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SAS/STAT® 14.3 User's Guide

The PLS Procedure

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Chapter 90
The PLS Procedure

Contents

Overview: PLS Procedure

The PLS procedure fits models by 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*, *latent vectors*, or *latent variables*), 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 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 as follows:

- 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 predictive 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 *overfitting*—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, minimizing the prediction error for the unfitted part, and iterating with different portions of the data in the roles of fitted and unfitted. Various methods of cross validation are available, including one-at-a-time validation and splitting the data into blocks. The PLS procedure also offers test set validation, where the model is fit to the entire primary input data set and the fit is evaluated over a distinct test data set.

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.

The PLS procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, "Statistical Graphics Using ODS." For specific information about the statistical graphics available with the PLS procedure, see the PLOTS options in the PROC PLS statements and the section "ODS Graphics" on page 7325.

Getting Started: PLS Procedure

Spectrometric Calibration

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 seawater 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 by 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 90.1.

Figure 90.1 PLS Variation Summary

The PLS Procedure

Percent Variation Accounted for by Partial Least Squares Factors

	Model Effects		Dependent Variables	
Number of Extracted 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

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 important, 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

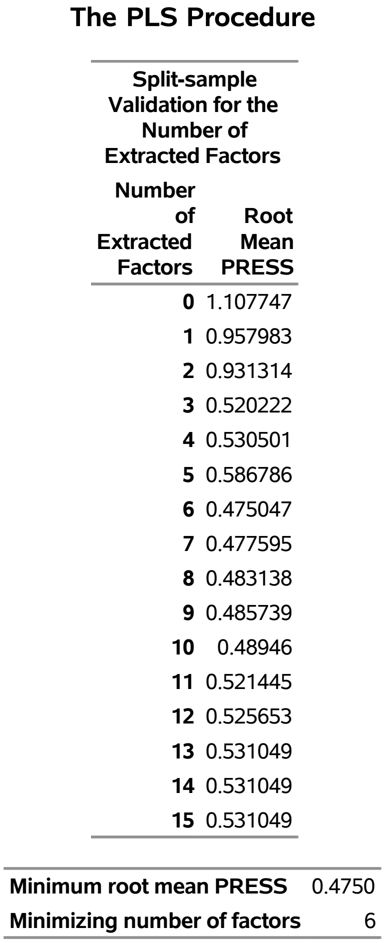
A PLS model is not complete until you choose the number of factors. You can choose the number of factors by using cross validation, in which the data set is divided into two or more groups. You fit the model to all groups except one, and then you check the capability of the model to predict responses 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 composed of every *n*th observation beginning with the first, every *n*th 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 90.2 and Figure 90.3.

Figure 90.2 Split-Sample Validated PRESS Statistics for Number of Factors



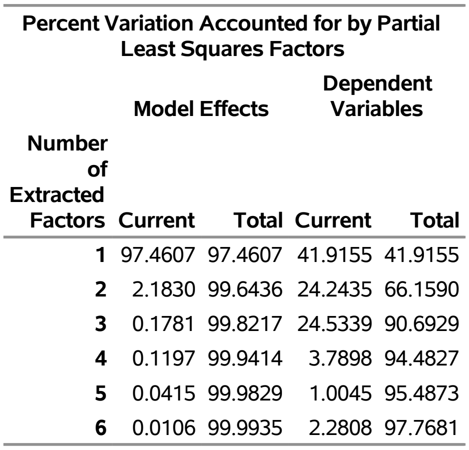
The PLS Procedure

Split-sample Validation for the Number of Extracted Factors

Number of Extracted Factors	Root Mean 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 90.3 PLS Variation Summary for Split-Sample Validated Model



Percent Variation Accounted for by Partial Least Squares Factors

	Model Effects		**Dependent Variables**	
Number of Extracted 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

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 90.4 and Figure 90.5.

Figure 90.4 Testing Split-Sample Validation for Number of Factors

The PLS Procedure

Split-sample Validation for the Number of Extracted Factors

Number of Extracted Factors	Root Mean PRESS	T**2	Prob > T**2
0	1.107747	9.272858	0.0010
1	0.957983	10.62305	<.0001
2	0.931314	8.950878	0.0010
3	0.520222	5.133259	0.1440
4	0.530501	5.168427	0.1340
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	0.0150
11	0.521445	6.666235	0.0130
12	0.525653	7.092861	0.0080
13	0.531049	7.538298	0.0030
14	0.531049	7.538298	0.0030
15	0.531049	7.538298	0.0030

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

Figure 90.5 PLS Variation Summary for Tested Split-Sample Validated Model

Percent Variation Accounted for by Partial Least Squares Factors

	Model Effects		Dependent Variables	
Number of Extracted 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

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;
run;

proc pls data=all nfac=3;
   model ls ha dt = v1-v27;
   output out=pred p=p_ls p_ha p_dt;
run;

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 90.6.

Figure 90.6 Predicted Concentrations for New Observations

Obs	obsnam	p_ls	p_ha	p_dt
17	EM17	2.54261	0.31877	81.4174
18	EM25	-0.24716	1.37892	46.3212

Finally, if ODS Graphics is enabled, PLS also displays by default a plot of the amount of variation accounted for by each factor, as well as a correlations loading plot that summarizes the first two dimensions of the PLS model. The following statements, which are the same as the previous split-sample validation analysis but with ODS Graphics enabled, additionally produce Figure 90.7 and Figure 90.8:

```
ods graphics on;

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

Figure 90.7 Split-Sample Cross Validation Plot

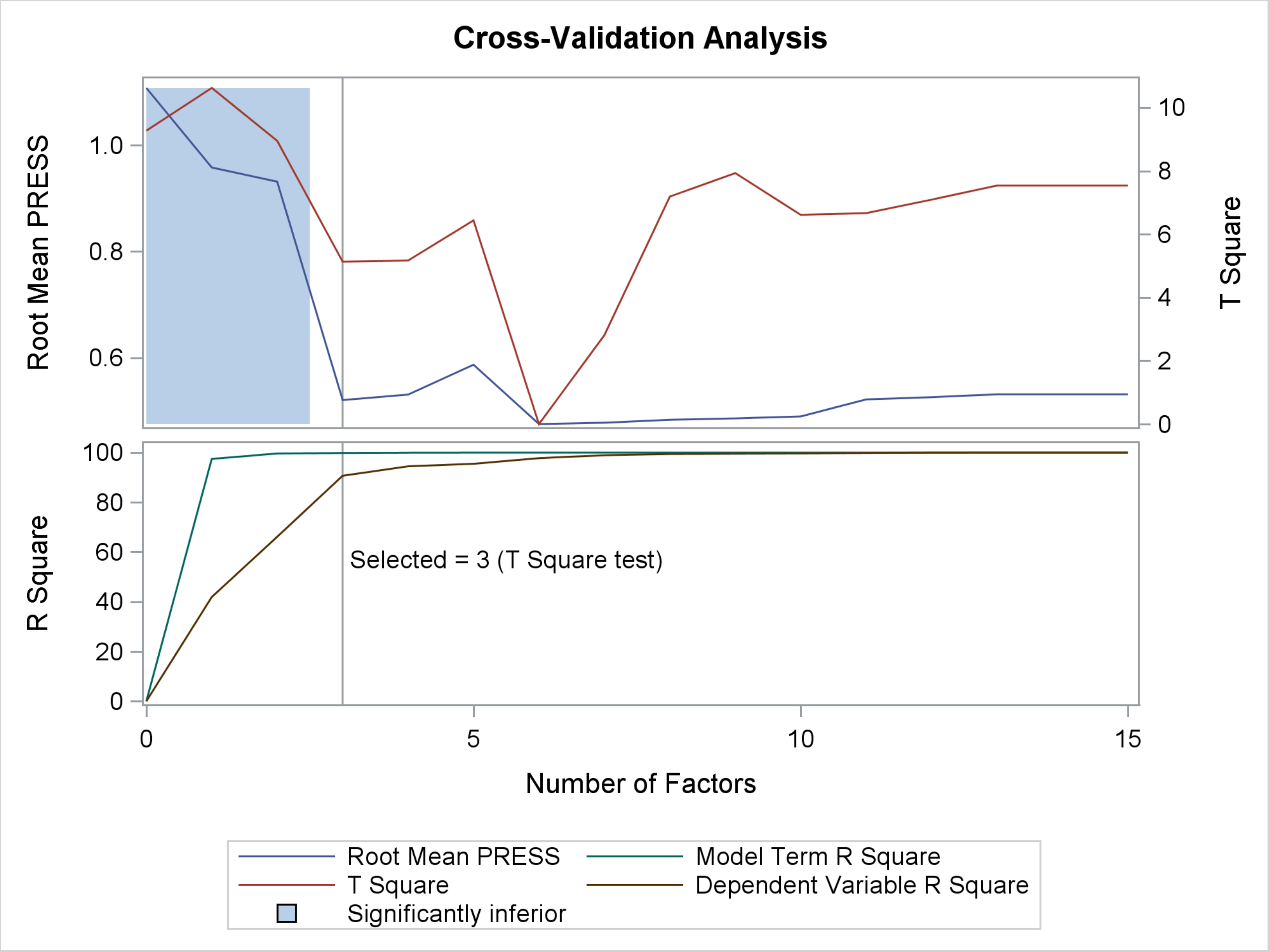
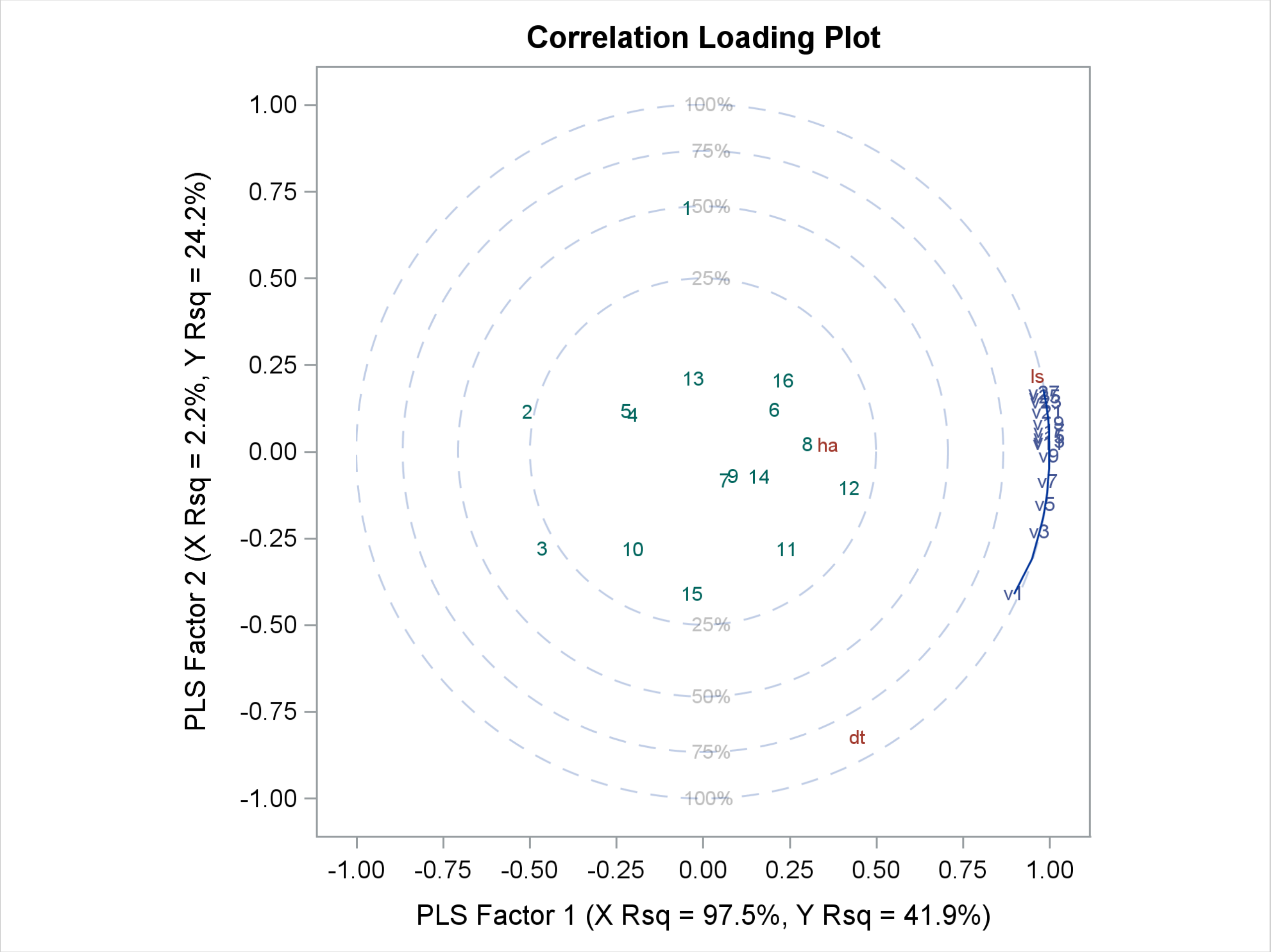


Figure 90.8 Correlation Loading Plot



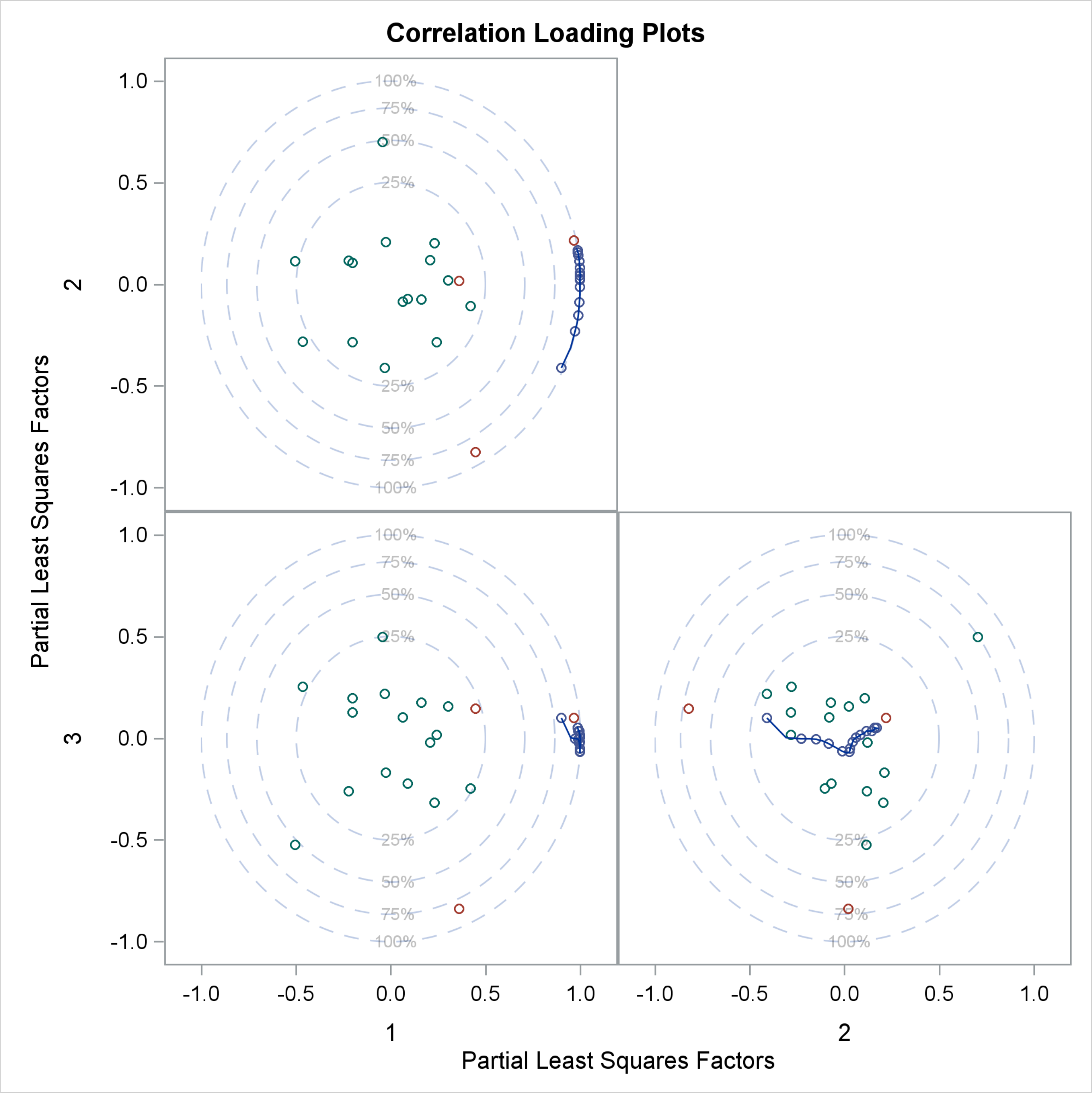
The cross validation plot in Figure 90.7 gives a visual representation of the selection of the optimum number of factors discussed previously. The correlation loading plot is a compact summary of many features of the PLS model. For example, it shows that the first factor is highly positively correlated with all spectral values, indicating that it is approximately an average of them all; the second factor is positively correlated with the lowest frequencies and negatively correlated with the highest, indicating that it is approximately a contrast between the two ends of the spectrum. The observations, represented by their number in the data set on this plot, are generally spaced well apart, indicating that the data give good information about these first two factors. For more details on the interpretation of the correlation loading plot, see the section "ODS Graphics" on page 7325 and Example 90.1.

The default correlation loading plot for just the first two factors depicts most of the model information. In order to see correlation loadings for all three of the selected factors, you use the NFAC= suboption for the PLOT=CORRLOAD option, as in the following:

```
proc pls data=sample nfac=3 plot=corrload(nfac=3);
   model ls ha dt = v1-v27;
run;
```

The resulting plot is shown in Figure 90.9.

Figure 90.9 Correlation Loading Plot Matrix



Syntax: PLS Procedure

The following statements are available in the PLS procedure. Items within the angle brackets are optional.

PROC PLS < *options* > **;**
BY *variables* **;**
CLASS *variables* < / *option* > **;**
EFFECT *name*=*effect-type* (*variables*< / *options* >) **;**
ID *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. CLASS and EFFECT statements, if present, must precede the MODEL statement.

PROC PLS Statement

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

The PROC PLS statement invokes the PLS procedure. Optionally, you can also indicate the analysis data and method in the PROC PLS statement. Table 90.1 summarizes the *options* available in the PROC PLS statement.

Table 90.1 PROC PLS Statement Options

Option	Description
CENSCALE	Displays the centering and scaling information
CV=	Specifies the cross validation method to be used
CVTEST	Specifies that van der Voet's (1994) randomization-based model comparison test be performed
DATA=	Names the SAS data set
DETAILS	Displays the details of the fitted model
METHOD=	Specifies the general factor extraction method to be used
MISSING=	Specifies how observations with missing values are to be handled in computing the fit
NFAC=	Specifies the number of factors to extract
NOCENTER	Suppresses centering of the responses and predictors before fitting
NOCVSTDIZE	Suppresses re-centering and rescaling of the responses and predictors when cross-validating
NOPRINT	Suppresses the normal display of results
NOSCALE	Suppresses scaling of the responses and predictors before fitting
PLOTS	Controls the plots produced through ODS Graphics
VARSCALE	Specifies that continuous model variables be centered and scaled
VARSS	Displays the amount of variation accounted for in each response and predictor

The following *options* are available.

CENSCALE

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

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 n blocks of consecutive 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 an integer used to start the pseudo-random number generator for selecting the random test set. If you do not specify a seed, or specify a value less than or equal to zero, the seed is by default generated from reading the time of day from the computer's clock.

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; for more information, see the section "Cross Validation" on page 7321. You can also specify the following *cv-test-options* in parentheses after the CVTEST option:

PVAL=*n*

specifies the cutoff 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).

DATA=*SAS-data-set*

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

DETAILS

lists the details of the fitted model for each successive factor. The details listed are different for different extraction methods; for more information, see the section "Displayed Output" on page 7323.

METHOD=PLS< (*PLS-options*) > | SIMPLS | PCR | 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 $\mathbf{X}'\mathbf{Y}$, EIG bases the extraction on the eigenvalue decomposition of $\mathbf{Y}'\mathbf{X}\mathbf{X}'\mathbf{Y}$, and RLGW is an iterative approach that is efficient when there are many predictors. 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}.

MISSING=NONE | AVG | EM < (*EM-options*) >

specifies how observations with missing values are to be handled in computing the fit. The default is MISSING=NONE, for which observations with any missing variables (dependent or independent) are excluded from the analysis. MISSING=AVG specifies that the fit be computed by filling in missing values with the average of the nonmissing values for the corresponding variable. If you specify MISSING=EM, then the procedure first computes the model with MISSING=AVG and then fills in missing values by their predicted values based on that model and computes the model again. For both methods of imputation, the imputed values contribute to the centering and scaling values, and the difference between the imputed values and their final predictions contributes to the percentage of variation explained. You can also specify the following optional *EM-options* in parentheses after MISSING=EM:

MAXITER=*n*

specifies the maximum number of iterations for the imputation/fit loop. The default value is 1. If you specify a large value of MAXITER=, then the loop will iterate until it converges (as controlled by the EPSILON= option).

EPSILON=*n*

specifies the convergence criterion for the imputation/fit loop. The default value is 10^{-8}. This option is effective only if you specify a large value for the MAXITER= option.

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 (observations). This is probably more than you need for most applications. Extracting too many factors can lead to an overfit 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.

NOCENTER

suppresses centering of the responses and predictors before fitting. This is useful if the analysis variables are already centered and scaled. For more information, see the section "Centering and Scaling" on page 7322.

NOCVSTDIZE

suppresses re-centering and rescaling of the responses and predictors before each model is fit in the cross validation. For more information, see the section "Centering and Scaling" on page 7322.

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); for more information, see Chapter 20, "Using the Output Delivery System."

NOSCALE

suppresses scaling of the responses and predictors before fitting. This is useful if the analysis variables are already centered and scaled. For more information, see the section "Centering and Scaling" on page 7322.

PLOTS < (*global-plot-options*) > < = *plot-request*< (*options*) > >

PLOTS < (*global-plot-options*) > < = (*plot-request*< (*options*) > < ... *plot-request*< (*options*) > >) >

controls the plots produced through ODS Graphics. When you specify only one *plot-request*, you can omit the parentheses from around the plot request. For example:

```
plots=none
plots=cvplot
plots=(diagnostics cvplot)
plots(unpack)=diagnostics
plots(unpack)=(diagnostics corrload(trace=off))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc pls data=pentaTrain;
   model log_RAI = S1-S5 L1-L5 P1-P5;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 615 in Chapter 21, "Statistical Graphics Using ODS."

If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC PLS produces by default a plot of the R-square analysis and a correlation loading plot summarizing the first two factors.

The *global-plot-options* include the following:

FLIP

interchanges the X-axis and Y-axis dimensions for the score, weight, and loading plots.

ONLY

suppresses the default plots. Only plots specifically requested are displayed.

UNPACKPANEL

UNPACK

suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACKPANEL to get each plot in a separate panel. You can specify PLOTS(UNPACKPANEL) to unpack only the default plots. You can also specify UNPACKPANEL as a suboption for certain specific plots, as discussed in the following.

The *plot-requests* include the following:

ALL

produces all appropriate plots. You can specify other options with ALL—for example, to request all plots and unpack only the residuals, specify PLOTS=(ALL RESIDUALS(UNPACK)).

CORRLOAD < (*options*) >

produces a correlation loading plot (default). You can specify the following *options*:

TRACE=OFF | ON

controls how points that correspond to the X-loadings are depicted. You can specify the following values:

OFF specifies that all X-loadings be depicted in the plot by their names plotted at the corresponding point on the graph.

ON specifies that the positions for all the X-loadings be depicted by a "trace" through the corresponding points.

By default, TRACE=ON if there are more than 20 predictors, and TRACE=OFF otherwise.

NFAC=*n*

specifies the number of factors for which to display correlation loading plots. By default, NFAC=2, which corresponds to a single plot for the first two factors. If you specify a value of n greater than 2, then the $n(n-1)/2$ plots are displayed together in a matrix of correlation loading plots. The maximum number of factors that can be displayed in such a matrix is 8.

UNPACK

requests that the $n(n-1)/2$ correlation loading plots be produced separately instead of in a matrix. This options has no effect unless the NFAC=*n* option is also specified, with a value of n greater than 2.

CVPLOT

produces a cross validation and R-square analysis. This plot requires the CV= option to be specified, and is displayed by default in this case.

DIAGNOSTICS < (UNPACK) >

produces a summary panel of the fit for each dependent variable. The summary by default consists of a panel for each dependent variable, with plots depicting the distribution of residuals and predicted values. You can use the UNPACK suboption to specify that the subplots be produced separately.

DMOD

produces the DMODX, DMODY, and DMODXY plots.

DMODX

produces a plot of the distance of each observation to the X model.

DMODXY

produces plots of the distance of each observation to the X and Y models.

DMODY

produces a plot of the distance of each observation to the Y model.

FIT

produces both the fit diagnostic panel and the ParmProfiles plot.

NONE

suppresses the display of graphics.

PARMPROFILES

produces profiles of the regression coefficients.

SCORES < (UNPACK | FLIP) >

produces the XScores, YScores, XYScores, and DModXY plots. You can use the UNPACK suboption to specify that the subplots for scores be produced separately, and the FLIP option to interchange their default X-axis and Y-axis dimensions.

RESIDUALS < (UNPACK) >

plots the residuals for each dependent variable against each independent variable. Residual plots are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately.

VIP

produces profiles of variable importance factors.

WEIGHTS < (UNPACK | FLIP) >

produces all X and Y loading and weight plots, as well as the VIP plot. You can use the UNPACK suboption to specify that the subplots for weights and loadings be produced separately, and the FLIP option to interchange their default X-axis and Y-axis dimensions.

XLOADINGPLOT < (UNPACK | FLIP) >

produces a scatter plot matrix of X-loadings against each other. Loading scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

XLOADINGPROFILES

produces profiles of the X-loadings.

XSCORES < (UNPACK | FLIP) >

produces a scatter plot matrix of X-scores against each other. Score scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

XWEIGHTPLOT < (UNPACK | FLIP) >

produces a scatter plot matrix of X-weights against each other. Weight scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

XWEIGHTPROFILES

produces profiles of the X-weights.

XYSCORES < (UNPACK) >

produces a scatter plot matrix of X-scores against Y-scores. Score scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately.

YSCORES < (UNPACK | FLIP) >

produces a scatter plot matrix of Y-scores against each other. Score scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

YWEIGHTPLOT < (UNPACK | FLIP) >

produces a scatter plot matrix of Y-weights against each other. Weight scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

VARSCALE

specifies that continuous model variables be centered and scaled prior to centering and scaling the model effects in which they are involved. The rescaling specified by the VARSCALE option is sometimes more appropriate if the model involves crossproducts between model variables; however, the VARSCALE option still might not produce the model you expect. For more information, see the section “Centering and Scaling” on page 7322.

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.

BY Statement

BY *variables* **;**

You can specify a BY statement with PROC PLS to obtain separate analyses of observations in groups that are 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. If you specify more than one BY statement, only the last one specified is used.

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

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option 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 by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *SAS Visual Data Management and Utility Procedures Guide*.

CLASS Statement

CLASS *variables* < / **TRUNCATE** > **;**

The CLASS statement names the classification variables to be used in the model. The PLS procedure uses a singular, GLM parameterization for effects involving CLASS variables, as discussed in the section "GLM Parameterization of Classification Variables and Effects" on page 391 in Chapter 19, "Shared Concepts and Topics." Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

NOTE: Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *SAS Visual Data Management and Utility Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Language Reference: Dictionary*.

You can specify the following *option* in the CLASS statement after a slash (/):

TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

EFFECT Statement

EFFECT *name***=***effect-type* **(***variables< / options >***) ;**

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects formed from continuous or classification variables, as discussed in the section "GLM Parameterization of Classification Variables and Effects" on page 391 in Chapter 19, "Shared Concepts and Topics."

The following *effect-types* are available.

COLLECTION
specifies a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.

LAG
specifies a classification effect in which the level that is used for a particular period corresponds to the level in the preceding period.

MULTIMEMBER | MM
specifies a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.

POLYNOMIAL | POLY
specifies a multivariate polynomial effect in the specified numeric variables.

SPLINE
specifies a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables.

Table 90.2 summarizes the *options* available in the EFFECT statement.

Table 90.2 EFFECT Statement Options

Option	Description
Collection Effects Options	
DETAILS	Displays the constituents of the collection effect
Lag Effects Options	
DESIGNROLE=	Names a variable that controls to which lag design an observation is assigned
DETAILS	Displays the lag design of the lag effect
NLAG=	Specifies the number of periods in the lag
PERIOD=	Names the variable that defines the period. This option is required.
WITHIN=	Names the variable or variables that define the group within which each period is defined. This option is required.

Table 90.2 *continued*

Option	Description
Multimember Effects Options	
NOEFFECT	Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns
WEIGHT=	Specifies the weight variable for the contributions of each of the classification effects
Polynomial Effects Options	
DEGREE=	Specifies the degree of the polynomial
MDEGREE=	Specifies the maximum degree of any variable in a term of the polynomial
STANDARDIZE=	Specifies centering and scaling suboptions for the variables that define the polynomial
Spline Effects Options	
BASIS=	Specifies the type of basis (B-spline basis or truncated power function basis) for the spline effect
DEGREE=	Specifies the degree of the spline effect
KNOTMETHOD=	Specifies how to construct the knots for the spline effect

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section "EFFECT Statement" on page 401 in Chapter 19, "Shared Concepts and Topics."

ID Statement

ID *variables* **;**

The ID statement names variables whose values are used to label observations in plots. If you do not specify an ID statement, then each observations is labeled in plots by its corresponding observation number.

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; for more information, see the section "Specification of Effects" on page 3773 in Chapter 48, "The GLM Procedure." 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, latent variables, 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: PLS Procedure

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 $\mathbf{X} = \mathbf{X}_0$ be the centered and scaled matrix of predictors and let $\mathbf{Y} = \mathbf{Y}_0$ be the centered and scaled matrix of response values. The PLS method starts with a linear combination $\mathbf{t} = \mathbf{X}_0\mathbf{w}$ of the predictors, where $\mathbf{t}$ is called a *score* vector and $\mathbf{w}$ is its associated *weight* vector. The PLS method predicts both $\mathbf{X}_0$ and $\mathbf{Y}_0$ by regression on $\mathbf{t}$:

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

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

The specific linear combination $\mathbf{t} = \mathbf{X}_0\mathbf{w}$ is the one that has maximum covariance $\mathbf{t}'\mathbf{u}$ with some response linear combination $\mathbf{u} = \mathbf{Y}_0\mathbf{q}$. 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 $\mathbf{X}_0'\mathbf{Y}_0$ or, equivalently, the first eigenvectors of $\mathbf{X}_0'\mathbf{Y}_0\mathbf{Y}_0'\mathbf{X}_0$ and $\mathbf{Y}_0'\mathbf{X}_0\mathbf{X}_0'\mathbf{Y}_0$, respectively.

This accounts for how the first PLS factor is extracted. The second factor is extracted in the same way by replacing $\mathbf{X}_0$ and $\mathbf{Y}_0$ with the X- and Y-residuals from the first factor:

$$\begin{array}{rcl} \mathbf{X}_1 & = & \mathbf{X}_0 - \hat{\mathbf{X}}_0 \\ \mathbf{Y}_1 & = & \mathbf{Y}_0 - \hat{\mathbf{Y}}_0 \end{array}$$

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

SIMPLS

Note that each extracted PLS factor is defined in terms of different X-variables $\mathbf{X}_i$. 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 $\mathbf{t}_i = \mathbf{X}\mathbf{r}_i$ in terms of the original (centered and scaled) predictors $\mathbf{X}$. The SIMPLS X-weight vectors r_i are similar to the eigenvectors of $\mathbf{S}\mathbf{S}' = \mathbf{X}'\mathbf{Y}\mathbf{Y}'\mathbf{X}$, 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

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

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

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

The SIMPLS scores are identical to the PLS scores for one response but slightly different for more than one response; see 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 $\mathbf{X}$, it is easy to compute the overall model coefficients $\mathbf{B}$:

$$\begin{aligned}\hat{\mathbf{Y}} &= \sum_i \mathbf{t}_i \mathbf{c}_i' \\ &= \sum_i \mathbf{X}\mathbf{r}_i \mathbf{c}_i' \\ &= \mathbf{X}\mathbf{B}, \text{ where } \mathbf{B} = \mathbf{R}\mathbf{C}'\end{aligned}$$

Principal Components Regression

Like the SIMPLS method, principal components regression (PCR) defines all the scores in terms of the original (centered and scaled) predictors $\mathbf{X}$. 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 $\mathbf{X}$ as possible; equivalently, the X-weights for the PCR method are the eigenvectors of the predictor covariance matrix $\mathbf{X}'\mathbf{X}$. 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 $\mathbf{Y}$ in terms of the original predictors $\mathbf{X}$.

Reduced Rank Regression

As discussed in the preceding sections, partial least squares depends on selecting factors $\mathbf{t} = \mathbf{X}\mathbf{w}$ of the predictors and $\mathbf{u} = \mathbf{Y}\mathbf{q}$ 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 $\hat{\mathbf{Y}}_{\mathrm{LS}}'\hat{\mathbf{Y}}_{\mathrm{LS}}$ of the responses predicted by ordinary least squares regression; the X-scores are the projections of the Y-scores $\mathbf{Y}\mathbf{q}_i$ 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 affects 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;
   model y = x1 x2;
run;

proc pls data=data nfac=1 method=pcr;
   model y = x1 x2;
run;

proc pls data=data nfac=1 method=pls;
   model y = x1 x2;
run;
```

The amount of model and response variation explained by the first factor for each method is shown in Figure 90.10 through Figure 90.12.

Figure 90.10 Variation Explained by First Reduced Rank Regression Factor

The PLS Procedure

Percent Variation Accounted for by Reduced Rank Regression Factors

	Model Effects		Dependent Variables	
Number of Extracted Factors	Current	Total	Current	Total
1	15.0661	15.0661	100.0000	100.0000

Figure 90.11 Variation Explained by First Principal Components Regression Factor

The PLS Procedure

Percent Variation Accounted for by Principal Components

	Model Effects		Dependent Variables	
Number of Extracted Factors	Current	Total	Current	Total
1	92.9996	92.9996	9.3787	9.3787

Figure 90.12 Variation Explained by First Partial Least Squares Regression Factor

The PLS Procedure

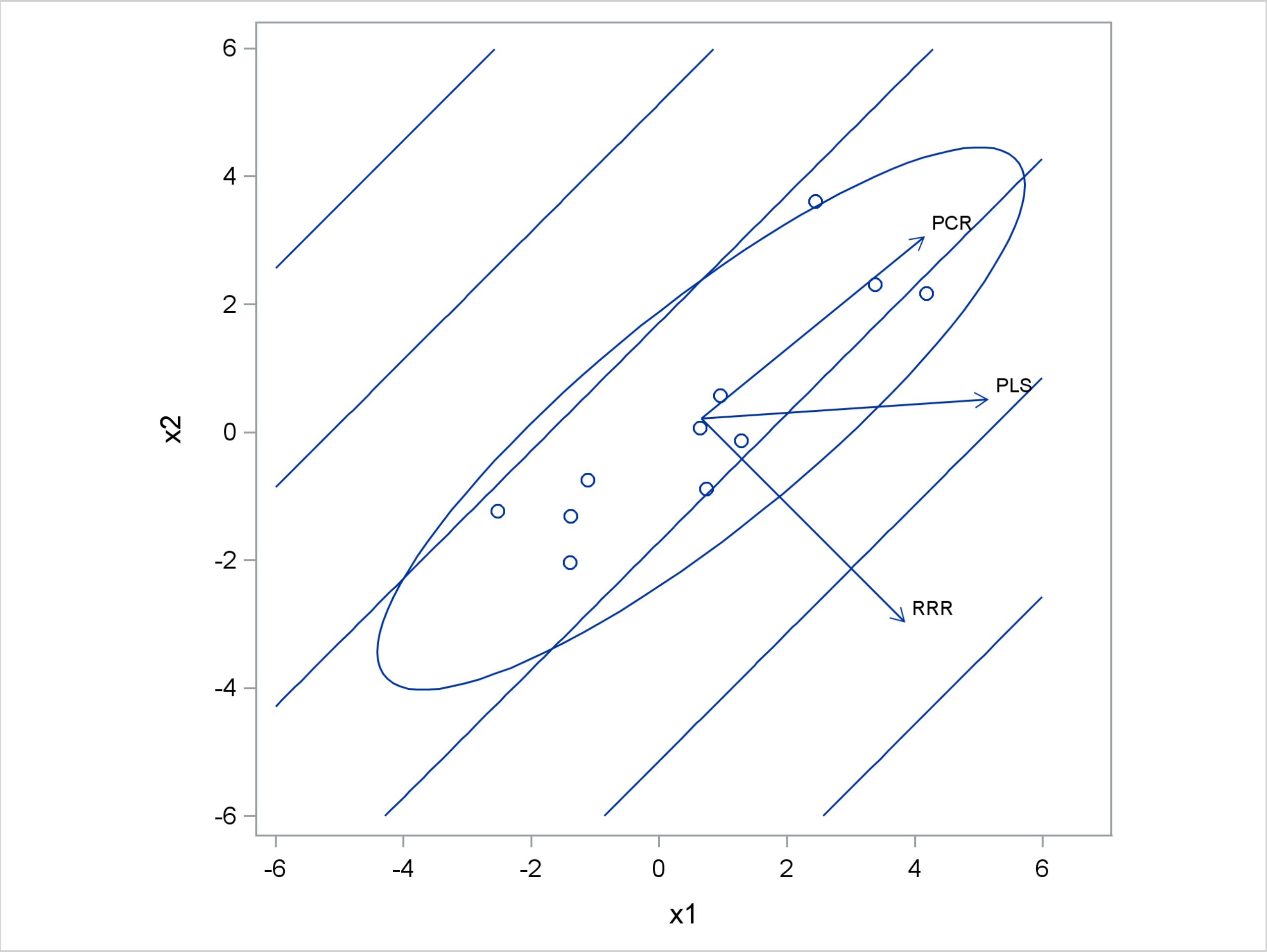
Percent Variation Accounted for by Partial Least Squares Factors

	Model Effects		Dependent Variables	
Number of Extracted Factors	Current	Total	Current	Total
1	88.5357	88.5357	26.5304	26.5304

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

Figure 90.13 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 *overfit* 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 are serially correlated, in which case either blocked or split-sample validation might be more appropriate (CV=BLOCK or CV=SPLIT); you can specify the number of 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 might 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 $\sum_{jk} R^2_{i,jk}$. 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 $C_i = \mathbf{d}'_{i,\cdot}\mathbf{S}_i^{-1}\mathbf{d}_{i,\cdot}$, where $\mathbf{d}_{i,\cdot}$ is the sum of the vectors $\mathbf{d}_{i,j} = \{D_{i,j1},\ldots,D_{i,jN_y}\}'$ and $\mathbf{S}_i$ is the sum of squares and crossproducts matrix

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

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 section "Regression Methods" on page 7317 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 std(Time) in Time is roughly equivalent to a change of std(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 crossproduct. That is, if the ith values of two predictors are denoted x^1_i and x^2_i, then the default standardized ith value of the crossproduct is

$$\frac{x^1_i x^2_i - \mathrm{mean}_j(x^1_j x^2_j)}{\mathrm{std}_j(x^1_j x^2_j)}$$

If you want the crossproduct 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 $m^k = \mathrm{mean}_j(x_j^k)$ and $s^k = \mathrm{std}_j(x_j^k)$ 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 crossproducts nested within each term, the resulting model might not be equivalent to a simple linear model in the same terms. To see this, note that a model involving the crossproduct 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

By default, PROC PLS handles missing values very simply. Observations with any missing independent variables (including all classification 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.

However, the MISSING= option in the PROC PLS statement provides more sophisticated ways of modeling in the presence of missing values. If you specify MISSING=AVG or MISSING=EM, then all observations in the input data set contribute to both the analysis and the OUTPUT OUT= data set. With MISSING=AVG, the fit is computed by filling in missing values with the average of the nonmissing values for the corresponding variable. With MISSING=EM, the procedure first computes the model with MISSING=AVG, then fills in missing values with their predicted values based on that model and computes the model again. Alternatively, you can specify MISSING=EM(MAXITER=*n*) with a large value of *n* in order to perform this imputation/fit loop until convergence.

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 in 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 in the PROC PLS statement, then details of the fitted model are displayed for each successive factor. These details for each number of factors include the following:

- 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 in the PROC PLS statement, then centering and scaling information for each response and predictor is displayed.

If you specify the VARSS option in 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 in 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 Table 90.3. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 90.3 ODS Tables Produced by 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
MissingIterations	Iterations for missing value imputation	PROC	MISSING=EM
ModelInfo	Model information	PROC	default
NObs	Number of observations	PROC	default
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

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, "Statistical Graphics Using ODS."

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 615 in Chapter 21, "Statistical Graphics Using ODS."

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section "A Primer on ODS Statistical Graphics" on page 614 in Chapter 21, "Statistical Graphics Using ODS."

When ODS Graphics is enabled, by default the PLS procedure produces a plot of the variation accounted for by each extracted factor, as well as a *correlation loading plot* for the first two extracted factors (if the final model has at least two factors). The plot of the variation accounted for can take several forms:

- If the PLS analysis does not include cross validation, then the plot shows the total R square for both model effects and the dependent variables against the number of factors.
- If you specify the CV= option to select the number of factors in the final model by cross validation, then the plot shows the R-square analysis discussed previously as well as the root mean PRESS from the cross validation analysis, with the selected number of factors identified by a vertical line.

The correlation loading plot for the first two factors summarizes many aspects of the two most significant dimensions of the model. It consists of overlaid scatter plots of the scores of the first two factors, the loadings of the model effects, and the loadings of the dependent variables. The loadings are scaled so that the amount of variation in the variables that is explained by the model is proportional to the distance from the origin; circles indicating various levels of explained variation are also overlaid on the correlation loading plot. Also, the correlation between the model approximations for any two variables is proportional to the length of the projection of the point corresponding to one variable on a line through the origin passing through the point corresponding to the other variable; the sign of the correlation corresponds to which side of the origin the projected point falls on.

The R square and the first two correlation loadings are plotted by default when ODS Graphics is enabled, but you can produce many other plots for the PROC PLS analysis.

ODS Graph Names

PROC PLS assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in Table 90.4.

Table 90.4 Graphs Produced by PROC PLS

ODS Graph Name	Plot Description	Option
CorrLoadPlot	Correlation loading plot (default)	PLOT=CORRLOAD(*option*)
CVPlot	Cross validation and R-square analysis (default, as appropriate)	CV=

Table 90.4 *continued*

ODS Graph Name	Plot Description	Option
DModXPlot	Distance of each observation to the X model	PLOT=DMODX
DModXYPlot	Distance of each observation to the X and Y models	PLOT=DMODXY
DModYPlot	Distance of each observation to the Y model	PLOT=DMODY
DiagnosticsPanel	Panel of diagnostic plots for the fit	PLOT=DIAGNOSTICS
AbsResidualByPredicted	Absolute residual by predicted values	PLOT=DIAGNOSTICS(UNPACK)
ObservedByPredicted	Observed by predicted	PLOT=DIAGNOSTICS(UNPACK)
QQPlot	Residual Q-Q plot	PLOT=DIAGNOSTICS(UNPACK)
ResidualByPredicted	Residual by predicted values	PLOT=DIAGNOSTICS(UNPACK)
ResidualHistogram	Residual histogram	PLOT=DIAGNOSTICS(UNPACK)
RFPlot	RF plot	PLOT=DIAGNOSTICS(UNPACK)
ParmProfiles	Profiles of regression coefficients	PLOT=PARMPROFILES
R2Plot	R-square analysis (default, as appropriate)	
ResidualPlots	Residuals for each dependent variable	PLOT=RESIDUALS
VariableImportancePlot	Profile of variable importance factors	PLOT=VIP
XLoadingPlot	Scatter plot matrix of X-loadings against each other	PLOT=XLOADINGPLOT
XLoadingProfiles	Profiles of the X-loadings	PLOT=XLOADINGPROFILES
XScorePlot	Scatter plot matrix of X-scores against each other	PLOT=XSCORES
XWeightPlot	Scatter plot matrix of X-weights against each other	PLOT=XWEIGHTPLOT
XWeightProfiles	Profiles of the X-weights	PLOT=XWEIGHTPROFILES
XYScorePlot	Scatter plot matrix of X-scores against Y-scores	PLOT=XYSCORES
YScorePlot	Scatter plot matrix of Y-scores against each other	PLOT=YSCORES
YWeightPlot	Scatter plot matrix of Y-weights against each other	PLOT=YWEIGHTPLOT

Examples: PLS Procedure

Example 90.1: Examining Model Details

This 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 pentaTrain, which contains these data.

```
data pentaTrain;
   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
   ;
```

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 (see 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=pentaTrain;
      model log_RAI = S1-S5 L1-L5 P1-P5;
   run;
```

The PLS procedure displays a table, shown in Output 90.1.1, showing how much predictor and response variation is explained by each PLS factor.

Output 90.1.1 Amount of Training Set Variation Explained

The PLS Procedure

Percent Variation Accounted for by Partial Least Squares Factors

	Model Effects		Dependent Variables	
Number of Extracted Factors	**Current**	**Total**	**Current**	**Total**
1	16.9014	16.9014	89.6399	89.6399
2	12.7721	29.6735	7.8368	97.4767
3	14.6554	44.3289	0.4636	97.9403
4	11.8421	56.1710	0.2485	98.1889
5	10.5894	66.7605	0.1494	98.3383
6	5.1876	71.9481	0.2617	98.6001
7	6.1873	78.1354	0.2428	98.8428
8	7.2252	85.3606	0.1926	99.0354
9	6.7285	92.0891	0.0725	99.1080
10	7.9076	99.9967	0.0000	99.1080
11	0.0033	100.0000	0.0099	99.1179
12	0.0000	100.0000	0.0000	99.1179
13	0.0000	100.0000	0.0000	99.1179
14	0.0000	100.0000	0.0000	99.1179
15	0.0000	100.0000	0.0000	99.1179

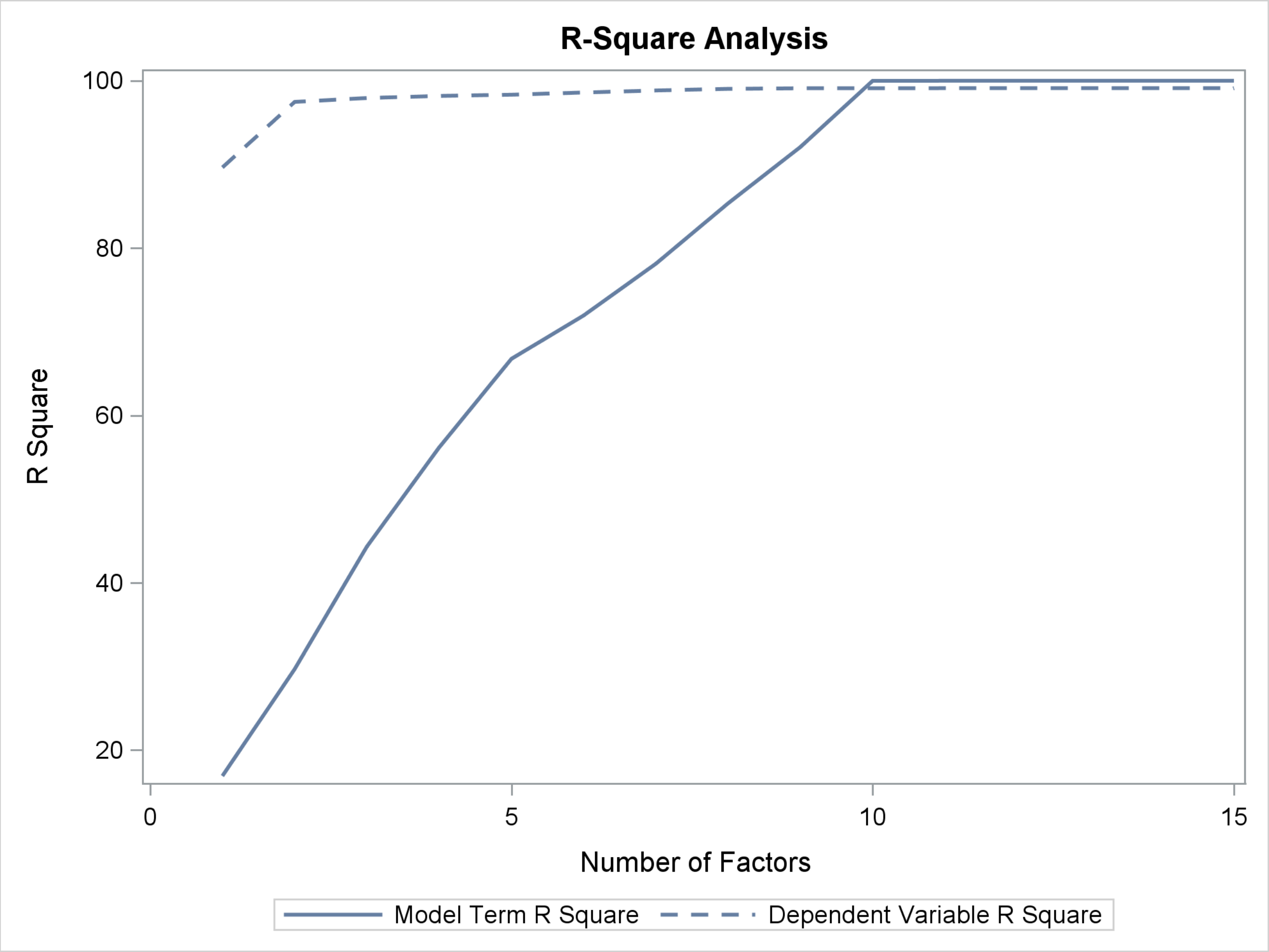
From Output 90.1.1, note that 97% of the response variation is already explained by just two factors, but only 29% of the predictor variation is explained.

The graphics in PROC PLS, available when ODS Graphics is enabled, make it easier to see features of the PLS model.

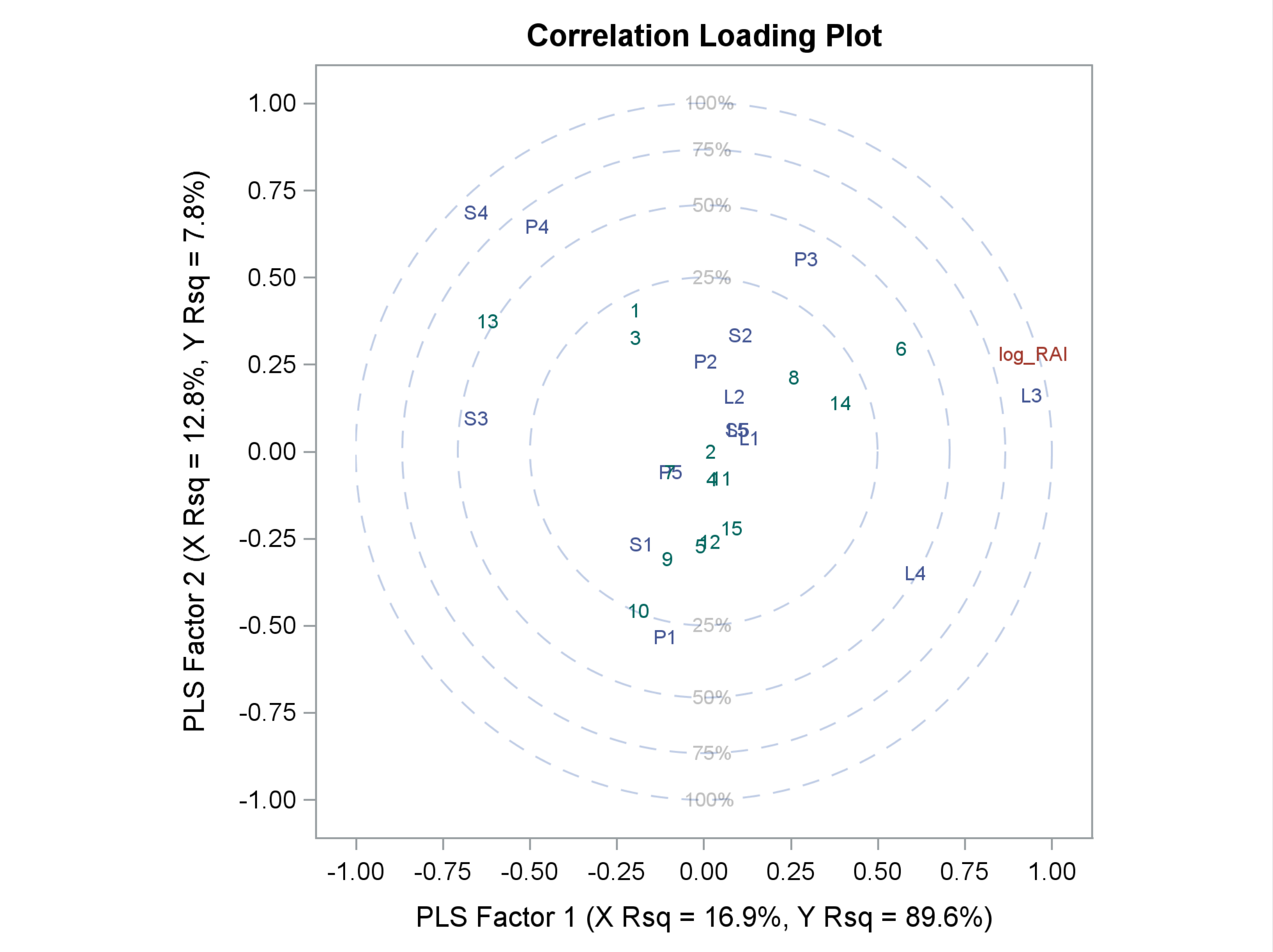
If ODS Graphics is enabled, then in addition to the tables discussed previously, PROC PLS displays a graphical depiction of the R-square analysis as well as a correlation loading plot summarizing the model based on the first two PLS factors. The following statements perform the previous analysis with ODS Graphics enabled, producing Output 90.1.2 and Output 90.1.3.

```
ods graphics on;

proc pls data=pentaTrain;
   model log_RAI = S1-S5 L1-L5 P1-P5;
run;
```

Output 90.1.2 Plot of Proportion of Variation Accounted For



Output 90.1.3 Correlation Loading Plot



The plot in Output 90.1.2 of the proportion of variation explained (or R square) makes it clear that there is a plateau in the response variation after two factors are included in the model. The correlation loading plot in Output 90.1.3 summarizes many features of this two-factor model, including the following:

- The X-scores are plotted as numbers for each observation. You should look for patterns or clearly grouped observations. If you see a curved pattern, for example, you might 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. 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.

- The loadings show how much variation in each variable is accounted for by the first two factors, jointly by the distance of the corresponding point from the origin and individually by the distance for the projections of this point onto the horizontal and vertical axes. That the dependent variable is well explained by the model is reflected in the fact that the point for log_RAI is near the 100% circle.

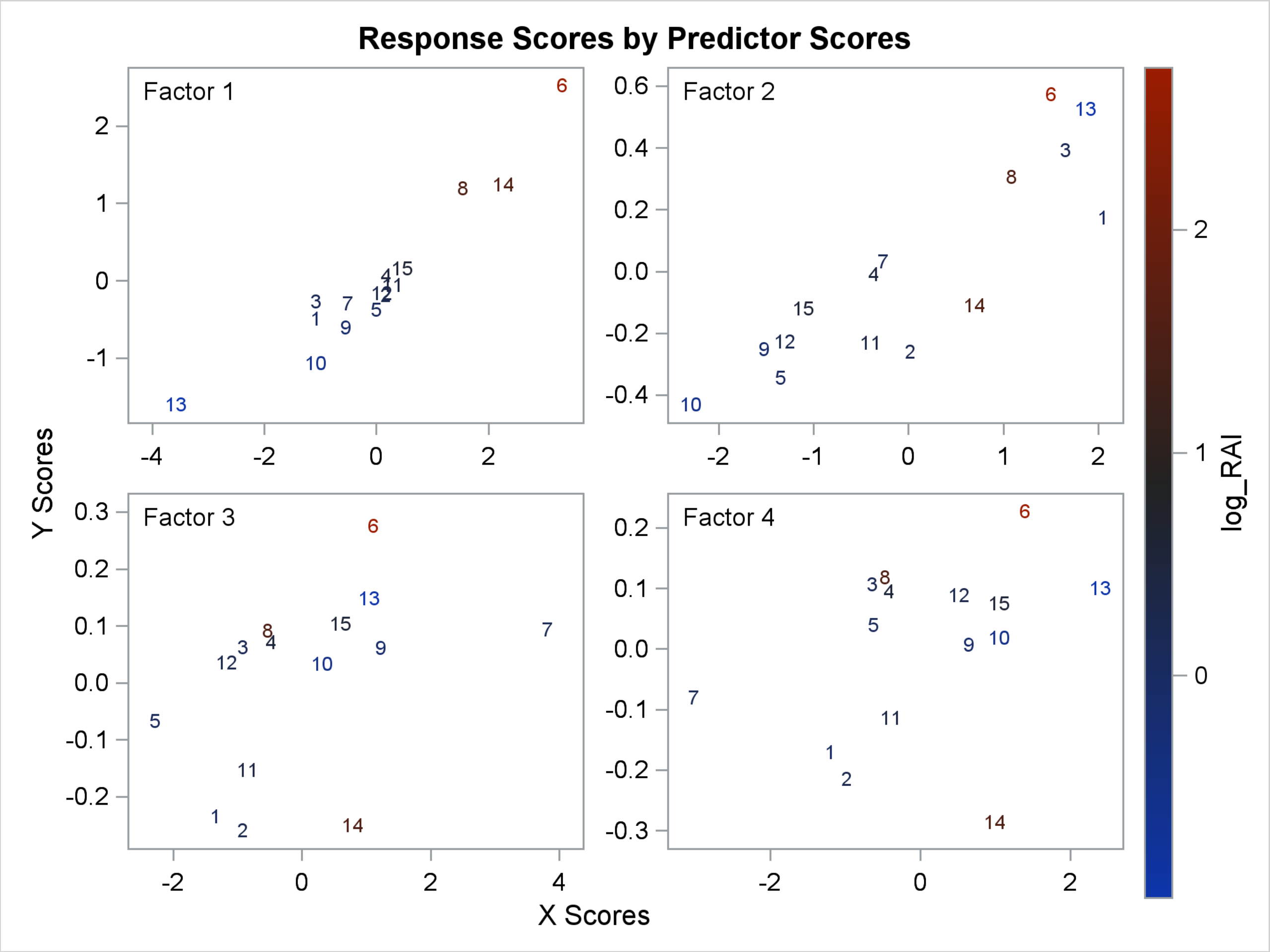
- You can also use the projection interpretation to relate variables to each other. For example, projecting other variables' points onto the line that runs through the log_RAI point and the origin, you can see that the PLS approximation for the predictor L3 is highly positively correlated with log_RAI, S3 is somewhat less correlated but in the negative direction, and several predictors including L1, L5, and S5 have very little correlation with log_RAI.

Other graphics enable you to explore more of the features of the PLS model. For example, you can examine the X-scores versus the Y-scores to explore how partial least squares chooses successive factors. 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. When ODS Graphics is enabled, you can plot the X-scores versus the Y-scores by using the PLOT=XYSCORES option, as shown in the following statements.

```
proc pls data=pentaTrain nfac=4 plot=XYScores;
   model log_RAI = S1-S5 L1-L5 P1-P5;
run;
```

The plot of the X-scores versus the Y-scores for the first four factors is shown in Output 90.1.4.

Output 90.1.4 X-Scores versus Y-Scores



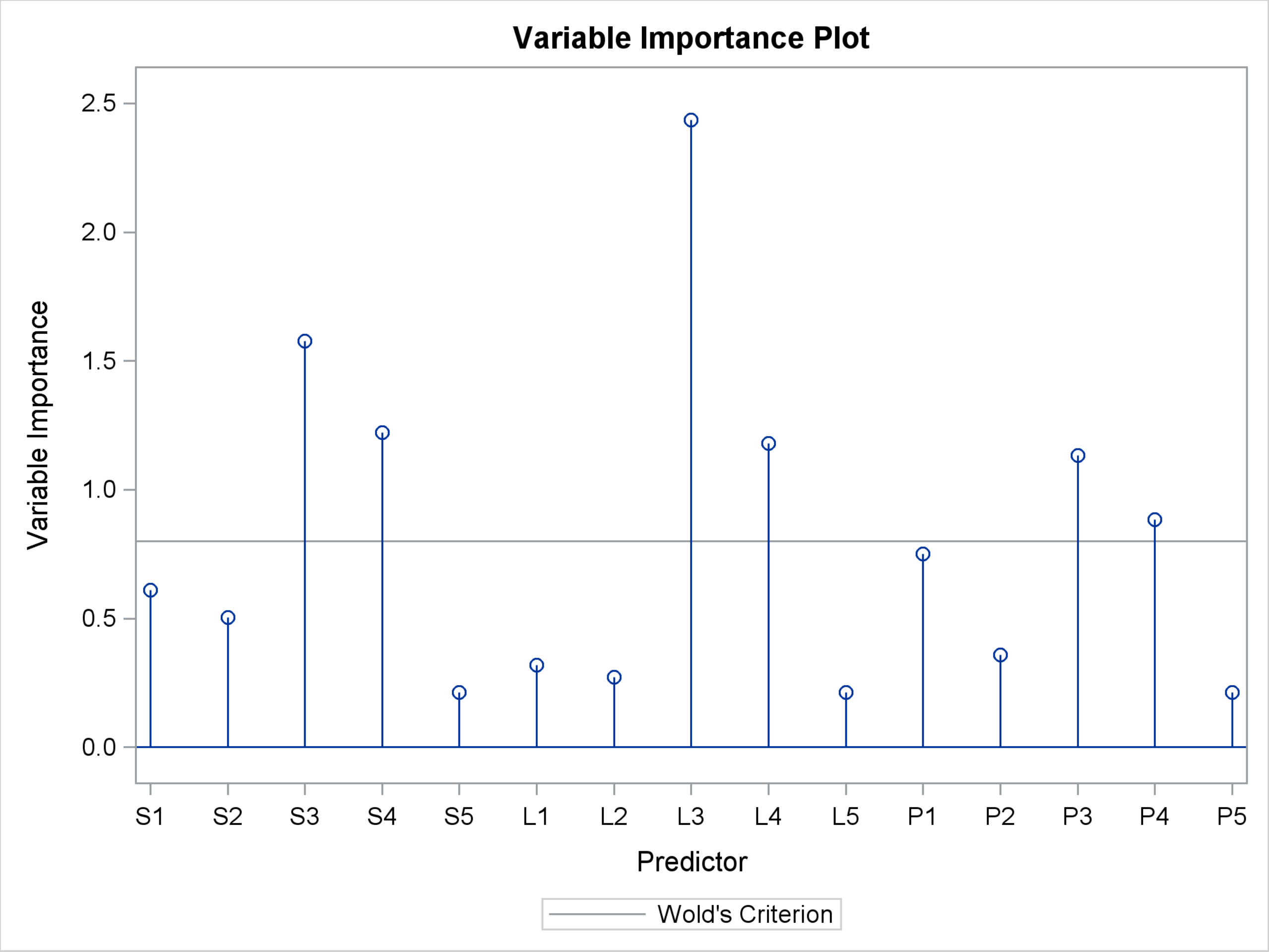
For this example, Output 90.1.4 shows high correlation between X- and Y-scores for the first factor but somewhat lower correlation for the second factor and sharply diminishing correlation after that. This adds strength to the judgment that NFAC=2 is the right number of factors for these data and this model. Note that observation 13 is again extreme in the first two plots. This run might be overly influential for the PLS analysis; thus, you should check to make sure it is reliable.

As explained earlier, you can draw some inferences about the relationship between individual predictors and the dependent variable from the correlation loading plot. However, the regression coefficient profile and the variable importance plot give a more direct indication of which predictors are most useful for predicting the dependent variable. The regression coefficients represent the importance each predictor has in the prediction of just the response. The variable importance plot, on the other hand, represents the contribution of each predictor in fitting the PLS model for both predictors and response. It is based on the *Variable Importance for Projection* (VIP) statistic of Wold (1994), which summarizes the contribution a variable makes to the model. 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 in Umetrics (1995) considers a value less than 0.8 to be "small" for the VIP. The following statements fit a two-factor PLS model and display these two additional plots.

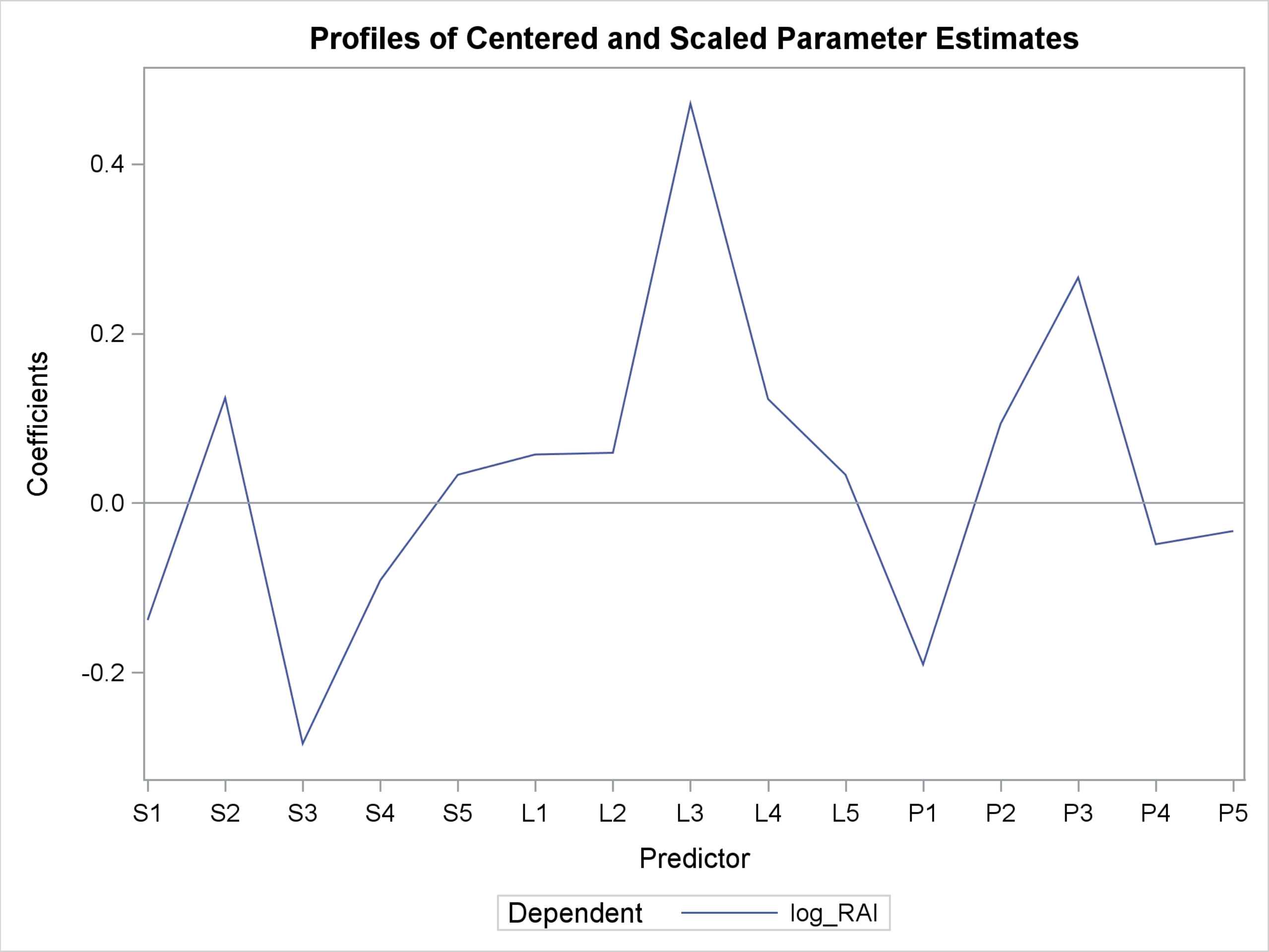
```
proc pls data=pentaTrain nfac=2 plot=(ParmProfiles VIP);
   model log_RAI = S1-S5 L1-L5 P1-P5;
run;

ods graphics off;
```

The additional graphics are shown in Output 90.1.5 and Output 90.1.6.

Output 90.1.5 Variable Importance Plots



Output 90.1.6 Regression Parameter Profile



In these two plots, the variables L1, L2, P2, S5, L5, and P5 have small absolute coefficients and small VIP. Looking back at the correlation loading plot in Output 90.1.2, 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 90.2: Examining Outliers

This example is a continuation of Example 90.1.

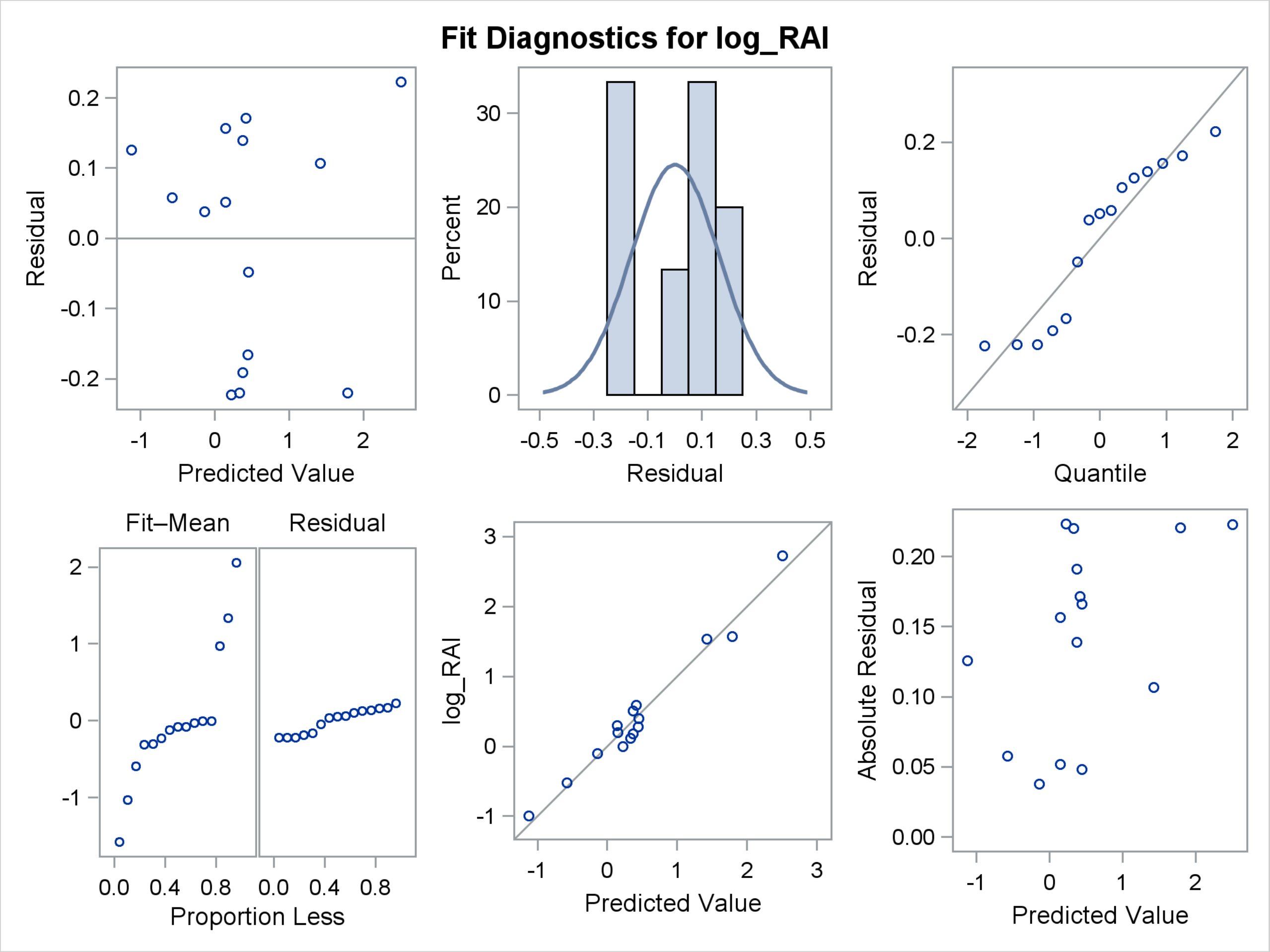
Standard diagnostics for statistical models focus on the response, allowing you to look for patterns that indicate the model is inadequate or for outliers that do not seem to follow the trend of the rest of the data. However, partial least squares effectively models the predictors as well as the responses, so you should consider the pattern of the fit for both. The DModX and DModY statistics give the distance from each point to the PLS model with respect to the predictors and the responses, respectively, and ODS Graphics enables you to plot these values. 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 might have something in common, in which case they should be analyzed separately.

The following statements fit a reduced model to the data discussed in Example 90.1 and plot a panel of standard diagnostics as well as the distances of the observations to the model.

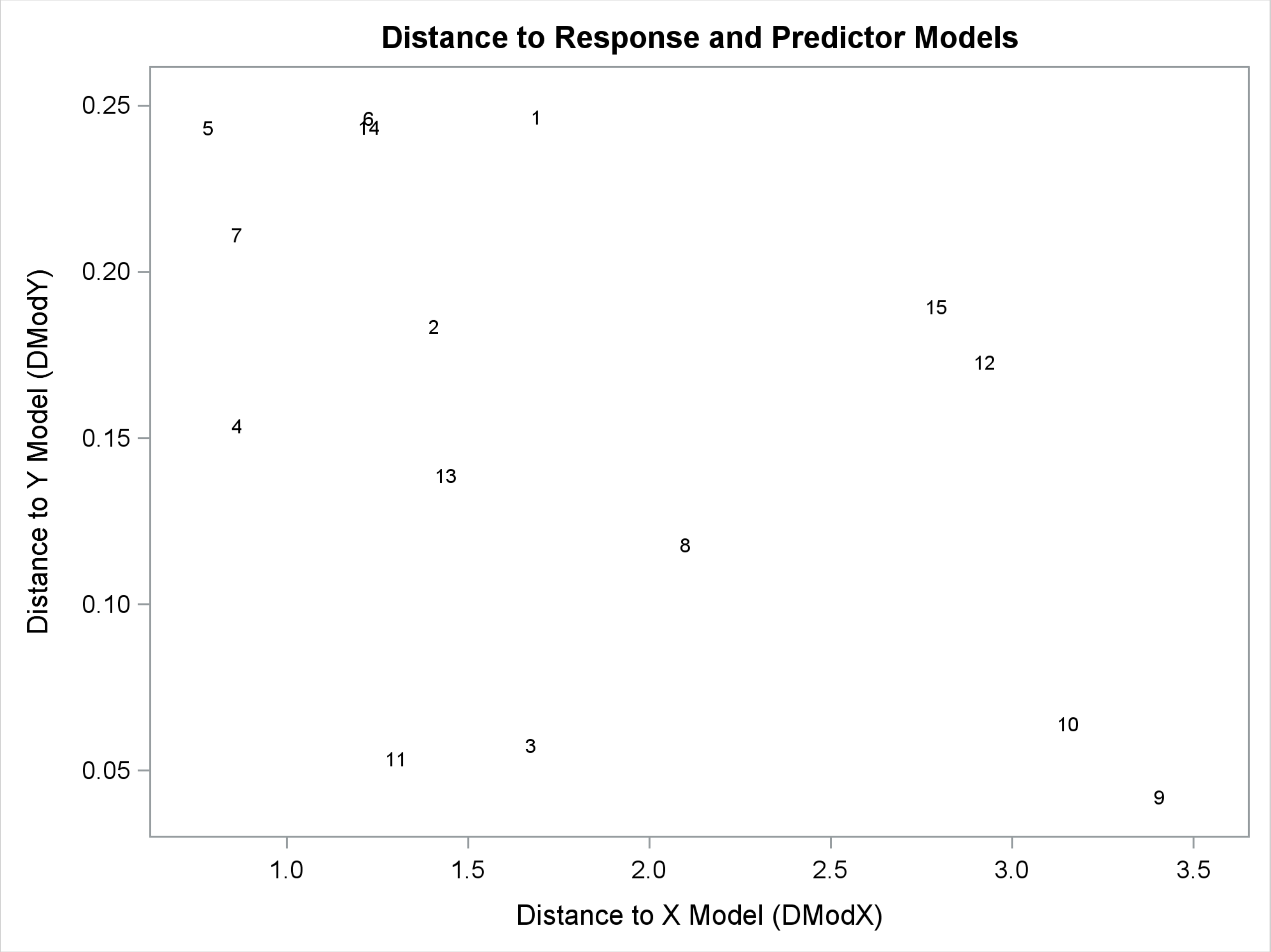
```
ods graphics on;

proc pls data=pentaTrain nfac=2 plot=(diagnostics dmod);
   model log_RAI = S1    P1
                   S2
                   S3 L3 P3
                   S4 L4   ;
run;
```

The plots are shown in Output 90.2.1 and Output 90.2.2.

Output 90.2.1 Model Fit Diagnostics



Output 90.2.2 Predictor versus Response Distances to the Model

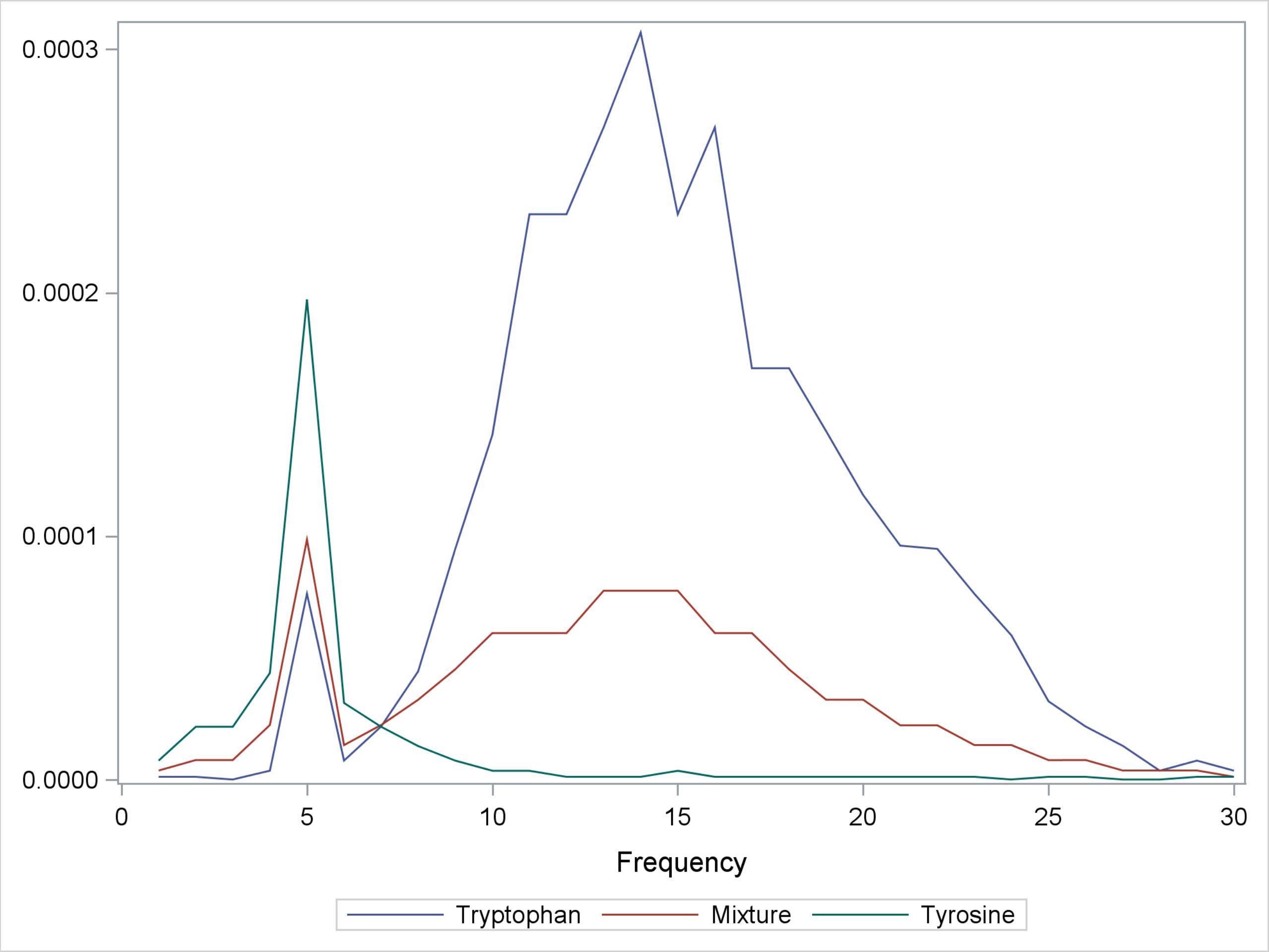


There appear to be no profound outliers in either the predictor space or the response space.

Example 90.3: Choosing a PLS Model by Test Set Validation

This 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 90.3.1 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 90.3.1 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

   ... more lines ...

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

   ... more lines ...

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 90.3.2 indicates that only three or four factors are required to explain almost all of the variation in both the predictors and the responses.

Output 90.3.2 Amount of Training Set Variation Explained

The PLS Procedure

Percent Variation Accounted for by Partial Least Squares Factors

	Model Effects		Dependent Variables	
Number of Extracted 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. The following statements also employ the ODS Graphics features in PROC PLS to display the cross validation results in a plot.

```
ods graphics on;

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 tabular results of the test set validation are shown in Output 90.3.3, and the graphical results are shown in Output 90.3.4. 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 90.3.3 Test Set Validation for the Number of PLS Factors

The PLS Procedure

Test Set Validation for the Number of Extracted Factors

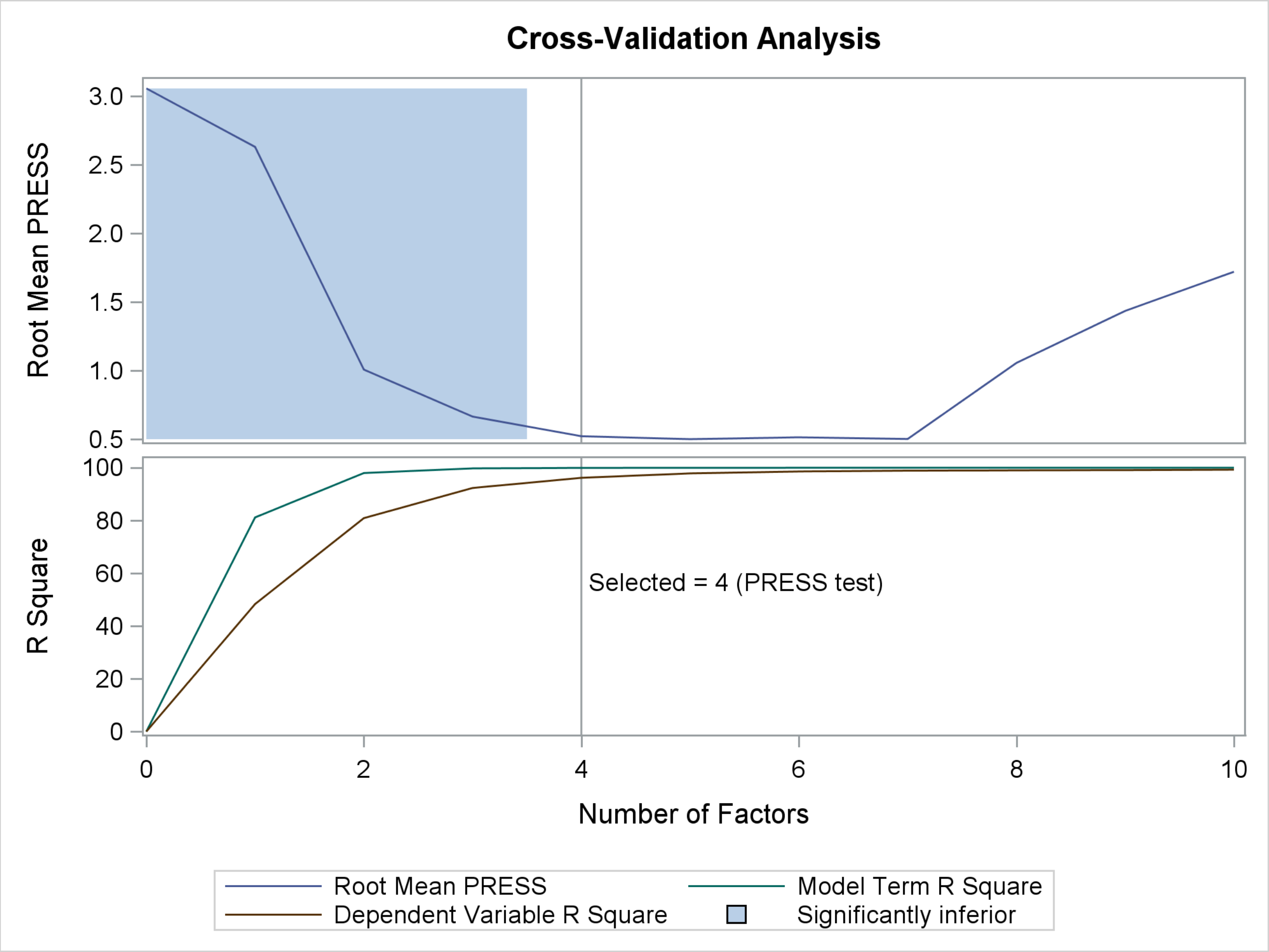
Number of Extracted Factors	Root Mean PRESS	Prob > PRESS
0	3.056797	<.0001
1	2.630561	<.0001
2	1.00706	0.0070
3	0.664603	0.0020
4	0.521578	0.3800
5	0.500034	1.0000
6	0.513561	0.5100
7	0.501431	0.6870
8	1.055791	0.1530
9	1.435085	0.1010
10	1.720389	0.0320

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

Percent Variation Accounted for by Partial Least Squares Factors

	Model Effects		Dependent Variables	
Number of Extracted 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

Output 90.3.4 Test Set Validation Plot

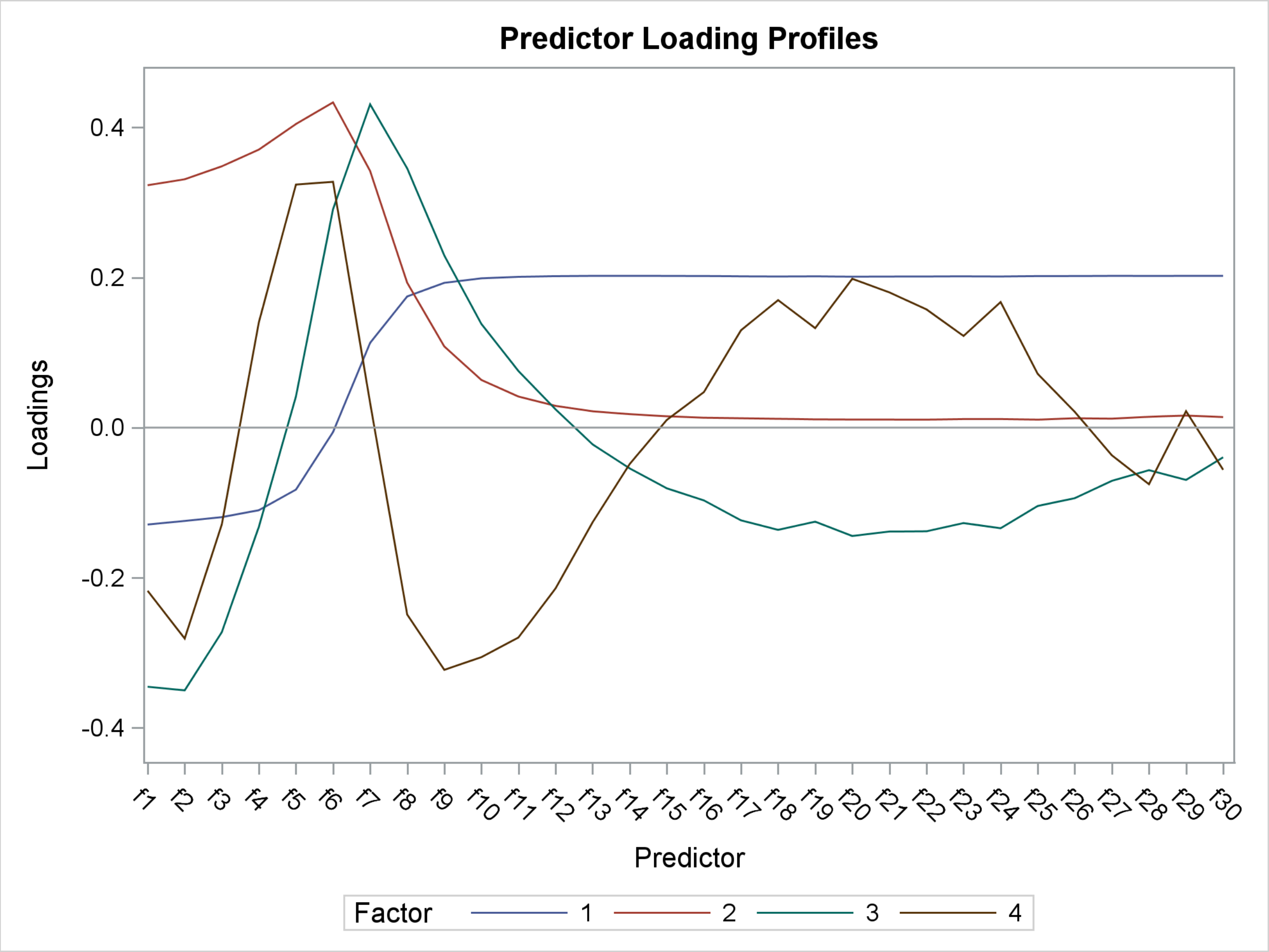


The factor loadings show how the PLS factors are constructed from the centered and scaled predictors. For spectral calibration, it is useful to plot the loadings against the frequency. In many cases, the physical meanings that can be attached to factor loadings help to validate the scientific interpretation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

```
proc pls data=ftrain nfac=4 plot=XLoadingProfiles;
   model tot_log tyr_log try_log = f1-f30;
run;

ods graphics off;
```

The resulting plot is shown in Output 90.3.5.

Output 90.3.5 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 approximately a weighted sum of only the frequencies in the first set.

Example 90.4: Partial Least Squares Spline Smoothing

The EFFECT statement makes it easy to construct a wide variety of linear models. In particular, you can use the spline effect to add smoothing terms to a model. A particular benefit of using spline effects in PROC PLS is that, when operating on spline basis functions, the partial least squares algorithm effectively chooses the amount of smoothing automatically, especially if you combine it with cross validation for the selecting the number of factors. This example employs the EFFECT statement to demonstrate partial least squares spline smoothing of agricultural data.

Weibe (1935) presents data from a study of uniformity of wheat yields over a certain rectangular plot of land. The following statements read these wheat yield measurements, indexed by row and column distances, into the SAS data set Wheat:

```
data Wheat;
   keep Row Column Yield;
   input Yield @@;
   iRow = int((_N_-1)/12);
   iCol = mod( _N_-1 ,12);
   Column = iCol*15 + 1; /* Column distance, in feet */
   Row    = iRow* 1 + 1; /* Row    distance, in feet */
   Row = 125 - Row + 1;  /* Invert rows              */
   datalines;
 715 595 580 580 615 610 540 515 557 665 560 612
 770 710 655 675 700 690 565 585 550 574 511 618
 760 715 690 690 655 725 665 640 665 705 644 705
 665 615 685 555 585 630 550 520 553 616 573 570
 755 730 670 580 545 620 580 525 495 565 599 612
 745 670 585 560 550 710 590 545 538 587 600 664
 645 690 550 520 450 630 535 505 530 536 611 578
 585 495 455 470 445 555 500 450 420 461 531 559

   ... more lines ...

 570 585 635 765 550 675 765 620 608 705 677 660
 505 500 580 655 470 565 570 555 537 585 589 619
 465 430 510 680 460 600 670 615 620 594 616 784
;
```

The following statements use the PLS procedure to smooth these wheat yields using two spline effects, one for rows and another for columns, in addition to their crossproduct. Each spline effect has, by default, seven basis columns; thus their crossproduct has $49 = 7^2$ columns, for a total of 63 parameters in the full linear model. However, the predictive PLS model does not actually need to have 63 degrees of freedom. Rather, the degree of smoothing is controlled by the number of PLS factors, which in this case is chosen automatically by random subset validation with the CV=RANDOM option.

```
ods graphics on;

proc pls data=Wheat cv=random(seed=1) cvtest(seed=12345)
         plot(only)=contourfit(obs=gradient);
   effect splCol = spline(Column);
   effect splRow = spline(Row   );
   model Yield = splCol|splRow;
run;
```

These statements produce the output shown in Output 90.4.1 through Output 90.4.4.

Output 90.4.1 Default Spline Basis: Model and Data Information

The PLS Procedure

Data Set	WORK.WHEAT
Factor Extraction Method	Partial Least Squares
PLS Algorithm	NIPALS
Number of Response Variables	1
Number of Predictor Parameters	63
Missing Value Handling	Exclude
Maximum Number of Factors	15
Validation Method	10-fold Random Subset Validation
Random Subset Seed	1
Validation Testing Criterion	Prob T**2 > 0.1
Number of Random Permutations	1000
Random Permutation Seed	12345

Number of Observations Read	1500
Number of Observations Used	1500

Output 90.4.2 Default Spline Basis: Random Subset Validated PRESS Statistics for Number of Factors

Random Subset Validation for the Number of Extracted Factors

Number of Extracted Factors	Root Mean PRESS	T**2	Prob > T**2
0	1.066355	251.8793	<.0001
1	0.826177	123.8161	<.0001
2	0.745877	61.6035	<.0001
3	0.725181	44.99644	<.0001
4	0.701464	23.20199	<.0001
5	0.687164	8.369711	0.0030
6	0.683917	8.775847	0.0010
7	0.677969	2.907019	0.0830
8	0.676423	2.190871	0.1340
9	0.676966	3.191284	0.0600
10	0.675026	1.334638	0.2390
11	0.673906	0.556455	0.4470
12	0.673653	1.257292	0.2790
13	0.672669	0	1.0000
14	0.673596	2.386014	0.1190
15	0.672828	0.02962	0.8820

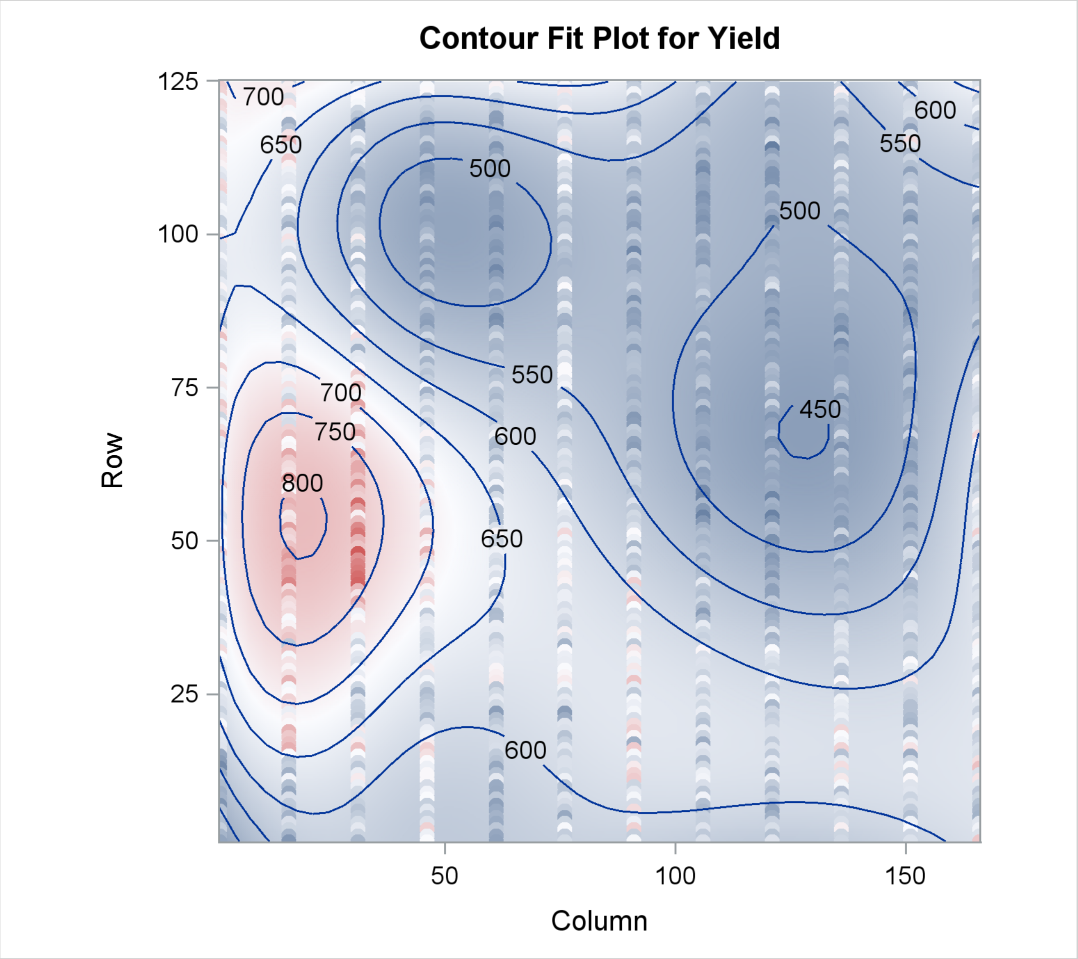
Minimum root mean PRESS	0.6727
Minimizing number of factors	13
Smallest number of factors with p > 0.1	8

Output 90.4.3 Default Spline Basis: PLS Variation Summary for Split-Sample Validated Model

Percent Variation Accounted for by Partial Least Squares Factors

	Model Effects		Dependent Variables	
Number of Extracted Factors	**Current**	**Total**	**Current**	**Total**
1	11.5269	11.5269	40.2471	40.2471
2	7.2314	18.7583	10.4908	50.7379
3	6.9147	25.6730	2.6523	53.3902
4	3.8433	29.5163	2.8806	56.2708
5	6.4795	35.9958	1.3197	57.5905
6	7.6201	43.6159	1.1700	58.7605
7	7.3214	50.9373	0.7186	59.4790
8	4.8363	55.7736	0.4548	59.9339

Output 90.4.4 Default Spline Basis: Smoothed Yield



The cross validation results in Output 90.4.2 point to a model with eight PLS factors; this is the smallest model whose predicted residual sum of squares (PRESS) is insignificantly different from the model with the absolute minimum PRESS. The variation summary in Output 90.4.3 shows that this model accounts for about 60% of the variation in the Yield values. The OBS=GRADIENT suboption for the PLOT=CONTOURFIT option specifies that the observations in the resulting plot, Output 90.4.4, be colored according to the same scheme as the surface of predicted yield. This coloration enables you to easily tell which observations are above the surface of predicted yield and which are below.

The surface of predicted yield is somewhat smoother than what Weibe (1935) settled on originally, with a predominance of simple, elliptically shaped contours. You can easily specify a potentially more granular model by increasing the number of knots in the spline bases. Even though the more granular model increases the number of predictor parameters, cross validation can still protect you from overfitting the data. The following statements are the same as those shown before, except that the spline effects now have twice as many basis functions:

```
ods graphics on;

proc pls data=Wheat cv=random(seed=1) cvtest(seed=12345)
         plot(only)=contourfit(obs=gradient);
   effect splCol = spline(Column / knotmethod=equal(14));
   effect splRow = spline(Row    / knotmethod=equal(14));
   model Yield = splCol|splRow;
run;
```

The resulting output is shown in Output 90.4.5 through Output 90.4.8.

Output 90.4.5 More Granular Spline Basis: Model and Data Information

The PLS Procedure

Data Set	WORK.WHEAT
Factor Extraction Method	Partial Least Squares
PLS Algorithm	NIPALS
Number of Response Variables	1
Number of Predictor Parameters	360
Missing Value Handling	Exclude
Maximum Number of Factors	15
Validation Method	10-fold Random Subset Validation
Random Subset Seed	1
Validation Testing Criterion	Prob T**2 > 0.1
Number of Random Permutations	1000
Random Permutation Seed	12345

Number of Observations Read	1500
Number of Observations Used	1500

Output 90.4.6 More Granular Spline Basis: Random Subset Validated PRESS Statistics for Number of Factors

Random Subset Validation for the Number of Extracted Factors

Number of Extracted Factors	Root Mean PRESS	T**2	Prob > T**2
0	1.066355	247.9268	<.0001
1	0.652658	20.68858	<.0001
2	0.615087	0.074822	0.7740
3	0.614128	0	1.0000
4	0.615268	0.197678	0.6490
5	0.618001	1.372038	0.2340
6	0.622949	5.035504	0.0180
7	0.626482	7.296797	0.0080
8	0.633316	13.66045	<.0001
9	0.635239	16.16922	<.0001
10	0.636938	18.02295	<.0001
11	0.636494	16.9881	<.0001
12	0.63682	16.83341	<.0001
13	0.637719	16.74157	<.0001
14	0.637627	15.79342	<.0001
15	0.638431	16.12327	<.0001

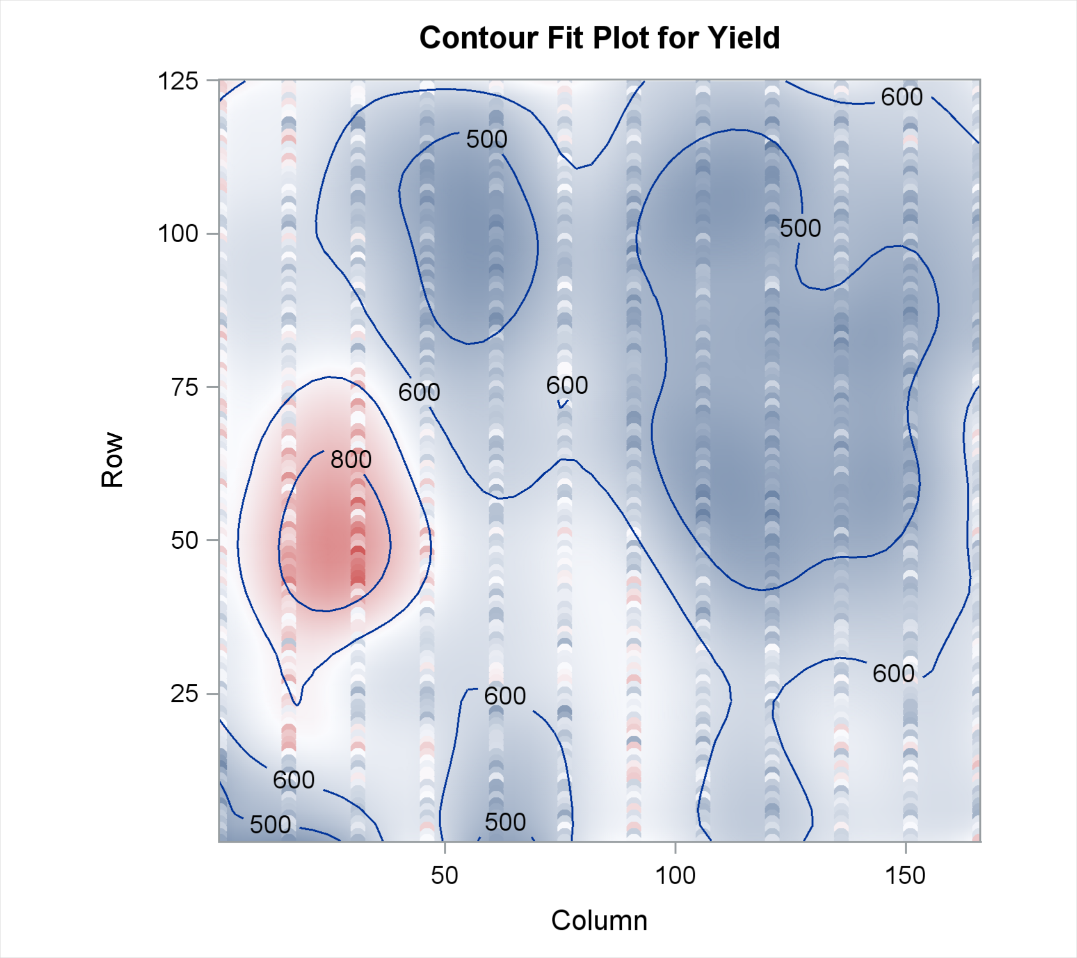
Minimum root mean PRESS	0.6141
Minimizing number of factors	3
Smallest number of factors with p > 0.1	2

Output 90.4.7 More Granular Spline Basis: PLS Variation Summary for Split-Sample Validated Model

Percent Variation Accounted for by Partial Least Squares Factors

	Model Effects		Dependent Variables	
Number of Extracted Factors	**Current**	**Total**	**Current**	**Total**
1	1.7967	1.7967	64.7792	64.7792
2	1.3719	3.1687	6.3163	71.0955

Output 90.4.8 More Granular Spline Basis: Smoothed Yield



Output 90.4.5 shows that the model now has 360 parameters, many more than before. In Output 90.4.6 you can see that with more granular spline effects, fewer PLS factors are required—only two, in fact. However, Output 90.4.7 shows that this model now accounts for over 70% of the variation in the Yield values, and the contours of predicted values in Output 90.4.8 are less inclined to be simple elliptical shapes.

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