# Informative score-loading-contribution plots for multi-response process monitoring

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### Abstract

The projection based multivariate data methods of principal component regression (PCR) and partial least squares regression (PLSR) are well established in the field of process monitoring. Use of score and loading plots for visualization is, however, complicated when many components are required for good predictions, and the information is therefore often compressed into less informative $T^2$ and contribution plots. The score information may, however, be further compressed by projection onto subspaces spanned by the vectors of prediction coefficients for the response variables. This is especially attractive in the case of two response variables, i.e. when the model reduction results in a single score-loading biplot. Contribution vectors for the process variables, as well as a confidence ellipse, may also be included in such a plot. As illustrated in an industrial data example, such a score-loading-contribution plot provides means of both failure detection and fault diagnosis.

**Keywords:** process monitoring, model reduction, score-loading-contribution plots

## 1 Introduction

The projection based multivariate data methods of principal component regression (PCR) and partial least squares regression (PLSR) are well established in the field of process monitoring [1,2]. The basic problem is then to predict one or more primary response variables from a number of measured secondary process variables. These response variables are typically product qualities that cannot be measured online, and due to many correlated process measurements the regression problem is often ill-posed.

The strength of PCR and PLSR as compared with other regression methods, is the visualization possibilities given by use of score and loading plots, often combined in score-loading biplots with corresponding score and loading directions [3]. Such visualizations are absolutely essential in process monitoring applications, where causes for process upsets and not only prediction of the responses are of interest. The interpretation of these plots are, however, often made difficult by the fact that more than two PCR or PLSR components are necessary in order to obtain good predictions. Thus many biplots may have to be monitored simultaneously, and the coordination of this information is obviously difficult. Another possibility is to compress the process data into less informative Hotelling's $T^2$ plots. In order to see which process variables that are involved in detected process upsets, intricate contribution plots also have to be designed and interpreted [1,2].

The basic insight utilized in the present paper is that the number of components for prediction and visualization need not be the same. The reduction of number of components is the major result of the often rather cumbersome orthogonal signal correction (OSC) methods, e.g. the OPLS algorithm [4], or

equivalent and more straightforward similarity transformation methods [5]. As a result of the similarity transformation in Reference [5], the original loadings are projected onto the subspace spanned by the fitted response vectors in $\hat{\mathbf{Y}}$. Another possibility for model reduction is to project all original PCR or PLSR scores onto subspaces spanned by the vectors of prediction coefficients in $\hat{\mathbf{B}}$. This was suggested already in Reference [6], and it has been used in definitions of the net analytic signal (NAS) [7,8,9]. An example related to process monitoring is the 2PLS algorithm presented in Reference [10], where the projection subplane includes $\hat{\mathbf{b}}$, and a more general treatment is given in Reference [11]. Such score projections are especially attractive with two responses, in which case the minimum number of two components is obtained by projection upon the plane spanned by the two coefficient vectors, and the present paper focuses on this case. A process monitoring application of the 2PLS algorithm is presented earlier [12], and the present paper may be seen as an extension of that. A similar example, also with one response variable only, is given in Reference [13].

In the present paper I will first recapitulate how any number of PCR or PLSR components can be reduced to the number of responses, without loss of prediction capability. Specifically will two responses require two final components only, and thus one final score plot and one final loading plot only. Using correspondence properties [3], I will then show how these plots may be combined in an informative score-loading biplot, where the contribution to scores from the different regressor variables can also be shown as contribution vectors. The result is an informative score-loading-contribution plot, where also axes for the two responses and a confidence ellipse for the score positions may be included.

In summary the proposed monitoring method for industrial processes with two response variables involves projections in two steps:

1. Projection of objects (rows) in the $\mathbf{X}$ matrix onto space defined by loading or loading weights vectors found by PCR or PLSR. With more than two components, we may here have deviations in several dimensions. As a result there is a need for a statistical $T^2$-plot in order to find out-of-control situations, and a special contribution plot in order to see which variables that are causing the deviations.

2. Further projections of the PCR or PLSR scores onto plane defined by $\hat{\mathbf{b}}_1$ and $\hat{\mathbf{b}}_2$. Here we will have deviations in two dimensions only, and the $T^2$-plot may thus be replaced by a confidence ellipse in the score-loading plot, while the influence from the different variables may be shown by contribution vectors in the same plot.

The theoretical development is finally illustrated by use of industrial data from a mineral processing plant.

## 2  Theory

**Latent variables model**

With several responses $y_1$, $y_2$ ... $y_m$ and any number of process variables $x_1$, $x_2$, ... $x_p$, a principal component decomposition of the calibration $\mathbf{X}$ data results in the latent variables PCR model

$$\mathbf{Y} = \mathbf{TQ}^T + \mathbf{F} \tag{1}$$
$$\mathbf{X} = \mathbf{TP}^T + \mathbf{E}. \tag{2}$$

Alternatively one may use a non-orthogonalized PLSR model with different matrices $\mathbf{T}$, $\mathbf{Q}$, $\mathbf{F}$ and $\mathbf{E}$, and with $\mathbf{P}$ replaced by $\mathbf{W}$ [14]. These two models exhibit total score-loading correspondence, as opposed to the standard PLSR model using orthogonalized scores [3]. With more than one response variable a PLSR model must be of the PLS2 type, which will often result in inferior predictions as compared with a PCR model. The drawback with PCR, on the other hand, is traditionally considered to be the normally higher number of components. Since we in either case will reduce the number of components to two, we here assume the PCR model (1,2). With few calibration samples, however, the parameter bias will be

lower with few original components [15], and with comparable prediction capabilities a PLS2 model may then be the best choice.

From Eqs. (1) and (2) follow the least squares (LS) solutions $\hat{\mathbf{Q}}^T = \left(\mathbf{T}^T\mathbf{T}\right)^{-1}\mathbf{T}^T\mathbf{Y}$ and $\hat{\mathbf{T}} = \mathbf{XP}\left(\mathbf{P}^T\mathbf{P}\right)^{-1} = \mathbf{XP}$, and with $\hat{\mathbf{Y}} = \mathbf{X}\hat{\mathbf{B}}$ thus follows that the regression coefficients are given by

$$\hat{\mathbf{B}} = \mathbf{P}\left(\mathbf{P}^T\mathbf{X}^T\mathbf{XP}\right)^{-1}\mathbf{P}^T\mathbf{X}^T\mathbf{Y}. \tag{3}$$

**Model reduction**

We shall now focus on the specific case with two response variables, and thus two coefficient vectors, and use the plane spanned by $\hat{\mathbf{b}}_1$ and $\hat{\mathbf{b}}_2$ as projection subspace. In this plane we may define two new unit loading vectors $\tilde{\mathbf{p}}_1$ and $\tilde{\mathbf{p}}_2$, as shown in Fig. 1.
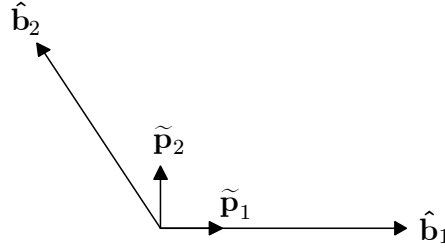


Figure 1. New unit loading vectors in subspace spanned by $\hat{b}_1$ and $\hat{b}_2$.

Projection of the original scores onto the plane spanned by $\tilde{\mathbf{P}} = \left[\begin{array}{cc} \tilde{\mathbf{p}}_1 & \tilde{\mathbf{p}}_2 \end{array}\right]$ results in a reduced model with two components only,

$$\mathbf{Y} = \tilde{\mathbf{T}}\tilde{\mathbf{Q}}^T + \mathbf{F} \tag{4}$$

$$\mathbf{X} = \tilde{\mathbf{T}}\tilde{\mathbf{P}}^T + \mathbf{E}, \tag{5}$$

where $\tilde{\mathbf{T}} = \mathbf{X}\tilde{\mathbf{P}}$, just as we for the original model (1,2) have $\mathbf{T} = \mathbf{XP}$. In the same way as $\hat{\mathbf{B}}$ in Eq. (3) is found from the original model (1,2), the reduced model (4,5) gives

$$\tilde{\mathbf{B}} = \left[\begin{array}{cc} \tilde{\mathbf{b}}_1 & \tilde{\mathbf{b}}_2 \end{array}\right] = \tilde{\mathbf{P}}\left(\tilde{\mathbf{P}}^T\mathbf{X}^T\mathbf{X}\tilde{\mathbf{P}}\right)^{-1}\tilde{\mathbf{P}}^T\mathbf{X}^T\left[\begin{array}{cc} \mathbf{y}_1 & \mathbf{y}_2 \end{array}\right]. \tag{6}$$

It is, however, straightforward to show that $\tilde{\mathbf{B}} = \hat{\mathbf{B}}$:

**Theorem 1** *The coefficient matrix $\tilde{\mathbf{B}}$ in Eq. (6) is identical with the coefficient matrix $\hat{\mathbf{B}}$ in Eq. (3).*

**Proof.** From the definition of $\tilde{\mathbf{P}}$ according to Fig. 1 follows that $\tilde{\mathbf{P}} = \hat{\mathbf{B}}\mathbf{M}$, where $\mathbf{M}$ is an invertible transformation matrix. From Eqs. (6) and (3), with $\left(\mathbf{P}^T\mathbf{X}^T\mathbf{XP}\right)^{-1} = (\cdot)^{-1}$, thus follows

$$\begin{aligned} \tilde{\mathbf{B}} &= \hat{\mathbf{B}}\mathbf{M}\left(\mathbf{M}^T\hat{\mathbf{B}}^T\mathbf{X}^T\mathbf{X}\hat{\mathbf{B}}\mathbf{M}\right)^{-1}\mathbf{M}^T\hat{\mathbf{B}}^T\mathbf{X}^T\mathbf{Y} = \hat{\mathbf{B}}\left(\hat{\mathbf{B}}^T\mathbf{X}^T\mathbf{X}\hat{\mathbf{B}}\right)^{-1}\hat{\mathbf{B}}^T\mathbf{X}^T\mathbf{Y} \\ &= \mathbf{P}\left(\cdot\right)^{-1}\mathbf{P}^T\mathbf{X}^T\mathbf{Y}\left(\mathbf{Y}^T\mathbf{XP}\left(\cdot\right)^{-1}\mathbf{P}^T\mathbf{X}^T\mathbf{XP}\left(\cdot\right)^{-1}\mathbf{P}^T\mathbf{X}^T\mathbf{Y}\right)^{-1}\mathbf{Y}^T\mathbf{XP}\left(\cdot\right)^{-1}\mathbf{P}^T\mathbf{X}^T\mathbf{Y} \\ &= \mathbf{P}\left(\mathbf{P}^T\mathbf{X}^T\mathbf{XP}\right)^{-1}\mathbf{P}^T\mathbf{X}^T\mathbf{Y} = \hat{\mathbf{B}}. \end{aligned} \tag{7}$$

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Note that although the theorem is valid also for PLS2 models, it is not valid for a set of PLS1 models for the different responses. The reason for this is that the coefficient vectors then are located in different subspaces. For the same reason the theorem is not valid for a set of individual PCR models with different numbers of components. For a more thorough discussion and a more general theorem, see Reference [11].

**Score-loading correspondence and contribution vectors**

Since $\tilde{\mathbf{T}} = \mathbf{X}\tilde{\mathbf{P}}$, where $\tilde{\mathbf{P}}$ is orthonormal, there is total score-loading correspondence [3]. A future process deviation $\Delta\mathbf{x}^T = \begin{bmatrix} 0 & \cdots & 0 & \Delta x_{ij} & 0 & \cdots & 0 \end{bmatrix}$ caused by a single variable will thus result in a score position

$$\begin{bmatrix} \Delta t_{i1} & \Delta t_{i2} \end{bmatrix} = \Delta x_{ij} \begin{bmatrix} \tilde{p}_{i1} & \tilde{p}_{i2} \end{bmatrix}. \tag{8}$$

From this follows that the size of the deviation is determined by the value of $\Delta x_{ij}$ (including sign) and the corresponding loadings in $\begin{bmatrix} \tilde{\mathbf{p}}_1 & \tilde{\mathbf{p}}_2 \end{bmatrix}$, while the direction is determined by the loadings only. This may be visualized by use of contribution vectors in the score-loading biplot, as illustrated in the industrial data example in Section 3.

**Score statistics**

A comparison of a new sample with the calibration data set can be done by use of the Hotelling's $T^2$ statistic [16] based on the estimated score covariance matrix, which with centered data and use of the model (4,5) is

$$S = \frac{1}{N-1}\tilde{\mathbf{T}}^T\tilde{\mathbf{T}}. \tag{9}$$

With centered data the $T^2$ statistic for a new sample is

$$T^2 = \mathbf{t}_{new}^T S^{-1}\mathbf{t}_{new}, \tag{10}$$

while the upper control limit for a new score based on $N$ past samples is

$$T_{UCL}^2 = \frac{2\left(N^2-1\right)}{N(N-2)}F_\alpha(2, N-2), \tag{11}$$

where $F_\alpha(2, N-2)$ is the upper $100\alpha$ % critical point of the F distribution with $(2, N-2)$ degrees of freedom [1,2].

With two components only, the upper control limit can be shown as a confidence ellipse in the score-loading-contribution plot, as illustrated in the industrial data example in Section 3. The confidence ellipse and the contribution vectors thus give both failure detection and fault diagnosis.

# 3  Industrial data example

The following example uses multivariate regression data from a mineral processing plant [17] (the 'cleaner' data, originally published in Reference [18]). The problem considered here is to predict two given response variables from twelve known process variables. For the purpose of finding an initial PCR factorization, samples 1 to 120 in the data sets xce and yce [17] were used for modeling, while samples 151 to 240 in the same data sets were used for validation. The data were centered and scaled to unit variance (autoscaled), and the result was a PCR model with $A = 10$ components, resulting in validation root mean square errors $RMSEP = 0.21$ and $RMSEP = 0.28$ for the two responses respectively (as compared with $RMSEP = 1$ for $A = 0$). The model (1,2) was finally compressed into the two-component model (4,5), resulting in a new loading matrix $\tilde{\mathbf{P}} = \begin{bmatrix} \tilde{\mathbf{p}}_1 & \tilde{\mathbf{p}}_2 \end{bmatrix}$ according to Fig. 1.

Before proceeding with the example it is appropriate with a note on abnormal samples. When an ordinary PCR or PLSR model is used in a process monitoring application, there is a need to check that new objects are not too far away from the projection subspace, as compared with the modeling samples. This is often done by use of a squared projection error (SPE) plot [12]. The situation is the same in the reduced model case, only that the subspace is now the plane defined by $\tilde{\mathbf{P}}$. As shown in reference [12], no such abnormal samples are present in the data used here.

A score-loading-contribution plot as described in Section 2 is shown in Fig. 2, with skewed axes according to the true covariance between the response variables $\hat{\mathbf{y}}_1$ and $\hat{\mathbf{y}}_2$ (the vertical axis to the left is thus irrelevant). The directions of the loadings are here shown by asterisks placed in a normalized

distance from the origin, while the variable contributions are shown by radial vector lines out from the origin. In the projection plane according to Fig. 1, only variables number 1, 2, 3 and 8 give significant contributions to the score, while the rest of the twelve variables have very little to say (for clarity they are therefore omitted in Fig. 2). The confidence ellipse is computed according Eq. (11), with $\alpha = 0.01$. The score for sample number 207 is marked by a dot-filled square, while older scores are shown by dots connected by dashed lines. The asterisk-filled circles show the response variable values for the last sample. For this specific sample, variables number 1 and 3 have negative values (pushing the score away from the loadings), while variables number 2 and 8 have positive values (attracting the score towards the loadings). Note that the sum of the contribution vectors gives the score position (exactly when all the twelve contribution vectors are included).
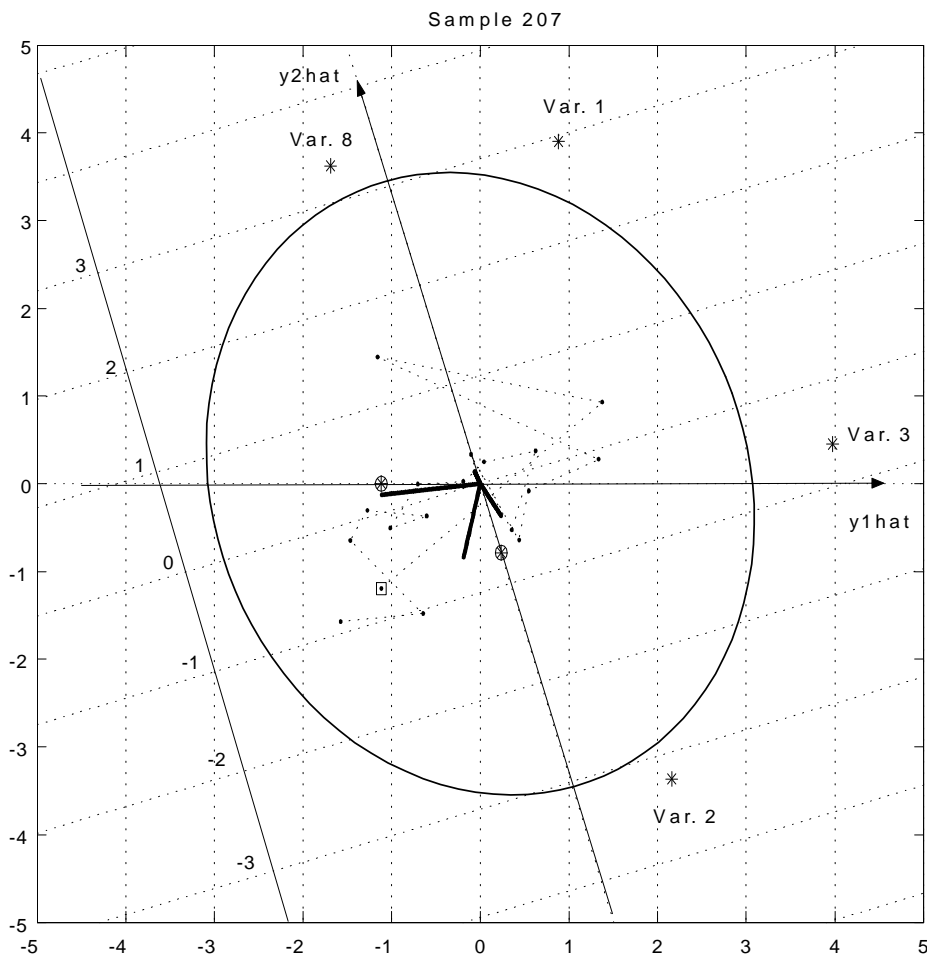


Figure 2. Score-loading-contribution plot for in-control situation, with skewed axes according to the true covariance between the response variables (the vertical axis to the left is irrelevant). See also explanation in text.

The plot two samples later is shown in Fig. 3. A process operator will now see that the score is moving outside the confidence ellipse, and that this primarily is caused by large positive values of variables 2 and 3. If this is the situation also for scores that follow, corrective action has to be taken.
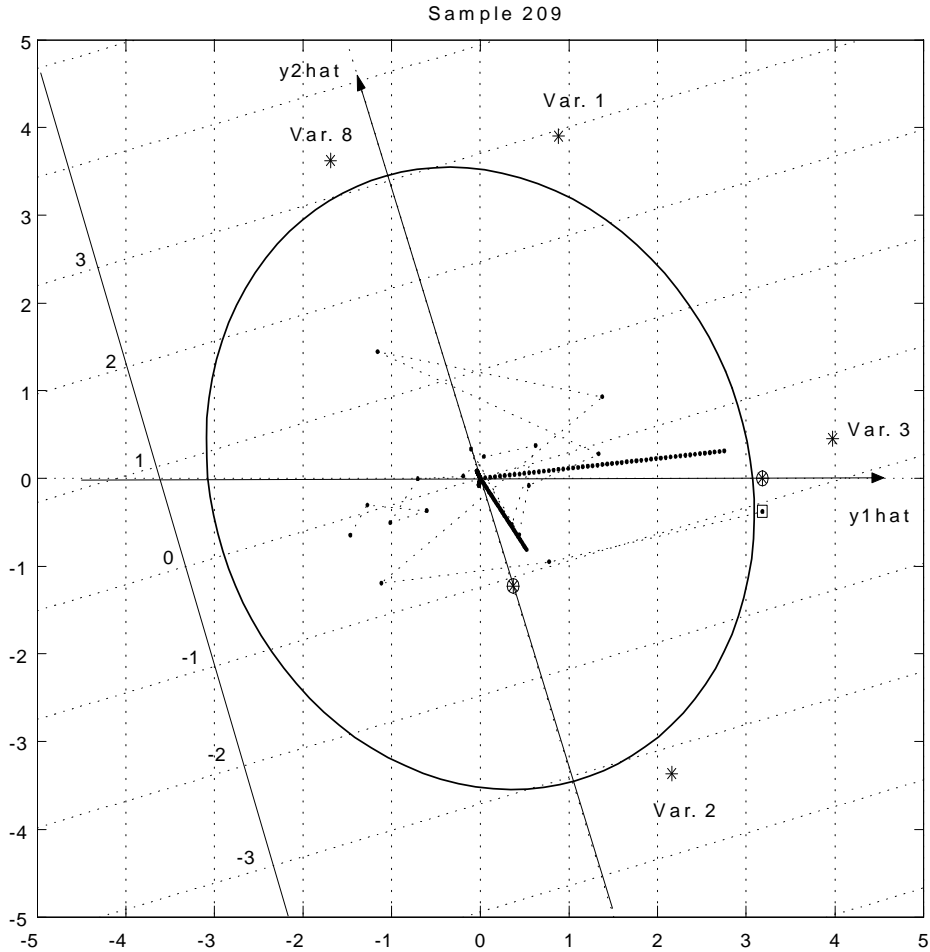
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Figure 3. Score-loading-contribution plot for potential out-of-control situation.

Finally note that the plots in Figs. 2 and 3 could be shown with orthogonal axes for the two response variables, which might make the situation easier for a process operator. That would, however, give a false impression of independent response variables.

# 4 Conclusions

For the case with two response variables, score projections onto a plane spanned by the two PCR coefficient vectors and use of two orthogonal loading vectors in that plane, result in a reduced model with two components and single score and loading plots with exact correspondence. In the score-loading biplot the position of the score will thus be exactly determined by contribution vectors for the regressor variables. For the general case with $m$ response variables, the corresponding projection subspace is spanned by the $m$ coefficient vectors.

With two response variables, a confidence ellipse for failure detection may be added to the score-loading-contribution plot. When a failure is detected, the contribution vectors provide fault diagnosis.

The theory is valid also for non-orthogonalized PLS2 models, while use of separate non-orthogonalized PLS1 models give only approximate results. The reason for this is that the two coefficient vectors then will be located in different subspaces. This is the case also for a set of individual PCR models using different numbers of components.

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