## PLS회귀를 이용한 포지셔닝맵의 구축

Building Positioning Map by PLS Regression

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## PLS회귀를 이용한 포지셔닝맵의 구축

## Building Positioning Map by PLS Regression

이성근•Yi, Seong Keun, 최지호•Choi, Jiho, 이종호•Lee, Jong-Ho

Partial Least Squares (PLS) 회귀 방법은 관찰치의 수보다 변수의 수가 더 많을 때 사용할 수 있는 다변량 분석기법이다. 뿐만 아니라 PLS회귀는 주성분을 추출할 때 반응변수와 설명변수를 동시에 고려하기 때문에 주 성분회귀분석보다 예측력이 더 우월하다. 이 논문에서는 PLS방법으로 얻어진 주성분에 각 변수(속성)를 회귀시 켜 각 변수의 벡터를 구하였으며, 각 주성분점수를 활용하여 관찰치(브랜드)들의 좌표를 구하여 각 관찰치들의 포지션을 지도상에 표시할 수 있도록 하였다. 얻어진 관찰치들의 포지션은 각 변수의 위치와 교차하여 해석할 수 있어 각 관찰치의 특성을 파악할 수 있으며, 각 설명변수들도 각 반응변수들과 어떻게 관계를 가질 수 있는가도 지도상에서 해석이 가능하다.

핵심주제어: PLS, Partial Least Squares, PLSR, PLS Regression, singular value decomposition PCR, Principal Component Regression

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#### Abstract

Partial Least Squares regression(PLSR) proposed by Herman Wold in 1966 has been used as very valuable method to predict a set of response variables by a set of explanatory variables. PLSR is very useful for building a predictive model when variables are many and highly correlated. Multiple regression analysis also useful tool for building a prediction model. But it has much limitation when variables are many and highly correlated. In such cases, even though we can build a prediction model, it will fail to predict new data well (Tobias, 2007). Especially when the number of variables is much larger than the number of observations, the phenomenon of so-called 'overfitting' occurs. When the explanatory variables are highly correlated, one approach to overcome the problem is to remove the some of highly correlated explanatory variables. Another approach is to reduce the explanatory variables into small number of variables which have no correlations. The concept of PLS is to extract small numbers of latent variables which explain for highly correlated many variables. In that sense, PLS is a indirect modelling. But the way of extracting latent variables is different from the traditional method,

The superiority of PLSR to PCR(Principal Component Regression) is very well known. Ryan et. al (1999) showed empirically that PLSR is better than PCR in prediction the response variable. They compared three models with mediators and collinearity among the response variables, for example, regression, PCR, and PLSR. As the hypothesized conceptual model had moderators and collinearity in their study, the regression model was not germane to the research objective. Hence their focus was on the comparison of PCR, with PLSR. Even though the fact that there was a difference in estimating the coefficients between PCR and PLSR was very confusing, But prediction of PLSR was better than PCR.

Even though PLSR began in social sciences, it's uses are extended to the various fields like chemometrics (Westerhuis 1998; Wagon \& Kowalski 1988; Geladi \& Kowalski 1986) or sensory evaluation (Martens \& Naes 1989), marketing (Abdi 2003; Chin et al. 2003; Graver, et al 2002; Ryan et al 1999; Fornell and Bookstein 1982; Japal 1982) and design (Han and Yang 2004). Interestingly, similarly to this research, Husson \& Pages (2005) proposed the way of corresponding additional variables by the use of PLSR coefficients instead of the linear regression coefficients in Prefmap technique. Huh and colleagues proposed several quantification methods using traditional multivariate data analysis techniques (Kim, 2000; Yang, 1998; Park and Huh 1996a, b; Han, 1995). The quantification methods proposed by them are endeavors to reduce the multivariate data with interrelationship and to represent or to plot them onto the low dimensional space. Projection pursuit stands for those methods. It aims to analyze the characteristics and structure of data through projecting the multivariate data onto the lower dimensional space and through analyzing the projection. In that sense, quantification method means a technique for building map in marketing.


The purpose of this research is to propose the algorithm for building positioning map by PLSR. The
basis of the algorithm is a singular value decomposition. To derive the form of singular value decomposition, Lagrange multiplier method function was adopted. After components are extracted via singular value decomposition, the relationships between components and variables can be gotten by regressing variables on the components. The regression coefficients are the coordinates of the variables. Additionally we can get score vectors of components for observations from the same process. They are the coordinates of the observations. That is, The variables and observations can be positioned on the simple space generated by PLSR.
The quantification technique for PLS method gives us the better understanding of structure of variables and observations. The limitation of this study is the situation when there are more than 2 sets of data. In that case it is very to difficult to solve the Lagrange multiplier method function due to the many constraints in the equation. Thus we should consider another method of extracting the principal components due to the many constraints in the equation.

Key words: PLS, Partial Least Squares, PLSR, PLS Regression, singular value decomposition,
PCR, Principal Component Regression

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## I. Backgrounds and Purposes

Partial Least Squares (PLS) proposed by Herman Wold in 1966 has been used as very valuable method to predict a set of response variables by a set of explanatory variables. Even though PLS began in social sciences, it's uses are expanded to various fields like chemometrics (Westerhuis 1998; Wagen \& Kowalski 1987; Geladi \& Kowalski 1986) or sensory evaluation (Martens \& Naes 1989), marketing (Abdi 2003; Chin et al. 2003; Graber, et al 2002; Ryan et al 1999; Fornell and Bookstein 1982; Japal 1982) and design (Han and Yang 2004). Interestingly, similarly to this research, Husson \& Pages (2005) proposed the way of corresponding additional variables by the use of PLS regression coefficients instead of the linear regression coefficients in Prefmap technique.

Basically PLS is a regression method in the sense that it deals the relationship between response variable and explanatory variables. But it is comparatively different method that it can be used when explanatory variables have collinearity, and when the number of observation is smaller than the number of explanatory variables. That is, univariate PLS, which deals one response variable has much similarity with traditional regression.

To avoid collinearity in PLS, it uses a kind of principal component analysis, which tries to reduce many mutually interrelated variables into small number of irrelevant variables. From that point of view, PLS can be compared to Principal Component Regression (PCR). The idea of PCR is similar to PLS. Both PCR and PLS consider collinearity or interrelationship among the explanatory variables. Whereas PCR considers only collinearity or interrelationship among the explanatory variables, PLS considers both response variables and explanatory variables when it determines the principle component. That is, PCR considers solely
explanatory variables when it determines principle component, whereas, in PLS the information of response variables is considered when it determines principle component.

PLS is very similar to canonical correlation analysis(CCA) from the point of view that they deal the relationship of sets of variables and use a kind of principle component analysis (PCA).

Huh and his colleagues proposed several positioning map methods using traditional multivariate data analysis techniques (Kim 2000; Yang 1998; Park and Huh 1996a, b; Han 1995). They called it as 'quantification method'. The quantification methods proposed by them are endeavors to reduce the multivariate data with interrelationship and to represent or to plot them onto the lower dimensional space. Projection pursuit stands for those methods. It aims to analyze the characteristics and structure of data through projecting the multivariate data onto the lower dimensional space and through analyzing the projection. In that sense, quantification method means a technique for building map in marketing. Based on the above ideas, the purposes of this research is to propose an algorithm for building positioning map by partial least squares regression.

## II. Basic Ideas of the Study

## 1. Singular Value Decomposition

As told, the basis of the study is singular value decomposition (SVD). Let's consider the $n \times p$ data matrix $X$ with rank $r$ ( $r<p$ ) (Huh 1995). $X$ can be written as

$$
\begin{equation*}
X=U D V^{t}, \tag{2.1}
\end{equation*}
$$

where $U=\left(u_{1}, u_{2}, \ldots u_{r}\right)$ and $V=\left(v_{1}, v_{2}, \ldots v_{r}\right)$ are the column orthogonal matrics of size $n \times r$ and $p \times r$
respectively $\left(U^{t} U=I_{r}, V^{t} V=I_{r}\right)$, and $D$ is $r \times r$ diagonal matrix with singular value $\mu_{1} \geq \mu_{2} \ldots \geq \mu_{r}(>0)$ as its diagonal elements. The left singular vectors $U=\left(u_{1}, u_{2}, \ldots u_{r}\right)$ form an orthogonal basis for the columns of $X$ in $R^{n}$ and the right singular vectors $V=\left(v_{1}, v_{2}, \ldots v_{r}\right)$ form an orthogonal basis for the rows of $X$ in $R^{p}$.

SVD has very close relationship with eigen system. Let's consider the data matrix $X^{t} X(p \times p)$ where $X$ is $n \times p$ matrix. $X^{t} X$ can be written as

$$
\begin{equation*}
X^{t} X=V D^{2} V^{t} \tag{2.2}
\end{equation*}
$$

We can find that the right singular vectors are eigen vectors of $X^{t} X$ and the squared singular values are eigen values, $\lambda_{1}, \lambda_{2} \cdots \lambda_{r}$. So we can get eigen values and eigen vectors of $X^{t} X$ through SVD of $X$.

## 2. Partial Least Squares Regression

Partial least squares regression(PLSR) is very useful for building a predictive model when variables are many and highly correlated. Multiple regression analysis also useful tool for building a prediction model. But it has much limitation when variables are many and highly correlated. In such cases, even though we can build a prediction model, it will fail to predict new data well (Tobias 2007). Especially when the number of variables is much larger than the number of observations, the phenomenon of so-called 'overfitting' occurs.
When the explanatory variables are highly correlated, one approach to overcome the problem is to remove the some of highly correlated explanatory variables. Another approach is to reduce the explanatory variables into small number of variables which have no correlations.

The concept of PLS is to extract small numbers of latent
variables which explain for highly correlated many variables. In that sense, PLS is a indirect modelling. But the way of extracting latent variables is different from the traditional method, It will be explained later.

〈FIGURE 2.1〉 Indirect Modelling


PLS extracts the latent variables to maximize the relationship between the successive pairs of latent variables. So, it has interest in SVD of $X^{t} Y$. Originally PLS method means PLS regression. Usually we can get better predicted value through PLS regression than any other analysis. In PLS $Y$ is a matrix of response variables and $X$, a matrix of explanatory variables. It menas that $Y$ depends on $X$.

PLS proposed by Herman Wold in 1966, was improved by Naes and Martens (1985). Let's consider their original concept. Like PCR, PLS regression (PLSR) is a dependency model. For convenience, I will suggest such a case that $X$ is a set of variables(or a matrix) and $y$ is a single variable (or a vector). The $X$-variables and $y$-variables are scaled and centered, yielding $X_{0}$ and $y_{0}$. Then step 1 to 5 are performed for each component $a=1,2, \ldots, A_{\max }$ where $A_{\max }$ is the maximum number of PLSR component to be computed.

Step 1. Find weight vector $\widehat{w}_{a}$ by maximizing the
covariance between the linear combination $X_{a-1} w_{a}$ and $y$ under the constraint that $w_{a}^{t} w_{a}=1$.
Step 2. Find factor scores, $\hat{t_{k}}$ as the projection of $X_{a-1}$ on $\widehat{w_{a}}$, i.e. $\hat{t_{a}}=X_{a-1} \widehat{w_{a}}$
Step 3. Regress $X_{a-1}$ on $t_{a}$ to find the loading $\hat{p}_{a}^{t}$, i.e. $\hat{p_{a}}=X_{a-1}^{t} \hat{t_{a}} / \hat{t}_{a}^{t} \hat{t_{a}}$
Step 4. Regress $y_{a-1}$ on $t_{a}$ to find the loading $\hat{q_{a}}$, i.e. $\hat{q_{a}}=y_{a-1} \hat{t_{a}} / \hat{t}_{a}^{t} \hat{t_{a}}$
Step 5. Subtract $\hat{t_{a}} \hat{p}_{a}^{t}$ from $X_{a-1}$ and call the new matrix $X_{a}$.
Subtract $\hat{t_{a}} \hat{q_{a}}$ from $y_{a-1}$ and call the new matrix $y_{a}$.

After repeating the above steps until the maximum number of component, $A_{\max }$.

The superiority of PLSR to PCR is very well known. Ryan et.al(1999) showed empirically that PLSR is better than PCR in prediction the response variable. They compared three models with mediators and collinearity among the response variables, for example, regression, PCR, and PLSR. As the hypothesized conceptual model had moderators and collinearity in their study, the regression model was not germane to the research objective. Hence their focus was on the comparison of PCR, with PLSR. Even though the fact that there was a difference in estimating the coefficients between PCR and PLSR was very confusing, But prediction of PLSR was better than PCR.

## III. Suggesting Algorithm and Numerical Example

## 1. Basic Concept

As discussed earlier, the purpose of PLS regression is a
prediction of response variable(s). Let's consider data matrix $K$ with $p$ explanatory variables, $q$ response variables and $n$ observations. Data matrix $K$ consists of $X(n \times p)$ and $Y(n \times q)$. Here, I assume that data matrix $X$ and $Y$ are scaled and centered, but no such transformation mandatory (Huh et al 2007; Yi 2007).
The aim of PLS regression is to find linear combination of $p$-explanatory variables ( $X$ ) and $q$-response variables ( $Y$ ) which maximizes the covariance between the projections of each sets of variables. The problem of maximization can be written as

$$
\begin{align*}
& \text { maximize (w.r.t. } a \text { and } b) \operatorname{Cov}(X a, Y b)  \tag{3.1}\\
& \text { subject to } a^{t} a=b^{t} b=1,
\end{align*}
$$

where $X a$ and $Y b$ are projections of each data matrix $X$ and data matrix $Y$ (Huh, Lee, and Yi, 2007).

As the covariance of (3.1) is dependent on both direction and norm of $a$ and $b$, two constraints $a^{t} a=1$ and $b^{t} b=1$ are considered. Lagrangian function can be used to get the solution of (3.1) under the constraints. The function $L$ is defined as

$$
\begin{equation*}
L\left(a, b, \lambda_{1}, \lambda_{2}\right)=a^{t} X^{t} Y b-\lambda_{1}\left(a^{t} a-1\right)-\lambda_{2}\left(b^{t} b-1\right) \tag{3.2}
\end{equation*}
$$

subject to $a^{t} a=1$ and $b^{t} b=1$.

By setting the partial differential of $L$ to $0_{p}$ and $0_{q}$, (3.3) and (3.4) are obtained.

$$
\begin{align*}
& X^{t} Y b-2 \lambda_{1} a=0_{p},  \tag{3.3}\\
& Y^{t} X a-2 \lambda_{2} b=0_{q} \tag{3.4}
\end{align*}
$$

By solving the simultaneous equations of (3.3) and (3.4), with respect to $a, b$ is eliminated, Consequently, we have

$$
\begin{equation*}
X^{t} Y Y^{t} X a=4 \lambda_{1} \lambda_{2} a \tag{3.5}
\end{equation*}
$$

Here, the solution of $a$ is an eigen vector of $p \times p$ non-negative matrix $X^{t} Y Y^{t} X$. In the same manner, the solution of $b$ is an eigen vector of $q \times q$ non-negative matrix $Y^{t} X X^{t} Y$. Therefore, both $a$ and $b$ can be obtained from SVD (singular value decomposition) of $p \times q$ matrix $X^{t} Y$. That is, by the use of (3.5), $X^{t} Y Y^{t} X$ $=U D_{\mu} V^{t} V D_{\mu} U^{t}$ is obtained. Since $V^{t} V=I_{q}, X^{t} Y$ $Y^{t} X$ is equal to $U D_{\mu^{2}} U^{t}$. So, by decomposing $X^{t} Y Y^{t} X$, eigen value $\lambda=\mu^{2}$ and each eigen vector of matrix $X^{t} Y Y^{t} X$ is obtained.
Similarly, matrix $Y^{t} X X^{t} Y$ is decomposed into $V D_{\mu^{2}} V^{t}$, and eigen value $\lambda=\mu^{2}$ and each corresponding eigen vector of matrix $Y^{t} X X^{t} Y$ is obtained. Thus, we can find that weight vector $a$ of matrix $X$ is $u_{1}$ and weight vector $b$ of matrix $Y$ is $v_{1}$ from

$$
\begin{gather*}
X^{t} Y=U D_{\mu} V^{t}, U=\left(u_{1}, u_{2}, \cdots\right), V=\left(v_{1}, v_{2}, \cdots\right) \\
\mu_{1} \geq \mu_{2} \geq \cdots \tag{3.6}
\end{gather*}
$$

where $U^{t} U=V^{t} V=I_{q}$ and $D_{\mu}$ is a matrix with singular values $\mu_{1} \geq \mu_{2} \geq \cdots$ on the diagonal, the columns $u_{1}, u_{2}, \cdots$ of $U$ are left singular vectors, and the columns $v_{1}, v_{2}, \cdots$ of $V$ are right eigen vectors. Usually eigenvalues $\lambda_{i}$ is referred to $\mu_{i}^{2}$.
Consider the case that $Y$ is a vector $(=y)$. In PLS method, $b$ is obtained as $X^{t} y /\left\|X^{t} y\right\|$, when we consider the constraint ( $b^{t} b=1$ ) in (3.1). Accordingly SVD for $Y$ is not needed.

## 2. Positioning Algorithm for PLS regression

Let's consider data matrix $K$ with $p$ explanatory variables, $q$ response variables and $n$ observations. $X a$ will be transcribed as $s(n \times 1)$ and call it as score vector. By
regressing $Y$ on $s, Y$ fit, $\hat{Y}$ can be obtained as

$$
\begin{align*}
& \hat{Y}=s\left(s^{t} s\right)^{-1} s^{t} Y=s g_{Y}^{t} \\
& \text { where } g_{Y}^{t}=\left(s^{t} s\right)^{-1} s^{t} Y \tag{3.7}
\end{align*}
$$

$g_{Y}(q \times 1)$, regression coefficients of $s$, can be called $Y$ -loading vector. As shown in (3.7), PLS regression is a simple linear regression method in which $Y$ is regressed on an explanatory variable $s$.

When we determine coefficient vector $b$ (in $s=X b$ ), we should consider $Y$ as well as $X$ simultaneously. Determining the regression coefficient $g_{Y}^{t}$ is very complicated, since $\hat{Y}$ $=A Y$, where $A=A(Y)$ or $s\left(s^{t} s\right)^{-1} s^{t}$. Accordingly, distribution of $\hat{Y}$ can not be obtained easily in PLS regression, contrary to linear regression.

Above procedure is the first step in PLS regression. We can identify that rank of transformational matrix $A$ of $Y$ is 1. To obtain the improved fit, the rank of $A$ can be increased by the use of technique which will be shown in the quantification step. For convenience, I will suggest one more step in this algorithm. I will use the following notations for convenience.

## Notations

- $K$ : data matrix with several sub data matrix
- $X, Y$ : sub data matrix
- $a, b$ : weight vectors obtained from SVD
- $s, t$ : score vectors of sub data matrix $X, Y$
- $g_{X}$ : loading vector for sub data matrix $X$
- $g_{Y}$ : loading vector for sub data matrix $Y$
- $\hat{X}$ : predicted value of sub matrix $X$
- $\hat{Y}$ : predicted value of sub matrix $Y$
- number in subscript : PLS cycle

For the further steps, I will denote $s \rightarrow s_{1}, g_{Y} \rightarrow g_{1, Y}$,
$X \rightarrow X_{1}, \hat{X} \rightarrow \widehat{X}_{1}$ and $\hat{Y} \rightarrow \hat{Y}_{1}$. Following steps can be put in order for quantification of PLS regression.

- Data are centered and scaled

Cycle 1
Step 1 : Find weight vectors and score vectors
Find $a_{1}$ and $b_{1}$ in the manner of maximizing (3.1) under the these constraints $a^{t} a=1, b^{t} b=1$. Accordingly, we can obtain score vectors ( $X_{1} a_{1}=s_{1}$ and $Y_{1} b_{1}=t_{1}$ ) of data matrix $X_{1}$ and $Y_{1}$.

## Step 2 : Find loading vectors

Obtain $\widehat{X}_{1}$ and $\widehat{Y}_{1}, \widehat{X}_{1}$ can be obtained by regressing $X_{1}$ on $s_{1}$ and $\widehat{Y}_{1}$ can be obtained by regressing $Y_{1}$ on $s_{1}$. Thus, $\widehat{Y}_{1}$ is $s_{1}\left(s_{1}^{t} s_{1}\right)^{-1} s_{1}^{t} Y_{1}\left(=s_{1} g_{1 . Y}^{t}\right)$, where $g_{1 . Y}^{t}=$ $\left(s_{1}^{t} s_{1}\right)^{-1} s_{1}^{t} Y_{1} \quad$ and $\widehat{X}_{1}$ is $s_{1}\left(s_{1}^{t} s_{1}\right)^{-1} s_{1}^{t} X_{1} \quad\left(=s_{1} g_{1 . X}^{t}\right)$. where $g_{1 . Y}^{t}=\left(s_{1}^{t} s_{1}\right)^{-1} s_{1}^{t} X_{1}$.
If $X_{1}^{t} s_{1}\left(s_{1}^{t} s_{1}\right)^{-1}$ is denoted to $g_{1 . X}$, then $\widehat{X}_{1}$ become $s_{1}$ $g_{1 . X}^{t}$. Here $g_{1 . X}^{*}(p \times 1)\left(=X_{1}^{t} s_{1} /\left\|s_{1}\right\|\right)$ is called $X$ -loading vector. Similarly, $g_{1 . Y}(q \times 1)$ can be called $Y$ -loading vector.

## Step 3 : Deflate the data

Deflate $X_{1}$ and $Y_{1}$ with a following manner.

$$
Y_{2}=Y_{1}-\hat{Y}_{1}, X_{2}=X_{1}-\hat{X}_{1}
$$

## Cycle 2

## Step 4 : Finding weight vectors and score vectors

Find $a_{2}$ and $b_{2}$ in the manner of maximizing $\operatorname{Cov}\left(X_{2} a_{2}\right.$, $Y_{2} b_{2}$ ) under the constraints $a_{2}^{t} a_{2}=1$ and $b_{2}^{t} b_{2}=1$. Compute new score vector $s_{2}$ and $t_{2}$.

## Step 5 : Find loading vectors

Obtain $\widehat{X}_{2}$ and $\widehat{Y}_{2} \cdot \widehat{X}_{2}$ can be obtained by regressing $X_{2}$
on $s_{2}$ and $\widehat{Y}_{2}$ can be obtained by regressing $Y_{2}$ on $s_{2}$, where $s_{2}=X_{2} a_{2}, t_{2}=Y_{2} b_{2}$.

$$
\begin{aligned}
& \widehat{Y}_{2}=s_{2}\left(s_{2}^{t} s_{2}\right)^{-1} s_{2}^{t} Y_{2}=s_{2} g_{2 . Y}^{t}, \\
& \widehat{X}_{2}=s_{2}\left(s_{2}^{t} s_{2}\right)^{-1} s_{2}^{t} X_{2}=s_{2} g_{2 . X}^{t}
\end{aligned}
$$

Consequently, $\hat{Y}$ and $\hat{X}$ can be expressed as follows.

$$
\begin{aligned}
& \begin{aligned}
\hat{Y} & =\widehat{Y}_{1}+\widehat{Y}_{2} \\
\quad= & s_{1}\left(s_{1}^{t} s_{1}\right)^{-1} s_{1}^{t} Y_{1}+s_{2}\left(s_{2}^{t} s_{2}\right)^{-1} s_{2}^{t} Y_{2} \\
\quad & =s_{1} g_{1 . Y}^{t}+s_{2} g_{2 . Y}^{t},
\end{aligned} \\
& \begin{aligned}
\hat{X} & =\widehat{X}_{1}+\widehat{X}_{2} \\
& =s_{1}\left(s_{1}^{t} s_{1}\right)^{-1} s_{1}^{t} X_{1}+s_{2}\left(s_{2}^{t} s_{2}\right)^{-1} s_{2}^{t} X_{2} \\
& =s_{1} g_{1 . X}^{t}+s_{2} g_{2 . X}^{t},
\end{aligned} \\
& \text { where } g_{2 . Y}^{t}=\left(s_{2}^{t} s_{2}\right)^{-1} s_{2}^{t} Y_{2} \\
& \text { and } g_{2 . X}^{t}=\left(s_{2}^{t} s_{2}\right)^{-1} s_{2}^{t} X_{2} .
\end{aligned}
$$

By the use of above procedure, the prediction value of subject $y^{*}(q \times 1)$ that has $x^{*}(p \times 1)$ is possible. The procedure extends iteratively in a natural way to give $r$ ( $r$ $=1,2,3, \cdots$ ) number of components of $\hat{X}$ and $\hat{Y}$. To determine the number of components which will be included in regression model, cross validation technique is usually used.

The focus of this paper lies in the suggesting positioning method using PLS regression. Consider multivariate data matrix $K$ which consists of data matrix $X$ with $p$ explanatory variables and data matrix $Y$ with $q$-response variables again. I assume that data matrix $X$ and data matrix $Y$ are scaled and centered. According to PLS regression, score vectors of $X, s_{1}, s_{2}(=n \times 1)$ are orthogonal and they can generate the base of projection space.

For positioning of multivariate data matrix $(X, Y)$ by PLS in the reduced space, determination of the coordinates is needed. In step 2 and step 5 of the algorithm, as previously showed, we obtained $X$-loading vectors and $Y$-loading

〈TABLE 3．1〉 Quantification formulas of PLS regression for columns（variables）

|  | Dimension 1 | Dimension 2 |
| :---: | :---: | :---: |
| $X$ variables | $x_{j}^{t} s_{1}^{*}$ | $x_{j}^{t} s_{2}^{*}$ |
| $Y$ variables | $y_{k}^{t} s_{1}^{*}$ | $y_{k}^{t} s_{2}^{*}$ |

$$
\text { Note : } s_{1}^{*}=s_{1} /\left\|s_{1}\right\|, s_{2}^{*}=s_{2} /\left\|s_{2}\right\|
$$

〈TABLE 3．2〉 Quantification formulas of PLS regression for rows（observations）

|  | Dimension 1 | Dimension 2 |
| :---: | :---: | :---: |
| Observations <br> in data matrix $X$ | $X_{1} a_{1}=s_{1}$ | $X_{2} a_{2}=s_{2}$ |
| Observations <br> in data matrix $Y$ | $Y_{1} b_{1}=t_{1}$ | $Y_{2} b_{2}=t_{2}$ |

vectors．Each loading vectors for $X(=n \times p)$ variables and $Y(n \times q)$ variables can be used as coordinates．Thus， columns $x_{j}(j=1,2, \ldots p)$ of data matrix $X$ can be pointed on the linear space $P_{j}:\left(x_{j}^{t} s_{1}^{*}, x_{j}^{t} s_{2}^{*} \cdots\right)$ generated by $s_{1}, s_{2}$ ， ． －．And columns $y_{k}(k=1,2, \ldots q)$ of data matrix $Y$ can be pointed on the linear space $Q_{k}:\left(y_{k}^{t} s_{1}^{*}, y_{j}^{k} s_{2}^{*} \cdots\right)$ generated by $s_{1}, s_{2}$ ，• • Here $s_{1}^{*}$ is $s_{1}^{*}=s_{1} /\left\|s_{1}\right\|$ and $s_{2}^{*}$ is $s_{2}^{*}=s_{2} /\left\|s_{2}\right\|$ ．The coordinates of each columns for dimension 1 and for dimension 2 are suggested in Table 3.1 and Table 3.2

## 3．Numerical Example

## Data description

The data shown as an example here are the survey results of the automobile market in China．I am interested in how the property of automobile has an effect on the consumer＇s attitude toward brand．Thus I considered the data for property evaluation of the automobile and the data for attitude toward brand which are collected from the survey done in 2006.

Thus，I consider the data matrix $K$ with thirty six
variables and fifty observations（companies）．Data matrix $K$ consists of two sets of variables denoted by $X(=50 \times 34)$ and $Y(=50 \times 2)$ ．Here，$X$ is a data set for consumers＇ evaluation of automobile＇s property for companies．And $Y$ is a data set for consumers＇attitude toward brand．Here，data set $X$ and $Y$ are collected in a seven point scale（from point 1 to point 7）and they are scaled and centered for the analysis．The brands and properties evaluated are listed in Table 3.1 and Table 3．2．Attitude toward brand used as a data set $Y$ are＇overall satisfaction $(=Y 1)$＇and＇repurchase intention（ $=Y 2$ ），

## Interpretation of the result

Loading vectors of $X, Y$ variables are listed in Table 3.5 and in Table 3．6，and score vectors are listed in Table 3．7． Quantification plots are showed in Figure 3.1 based on the Table 3.5 and Table 3．6．
Two components were extracted for convenience in this analysis．The total amount of the variance which was explained by two components was $56.3 \%$ ．The first component explained the variance by $37.2 \%$ and the second component did 19．0\％．
The $X$－variables are divided into two groups on the

〈TABLE 3．3〉Automobile brands surveyed in China

```
1．Beijing Hyundai 2．Beijing Jeep 3．Changan Ford 4．Changan Suzuki 5．Dongfeng Citroen 6．Dongfeng honda 7．Dongfeng Nissan 8．DYK 9．Southeast Motor 10．Faw Hainan Mazda 11．Faw Mazda 12．Faw－VW
13．Guangzhou Honda 14．Guangzhou Toyota 15．Geely 16．Nanjing Fiat
17．Chery 18．Shanghai GM 19．SVE 20．Tianjin Faw 21．Faw Toyota
22．Korean Hyundai 23．Korean Kia 24．Hafei Motor 25．Changhe Suzuki
26．Changan Motor 27．Biyadi 28．Jiangnan Auto 29．Faw Huali 30．Jilin Tongtian 31．Dongfeng Liuzhou 32．Nanjing Motor 33．Dongfeng Peugeot 34．SGM Wuling 35．Shanghai Maple 36．Beijing Benz 37．Huachen BMW
38．Huachen Motor 39．Faw Motor 40．Changcheng Auto 41．Changfeng Auto
42．Jiangling Auto 43．Zhengzhou Nissan 44．Jiao Auto 45．Huatai Hyundai 46. Beijing Futon 47．Beijing Auto 48．Jianghuai Auto
49．Baolong Auto 50．Mercedes－Benz
```

〈TABLE 3．4〉 Property list of automobile brands

```
1. proper engine displacement/ power
2. engine type (v6,diesel engine, etc.)
3. good acceleration 4. good performance in cross country running.
5. stability at steering 6 . convenience for parking
7. durability of the whole 8. type of drive (two-wheel/four-wheel drive)
9. gear type (manual/auto) 10. overall exterior styling
11. overall interior 12. broad vision 13. car size
14. convenience to get in and out
15. convenience to load and unload cargoes 16. space of the front seats
17. space of the second row 18 . overall quietness
19. standard features 20 . price 21 . scope of quality guarantee
22. future trading price 23. efficiency of fuel
24. efficiency of maintenance 25. manufacturer impression
26. place of origin 27. availability of parts 28 . cargo capacity
29. guard against theft 30 . overall safety 31 . environmental protection
32. sales service 33 . after-sales service 34 . lead time
```

direction．The variables of the first group gather around variable 30 （overall safety）．The first group consist of variable 30 （overall safety），variable 25 （manufacturer＇s impression），variable 13 （car size），variable 10 （overall exterior styling）and so forth．The variables of the second group gather around variable 22 （future trading price）．The second group consist of variable 22 （future trading price）， variable 20 （price），variable 15 （convenience to load and unload cargoes），variable 29 （guard against theft）and so forth．We can interpret that the first group is on＇the basic performance or the function of the automobile＇and the second one is on＇the additional value of the automobile＇．

The observations（brands）are dense around the second axis and scattered along the first axis．We can interpret that
there is no substantial difference in the second axis and some difference in the first axis among the observations （brands）．That is，the difference among the brands occur only in the first axis．

By the use of the loading vectors and score vectors， variables and observations are plotted onto the space generated by each score vectors．They are Figure 3.1 and Figure 3．2．As shown in Figure 3．1，variable 7 in $X$－ variables（＇durability of the whole＇）has same direction with variables 1 （＇overall satisfaction＇）of $Y$－variables．It means that＇durability of the whole＇has a relationship with＇overall satisfaction＇．Similarly variable 18 （＇overall quietness＇）and variable 10 （＇overall exterior styling＇）of $X$ variables are very close to variable 2 （＇repurchase intention＇）of $Y$ variables．

〈TABLE 3．5〉 Loading vectors of $X$ variables

| variables | Loading vectors of $X$ variables |  |
| :---: | :---: | :---: |
|  | dimension 1 | dimension 2 |
| X1 | －4．582 | －0．726 |
| $\times 2$ | －4．013 | 1.195 |
| X3 | －5．303 | －0．001 |
| $\times 4$ | －3．256 | －2．100 |
| $\times 5$ | －5．859 | －1．520 |
| $\times 6$ | －1．046 | －3．036 |
| $\times 7$ | －3．703 | 3.934 |
| X8 | －4．628 | －2．451 |
| X9 | －0．177 | 0.614 |
| $\times 10$ | －3．890 | 1.458 |
| $\times 11$ | －4．666 | －0．967 |
| $\times 12$ | －3．804 | 1.291 |
| $\times 13$ | －4．183 | －0．545 |
| $\times 14$ | －3．747 | －3．169 |
| $\times 15$ | －2．611 | －4．947 |
| $\times 16$ | －5．642 | －1．613 |
| $\times 17$ | －1．802 | 1.425 |
| $\times 18$ | －5．230 | 1.758 |
| $\times 19$ | －3．796 | －1．001 |
| $\times 20$ | 0.436 | －3．327 |
| $\times 21$ | －3．799 | －2．655 |
| $\times 22$ | －1．648 | －5．133 |
| $\times 23$ | －1．693 | －3．586 |
| $\times 24$ | －3．694 | 0.636 |
| $\times 25$ | －5．302 | －0．830 |
| $\times 26$ | －4．799 | －2．719 |
| $\times 27$ | －2．566 | －4．022 |
| $\times 28$ | －4．223 | －2．094 |
| $\times 29$ | －4．316 | －1．756 |
| $\times 30$ | －5．704 | 1.072 |
| $\times 31$ | －2．245 | －3．852 |
| $\times 32$ | －5．429 | －2．204 |
| $\times 33$ | －3．836 | －2．860 |
| X34 | －4．817 | －3．710 |

We can interpret the plots in Figure 3.1 and Figure 3.2 jointly．To the direction of＇overall satisfaction＇，observation 49 （＇Baolong auto＇）and observation 36 （＇Beijing Benz＇） locate．Observation 37 （＇Huachen BMW＇）and 43 （＇Zhengzhou Nissan）have very close relationship（＇repurchase intention＇）． That is to say，we can infer that those brands are well evaluated in the＇attitude toward brand＇．

We can combine the plots of $X$－variables with and $X$－ observations．Brand 46 （Beijing Futon），brand 47 （Beijing Auto）and brand 30 （Jilin Tongtian）have the direction with the second group of the $X$－variables．It can be interpreted that Brand 46 is evaluated most positively in the second

〈TABLE 3．6〉 The loading vectors of $Y$ variables

| variables | Loading vectors of $Y$ variables |  |
| :---: | :---: | :---: |
|  | dimension 1 | dimension 2 |
| Y1 | -4.018 | 3.843 |
| Y2 | -4.061 | 1.926 |

〈TABL 3．7〉The score vectors of $X$ and $Y$

| brands | Score vectors of $X$ |  | Score vectors of $Y$ |  |
| :---: | ---: | ---: | ---: | ---: |
|  | score 1 | score 2 | score 1 | score 2 |
| 1 | 0.2573 | 0.6153 | -0.1716 | 0.1950 |
| 2 | -1.5322 | -0.2144 | -0.7644 | 0.4854 |
| 3 | -0.2506 | 0.4663 | -1.1950 | 1.0885 |
| 4 | 3.6472 | -0.6619 | 0.8696 | 0.1628 |
| 5 | 0.1907 | 0.1543 | -0.0462 | 0.2253 |
| 6 | -2.1338 | -0.0873 | -0.1893 | -0.5392 |
| 7 | -3.2126 | -0.0604 | -0.7998 | -0.1804 |
| 8 | 2.821 | -0.2684 | 0.1691 | 0.7810 |
| 9 | -1.1962 | 0.1422 | 0.5466 | -0.8871 |
| 10 | 1.6745 | 0.8386 | 0.2413 | 0.1749 |
| 11 | -0.5950 | -0.0872 | -0.6022 | 0.2459 |
| 12 | -0.8816 | 0.4228 | -0.9075 | 0.4908 |
| 13 | -1.5963 | 0.5584 | -0.7998 | 0.2379 |
| 14 | -2.4841 | 5.2791 | -2.9721 | 2.0106 |
| 15 | 1.6042 | -0.8362 | 1.6055 | -0.9565 |
| 16 | 1.4725 | -0.3022 | 0.4567 | -0.0131 |
| 17 | 1.9291 | -0.9091 | 0.8696 | -0.2819 |
| 18 | -0.9682 | 0.7146 | -0.6921 | 0.3326 |
| 19 | -1.1885 | 0.1760 | -0.6921 | 0.2756 |
| 20 | 1.6584 | -1.1367 | 0.2591 | 0.2862 |
| 21 | -1.8311 | 0.2621 | -0.6022 | -0.0740 |
| 22 | 2.1013 | 2.4058 | -1.1051 | 1.5139 |
| 23 | -1.3366 | 2.8859 | 0.1691 | -0.3057 |
| 24 | 4.0785 | 0.8092 | 1.4624 | -0.4791 |
| 25 | 1.8296 | -0.8445 | 0.3490 | 0.1472 |
| 26 | 4.8526 | -1.3732 | 1.4978 | -0.0479 |
| 27 | 2.1274 | -0.5577 | 0.9050 | 0.0003 |
| 28 | 9.3323 | 0.5278 | 2.2514 | 0.6364 |
| 29 | -1.3013 | 1.9018 | -0.8366 | 0.8439 |
| 30 | -1.0190 | -7.4022 | 1.1408 | -2.3552 |
| 31 | 0.845 | -0.3278 | -0.0639 | 0.2714 |
| 32 | 0.4360 | -0.6694 | 0.1337 | -0.0778 |
| 33 | -0.8699 | 0.5462 | -0.2615 | 0.0866 |
| 34 | 8.5661 | 0.3622 | 2.9710 | -1.0283 |
| 35 | 1.4476 | -0.8746 | 1.7131 | -1.0649 |
| 36 | -2.0491 | 2.6768 | -1.2658 | 0.1614 |
| 37 | -3.9161 | 1.2294 | -1.2127 | 0.0244 |
| 38 | -0.9434 | 0.9541 | -0.7821 | 0.5223 |
| 39 | -1.8564 | 2.2781 | -2.0209 | 1.4468 |
| 40 | 0.2288 | -0.3174 | 0.4744 | -0.2196 |
| 41 | -2.2228 | 0.7235 | -0.5668 | 0.0555 |
| 42 | -1.3820 | 0.4531 | 1.0672 | -1.3900 |
| 43 | -2.5655 | 1.4262 | -0.2615 | -0.3522 |
| 44 | 3.4582 | -0.3356 | 1.4978 | -0.4088 |
| 45 | -0.4757 | -1.8626 | 1.1203 | -0.8091 |
| 46 | -8.1641 | -4.3247 | -0.2084 | -1.4549 |
| 47 | -4.6658 | -2.0445 | -1.2850 | 0.1292 |
| 48 | -0.9320 | -0.9416 | 0.6543 | -0.8866 |
| 49 | -2.7140 | 3.4292 | -2.8113 | 2.2295 |
| 50 | -0.2852 | -5.7993 | 0.6911 | -1.2488 |
|  |  |  |  |  |

〈FIGURE 3．1〉 Plots of variables by PLS regression


〈FIGURE 3．2〉 Plots of observations by PLS regression

group of variables．But as the variables of the second group has no relationship with the＇attitude toward brand＇，it seems
that the good evaluation of those brands will not be associated with the direct selling．On the other hand，brand

37 （Huachen BMW）has a same direction with the first group of variables．Thus it seems that brand can get good performance in the market．

On the contrary，brand 34 （SGM Wuling）and brand 28 （Jiangnan Auto）have a opposite direction to the other variables．It seems that they are badly evaluated in the properties of $X$－variables．Brand 44 （Jiao Auto）and brand 26 （Changan Motor）have similar position with brand 34 and brand 28.

To get the visual image I suggested in this paper，I used ＇R＇language．

## IV．Summary and Discussions

The purpose of this research is to propose the positioning algorithm for PLS regression．In this study I proposed how to position the variables and the observations onto the simple space by PLS regression．The basis of the algorithm is in the singular value decomposition．But the problem exists in the way of deriving the singular value composition．

To derive the form of singular value decomposition， Lagrange multiplier method function was adopted．After components are extracted via singular value decomposition， the relationships between components and variables can be derived by regressing variables on the components．The regression coefficients are the coordinates of the variables． Additionally we can get score vectors of components for observations．They are the coordinates of the observations． Based on the coordinates，the variables and observations can be positioned on the simple space generated by PLS regression．

The quantification technique for PLS method gives us the better understanding of structure of variables and observations． Especially when there are so many sets of variables，
quantification technique proposed here is very useful．As we mentioned above，the key idea of this algorithm lies in the way of building the singular value composition format． When there are two sets of data，using Lagrange multiplier method function may be a good way of building the singular value composition format．But，given the over 3 sets of data， it is very to difficult to solve the Lagrange multiplier method function due to the many constraints in the equation．
Let＇s consider 3 sets of variables $X(=n \times p), Y(=n \times q)$ ， and $Z(=n \times r)$ ．Let denote $X a, Y b$ ，and $Z c$ be the projections of each data matrix $X, Y$ ，and $Z$ ．Unlike objective function suggested in the case of two sets of variables，we have to use the constraints $a^{t} a=1, b^{t} b=1$ ，and $c^{t} c=1$ for obtaining solution．In this case，the method we used in the two data sets case has problem in solving the problem．Of course，alternatively，the constraint $a^{t} a+b^{t} b+c^{t} c=3$ can be used for the simple process．Strictly we can not be sure that it should be a correct way of solving problem．For that reason，it is very needful to find a way of solving the problem in the case of many data sets．

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