus, if you use the default NFAC= specification, you should also either use the CV= option to select the appropriate number of factors for the final model or consider the analysis to be preliminary and examine the results to determine the appropriate number of factors for a subsequent analysis.

NOPRINT

suppresses the normal display of results. This is useful when you want only the output statistics saved in a data set. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 15, “Using the Output Delivery System,” for more information.

NOSCALE

suppresses scaling of the responses and predictors before fitting. This is useful if the analysis variables are already centered and scaled. See the “Centering and Scaling” section on page 2711 for more information.

NOCENTER

suppresses centering of the responses and predictors before fitting. This is useful if the analysis variables are already centered and scaled. See the “Centering and Scaling” section on page 2711 for more information.

NOCVSTDIZE

suppresses re-centering and re-scaling of the responses and predictors before each model is fit in the cross validation. See the “Centering and Scaling” section on page 2711 for more information.

CENSCALE

lists the centering and scaling information for each response and predictor.

VARSCALE

specifies that continuous model variables should be centered and scaled prior to centering and scaling the model effects in which they are involved. The rescaling specified by the VARSCALE option may be more appropriate if the model involves cross products between model variables; however, the VARSCALE option still may not produce the model you expect. See the “Centering and Scaling” section on page 2711 for more information.

VARSS

lists, in addition to the average response and predictor sum of squares accounted for by each successive factor, the amount of variation accounted for in each response and predictor.

DETAILS

lists the details of the fitted model for each successive factor. The details listed are different for different extraction methods: see the “Displayed Output” section on page 2712 for more information.

BY Statement

BY *variables* **;**

You can specify a BY statement with PROC PLS to obtain separate analyses on observations in groups defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. The *variables* are one or more variables in the input data set.

If you specify more than one BY statement, the procedure uses only the latest BY statement and ignores any previous ones.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data using the SORT procedure with a similar BY statement.
- Specify the BY statement option NOTSORTED or DESCENDING in the BY statement for the PLS procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables using the DATASETS procedure (in base SAS software).

For more information on the BY statement, refer to the discussion in *SAS Language Reference: Concepts*. For more information on the DATASETS procedure, refer to the discussion in the *SAS Procedures Guide*.

CLASS Statement

CLASS *variables* **;**

The CLASS statement names the classification variables to be used in the analysis. If the CLASS statement is used, it must appear before the MODEL statement.

Classification variables can be either character or numeric. The procedure uses only the first 16 characters of a character variable. Class levels are determined from the formatted values of the CLASS variables. Thus, you can use formats to group values into levels. Refer to the discussion of the FORMAT procedure in the *SAS Procedures Guide* and to the discussions of the FORMAT statement and SAS formats in *SAS Language Reference: Dictionary*. 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 *response-variables* **=** *predictor-effects* < **/** *options* >**;**

The MODEL statement names the responses and the predictors, which determine the **Y** and **X** matrices of the model, respectively. Usually you simply list the names of the predictor variables as the model effects, but you can also use the effects notation of PROC GLM to specify polynomial effects and interactions; see the "Specification of Effects" section on page 1517 in Chapter 30, "The GLM Procedure," for further details. The MODEL statement is required. You can specify only one MODEL statement (in contrast to the REG procedure, for example, which allows several MODEL statements in the same PROC REG run).

You can specify the following options in the MODEL statement after a slash (/).

INTERCEPT
By default, the responses and predictors are centered; thus, no intercept is required in the model. You can specify the INTERCEPT option to override the default.

SOLUTION
lists the coefficients of the final predictive model for the responses. The coefficients for predicting the centered and scaled responses based on the centered and scaled predictors are displayed, as well as the coefficients for predicting the raw responses based on the raw predictors.

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 predictors
XSCORE	extracted factors (X-scores, latent vectors, T)
YSCORE	extracted responses (Y-scores, U)
STDY	standardized (centered and scaled) responses
STDX	standardized (centered and scaled) predictors
H	approximate leverage

PRESS	approximate predicted residuals
TSQUARE	scaled sum of squares of score values
STDXSSE	sum of squares of residuals for standardized predictors
STDYSSE	sum of squares of residuals for standardized responses

Suppose that there are N_x predictors and N_y responses and that the model has N_f selected factors.

- The keywords XRESIDUAL and STDX define an output variable for each predictor, so N_x names are required after each one.
- The keywords PREDICTED, YRESIDUAL, STDY, and PRESS define an output variable for each response, so N_y names are required after each of these keywords.
- The keywords XSCORE and YSCORE specify an output variable for each selected model factor. For these keywords, you provide only one base name, and the variables corresponding to each successive factor are named by appending the factor number to the base name. For example, if $N_f = 3$ then a specification of XSCORE=T would produce the variables T1, T2, and T3.
- Finally, the keywords H, TSQUARE, STDXSSE, and STDYSSE each specify a single output variable, so only one name is required after each of these keywords.

Details

Regression Methods

All of the predictive methods implemented in PROC PLS work essentially by finding linear combinations of the predictors (factors) to use to predict the responses linearly. The methods differ only in how the factors are derived, as explained in the following sections.

Partial Least Squares

Partial least squares (PLS) works by extracting one factor at a time. Let $X = X_0$ be the centered and scaled matrix of predictors and $Y = Y_0$ the centered and scaled matrix of response values. The PLS method starts with a linear combination $\mathbf{t} = X_0\mathbf{w}$ of the predictors, where $\mathbf{t}$ is called a *score* vector and $\mathbf{w}$ is its associated *weight* vector. The PLS method predicts both X_0 and Y_0 by regression on $\mathbf{t}$:

$$\begin{aligned} \hat{X}_0 &= \mathbf{t}\mathbf{p}', \text{ where } \mathbf{p}' = (\mathbf{t}'\mathbf{t})^{-1}\mathbf{t}'X_0 \\ \hat{Y}_0 &= \mathbf{t}\mathbf{c}', \text{ where } \mathbf{c}' = (\mathbf{t}'\mathbf{t})^{-1}\mathbf{t}'Y_0 \end{aligned}$$

The vectors $\mathbf{p}$ and $\mathbf{c}$ are called the X- and Y-*loadings*, respectively.

The specific linear combination $\mathbf{t} = X_0\mathbf{w}$ is the one that has maximum covariance $\mathbf{t}'\mathbf{u}$ with some response linear combination $\mathbf{u} = Y_0\mathbf{q}$. Another characterization is that the X- and Y-weights $\mathbf{w}$ and $\mathbf{q}$ are proportional to the first left and right singular vectors of the covariance matrix $X_0'Y_0$ or, equivalently, the first eigenvectors of $X_0'Y_0Y_0'X_0$ and $Y_0'X_0X_0'Y_0$, respectively.

This accounts for how the first PLS factor is extracted. The second factor is extracted in the same way by replacing X_0 and Y_0 with the X- and Y-residuals from the first factor

$$\begin{aligned} X_1 &= X_0 - \hat{X}_0 \\ Y_1 &= Y_0 - \hat{Y}_0 \end{aligned}$$

These residuals are also called the *deflated* X and Y blocks. The process of extracting a score vector and deflating the data matrices is repeated for as many extracted factors as are desired.

SIMPLS

Note that each extracted PLS factor is defined in terms of different X-variables X_i. This leads to difficulties in comparing different scores, weights, and so forth. The SIMPLS method of de Jong (1993) overcomes these difficulties by computing each score $\mathbf{t}_i = X\mathbf{r}_i$ in terms of the original (centered and scaled) predictors X. The SIMPLS X-weight vectors r_i are similar to the eigenvectors of $SS' = X'YY'X$, but they satisfy a different orthogonality condition. The $\mathbf{r}_1$ vector is just the first eigenvector $\mathbf{e}_1$ (so that the first SIMPLS score is the same as the first PLS score), but whereas the second eigenvector maximizes

$$\mathbf{e}_1'SS'\mathbf{e}_2 \text{ subject to } \mathbf{e}_1'\mathbf{e}_2 = 0$$

the second SIMPLS weight $\mathbf{r}_2$ maximizes

$$\mathbf{r}_1'SS'\mathbf{r}_2 \text{ subject to } \mathbf{r}_1'X'X\mathbf{r}_2 = \mathbf{t}_1'\mathbf{t}_2 = 0$$

The SIMPLS scores are identical to the PLS scores for one response but slightly different for more than one response; refer to de Jong (1993) for details. The X- and Y-loadings are defined as in PLS, but since the scores are all defined in terms of X, it is easy to compute the overall model coefficients B:

$$\begin{aligned} \hat{Y} &= \sum_i \mathbf{t_i c_i}' \\ &= \sum_i X\mathbf{r_i c_i}' \\ &= XB, \text{ where } B = RC' \end{aligned}$$

Principal Components Regression

Like the SIMPLS method, principal components regression (PCR) defines all the scores in terms of the original (centered and scaled) predictors X. However, unlike both the PLS and SIMPLS methods, the PCR method chooses the X-weights/X-scores without regard to the response data. The X-scores are chosen to explain as much variation in X as possible; equivalently, the X-weights for the PCR method are the eigenvectors of the predictor covariance matrix $X'X$. Again, the X- and Y-loadings are defined as in PLS; but, as in SIMPLS, it is easy to compute overall model coefficients for the original (centered and scaled) responses Y in terms of the original predictors X.

Reduced Rank Regression

As discussed in the preceding sections, partial least squares depends on selecting factors $\mathbf{t} = X\mathbf{w}$ of the predictors and $\mathbf{u} = Y\mathbf{q}$ of the responses that have maximum covariance, whereas principal components regression effectively ignores $\mathbf{u}$ and selects $\mathbf{t}$ to have maximum variance, subject to orthogonality constraints. In contrast, reduced rank regression selects $\mathbf{u}$ to account for as much variation in the *predicted* responses as possible, effectively ignoring the predictors for the purposes of factor extraction. In reduced rank regression, the Y-weights $\mathbf{q}_i$ are the eigenvectors of the covariance matrix $\hat{Y}_{\mathrm{LS}}'\hat{Y}_{\mathrm{LS}}$ of the responses predicted by ordinary least squares regression; the X-scores are the projections of the Y-scores $Y\mathbf{q}_i$ onto the X space.

Relationships Between Methods

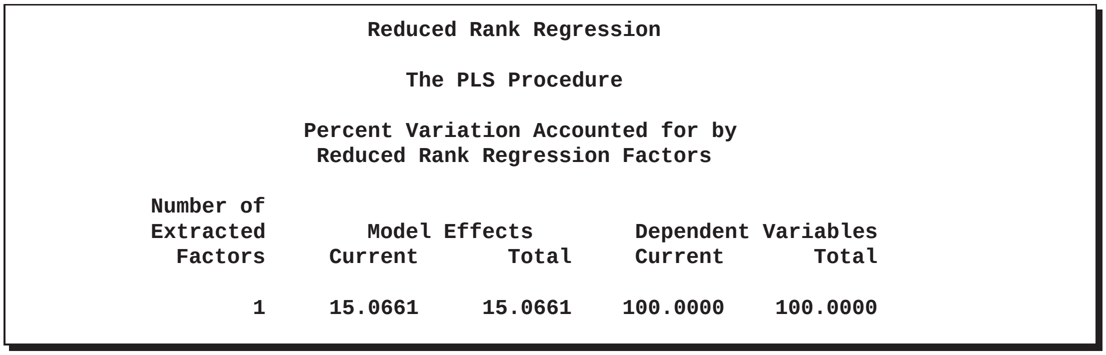
When you develop a predictive model, it is important to consider not only the explanatory power of the model for current responses, but also how well sampled the predictive functions are, since this impacts how well the model can extrapolate to future observations. All of the techniques implemented in the PLS procedure work by extracting successive factors, or linear combinations of the predictors, that optimally address one or both of these two goals—explaining response variation and explaining predictor variation. In particular, principal components regression selects factors that explain as much predictor variation as possible, reduced rank regression selects factors that explain as much response variation as possible, and partial least squares balances the two objectives, seeking for factors that explain both response and predictor variation.

To see the relationships between these methods, consider how each one extracts a single factor from the following artificial data set consisting of two predictors and one response:

```
data data;
   input x1 x2 y;
   datalines;
    3.37651  2.30716        0.75615
    0.74193 -0.88845        1.15285
    4.18747  2.17373        1.42392
    0.96097  0.57301        0.27433
   -1.11161 -0.75225       -0.25410
   -1.38029 -1.31343       -0.04728
    1.28153 -0.13751        1.00341
   -1.39242 -2.03615        0.45518
    0.63741  0.06183        0.40699
   -2.52533 -1.23726       -0.91080
    2.44277  3.61077       -0.82590
   ;
```

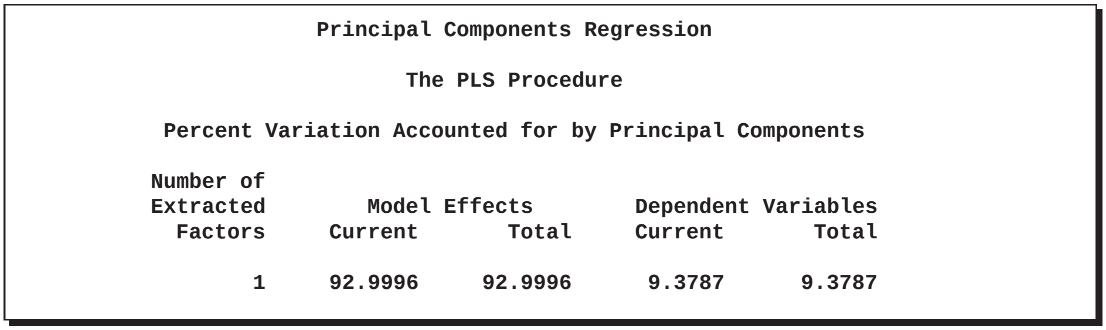
```
proc pls data=data nfac=1 method=rrr;
   title "Reduced Rank Regression";
   model y = x1 x2;
proc pls data=data nfac=1 method=pcr;
   title "Principal Components Regression";
   model y = x1 x2;
proc pls data=data nfac=1 method=pls;
   title "Partial Least Squares Regression";
   model y = x1 x2;
run;
```

The amount of model and response variation explained by the first factor for each method is shown in Figure 51.7 through Figure 51.9.



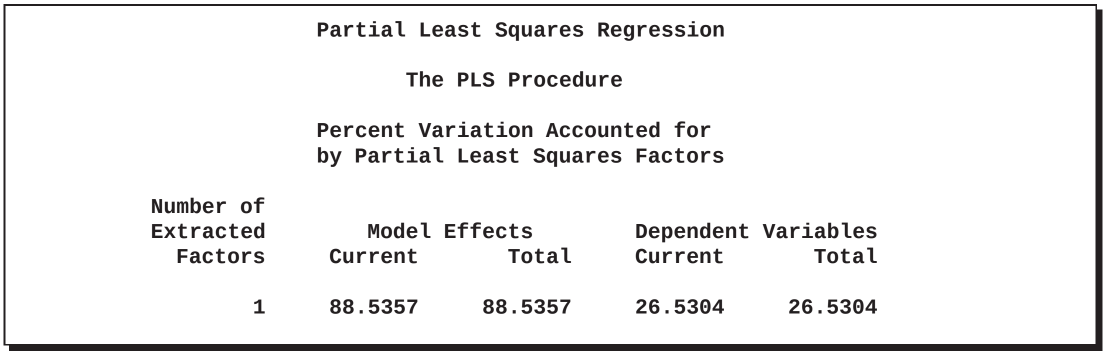
```
                 Reduced Rank Regression

                    The PLS Procedure

            Percent Variation Accounted for by
             Reduced Rank Regression Factors

Number of
Extracted        Model Effects        Dependent Variables
  Factors     Current       Total     Current       Total

        1     15.0661     15.0661    100.0000    100.0000
```

Figure 51.7. Variation Explained by First Reduced Rank Regression Factor



```
             Principal Components Regression

                    The PLS Procedure

 Percent Variation Accounted for by Principal Components

Number of
Extracted        Model Effects        Dependent Variables
  Factors     Current       Total     Current       Total

        1     92.9996     92.9996      9.3787      9.3787
```

Figure 51.8. Variation Explained by First Principal Components Regression Factor



```
             Partial Least Squares Regression

                    The PLS Procedure

             Percent Variation Accounted for
             by Partial Least Squares Factors

Number of
Extracted        Model Effects        Dependent Variables
  Factors     Current       Total     Current       Total

        1     88.5357     88.5357     26.5304     26.5304
```

Figure 51.9. Variation Explained by First Partial Least Squares Regression Factor

Notice that, while the first reduced rank regression factor explains *all* of the response variation, it accounts for only about 15% of the predictor variation. In contrast, the first principal components regression factor accounts for most of the predictor variation (93%) but only 9% of the response variation. The first partial least squares factor accounts for only slightly less predictor variation than principal components but about three times as much response variation.

Figure 51.10 illustrates how partial least squares balances the goals of explaining response and predictor variation in this case.

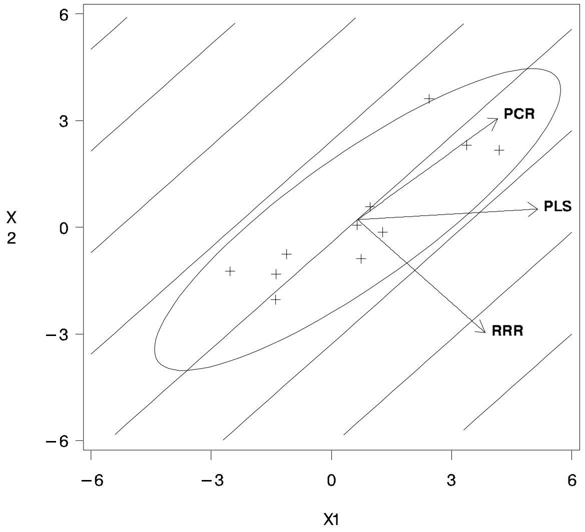


Figure 51.10. Depiction of First Factors for Three Different Regression Methods

The ellipse shows the general shape of the 11 observations in the predictor space, with the contours of increasing y overlaid. Also shown are the directions of the first factor for each of the three methods. Notice that, while the predictors vary most in the x1 = x2 direction, the response changes most in the orthogonal x1 = -x2 direction. This explains why the first principal component accounts for little variation in the response and why the first reduced rank regression factor accounts for little variation in the predictors. The direction of the first partial least squares factor represents a compromise between the other two directions.

Cross Validation

None of the regression methods implemented in the PLS procedure fit the observed data any better than ordinary least squares (OLS) regression; in fact, all of the methods approach OLS as more factors are extracted. The crucial point is that, when there are many predictors, OLS can *over-fit* the observed data; biased regression methods with fewer extracted factors can provide better predictability of *future* observations. However, as the preceding observations imply, the quality of the observed data fit cannot be used to choose the number of factors to extract; the number of extracted factors must be chosen on the basis of how well the model fits observations not involved in the modeling procedure itself.

One method of choosing the number of extracted factors is to fit the model to only part of the available data (the *training set*) and to measure how well models with different numbers of extracted factors fit the other part of the data (the *test set*). This is called *test set validation*. However, it is rare that you have enough data to make both parts large enough for pure test set validation to be useful. Alternatively, you can make several different divisions of the observed data into training set and test set. This is called *cross validation*, and there are several different types. In *one-at-a-time* cross validation, the first observation is held out as a single-element test set, with all other observations as the training set; next, the second observation is held out, then the third, and so on. Another method is to hold out successive blocks of observations as test sets, for example, observations 1 through 7, then observations 8 through 14, and so on; this is known as *blocked* validation. A similar method is *split-sample* cross validation, in which successive groups of widely separated observations are held out as the test set, for example, observations {1, 11, 21, . . . }, then observations {2, 12, 22, . . . }, and so on. Finally, test sets can be selected from the observed data randomly; this is known as *random sample* cross validation.

Which validation you should use depends on your data. Test set validation is preferred when you have enough data to make a division into a sizable training set and test set that represent the predictive population well. You can specify that the number of extracted factors be selected by test set validation by using the CV=TESTSET(*data set*) option, where *data set* is the name of the data set containing the test set. If you do not have enough data for test set validation, you can use one of the cross validation techniques. The most common technique is one-at-a-time validation (which you can specify with the CV=ONE option or just the CV option), unless the observed data is serially correlated, in which case either blocked or split-sample validation may be more appropriate (CV=BLOCK or CV=SPLIT); you can specify the size of the test sets in blocked or split-sample validation with a number in parentheses after the CV= option. Note that CV=ONE is the most computationally intensive of the cross validation methods, since it requires a recomputation of the PLS model for every input observation. Also, note that using random subset selection with CV=RANDOM may lead two different researchers to produce different PLS models on the same data (unless the same seed is used).

Whichever validation method you use, the number of factors chosen is usually the one that minimizes the predicted residual sum of squares (PRESS); this is the default choice if you specify any of the CV methods with PROC PLS. However, often models with fewer factors have PRESS statistics that are only marginally larger than the absolute minimum. To address this, van der Voet (1994) has proposed a statistical test for comparing the predicted residuals from different models; when you apply van der Voet's test, the number of factors chosen is the fewest with residuals that are insignificantly larger than the residuals of the model with minimum PRESS.

To see how van der Voet's test works, let $R_{i,jk}$ be the jth predicted residual for response k for the model with i extracted factors; the PRESS statistic is $\sum_{jk} R_{i,jk}^2$. Also, let $i_{\min}$ be the number of factors for which PRESS is minimized. The critical value for van der Voet's test is based on the differences between squared predicted residuals

$$D_{i,jk} \quad = \quad R^2_{i,jk} - R^2_{i_{\min},jk}$$

One alternative for the critical value is $C_i = \sum_{jk} D_{i,jk}$, which is just the difference between the PRESS statistics for i and $i_{\min}$ factors; alternatively, van der Voet suggests Hotelling's T^2 statistic $C_i = \mathbf{d}'_{i,\cdot} S_i^{-1} \mathbf{d}_{i,\cdot}$ where $\mathbf{d}_{i,\cdot}$ is the sum of the vectors $\mathbf{d}_{i,j} = \{D_{i,j1}, \ldots, D_{i,jN_y}\}'$ and S_i is the sum of squares and crossproducts matrix

$$S_i \quad = \quad \sum_j \mathbf{d}_{i,j} \mathbf{d}'_{i,j}$$

Virtually, the significance level for van der Voet's test is obtained by comparing C_i with the distribution of values that result from randomly exchanging $R^2_{i,jk}$ and $R^2_{i_{\min},jk}$. In practice, a Monte Carlo sample of such values is simulated and the significance level is approximated as the proportion of simulated critical values that are greater than C_i. If you apply van der Voet's test by specifying the CVTEST option, then, by default, the number of extracted factors chosen is the least number with an approximate significance level that is greater than 0.10.

Centering and Scaling

By default, the predictors and the responses are centered and scaled to have mean 0 and standard deviation 1. Centering the predictors and the responses ensures that the criterion for choosing successive factors is based on how much *variation* they explain, in either the predictors or the responses or both. (See the "Regression Methods" section on page 2705 for more details on how different methods explain variation.) Without centering, both the mean variable value and the variation around that mean are involved in selecting factors. Scaling serves to place all predictors and responses on an equal footing relative to their variation in the data. For example, if Time and Temp are two of the predictors, then scaling says that a change of $\mathrm{std}(\text{Time})$ in Time is roughly equivalent to a change of $\mathrm{std}(\text{Temp})$ in Temp.

Usually, both the predictors and responses should be centered and scaled. However, if their values already represent variation around a nominal or target value, then you can use the NOCENTER option in the PROC PLS statement to suppress centering. Likewise, if the predictors or responses are already all on comparable scales, then you can use the NOSCALE option to suppress scaling.

Note that, if the predictors involve crossproduct terms, then, by default, the variables are *not* standardized before standardizing the cross product. That is, if the ith values of two predictors are denoted x_i^1 and x_i^2, then the default standardized ith value of the cross product is

$$\frac{x_i^1 x_i^2 - \mathrm{mean}(x_j^1 x_j^2)}{\mathrm{std}(x_j^1 x_j^2)}$$

If you want the cross product to be based instead on standardized variables

$$\frac{x_i^1 - m^1}{s^1} \times \frac{x_i^2 - m^2}{s^2}$$

where $m^k = \mathrm{mean}(x_j^k)$ and $s^k = \mathrm{std}(x_j^k)$ for $k = 1, 2$, then you should use the VARSCALE option in the PROC PLS statement. Standardizing the variables separately is usually a good idea, but unless the model also contains all cross products nested within each term, the resulting model may not be equivalent to a simple linear model in the same terms. To see this, note that a model involving the cross product of two standardized variables

$$\frac{x_i^1 - m^1}{s^1} \times \frac{x_i^2 - m^2}{s^2} = x_i^1 x_i^2 \frac{1}{s^1 s^2} - x_i^1 \frac{m^2}{s^1 s^2} - x_i^2 \frac{m^1}{s^1 s^2} + \frac{m^1 m^2}{s^1 s^2}$$

involves both the crossproduct term and the linear terms for the unstandardized variables.

When cross validation is performed for the number of effects, there is some disagreement among practitioners as to whether each cross validation training set should be retransformed. By default, PROC PLS does so, but you can suppress this behavior by specifying the NOCVSTDIZE option in the PROC PLS statement.

Missing Values

PROC PLS handles missing values very simply. Observations with any missing independent variables (including all class variables) are excluded from the analysis, and no predictions are computed for such observations. Observations with no missing independent variables but any missing dependent variables are also excluded from the analysis, but predictions are computed.

Displayed Output

By default, PROC PLS displays just the amount of predictor and response variation accounted for by each factor.

If you perform a cross validation for the number of factors by specifying the CV option on the PROC PLS statement, then the procedure displays a summary of the cross validation for each number of factors, along with information about the optimal number of factors.

If you specify the DETAILS option on the PROC PLS statement, then details of the fitted model are displayed for each successive factor. These details include for each number of factors

- the predictor loadings
- the predictor weights
- the response weights
- the coded regression coefficients (for METHOD = SIMPLS, PCR, or RRR)

If you specify the CENSCALE option on the PROC PLS statement, then centering and scaling information for each response and predictor is displayed.

If you specify the VARSS option on the PROC PLS statement, the procedure displays, in addition to the average response and predictor sum of squares accounted for by each successive factor, the amount of variation accounted for in each response and predictor.

If you specify the SOLUTION option on the MODEL statement, then PROC PLS displays the coefficients of the final predictive model for the responses. The coefficients for predicting the centered and scaled responses based on the centered and scaled predictors are displayed, as well as the coefficients for predicting the raw responses based on the raw predictors.

ODS Table Names

PROC PLS assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information on ODS, see Chapter 15, "Using the Output Delivery System."

Table 51.1. ODS Tables Produced in PROC PLS

ODS Table Name	Description	Statement	Option
CVResults	Results of cross validation	PROC	CV
CenScaleParms	Parameter estimates for centered and scaled data	MODEL	SOLUTION
CodedCoef	Coded coefficients	PROC	DETAILS
ParameterEstimates	Parameter estimates for raw data	MODEL	SOLUTION
PercentVariation	Variation accounted for by each factor	PROC	default
ResidualSummary	Residual summary from cross validation	PROC	CV
XEffectCenScale	Centering and scaling information for predictor effects	PROC	CENSCALE
XLoadings	Loadings for independents	PROC	DETAILS
XVariableCenScale	Centering and scaling information for predictor variables	PROC	CENSCALE and VARSCALE
XWeights	Weights for independents	PROC	DETAILS
YVariableCenScale	Centering and scaling information for responses	PROC	CENSCALE
YWeights	Weights for dependents	PROC	DETAILS

Examples

Example 51.1. Examining Model Details

The following example, from Umetrics (1995), demonstrates different ways to examine a PLS model. The data come from the field of drug discovery. New drugs are developed from chemicals that are biologically active. Testing a compound for biological activity is an expensive procedure, so it is useful to be able to predict biological activity from cheaper chemical measurements. In fact, computational chemistry makes it possible to calculate certain chemical measurements without even making the compound. These measurements include size, lipophilicity, and polarity at various sites on the molecule. The following statements create a data set named penta, which contains these data.

```
data penta;
   input obsnam $ S1 L1 P1 S2 L2 P2
                  S3 L3 P3 S4 L4 P4
                  S5 L5 P5  log_RAI @@;
   n = _n_;
   datalines;
VESSK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
          1.9607 -1.6324  0.5746  1.9607 -1.6324  0.5746
          2.8369  1.4092 -3.1398                    0.00
VESAK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
          1.9607 -1.6324  0.5746  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    0.28
VEASK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
          0.0744 -1.7333  0.0902  1.9607 -1.6324  0.5746
          2.8369  1.4092 -3.1398                    0.20
VEAAK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
          0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    0.51
VKAAK    -2.6931 -2.5271 -1.2871  2.8369  1.4092 -3.1398
          0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    0.11
VEWAK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
         -4.7548  3.6521  0.8524  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    2.73
VEAAP    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
          0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
         -1.2201  0.8829  2.2253                    0.18
VEHAK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
          2.4064  1.7438  1.1057  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    1.53
VAAAK    -2.6931 -2.5271 -1.2871  0.0744 -1.7333  0.0902
          0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                   -0.10
GEAAK     2.2261 -5.3648  0.3049  3.0777  0.3891 -0.0701
          0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                   -0.52
LEAAK    -4.1921 -1.0285 -0.9801  3.0777  0.3891 -0.0701
          0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    0.40
FEAAK    -4.9217  1.2977  0.4473  3.0777  0.3891 -0.0701
          0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    0.30
VEGGK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
          2.2261 -5.3648  0.3049  2.2261 -5.3648  0.3049
          2.8369  1.4092 -3.1398                   -1.00
VEFAK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
         -4.9217  1.2977  0.4473  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    1.57
VELAK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
         -4.1921 -1.0285 -0.9801  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    0.59
AAAAA     0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
          0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
          0.0744 -1.7333  0.0902                   -0.10
AAYAA     0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
         -1.3944  2.3230  0.0139  0.0744 -1.7333  0.0902
          0.0744 -1.7333  0.0902                    0.46
AAWAA     0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
         -4.7548  3.6521  0.8524  0.0744 -1.7333  0.0902
          0.0744 -1.7333  0.0902                    0.75
VAWAA    -2.6931 -2.5271 -1.2871  0.0744 -1.7333  0.0902
         -4.7548  3.6521  0.8524  0.0744 -1.7333  0.0902
          0.0744 -1.7333  0.0902                    1.43
VAWAK    -2.6931 -2.5271 -1.2871  0.0744 -1.7333  0.0902
         -4.7548  3.6521  0.8524  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    1.45
VKWAA    -2.6931 -2.5271 -1.2871  2.8369  1.4092 -3.1398
         -4.7548  3.6521  0.8524  0.0744 -1.7333  0.0902
          0.0744 -1.7333  0.0902                    1.71
VWAAK    -2.6931 -2.5271 -1.2871 -4.7548  3.6521  0.8524
          0.0744 -1.7333  0.0902  0.0744 -1.7333  0.0902
          2.8369  1.4092 -3.1398                    0.04
VAAWK    -2.6931 -2.5271 -1.2871  0.0744 -1.7333  0.0902
          0.0744 -1.7333  0.0902 -4.7548  3.6521  0.8524
          2.8369  1.4092 -3.1398                    0.23
EKWAP     3.0777  0.3891 -0.0701  2.8369  1.4092 -3.1398
         -4.7548  3.6521  0.8524  0.0744 -1.7333  0.0902
         -1.2201  0.8829  2.2253                    1.30
VKWAP    -2.6931 -2.5271 -1.2871  2.8369  1.4092 -3.1398
         -4.7548  3.6521  0.8524  0.0744 -1.7333  0.0902
         -1.2201  0.8829  2.2253                    2.35
RKWAP     2.8827  2.5215 -3.4435  2.8369  1.4092 -3.1398
         -4.7548  3.6521  0.8524  0.0744 -1.7333  0.0902
         -1.2201  0.8829  2.2253                    1.98
VEWVK    -2.6931 -2.5271 -1.2871  3.0777  0.3891 -0.0701
         -4.7548  3.6521  0.8524 -2.6931 -2.5271 -1.2871
          2.8369  1.4092 -3.1398                    1.71
PGFSP    -1.2201  0.8829  2.2253  2.2261 -5.3648  0.3049
         -4.9217  1.2977  0.4473  1.9607 -1.6324  0.5746
         -1.2201  0.8829  2.2253                    0.90
FSPFR    -4.9217  1.2977  0.4473  1.9607 -1.6324  0.5746
         -1.2201  0.8829  2.2253 -4.9217  1.2977  0.4473
```

```
          2.8827  2.5215 -3.4435                    0.64
RYLPT     2.8827  2.5215 -3.4435 -1.3944  2.3230  0.0139
         -4.1921 -1.0285 -0.9801 -1.2201  0.8829  2.2253
          0.9243 -2.0921 -1.3996                    0.40
GGGGG     2.2261 -5.3648  0.3049  2.2261 -5.3648  0.3049
          2.2261 -5.3648  0.3049  2.2261 -5.3648  0.3049
          2.2261 -5.3648  0.3049                     .
;
data ptrain; set penta; if (n <= 15);
data ptest ; set penta; if (n >  15);
run;
```

You would like to study the relationship between these measurements and the activity of the compound, represented by the logarithm of the relative Bradykinin activating activity (log_RAI). Notice that these data consist of many predictors relative to the number of observations. Partial least squares is especially appropriate in this situation as a useful tool for finding a few underlying predictive factors that account for most of the variation in the response. Typically, the model is fit for part of the data (the “training” or “work” set), and the quality of the fit is judged by how well it predicts the other part of the data (the “test” or “prediction” set). For this example, the first 15 observations serve as the training set and the rest constitute the test set (refer to Ufkes et al. 1978, 1982).

When you fit a PLS model, you hope to find a few PLS factors that explain most of the variation in both predictors and responses. Factors that explain response variation provide good predictive models for new responses, and factors that explain predictor variation are well represented by the observed values of the predictors. The following statements fit a PLS model with two factors and save predicted values, residuals, and other information for each data point in a data set named outpls.

```
proc pls data=ptrain nfac=2;
   model log_RAI = S1-S5 L1-L5 P1-P5;
   output out=outpls predicted = yhat1
                     yresidual = yres1
                     xresidual = xres1-xres15
                     xscore    = xscr
                     yscore    = yscr;
run;
```

The PLS procedure displays a table, shown in Output 51.1.1, showing how much predictor and response variation is explained by each PLS factor.

Output 51.1.1. Amount of Training Set Variation Explained

```
                              The PLS Procedure

                       Percent Variation Accounted for
                       by Partial Least Squares Factors

          Number of
          Extracted        Model Effects        Dependent Variables
            Factors     Current       Total     Current       Total

                  1     16.9014     16.9014     89.6399     89.6399
                  2     12.7721     29.6735      7.8368     97.4767
```

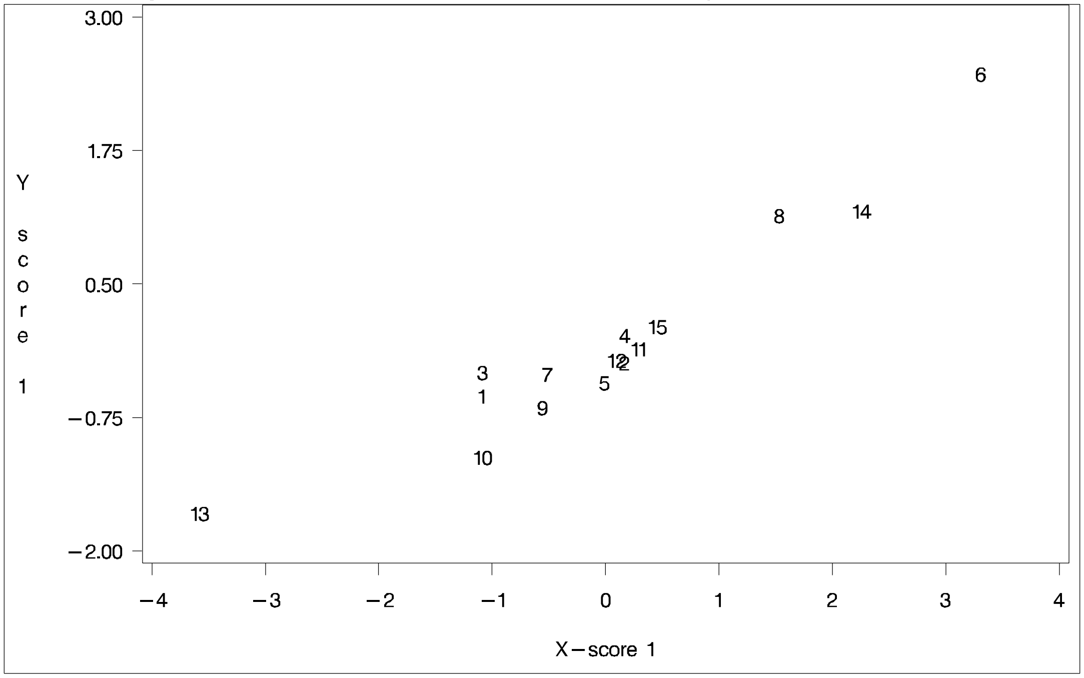
From Output 51.1.1, note that 97% of the response variation is already explained, but only 29% of the predictor variation is explained.

Partial least squares algorithms choose successive orthogonal factors that maximize the covariance between each X-score and the corresponding Y-score. For a good PLS model, the first few factors show a high correlation between the X- and Y-scores. The correlation usually decreases from one factor to the next. You can plot the X-scores versus the Y-scores for the first PLS factor using the following SAS statements.

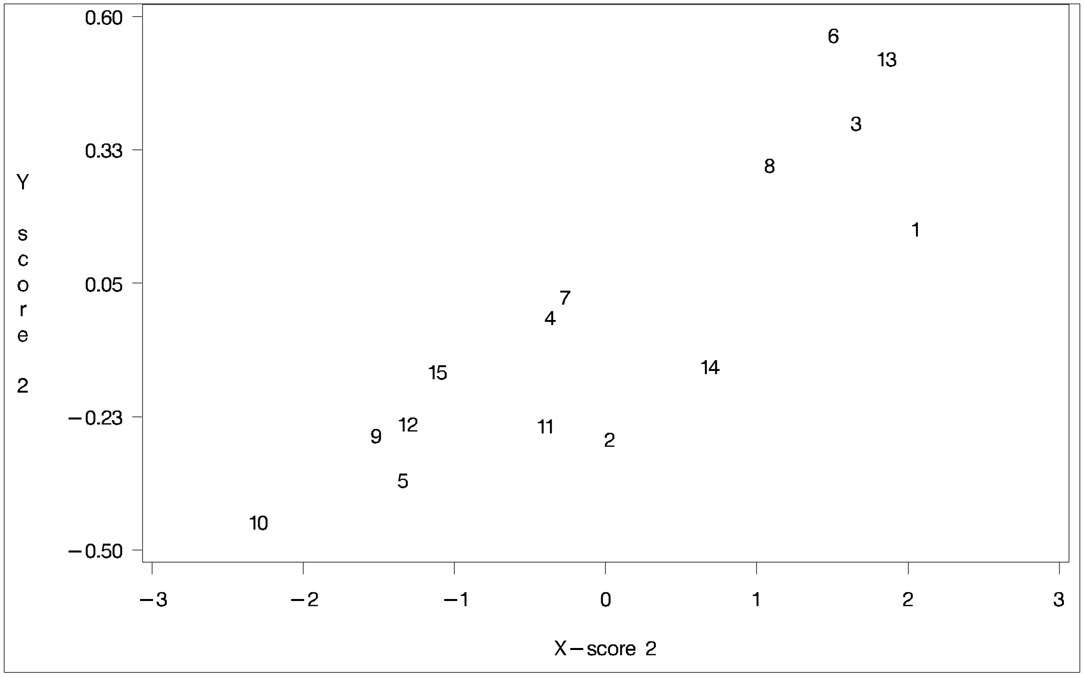
```
%let ifac = 1;
data pltanno; set outpls;
   length text $ 2;
   retain function ’label’ position ’5’ hsys ’3’ xsys ’2’ ysys ’2’
          color ’blue’ style ’swissb’;
   text=%str(n); x=xscr&ifac; y=yscr&ifac;
axis1 label=(angle=270 rotate=90 "Y score &ifac")
      major=(number=5) minor=none;
axis2 label=("X-score &ifac") minor=none;
symbol1 v=none i=none;
proc gplot data=outpls;
   plot yscr&ifac*xscr&ifac=1
      / anno=pltanno vaxis=axis1 haxis=axis2 frame cframe=ligr;
run;
```

By changing the macro variable ifac to 2 instead of 1, you can use the same statements to plot the X-scores versus the Y-scores for the second PLS factor. The resulting plots are shown in Output 51.1.2 and Output 51.1.3. The numbers on the plot represent the observation number in the penta data set.

Output 51.1.2. First X- and Y-scores for Penta-Peptide Model 1



Output 51.1.3. Second X- and Y-scores for Penta-Peptide Model 1



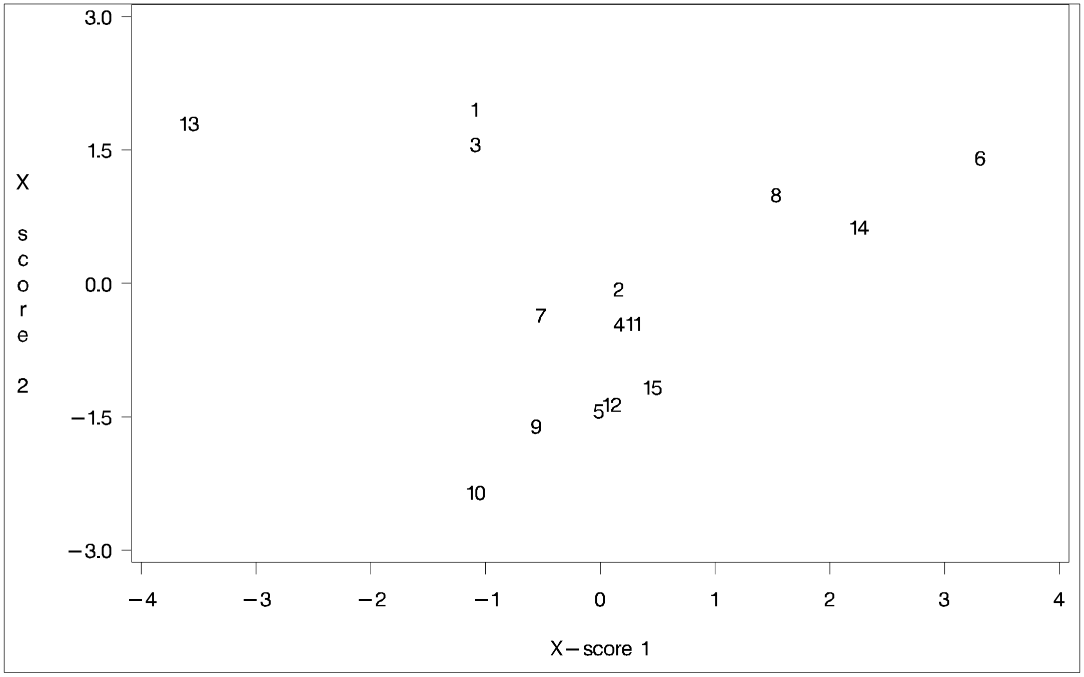
For this example, the figures show high correlation between X- and Y-scores for the first factor but somewhat lower correlation for the second factor.

You can also plot the X-scores against each other to look for irregularities in the data. You should look for patterns or clearly grouped observations. If you see a curved pattern, for example, you may want to add a quadratic term. Two or more groupings of observations indicate that it might be better to analyze the groups separately, perhaps by including classification effects in the model. The following SAS statements produce a plot of the first and second X-scores:

```
data pltanno; set outpls;
   length text $ 2;
   retain function 'label' position '5' hsys '3' xsys '2' ysys '2'
          color 'blue' style 'swissb';
   text=%str(n); x=xscr1; y=xscr2;
axis1 label=(angle=270 rotate=90 "X score 2")
      major=(number=5) minor=none;
axis2 label=("X-score 1") minor=none;
symbol1 v=none i=none;
proc gplot data=outpls;
   plot xscr2*xscr1=1
      / anno=pltanno vaxis=axis1 haxis=axis2 frame cframe=ligr;
run;
```

The plot is shown in Output 51.1.4.

Output 51.1.4. First and Second X-scores for Penta-Peptide Model 1



This plot appears to show most of the observations close together, with a few being more spread out with larger positive X-scores for factor 2. There are no clear grouping patterns, but observation 13 stands out; note that this observation is the most extreme on all three plots so far. This run may be overly influential in the PLS analysis; thus, you should check to make sure it is reliable.

Plots of the weights give the directions toward which each PLS factor projects. They show which predictors are most represented in each factor. Those predictors with small weights in absolute value are less important than those with large weights.

You can use the DETAILS option in the PROC PLS statement to display various model details, including the X-weights. You can then use the ODS statement to send the weights to an output data set, as follows:

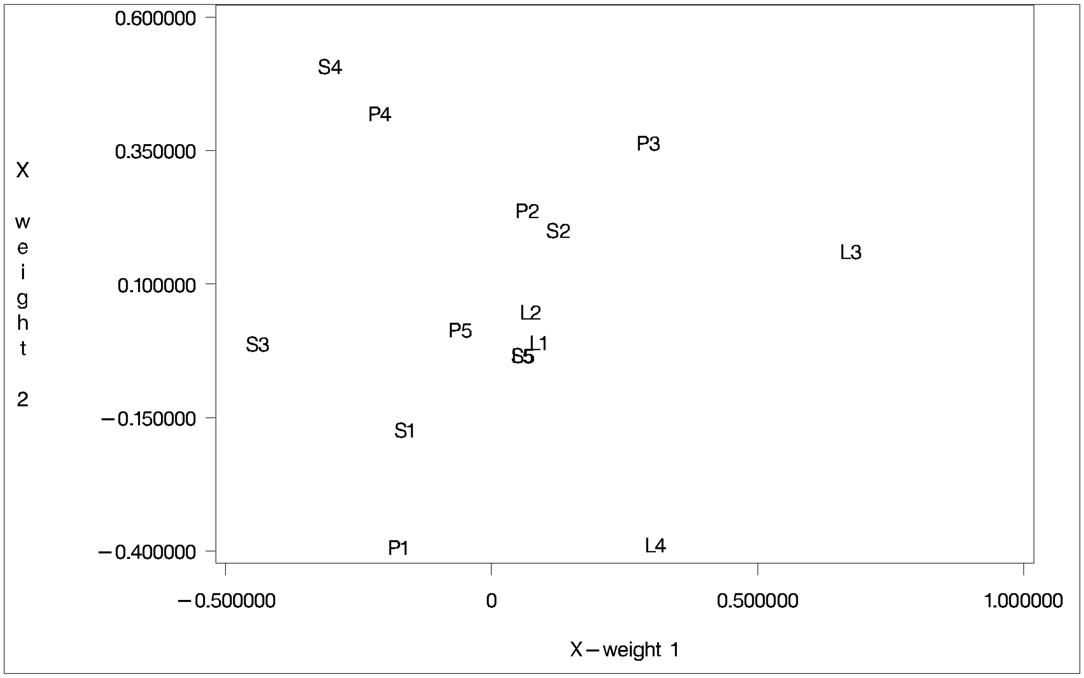
```
ods output XWeights=xweights;
proc pls data=ptrain nfac=2 details;
   model log_RAI = S1-S5 L1-L5 P1-P5;
run;
```

Once the X-weights are in a data set, you can use the following statements to plot the weights for the first two PLS factors against one another:

```
proc transpose data=xweights(drop=NumberOfFactors InnerRegCoef)
               out =xweights;
data xweights; set xweights;
   rename col1=w1 col2=w2;
data wt_anno; set xweights;
   length text $ 2;
   retain function ’label’
          position ’5’
          hsys     ’3’
          xsys     ’2’
          ysys     ’2’
          color    ’blue’
          style    ’swissb’;
   text=%str(_name_); x=w1; y=w2;
run;

axis1 label=(angle=270 rotate=90 "X weight 2")
      major=(number=5) minor=none;
axis2 label=("X-weight 1") minor=none;
symbol1 v=none i=none;
proc gplot data=xweights;
   plot w2*w1=1 / anno=wt_anno vaxis=axis1
                  haxis=axis2 frame cframe=ligr;
run; quit;
```

The plot of the X-weights is shown in Output 51.1.5.

Output 51.1.5. First and Second X-weights for Penta-Peptide Model 1



The weights plot shows a cluster of X-variables that are weighted at nearly zero for both factors. These variables add little to the model fit, and removing them may improve the model's predictive capability.

To explore further which predictors can be eliminated from the analysis, you can look at the regression coefficients for the standardized data. Predictors with small coefficients (in absolute value) make a small contribution to the response prediction. Another statistic summarizing the contribution a variable makes to the model is the *Variable Importance for Projection* (VIP) of Wold (1994). Whereas the regression coefficients represent the importance each predictor has in the prediction of just the response, the VIP represents the value of each predictor in fitting the PLS model for both predictors and response. If a predictor has a relatively small coefficient (in absolute value) *and* a small value of VIP, then it is a prime candidate for deletion. Wold (1994) considers a value less than 0.8 to be "small" for the VIP. The following statements produce coefficients and the VIP.

```
/*
/  Put coefficients, weights, and R**2’s into data sets.
/-------------------------------------------------------*/
ods listing close;
ods output PercentVariation  = pctvar
           XWeights          = xweights
           CenScaleParms     = solution;
proc pls data=ptrain nfac=2 details;
   model log_RAI = S1 L1 P1
                   S2 L2 P2
                   S3 L3 P3
                   S4 L4 P4
                   S5 L5 P5 / solution;
run;
ods listing;

/*
/  Just reformat the coefficients.
/-------------------------------------------------------*/
data solution; set solution;
   format log_RAI 8.5;
   if (RowName = ’Intercept’) then delete;
   rename RowName = Predictor log_RAI = B;
run;

/*
/  Transpose weights and R**2’s.
/-------------------------------------------------------*/
data xweights; set xweights; _name_=’W’||trim(left(_n_));
data pctvar  ; set pctvar  ; _name_=’R’||trim(left(_n_));
proc transpose data=xweights(drop=NumberOfFactors InnerRegCoef)
               out =xweights;
proc transpose data=pctvar(keep=_name_ CurrentYVariation)
               out =pctvar;
run;

/*
/  Sum the squared weights times the normalized R**2’s.
/  The VIP is defined as the square root of this
/  weighted average times the number of predictors.
/-------------------------------------------------------*/

proc sql;
   create table vip as
      select *
         from xweights left join pctvar(drop=_name_) on 1;
data vip; set vip; keep _name_ vip;
   array w{2};
   array r{2};
   VIP = 0;
   do i = 1 to 2;
      VIP = VIP + r{i}*(w{i}**2)/sum(of r1-r2);
      end;
   VIP = sqrt(VIP * 15);
```

```
data vipbpls; merge solution vip(drop=_name_);
proc print data=vipbpls;
run;
```

The output appears in Output 51.1.6.

Output 51.1.6. Estimated PLS Regression Coefficients and VIP (Model 1)

```
              Obs    Predictor          B       VIP

                1       S1        -0.13831    0.63084
                2       L1         0.05720    0.32874
                3       P1        -0.19064    0.77412
                4       S2         0.12383    0.52061
                5       L2         0.05909    0.28007
                6       P2         0.09361    0.36941
                7       S3        -0.28415    1.62992
                8       L3         0.47131    2.51518
                9       P3         0.26613    1.16839
               10       S4        -0.09145    1.26075
               11       L4         0.12265    1.21771
               12       P4        -0.04878    0.91090
               13       S5         0.03320    0.21989
               14       L5         0.03320    0.21989
               15       P5        -0.03320    0.21989
```

For this data set, the variables L1, L2, P2, P4, S5, L5, and P5 have small absolute coefficients and small VIP. Looking back at the weights plot in Output 51.1.5, you can see that these variables tend to be the ones near zero for both PLS factors. You should consider dropping these variables from the model.

Example 51.2. Examining Outliers

This example is a continuation of Example 51.1 on page 2714.

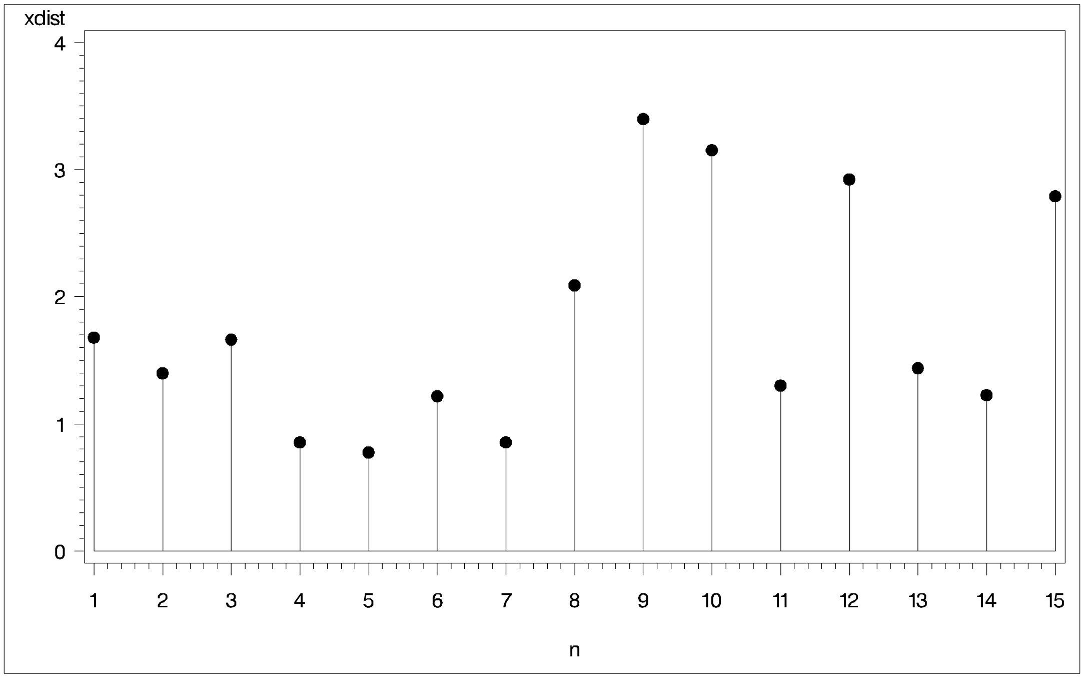
A PLS model effectively models both the predictors and the responses. In order to check for outliers, you should, therefore, look at the Euclidean distance from each point to the PLS model in both the standardized predictors and the standardized responses. No point should be dramatically farther from the model than the rest. If there is a group of points that are all farther from the model than the rest, they may have something in common, in which case they should be analyzed separately. The following statements compute and plot these distances to the reduced model, dropping variables L1, L2, P2, P4, S5, L5, and P5:

```
proc pls data=ptrain nfac=2 noprint;
   model log_RAI = S1    P1
                   S2
                   S3 L3 P3
                   S4 L4   ;
   output out=stdres stdxsse=stdxsse
                     stdysse=stdysse;
data stdres; set stdres;
   xdist = sqrt(stdxsse);
   ydist = sqrt(stdysse);
run;
```

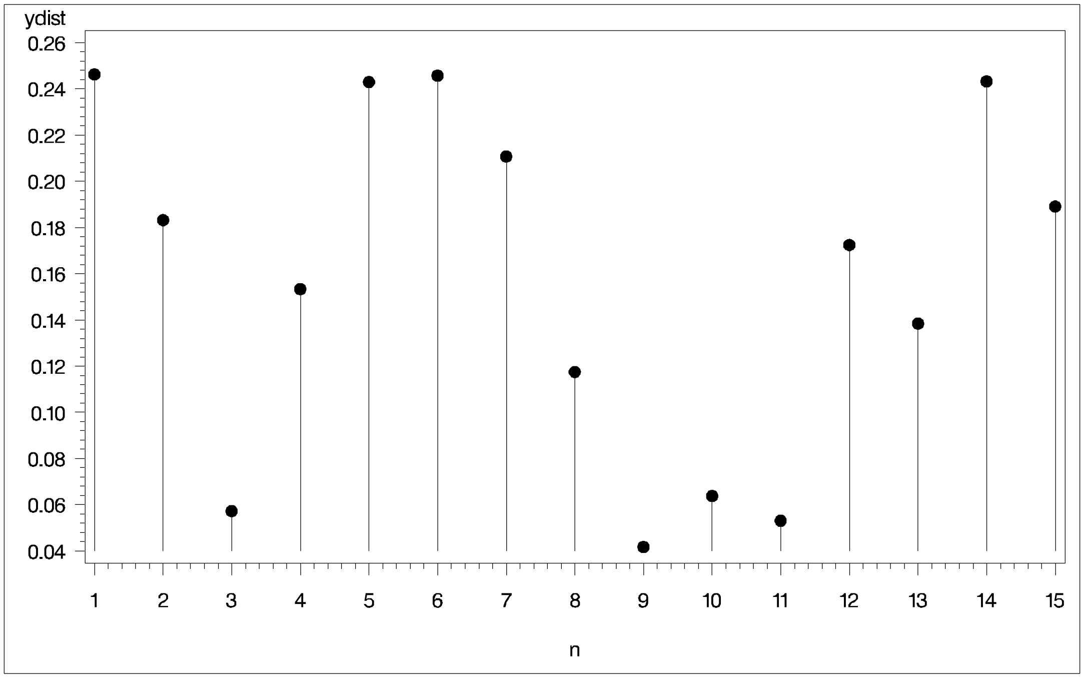
```
symbol1 i=needles v=dot c=blue;
proc gplot data=stdres;
   plot xdist*n=1 / cframe=ligr;
proc gplot data=stdres;
   plot ydist*n=1 / cframe=ligr;
run;
```

The plots are shown in Output 51.2.1 and Output 51.2.2.

Output 51.2.1. Distances from the X-variables to the Model (Training Set)



Output 51.2.2. Distances from the Y-variables to the Model (Training Set)

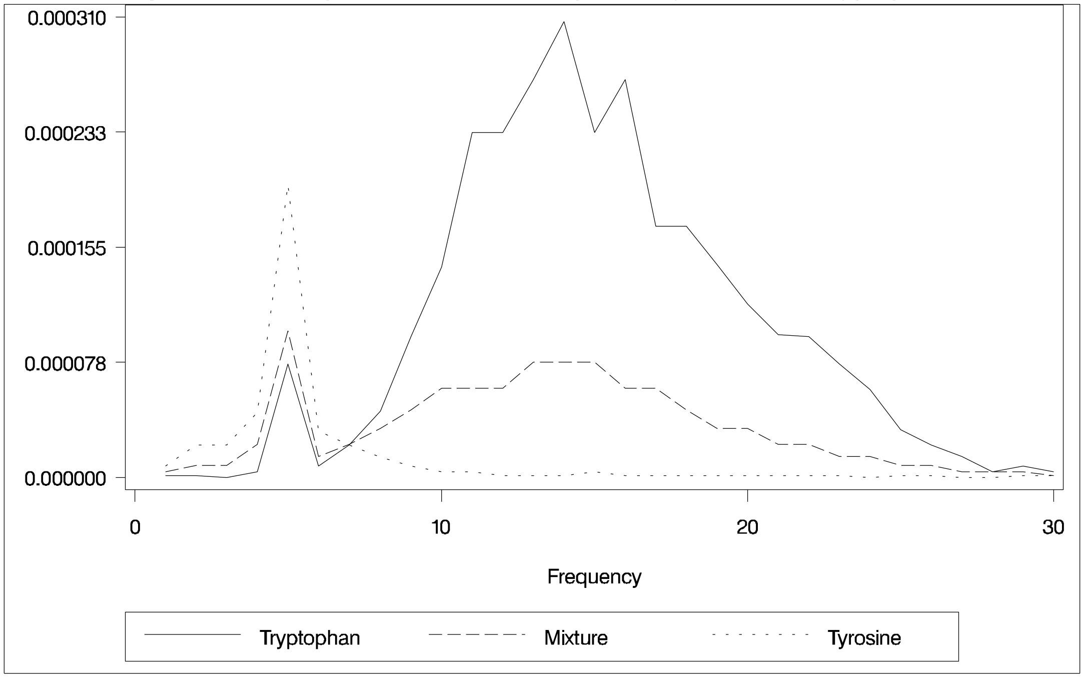


There appear to be no profound outliers in either the predictor space or the response space.

Example 51.3. Choosing a PLS Model by Test Set Validation

The following example demonstrates issues in spectrometric calibration. The data (Umetrics 1995) consist of spectrographic readings on 33 samples containing known concentrations of two amino acids, tyrosine and tryptophan. The spectra are measured at 30 frequencies across the overall range of frequencies. For example, Figure 51.3.1 shows the observed spectra for three samples, one with only tryptophan, one with only tyrosine, and one with a mixture of the two, all at a total concentration of 10^{-6}.

Output 51.3.1. Spectra for Three Samples of Tyrosine and Tryptophan



Of the 33 samples, 18 are used as a training set and 15 as a test set. The data originally appear in McAvoy et al. (1989).

These data were created in a lab, with the concentrations fixed in order to provide a wide range of applicability for the model. You want to use a linear function of the logarithms of the spectra to predict the logarithms of tyrosine and tryptophan concentration, as well as the logarithm of the total concentration. Actually, because of the possibility of zeros in both the responses and the predictors, slightly different transformations are used. The following statements create SAS data sets containing the training and test data, named ftrain and ftest, respectively:

```
data ftrain;
   input obsnam $ tot tyr f1-f30 @@;
   try = tot - tyr;
   if (tyr) then tyr_log = log10(tyr); else tyr_log = -8;
   if (try) then try_log = log10(try); else try_log = -8;
   tot_log = log10(tot);
   datalines;
17mix35 0.00003 0
 -6.215 -5.809 -5.114 -3.963 -2.897 -2.269 -1.675 -1.235
 -0.900 -0.659 -0.497 -0.395 -0.335 -0.315 -0.333 -0.377
 -0.453 -0.549 -0.658 -0.797 -0.878 -0.954 -1.060 -1.266
 -1.520 -1.804 -2.044 -2.269 -2.496 -2.714
19mix35 0.00003 3E-7
 -5.516 -5.294 -4.823 -3.858 -2.827 -2.249 -1.683 -1.218
 -0.907 -0.658 -0.501 -0.400 -0.345 -0.323 -0.342 -0.387
 -0.461 -0.554 -0.665 -0.803 -0.887 -0.960 -1.072 -1.272
 -1.541 -1.814 -2.058 -2.289 -2.496 -2.712
21mix35 0.00003 7.5E-7
 -5.519 -5.294 -4.501 -3.863 -2.827 -2.280 -1.716 -1.262
 -0.939 -0.694 -0.536 -0.444 -0.384 -0.369 -0.377 -0.421
 -0.495 -0.596 -0.706 -0.824 -0.917 -0.988 -1.103 -1.294
 -1.565 -1.841 -2.084 -2.320 -2.521 -2.729
23mix35 0.00003 1.5E-6
 -5.294 -4.705 -4.262 -3.605 -2.726 -2.239 -1.681 -1.250
 -0.925 -0.697 -0.534 -0.437 -0.381 -0.359 -0.369 -0.426
 -0.499 -0.591 -0.701 -0.843 -0.925 -0.989 -1.109 -1.310
 -1.579 -1.852 -2.090 -2.316 -2.521 -2.743
25mix35 0.00003 3E-6
 -4.600 -4.069 -3.764 -3.262 -2.598 -2.191 -1.680 -1.273
 -0.958 -0.729 -0.573 -0.470 -0.422 -0.407 -0.422 -0.468
 -0.538 -0.639 -0.753 -0.887 -0.968 -1.037 -1.147 -1.357
 -1.619 -1.886 -2.141 -2.359 -2.585 -2.792
27mix35 0.00003 7.5E-6
 -3.812 -3.376 -3.026 -2.726 -2.249 -1.919 -1.541 -1.198
 -0.951 -0.764 -0.639 -0.570 -0.528 -0.525 -0.550 -0.606
 -0.689 -0.781 -0.909 -1.031 -1.126 -1.191 -1.303 -1.503
 -1.784 -2.058 -2.297 -2.507 -2.727 -2.970
29mix35 0.00003 0.000015
 -3.053 -2.641 -2.382 -2.194 -1.977 -1.913 -1.728 -1.516
 -1.317 -1.158 -1.029 -0.963 -0.919 -0.915 -0.933 -0.981
 -1.055 -1.157 -1.271 -1.409 -1.505 -1.546 -1.675 -1.880
 -2.140 -2.415 -2.655 -2.879 -3.075 -3.319
28mix35 0.00003 0.0000225
 -2.626 -2.248 -2.004 -1.839 -1.742 -1.791 -1.786 -1.772
 -1.728 -1.666 -1.619 -1.591 -1.575 -1.580 -1.619 -1.671
 -1.754 -1.857 -1.982 -2.114 -2.210 -2.258 -2.379 -2.570
 -2.858 -3.117 -3.347 -3.568 -3.764 -4.012
26mix35 0.00003 0.000027
 -2.370 -1.990 -1.754 -1.624 -1.560 -1.655 -1.772 -1.899
 -1.982 -2.074 -2.157 -2.211 -2.267 -2.317 -2.369 -2.460
 -2.545 -2.668 -2.807 -2.951 -3.030 -3.075 -3.214 -3.376
 -3.685 -3.907 -4.129 -4.335 -4.501 -4.599
24mix35 0.00003 0.0000285
 -2.326 -1.952 -1.702 -1.583 -1.507 -1.629 -1.771 -1.945
 -2.115 -2.297 -2.448 -2.585 -2.696 -2.808 -2.913 -3.030
 -3.163 -3.265 -3.376 -3.534 -3.642 -3.721 -3.858 -4.012
 -4.262 -4.501 -4.704 -4.822 -4.956 -5.292
22mix35 0.00003 0.00002925
 -2.277 -1.912 -1.677 -1.556 -1.487 -1.630 -1.791 -1.969
 -2.203 -2.437 -2.655 -2.844 -3.032 -3.214 -3.378 -3.503
 -3.646 -3.812 -3.958 -4.129 -4.193 -4.262 -4.415 -4.501
 -4.823 -5.111 -5.113 -5.294 -5.290 -5.294
20mix35 0.00003 0.0000297
 -2.266 -1.912 -1.688 -1.546 -1.500 -1.640 -1.801 -2.011
 -2.277 -2.545 -2.823 -3.094 -3.376 -3.572 -3.812 -4.012
 -4.262 -4.415 -4.501 -4.705 -4.823 -4.823 -4.956 -5.111
 -5.111 -5.516 -5.524 -5.806 -5.806 -5.806
18mix35 0.00003 0.00003
```

```
 -2.258 -1.900 -1.666 -1.524 -1.479 -1.621 -1.803 -2.043
 -2.308 -2.626 -2.895 -3.214 -3.568 -3.907 -4.193 -4.423
 -4.825 -5.111 -5.111 -5.516 -5.516 -5.516 -5.516 -5.806
 -5.806 -5.806 -5.806 -5.806 -6.210 -6.215
trp2    0.0001 0
 -5.922 -5.435 -4.366 -3.149 -2.124 -1.392 -0.780 -0.336
 -0.002  0.233  0.391  0.490  0.540  0.563  0.541  0.488
  0.414  0.313  0.203  0.063 -0.028 -0.097 -0.215 -0.411
 -0.678 -0.953 -1.208 -1.418 -1.651 -1.855
mix5    0.0001 0.00001
 -3.932 -3.411 -2.964 -2.462 -1.836 -1.308 -0.796 -0.390
 -0.076  0.147  0.294  0.394  0.446  0.460  0.443  0.389
  0.314  0.220  0.099 -0.033 -0.128 -0.197 -0.308 -0.506
 -0.785 -1.050 -1.313 -1.529 -1.745 -1.970
mix4    0.0001 0.000025
 -2.996 -2.479 -2.099 -1.803 -1.459 -1.126 -0.761 -0.424
 -0.144  0.060  0.195  0.288  0.337  0.354  0.330  0.274
  0.206  0.105 -0.009 -0.148 -0.242 -0.306 -0.424 -0.626
 -0.892 -1.172 -1.425 -1.633 -1.877 -2.071
mix3    0.0001 0.00005
 -2.128 -1.661 -1.344 -1.160 -0.996 -0.877 -0.696 -0.495
 -0.313 -0.165 -0.042  0.032  0.069  0.079  0.050 -0.006
 -0.082 -0.179 -0.295 -0.436 -0.523 -0.584 -0.706 -0.898
 -1.178 -1.446 -1.696 -1.922 -2.128 -2.350
mix6    0.0001 0.00009
 -1.140 -0.757 -0.497 -0.362 -0.329 -0.412 -0.513 -0.647
 -0.772 -0.877 -0.958 -1.040 -1.104 -1.162 -1.233 -1.317
 -1.425 -1.543 -1.661 -1.804 -1.877 -1.959 -2.034 -2.249
 -2.502 -2.732 -2.964 -3.142 -3.313 -3.576
;

data ftest;
   input obsnam $ tot tyr f1-f30 @@;
   try = tot - tyr;
   if (tyr) then tyr_log = log10(tyr); else tyr_log = -8;
   if (try) then try_log = log10(try); else try_log = -8;
   tot_log = log10(tot);
   datalines;
43trp6  1E-6 0
 -5.915 -5.918 -6.908 -5.428 -4.117 -5.103 -4.660 -4.351
 -4.023 -3.849 -3.634 -3.634 -3.572 -3.513 -3.634 -3.572
 -3.772 -3.772 -3.844 -3.932 -4.017 -4.023 -4.117 -4.227
 -4.492 -4.660 -4.855 -5.428 -5.103 -5.428
59mix6  1E-6 1E-7
 -5.903 -5.903 -5.903 -5.082 -4.213 -5.083 -4.838 -4.639
 -4.474 -4.213 -4.001 -4.098 -4.001 -4.001 -3.907 -4.001
 -4.098 -4.098 -4.206 -4.098 -4.213 -4.213 -4.335 -4.474
 -4.639 -4.838 -4.837 -5.085 -5.410 -5.410
51mix6  1E-6 2.5E-7
 -5.907 -5.907 -5.415 -4.843 -4.213 -4.843 -4.843 -4.483
 -4.343 -4.006 -4.006 -3.912 -3.830 -3.830 -3.755 -3.912
 -4.006 -4.001 -4.213 -4.213 -4.335 -4.483 -4.483 -4.642
 -4.841 -5.088 -5.088 -5.415 -5.415 -5.415
49mix6  1E-6 5E-7
 -5.419 -5.091 -5.091 -4.648 -4.006 -4.846 -4.648 -4.483
 -4.343 -4.220 -4.220 -4.220 -4.110 -4.110 -4.110 -4.220
 -4.220 -4.343 -4.483 -4.483 -4.650 -4.650 -4.846 -4.846
 -5.093 -5.091 -5.419 -5.417 -5.417 -5.907
53mix6  1E-6 7.5E-7
```

```
 -5.083 -4.837 -4.837 -4.474 -3.826 -4.474 -4.639 -4.838
 -4.837 -4.639 -4.639 -4.641 -4.641 -4.639 -4.639 -4.837
 -4.838 -4.838 -5.083 -5.082 -5.083 -5.410 -5.410 -5.408
 -5.408 -5.900 -5.410 -5.903 -5.900 -6.908
57mix6  1E-6 9E-7
 -5.082 -4.836 -4.639 -4.474 -3.826 -4.636 -4.638 -4.638
 -4.837 -5.082 -5.082 -5.408 -5.082 -5.080 -5.408 -5.408
 -5.408 -5.408 -5.408 -5.408 -5.408 -5.900 -5.900 -5.900
 -5.900 -5.900 -5.900 -5.900 -6.908 -6.908
41tyro6 1E-6 1E-6
 -5.104 -4.662 -4.662 -4.358 -3.705 -4.501 -4.662 -4.859
 -5.104 -5.431 -5.433 -5.918 -5.918 -5.918 -5.431 -5.918
 -5.918 -5.918 -5.918 -5.918 -5.918 -5.918 -5.918 -6.908
 -5.918 -5.918 -6.908 -6.908 -5.918 -5.918
28trp5  0.00001 0
 -5.937 -5.937 -5.937 -4.526 -3.544 -3.170 -2.573 -2.115
 -1.792 -1.564 -1.400 -1.304 -1.244 -1.213 -1.240 -1.292
 -1.373 -1.453 -1.571 -1.697 -1.801 -1.873 -2.008 -2.198
 -2.469 -2.706 -2.990 -3.209 -3.384 -3.601
37mix5  0.00001 1E-6
 -5.109 -4.865 -4.501 -4.029 -3.319 -3.070 -2.569 -2.207
 -1.895 -1.684 -1.516 -1.423 -1.367 -1.348 -1.374 -1.415
 -1.503 -1.596 -1.718 -1.839 -1.927 -1.997 -2.118 -2.333
 -2.567 -2.874 -3.106 -3.313 -3.579 -3.781
33mix5  0.00001 2.5E-6
 -4.366 -4.129 -3.781 -3.467 -3.037 -2.939 -2.593 -2.268
 -1.988 -1.791 -1.649 -1.565 -1.520 -1.509 -1.524 -1.580
 -1.665 -1.758 -1.882 -2.037 -2.090 -2.162 -2.284 -2.465
 -2.761 -3.037 -3.270 -3.520 -3.709 -3.937
31mix5  0.00001 5E-6
 -3.790 -3.373 -3.119 -2.915 -2.671 -2.718 -2.555 -2.398
 -2.229 -2.085 -1.971 -1.902 -1.860 -1.837 -1.881 -1.949
 -2.009 -2.127 -2.230 -2.381 -2.455 -2.513 -2.624 -2.827
 -3.117 -3.373 -3.586 -3.785 -4.040 -4.366
35mix5  0.00001 7.5E-6
 -3.321 -2.970 -2.765 -2.594 -2.446 -2.548 -2.616 -2.617
 -2.572 -2.550 -2.508 -2.487 -2.488 -2.487 -2.529 -2.593
 -2.688 -2.792 -2.908 -3.037 -3.149 -3.189 -3.273 -3.467
 -3.781 -4.029 -4.241 -4.501 -4.669 -4.865
39mix5  0.00001 9E-6
 -3.142 -2.812 -2.564 -2.404 -2.281 -2.502 -2.589 -2.706
 -2.842 -2.964 -3.068 -3.103 -3.182 -3.268 -3.361 -3.411
 -3.517 -3.576 -3.705 -3.849 -3.932 -3.932 -4.029 -4.234
 -4.501 -4.664 -4.860 -5.104 -5.431 -5.433
26tyro5 0.00001 0.00001
 -3.037 -2.696 -2.464 -2.321 -2.239 -2.444 -2.602 -2.823
 -3.144 -3.396 -3.742 -4.063 -4.398 -4.699 -4.893 -5.138
 -5.140 -5.461 -5.463 -5.945 -5.461 -5.138 -5.140 -5.138
 -5.138 -5.463 -5.461 -5.461 -5.461 -5.461
tyro2   0.0001 0.0001
 -1.081 -0.710 -0.470 -0.337 -0.327 -0.433 -0.602 -0.841
 -1.119 -1.423 -1.750 -2.121 -2.449 -2.818 -3.110 -3.467
 -3.781 -4.029 -4.241 -4.366 -4.501 -4.366 -4.501 -4.501
 -4.668 -4.668 -4.865 -4.865 -5.109 -5.111
;
```

The following statements fit a PLS model with 10 factors.

```
proc pls data=ftrain nfac=10;
   model tot_log tyr_log try_log = f1-f30;
run;
```

The table shown in Output 51.3.2 indicates that only three or four factors are required to explain almost all of the variation in both the predictors and the responses.

Output 51.3.2. Amount of Training Set Variation Explained

```
                         The PLS Procedure

                  Percent Variation Accounted for
                  by Partial Least Squares Factors

     Number of
     Extracted        Model Effects        Dependent Variables
       Factors     Current       Total     Current       Total

             1     81.1654     81.1654     48.3385     48.3385
             2     16.8113     97.9768     32.5465     80.8851
             3      1.7639     99.7407     11.4438     92.3289
             4      0.1951     99.9357      3.8363     96.1652
             5      0.0276     99.9634      1.6880     97.8532
             6      0.0132     99.9765      0.7247     98.5779
             7      0.0052     99.9817      0.2926     98.8705
             8      0.0053     99.9870      0.1252     98.9956
             9      0.0049     99.9918      0.1067     99.1023
            10      0.0034     99.9952      0.1684     99.2707
```

In order to choose the optimal number of PLS factors, you can explore how well models based on the training data with different numbers of factors fit the test data. To do so, use the CV=TESTSET option, with an argument pointing to the test data set ftest, as in the following statements:

```
proc pls data=ftrain nfac=10 cv=testset(ftest)
                             cvtest(stat=press seed=12345);
   model tot_log tyr_log try_log = f1-f30;
run;
```

The results of the test set validation are shown in Output 51.3.3. They indicate that, although five PLS factors give the minimum predicted residual sum of squares, the residuals for four factors are insignificantly different from those for five. Thus, the smaller model is preferred.

Output 51.3.3. Test Set Validation for the Number of PLS Factors

```
                          The PLS Procedure

         Test Set Validation for the Number of Extracted Factors

                     Number of        Root
                     Extracted        Mean    Prob >
                       Factors       PRESS     PRESS

                             0    3.056797    <.0001
                             1    2.630561    <.0001
                             2     1.00706    0.0070
                             3    0.664603    0.0020
                             4    0.521578    0.3800
                             5    0.500034    1.0000
                             6    0.513561    0.5100
                             7    0.501431    0.6870
                             8    1.055791    0.1530
                             9    1.435085    0.1010
                            10    1.720389    0.0320


          Minimum root mean PRESS                     0.5000
          Minimizing number of factors                     5
          Smallest number of factors with p > 0.1          4



                          The PLS Procedure

                     Percent Variation Accounted for
                     by Partial Least Squares Factors

        Number of
        Extracted       Model Effects        Dependent Variables
          Factors     Current       Total     Current       Total

                1     81.1654     81.1654     48.3385     48.3385
                2     16.8113     97.9768     32.5465     80.8851
                3      1.7639     99.7407     11.4438     92.3289
                4      0.1951     99.9357      3.8363     96.1652
```

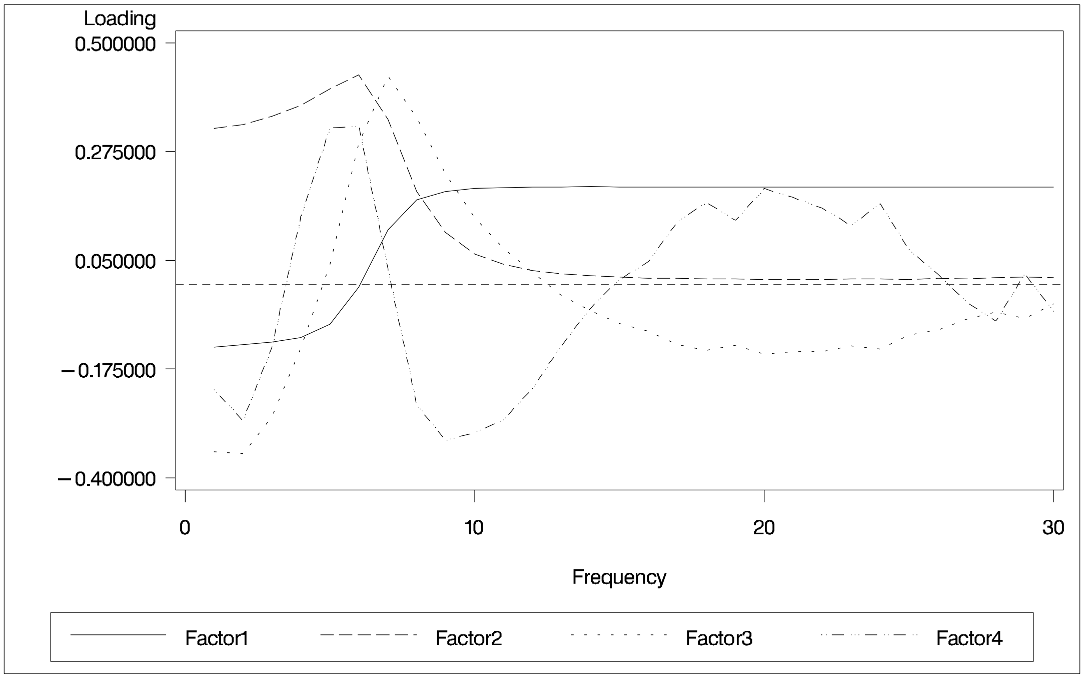
The factor loadings show how the PLS factors are constructed from the centered and scaled predictors. For spectral calibration, it is useful to plot the loadings against the frequency. In many cases, the physical meanings that can be attached to factor loadings help to validate the scientific interpretation of the PLS model. You can use the following statements to plot the loadings for the four PLS factors against frequency.

```
ods listing close;
ods output XLoadings=xloadings;
proc pls data=ftrain nfac=4 details method=pls;
   model tot_log tyr_log try_log = f1-f30;
run;
ods listing;
proc transpose data=xloadings(drop=NumberOfFactors)
               out =xloadings;


data xloadings; set xloadings;
```

```
   n = _n_;
   rename col1=Factor1 col2=Factor2
          col3=Factor3 col4=Factor4;
run;
goptions border;
axis1 label=("Loading"  ) major=(number=5) minor=none;
axis2 label=("Frequency")                  minor=none;
symbol1 v=none i=join c=red    l=1;
symbol2 v=none i=join c=green  l=1 /*l= 3*/;
symbol3 v=none i=join c=blue   l=1 /*l=34*/;
symbol4 v=none i=join c=yellow l=1 /*l=46*/;
legend1 label=none cborder=black;
proc gplot data=xloadings;
   plot (Factor1 Factor2 Factor3 Factor4)*n
      / overlay legend=legend1 vaxis=axis1
        haxis=axis2 vref=0 lvref=2 frame cframe=ligr;
run; quit;
```

The resulting plot is shown in Output 51.3.4.

Output 51.3.4. Predictor Loadings Across Frequencies



Notice that all four factors handle frequencies below and above about 7 or 8 differently. For example, the first factor is very nearly a simple contrast between the averages of the two sets of frequencies, and the second factor appears to be a weighted sum of only the frequencies in the first set.

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