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SHORT COMMUNICATION

Deflation in multiblock PLS

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SUMMARY

This paper describes some of the deflation problems in multiblock PLS. Deflation of **X** using block scores leads to inferior prediction of **Y**. Deflation of **X** using super scores gives the same predictions as standard PLS with all variables in one large *X*-block, but the information of the separate blocks gets mixed up owing to the deflation of **X**. If **Y** is deflated using the super score instead, these problems disappear. Copyright © 2001 John Wiley & Sons, Ltd.

KEY WORDS: multivariate regression; partial least squares; hierarchical model

INTRODUCTION

Multiblock PLS is an extension of standard PLS that can be used if additional information is available for blocking the variables into conceptually meaningful blocks. If process variables are obtained from different parts of the process, if two or more different spectroscopic methods have been used to analyze the same samples, or if two-way and three-way or multiway blocks of the same samples are combined for the prediction of **Y**, multiblock regression methods may be superior to single-block regression models with respect to interpretability. Multiblock PLS gives improved interpretation compared to standard PLS, where all variables are kept in one large block, because it is possible to zoom into separate blocks using the block scores calculated for each block. The block scores give information on the relation of the specific block with **Y** in the presence of the other blocks. If the only purpose of the model is to predict a future value of **Y** using predictor variables from several blocks, experience shows that no improvement is obtained if the variables are blocked. Geladi [1] already suggested that, in order to do predictions, it is better to combine all variables in one large *X*-block. In fact, Westerhuis *et al.* [2] showed that a specific variant of multiblock PLS equals the PLS model with all variables combined into a large *X*-block.

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In 1988, Wangen and Kowalski [3] introduced a multiblock PLS algorithm that was based on an algorithm originally presented by Wold *et al.* [4]. This algorithm can handle many types of pathway relationships between the blocks. Applications using this algorithm include the modeling of process variables that were blocked according to the part of the plant from which they were obtained [5], the modeling of contaminants in a river where samples of different sites were obtained [6], and the modeling of a pharmaceutical granulation process in which granule properties were separated from the composition of the powder mixture to predict physical properties of the final pharmaceutical tablets [7].

Different algorithms can be used to calculate the multiblock PLS model, and the deflation step plays a crucial part in the difference. Westerhuis *et al.* [2,7] showed that the block score deflation, as was suggested by Wangen and Kowalski [3], led to inferior prediction. They suggested a different way of deflation (super score deflation) and showed that this gave the same results as when all variables were kept in a large *X*-block and a standard PLS model was built [2]. The super scores summarize the information contained in all blocks, whereas the block scores summarize the information of a specific block. However, in the present paper it will be shown that the super score deflation method mixes variation between the separated blocks and therefore leads to interpretation problems. In order to overcome the mixing up of the blocks, it is necessary to only deflate **Y** using the super scores. This leads to the same predictions as with super score deflation of **X** [8], but because **X** is not deflated, the information in the blocks is not mixed up.

In the Theory section of this paper, three deflation methods (block score deflation of **X**, super score deflation of **X** and super score deflation of **Y**) will be discussed. Using data from a pharmaceutical granulation process, it will be shown how these deflation methods affect the prediction of **Y** and the interpretation of the different *X*-blocks.

THEORY

Many multiblock PLS algorithms have been presented in the literature [2,3,6,7,9–11]. Westerhuis *et al.* [7] presented algorithms for multiblock PLS using block score deflation of **X** as well as super score deflation of **X**. They showed that the block score deflation method leads to lower fit and poorer prediction of **Y** than the super score deflation method. Furthermore, it was proven that using the super score deflation in multiblock PLS is identical to performing a standard PLS with all predictor variables in one block [2]. The simplest and fastest way therefore to develop a multiblock PLS model is to first calculate the standard PLS model using all data and then calculate the multiblock parameters from this model. Algorithm 1 shows the way to calculate the multiblock PLS parameters from the standard PLS model.

Algorithm 1. Calculation of multiblock parameters from standard PLS model

1 Calculate a standard one-component PLS model between $\mathbf{X} = [\mathbf{X}_1,\ldots,\mathbf{X}_B]$ and **Y**. The scores **t** and **u**, weight **w** and loadings **p** and **q** are obtained. From these the multiblock PLS block weights $\mathbf{w}_b$, the super weights **ws** and the block scores $\mathbf{t}_b$ are obtained.
2 $\mathbf{w}_b = \mathbf{w}(b)/||\mathbf{w}(b)||^2$
3 $\mathbf{t}_b = \mathbf{X}_b\mathbf{w}_b$
4 $ws(b) = \mathbf{t}_b^{\mathrm{T}}\mathbf{u}/\mathbf{u}^{\mathrm{T}}\mathbf{u}$
5 $\mathbf{ws} = \mathbf{ws}/||\mathbf{ws}||^2$

Block score deflation
6a $\mathbf{p}_b = \mathbf{X}_b^{\mathrm{T}}\mathbf{t}_b/\mathbf{t}_b^{\mathrm{T}}\mathbf{t}_b$
7a $\mathbf{E}_b = \mathbf{X}_b - \mathbf{t}_b\mathbf{p}_b$

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8a $\mathbf{F} = \mathbf{Y} - \mathbf{tq}$

Super score deflation
6b $\mathbf{E}_b = \mathbf{X}_b - \mathbf{tp}(b)^{\mathrm{T}}$
7b $\mathbf{F} = \mathbf{Y} - \mathbf{tq}$

For additional components, set $\mathbf{X} = [\mathbf{E}_1,\ldots,\mathbf{E}_B]$ and $\mathbf{Y} = \mathbf{F}$ and go back to step 1.

Algorithm 1 assumes only one *Y*-block and multiple *X*-blocks, $\mathbf{X}_b$, $b = 1,\ldots,B$. The ideas can easily be extended to multiple *Y*-blocks. Here $\mathbf{X} = [\mathbf{X}_1,\ldots,\mathbf{X}_B]$, $\mathbf{E} = [\mathbf{E}_1,\ldots,\mathbf{E}_B]$ and $||\mathbf{w}(b)||^2$ equals the Frobenius norm of $\mathbf{w}(b)$, which is the only part of the standard PLS weight $\mathbf{w}$ that corresponds to the variables in block $\mathbf{X}_b$. Note that, in this notation, $\mathbf{p}(b)$ represent the part of the loading $\mathbf{p}$ that corresponds to block $\mathbf{X}_b$, and $\mathbf{p}_b$ represents the whole block loading for block $\mathbf{X}_b$.

The first step in building a multiblock PLS model is to calculate a standard one-component PLS with all variables combined in a single *X*-block. The scores $\mathbf{t}$ and $\mathbf{u}$, weights $\mathbf{w}$ and loadings $\mathbf{p}$ and $\mathbf{q}$ are obtained. It has been shown previously that the score of the standard PLS model, $\mathbf{t}$, equals the super score of the multiblock model [2]. From the PLS weights $\mathbf{w}$ the block weights $\mathbf{w}_b$ are obtained in step 2. In step 3 the block scores $\mathbf{t}_b$ for block $\mathbf{X}_b$ are calculated. In steps 4 and 5 the super weights $\mathbf{ws}$ are obtained. The super weights relate the block scores to the super score

$$\mathbf{t} = \sum_{b=1}^{B} ws(b)\mathbf{t}_b \tag{1}$$

Here $ws(b)$ is the element of $\mathbf{ws}$ that corresponds to block $\mathbf{X}_b$. After the first component has been determined, the *X*-blocks have to be deflated. For the super score deflation of block $\mathbf{X}_b$ (step 6b) the score $\mathbf{t}$ and the part of the PLS loading that corresponds to block $\mathbf{X}_b$, $\mathbf{p}(b)$, can be used. For the block score deflation, new block loadings $\mathbf{p}_b$ are calculated and these are used together with the block scores $\mathbf{t}_b$ to deflate block $\mathbf{X}_b$ (steps 6a and 7a). For additional components the algorithm has to be started again with the deflated $\mathbf{E}$ and $\mathbf{F}$ instead of $\mathbf{X}$ and $\mathbf{Y}$.

Deflation

In standard PLS, deflation is performed to remove the information from a specific PLS component from $\mathbf{X}$ and $\mathbf{Y}$. After deflation, this information cannot appear in another component and thus deflation inherently takes care of the orthogonality of the scores. Different types of deflation can be used. In PLS it is possible to deflate only $\mathbf{X}$ or $\mathbf{Y}$ without changing the predictions [8].

In multiblock PLS, two types of scores are present, block scores $\mathbf{t}_b$ and super scores $\mathbf{t}$. Both can be used for the deflation of $\mathbf{X}$, but they lead to different results. The deflation of only $\mathbf{Y}$ using super scores is also possible in multiblock PLS. The differences between these different deflation steps will only appear after the deflation. Thus the first component is the same for all methods, and the differences only appear starting from the second component.

Deflation of $\mathbf{X}$ *using block scores*

If the block scores $\mathbf{t}_b$ are used for the deflation of $\mathbf{X}_b$, the block scores are orthogonal but the super scores may be correlated. The super score $\mathbf{t}$, which is a linear combination of the block scores (Equation (1)), is used for the prediction and deflation of $\mathbf{Y}$. Deflation of $\mathbf{Y}$ in this case is necessary, as opposed to standard PLS, because different blocks may carry similar information. The deflation prevents the same variation in $\mathbf{Y}$ from being predicted in different components from different blocks.

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Since, in most cases, $ws(1),\ldots,ws(b-1),ws(b+1),\ldots,ws(B) \neq 0$, $\mathbf{t}_b$ is different from $\mathbf{t}$. This means that some variation in the $\mathbf{t}_b$ direction is not used for prediction of $\mathbf{Y}$ but is removed from $\mathbf{X}_b$. This direction cannot be attained from block $\mathbf{X}_b$ for future components. If this direction is also not available in the other blocks, then this may lead to inferior prediction of $\mathbf{Y}$ [2,7].

Deflation of $\mathbf{X}$ *using super scores*

If the super scores are used for the deflation of $\mathbf{X}$, this gives exactly the same predictions as a standard PLS with all predictor variables in one large X-block [2]. In this case the super scores are orthogonal but the block scores can be correlated. However, they can easily be rotated to become orthogonal. For interpretation the block scores are usually examined to discover what happened in each specific block. Therefore the block scores are expected to only describe the situation within the block. Equation (2) shows the deflation step for the case of two X-blocks for block $\mathbf{X}_1$ using the super score $\mathbf{t}$:

$$\begin{aligned}\mathbf{E}_1 &= \mathbf{X}_1 - \mathbf{t}\mathbf{p}(1)^{\mathrm{T}}\\ \mathbf{E}_1 &= \mathbf{X}_1 - (\mathbf{t}_1 ws(1) + \mathbf{t}_2 ws(2))\mathbf{p}(1)^{\mathrm{T}}\\ \mathbf{E}_1 &= \mathbf{X}_1 - \mathbf{t}_1 ws(1)\mathbf{p}(1)^{\mathrm{T}} - \mathbf{t}_2 ws(2)\mathbf{p}(1)^{\mathrm{T}}\end{aligned} \tag{2}$$

Here $\mathbf{p}(1)$ is the part of the loading $\mathbf{p}$ corresponding to the variables in block $\mathbf{X}_1$. Equation (2) clearly shows that, owing to the deflation step, information from block $\mathbf{X}_2$ ($\mathbf{t}_2 ws(2)\mathbf{p}(1)^{\mathrm{T}}$) is subtracted from block $\mathbf{X}_1$. This means that, after the first deflation step, information from block $\mathbf{X}_2$, which was not present in block $\mathbf{X}_1$, is introduced in block $\mathbf{X}_1$. Thus new block scores of block $\mathbf{X}_1$ may carry information that originally was not present in block $\mathbf{X}_1$. In general, this means that after the first deflation step the information in each block is not solely due to the variables in that block, but also due to the variables in other blocks. This makes interpretation of the block scores rather difficult.

Deflation of $\mathbf{Y}$ *using super scores*

Dayal and MacGregor [8] showed for standard PLS models that instead of deflating both $\mathbf{X}$ and $\mathbf{Y}$ it is possible to only deflate $\mathbf{Y}$. This can easily be extended to the multiblock PLS method. Thus instead of steps 6a and 7a or step 6b in Algorithm 1, only the following deflation step, 6c, is used:

$$\mathbf{F} = \mathbf{Y} - \mathbf{t}\mathbf{q}^{\mathrm{T}} \tag{3}$$

Then, for calculating an additional component, $\mathbf{F}$ is used instead of $\mathbf{Y}$, and $\mathbf{X}$ can be used repeatedly. However, if only $\mathbf{Y}$ is deflated, an extra step is necessary in the PLS algorithm to calculate $\mathbf{t}$ directly from $\mathbf{X}$:

$$\mathbf{t} = \mathbf{X}\mathbf{r} \tag{4}$$

where $\mathbf{r}$ can be obtained from $\mathbf{w}$ and $\mathbf{p}$:

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$$\begin{aligned}
\mathbf{r}^{(1)} &= \mathbf{w}^{(1)} \\
\mathbf{r}^{(2)} &= \left(\mathbf{I} - \mathbf{w}^{(1)}\mathbf{p}^{(1)^{\mathrm{T}}}\right)\mathbf{w}^{(2)} \\
&\vdots \\
\mathbf{r}^{(A)} &= \left(\mathbf{I} - \mathbf{w}^{(1)}\mathbf{p}^{(1)^{\mathrm{T}}}\right)\left(\mathbf{I} - \mathbf{w}^{(2)}\mathbf{p}^{(2)^{\mathrm{T}}}\right)\ldots\left(\mathbf{I} - \mathbf{w}^{(A-1)}\mathbf{p}^{(A-1)^{\mathrm{T}}}\right)\mathbf{w}^{(A)}
\end{aligned} \tag{5}$$

Here $\mathbf{r}^{(1)}$, $\mathbf{w}^{(1)}$ and $\mathbf{p}^{(1)}$ are the **r, w** and **p** vectors from the first PLS component respectively and **I** is the identity matrix. Now the PLS scores $\mathbf{t}^{(1)}$ until $\mathbf{t}^{(A)}$ can be calculated from **X** without deflation of **X**:

$$\begin{aligned}
\mathbf{t}^{(1)} &= \mathbf{X}\mathbf{r}^{(1)} \\
&\vdots \\
\mathbf{t}^{(A)} &= \mathbf{X}\mathbf{r}^{(A)}
\end{aligned} \tag{6}$$

for the first until the Ath PLS component. If, in the standard PLS model, **r** is calculated from **w** and **p**, then the block scores $\mathbf{t}_b$ are calculated from the new block weights $\mathbf{r}_b$ of the multiblock model. Steps 2 and 3 in Algorithm 1 need to be changed to

$$2\mathbf{r}_b = \mathbf{r}(b)/\|\mathbf{r}(b)\|^2$$

$$3\mathbf{t}_b = \mathbf{X}_b\mathbf{r}_b$$

where $\mathbf{r}(b)$ is the part of **r** that corresponds to block $\mathbf{X}_b$. The block scores $\mathbf{t}_b$ and the super weights **ws** will then be different from those presented in Algorithm 1. Because **X** is not deflated, no information from one block goes into another block, as was the case with the super score deflation of **X**. Therefore the block scores only give information of the corresponding block, which makes interpretation much easier. Deflation of **Y** using super scores gives super scores that are orthogonal, but the block scores may be correlated.

EXPERIMENTAL

In order to show the deflation problem in multiblock PLS, data from the production of pharmaceutical tablets will be used. These data were described previously in the literature [12,13]. The preparation of pharmaceutical tablets may include a granulation step to improve the tableting properties of the powder blend. In wet granulation the powder mixture is blended with a binding agent, which makes the small particles stick together and form larger granules. After the mixing step the granules are dried and can be processed further into pharmaceutical tablets. In order to study the granulation and tableting behavior of a new powder mixture consisting of microcrystalline cellulose (MCC) and mannitol, experiments were performed according to an experimental design [12]. In the granulation step the concentration of MCC, the amount of water added, the concentration of the binding agent and the mixing time were varied. For the tableting step the moisture percentage still present in the granules and the compression force were varied. The intermediate granules were analyzed and the

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Table I. Numbers of paired experiments with exactly equal values in block $\mathbf{X}_2$ but different compression forces in block $\mathbf{X}_1$. The first numbers represent experiments with a compression force of 10 kN and the last ones with 30 kN

8, 9	14, 15	46, 47
10, 11	16, 17	48, 49
12, 13	18, 19	50, 51
	20, 21	53, 52

particle size distribution, the flow rate and the poured and tapped volumes were determined. Finally, the crushing strength of the tablets was measured.

RESULTS

In the multiblock model the experimental design variables were collected in block $\mathbf{X}_1$ and the granule properties were collected in block $\mathbf{X}_2$. Fifty-three different types of tablets were produced. Because of the set-up of the experimental design, some of the granules produced were tableted at two different compression forces, 10 and 30 kN. This means that there are pairs of experiments for which all the variables in block $\mathbf{X}_2$ have exactly the same values, and in block $\mathbf{X}_1$ only the compression force is different. The numbers of these paired experiments are shown in Table I. Thus, in experiments 8 and 9, tablets are produced from exactly the same granules, but a different compression force is used. Since for these paired experiments all variables have exactly the same values, the block scores of block $\mathbf{X}_2$ for these experiments are expected to be exactly equal. These block scores of block $\mathbf{X}_2$ are being studied with the three deflation methods described in the Theory section.

In the multiblock model, block $\mathbf{X}_1$ (53×12) consists of the six design variables and their squared terms, and block $\mathbf{X}_2$ (53×14) consists of 14 granule properties as described above. The crushing strength of the tablets is used as the response vector $\mathbf{y}$ (53×1).

Different multiblock PLS models were built in which block score deflation of $\mathbf{X}$ (model 1), super score deflation of $\mathbf{X}$ (model 2) or super score deflation of $\mathbf{y}$ (model 3) was used. Attention will be focused on the prediction of the crushing strength of the tablets and on the score plots of block scores of block $\mathbf{X}_2$ with the granule properties. The first model is a multiblock PLS model where block score deflation was used. In this case the block scores of $\mathbf{X}_2$ are orthogonal but the super scores are somewhat correlated. Table II shows that the fit (%$\mathbf{Y}$) and prediction (Q^2) of the crushing strength using model 1 are worse than the fit and prediction using model 2 with super score deflation of $\mathbf{X}$ and model 3 with super score deflation of $\mathbf{Y}$. This effect has been described before [2,7].

Table II. Fit and prediction results of the modeling of the granulation data using multiblock PLS with block score deflation of $\mathbf{X}$ (model 1), super score deflation of $\mathbf{X}$ (model 2) and super score deflation of $\mathbf{Y}$ (model 3). The variation explained in $\mathbf{X}_1$ (design variables), $\mathbf{X}_2$ (granule properties) and $\mathbf{Y}$ (tablet crushing strength) and the prediction of $\mathbf{Y}$ (Q^2) are given

	Model 1				Model 2				Model 3			
#lv	%$\mathbf{X}_1$	%$\mathbf{X}_2$	%$\mathbf{Y}$	Q^2	%$\mathbf{X}_1$	%$\mathbf{X}_2$	%$\mathbf{Y}$	Q^2	%$\mathbf{X}_1$	%$\mathbf{X}_2$	%$\mathbf{Y}$	Q^2
1	19	30	69	0·64	15	26	69	0·64	15	26	69	0·64
2	30	74	87	0·80	21	43	89	0·82	21	43	89	0·82
3	37	83	90	0·84	31	72	94	0·89	31	72	94	0·89

#lv = latent vectors.

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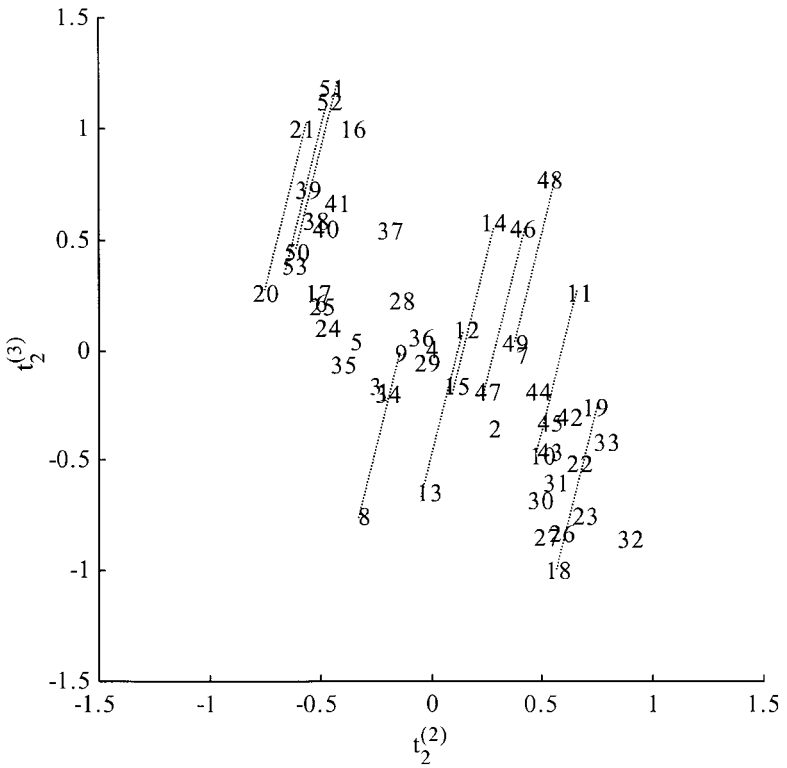


Figure 1. Score plot of block scores two and three of block $\mathbf{X}_2$ calculated using the super score deflation of $\mathbf{X}$. The dotted lines connect the pairs of experiments with exactly the same values for all variables in block $\mathbf{X}_2$. The score values for these pairs are different owing to the deflation method used.

Model 2 uses the super score deflation of $\mathbf{X}$, which produces correlated block scores, but now the super scores are orthogonal. This leads to the same fit as in the case of a standard PLS model, which is better than the fit of model 1. Figure 1 shows the score plot of block scores $\mathbf{t}_2^{(2)}$ and $\mathbf{t}_2^{(3)}$ of block $\mathbf{X}_2$. The particle size of the granules decreases from top left to bottom right in the score plot. The experiments with equal granule properties (see the pairs in Table I) have quite different score values in these block scores. The differences in score values between these pairs are marked in the figure with dotted lines. Experiments 8, 13 and 48 seem to be outside the main cluster, but they have exactly the same values for all variables in block $\mathbf{X}_2$ as experiments 9, 12 and 49 respectively. The only difference between these pairs is a compression force of 10 or 30 kN in block $\mathbf{X}_1$. Thus, owing to the deflation step, this difference in block $\mathbf{X}_1$ becomes visible in the score plot of block $\mathbf{X}_2$. The difference between the two experiments in each of the pairs is the same, because the only difference, which is the compression force in block $\mathbf{X}_1$, is constant for each of the paired observations. For other applications where the differences are not the same, the interpretation of the score plots becomes even more difficult.

The third model with super score deflation of only $\mathbf{y}$ gives exactly the same fit and prediction of $\mathbf{y}$ as model 2 with the super score deflation of $\mathbf{X}$. Figure 2 shows the block scores $\mathbf{t}_2^{(2)}$ and $\mathbf{t}_2^{(3)}$ for block $\mathbf{X}_2$ of model 3. This score plot is similar to the score plot using the super score deflation of $\mathbf{X}$ in Figure 1. Only small changes in the position of the experiments in the score plot can be observed. Again the particle size of the granules decreases from top left to bottom right in the score plot. However, the

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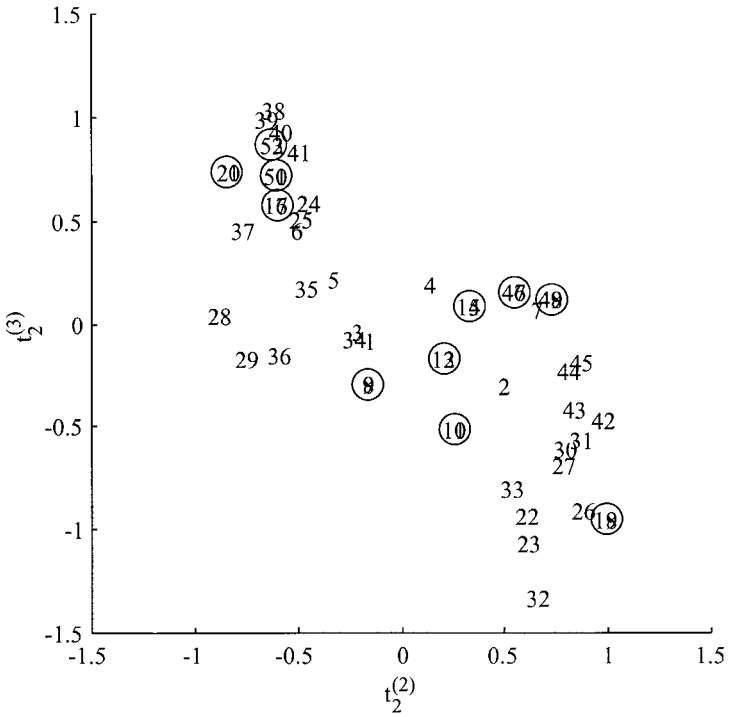


Figure 2. Score plot of block scores two and three of block $\mathbf{X}_2$ calculated using the super score deflation of $\mathbf{Y}$. The paired experiments now have exactly the same score values, indicated by circles. The information is not mixed up if deflation of $\mathbf{Y}$ is used.

difference is that with $\mathbf{y}$ deflation the experiments with the same values in block $\mathbf{X}_2$ (see Table I) also have exactly the same block score values. These pairs of experiments are marked with circles. The information of block $\mathbf{X}_1$ is not mixed up with the information of block $\mathbf{X}_2$. The paired experiments therefore are now correctly interpreted as being equal using this approach.

CONCLUSIONS

In this paper, some of the deflation problems of multiblock PLS have been addressed. If $\mathbf{X}$ is deflated using the block scores, inferior fit and predictions are obtained, because some information from the blocks is removed that is not used for prediction. If $\mathbf{X}$ is deflated using the super scores, then the information is mixed between the blocks. This leads to block scores that describe not only the information from their specific block but also information from other blocks. However, if, instead of $\mathbf{X}$, $\mathbf{Y}$ is deflated with the super scores, no information is mixed up and predictions remain equal to the standard PLS model with all variables in one large *X*-block. Therefore it is recommended that the deflation of $\mathbf{Y}$ is used in multiblock PLS models.

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