國立交通大學

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碩 士 論 文

調 控 式 的 部 份 最 小 平 方 法 之 研 究

Study on Partial Regularized Least Squares Method

研 究 生：邱郁仁

指導教授：蕭子健

中 華 民 國　九 十 七　年 七 月

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國 立 交 通 大 學

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調控式的部份最小平方法之研究

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摘要

本論文的目的在於建構一種分析法則，在未經處理的原始資料去除不必要的隱藏訊息。此新的學習法則稱之調控式的部份最小平方法，是合併部份最小平方法和規律法的優點，即使在雜訊的資料下，可避免過度配適的現象，得到較好的估算結果。

在模擬數據分析部份，調控式部份最小平方法用來分析三種不同的波型，並以均方根誤差做為判定的標準說明調控式部份最小平方法可得到較好的結果;實際的測量數據分析部份，利用實際的聲音檔案以及血糖濃度的光譜資料來驗證所提出的調控式部份最小平方法的確具備去除雜訊能力。

Study on Partial Regularized Least Squares Method

Student：Yu-Ren Chiou Advisor：Tzu-Chien Hsiao

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Abstract

The main purpose of this thesis is to develop a method of analyzing and reducing the unseen or noisy information from the source data without preprocessing. Here presents a novel learning algorithm—partial regularized least squares (PRLS). It combines the advantages of both the partial least squares (PLS) and regularization technique to provide an efficient procedure to avoid the circumstance of overfitting and attain better results when calibrating under noisy data.

In the simulated experiments, PRLS is applied to analyze the three different kinds of simulated waves. According to estimated standard of root mean square error, proving that PRLS has better performance than PLS. In real calibrated experiments, demonstrating PRLS certainly has the ability of noise reduction.

Acknowledgement

First of all, I would like to express my sincere appreciation to my advisor, Dr. TC Hsiao, for his helpful guidance, careful supervision and encourage throughout my Master degree. Under his guidance, he shows me a way how to treat and analyze the problem. And also thanks for Prof. Lin, as his professional approval that I have successfully adopt environment sound data for testing the performance of proposed scheme.

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Finally, thank my family for their understanding, supports and loves. Life is sometimes tough; however, there is nothing to defeat us with loves of family.

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中 華 民 國　97　年　7　月　24　日

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As members of the Final Examination Committee, we certify that we have read the thesis prepared by Yu-Ren Chiou entitled Study on Partial Regularized Least Squares Method

and recommend that it be accepted as fulfilling the thesis requirement for the Degree of Master of Science.

Committee Members:

Jiun-Hung Lin Tzu-Chien Hsiao

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Thesis Advisor: Tzu-Chien Hsiao

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Date: 2008/07/24

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Chapter 1. Introduction

1.1. Literature study

Multivariate analysis is successfully applied to process signal information. The application field includes spectrum analysis [1], bio-signal process [2] and image processing [3] etc. In general, it can be divided into two categories: regressor and value iteration also named as artificial neural network (ANN). The wildly used regressors are: Least Squares (LS), Principal Component Analysis (PCA) [4] and Partial Least Squares (PLS) [5]. And the most practical model in ANN is Multiple Layer Perceptron (MLP) [6]. Regressor and ANN analyze data in different processes and the analyzed results are suitable for different applications. For example, Wang [7] used ANN to solve the problem, classification of oral submucous fibrosis and oral carcinogenesis. Hsiao [8] apply regressor to classify the difference between normal and dyplasia tissues.

Hsiao [9] proposed a novel thought to hybrid regressive algorithm and ANN. In his study, the regressive algorithms can be treated as ANN architecture. For example, PLS can be treated as a three-layer ANN. For this view point, the research tracing path in this thesis will be illustrated in Figure 1.1.

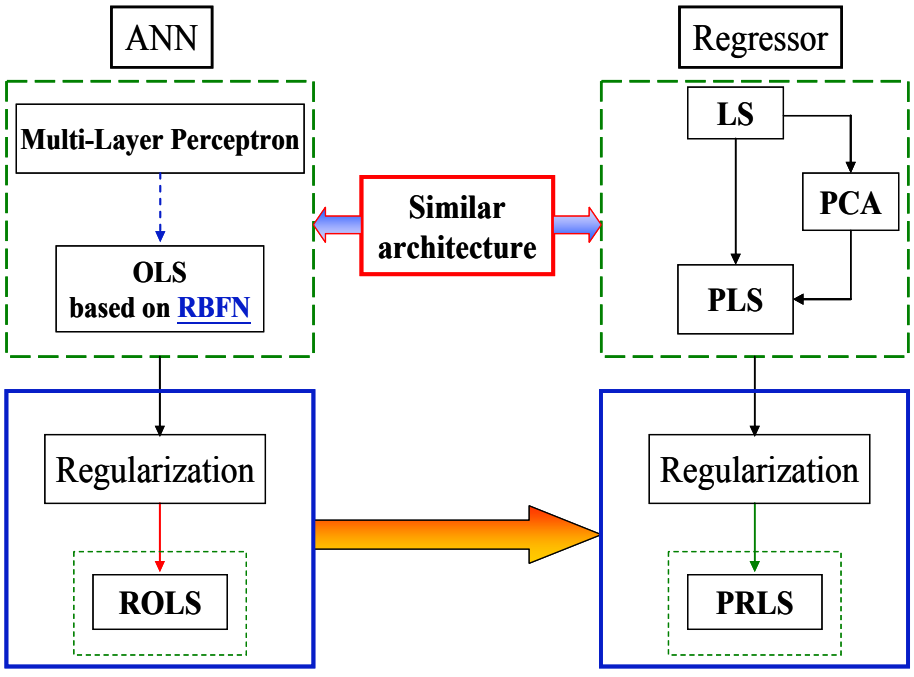


Figure 1.1 Research tracing diagram

Oja [4], [10] proposed PCA to reduce the dimension of input data by K-L transformation. However it has a main drawback which PCA lacks for information about which principal components are important for desired output and how many components are needed to compress the input data. PLS is a calibrated regression in common use. The concept of PLS was developed from LS. PLS also can compress the input data and solve the main drawback of PCA. But PLS estimation suffers from overfitting is more serious than PCA [5]. Chen [11] proposed Orthogonal Least Squares (OLS) based on radial basis function network (RBFN) also suffered from the same circumstance. By applying the regularization technique, Chen [12] also constructed Regularized Orthogonal Least Squares (ROLS) to solve the problem of overfitting.

In order to apply regularization technique to PLS, we represent PLS as three layer network. Following the example of ROLS computational architecture, we also modify the original PLS by combining the regularization to establish a novel calibrated model – partial regularized least squares (PRLS).

1.2. Motivation

PLS is a multivariate statistical technique that allows comparison between multiple response variables and multiple explanatory variables. It has been popular in many aspects. However there is a big problem that the predicted results would be influenced by outlier hidden in training data and lapse from output. The position is due to overtraining of system because we hope that executed outputs can approximate to desired outputs as far as possible. In ideal data, calibrated outcomes will be perfect but real data sets always have unseen information so that some results may reflect anomalies due to the information and poor accuracy for unseen examples. When training data goes along with noise, prediction often falls into a trap – overfitting [13]. Therefore we want to modify a usual method to acquire better performance than the original one when calibrating under noisy training data.

1.3. Related work

Pervious approaches have been proposed to solve the problem of overfitting.

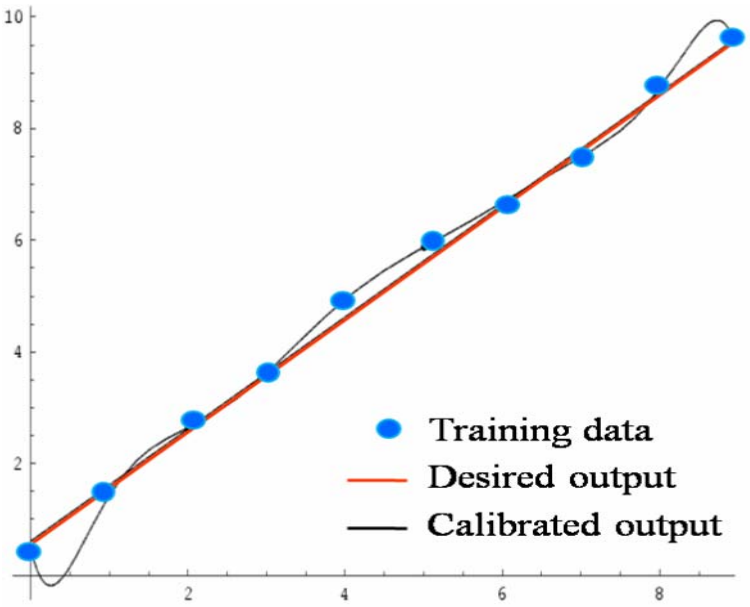


Figure 1.2 Illustration of overfitting.

The learner may adjust to specific features of the noisy training data that has no causal relation to calibration. To reduce the training error, the predicted curve would pass through each point possibly. At the same time, results would be influenced by the data with noise.

In general, three common techniques are selected to do:

1. Halt early – System would terminate training under a tolerant threshold. It is the simplest method but we have no idea when system must stop executing. If calculation process is terminated too early, results will be underfitting. Hence, it is difficult to determine when stopping working [6].
2. Postprocessing – System would select a validation data from original training data set and repeat until each observation in the set is used as validation data. The method also has the property of avoiding overfitting but it costs a large amount of computation [14].
3. Regularization – System would adopt iterative learning and calculate the probability distribution and acquiring the balance between overfitting and underfitting [12], [15], [16], [17], but it is hard to select regularized parameters appropriately.

1.4. Contribution

The contributions of this thesis can be summarized into two levels, as follow:

1. Here established a novel method combines a usual regression model with regularization, named PRLS. It combines the advantages of PLS and regularization.
2. Here also improved the accuracy of being calibrated by using PLS under the influence of noisy training data.

1.5. Thesis organization

Chapter 2 introduces the principle and architecture of several calibration models and further traces regularization technique [16], [17]. In Chapter 3, we discuss the relationship between PLS and regularization. Next, we propose a novel model - PRLS built by combining PLS with the technique. Chapter 4 shows the simulated experimental results of our purpose to evidence our theory. At last, the conclusion and further works are written down in Chapter 5.

Chapter 2. Methods and Materials

2.1. Least Squares (LS)

Classical least squares regression consists of minimizing the sum of the squared residuals. The linear model is given by $y_i = b_0 + x_{i1}b_1 + ... + x_{ip}b_p + \varepsilon_i$ (i = 1,…,n), where the error ε_i is usually assumed to be normally distributed with zero mean and standard deviation σ. The goal of multiple regression is to estimate $b = (b_0, b_1, ..., b_p)$ from the data $(1, x_{i1}, ..., x_{ip}, y_i)$. The sum of square error (*SSE*) is calculated as below:

$$SSE = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} (y_i - (b_0 + x_{i1}b_1 + ... + x_{ip}b_p))^2 \quad (2\text{-}1)$$

Partial difference by b_j, then we can derive (2-2)

$$\frac{\partial SSE}{\partial b_j} = 2\sum_{i=1}^{n} (y_i - (b_0 + x_{i1}b_1 + ... + x_{ip}b_p))(-1)x_{ij} = 0$$

(2-2)

where $j = 1,2,...,p$.

If we transform to matrix form, we can get a two layer multivariate analysis system illustrated as Figure 2.1. Then Y represents as matrix $[y_1, ..., y_n]^T$, real output $\hat{Y} = [\hat{y}_1, ..., \hat{y}_n]^T$ and $b = [b_0, b_1, ..., b_p]$.

The LS procedure in matrix form is defined as:

$$y = \mathbf{X}\, b + \varepsilon \quad (2\text{-}3)$$

We calculate the weighting coefficients due to (2-3).

$$\mathbf{X}^T y \approx \mathbf{X}^T \mathbf{X} b \quad (2\text{-}4)$$

$$b \approx (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T y) \quad (2\text{-}5)$$

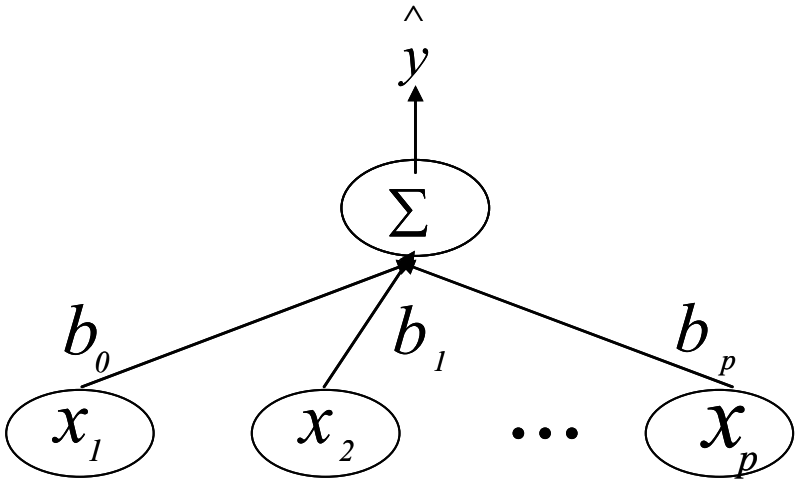


Figure 2.1 Two layer LS architecture.

In other words, LS method is to solve the approximated answer if there is no solution in geometry. We will use Figure 2.2, so as to explain

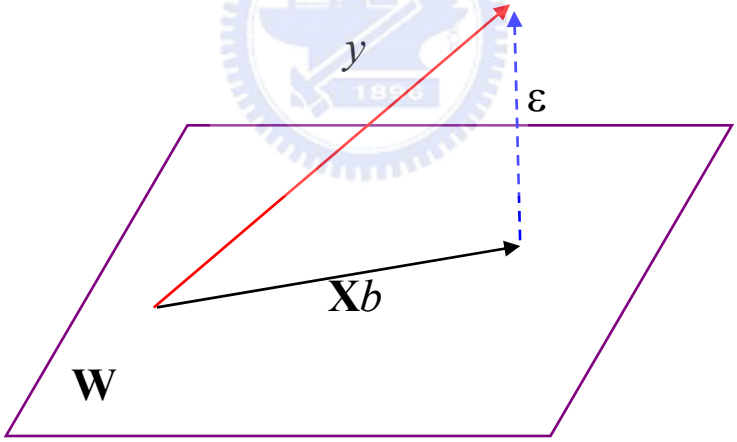


Figure 2.2 Illustration of LS in geometry

If $\mathbf{Y} \neq \mathbf{X}b$ express the column vectors of $\mathbf{X}$ can not span the vector $\mathbf{Y}$. We define the vector space $\mathbf{W} = span(col(\mathbf{X}))$ because the equation $\mathbf{Y} \neq \mathbf{X}b$ implies there is no solution. If we want to obtain the approximated answer, we have to reduce the residual ε. By the orthogonal projecting into vector space $\mathbf{W}$ acquiring the approximation because vector $\mathbf{Y}$ goes to space $\mathbf{W}$ takes straightly being apart from as the shortest.

2.2. Principal Component Analysis (PCA)

PCA is a self-organizing learning rule through Karhunen-Loeve (K-L) transformation mapping into feature space [10]. Adaptive eigenvectors which were chosen construct subspace of the space. And data reconstruction is also using K-L transformation mapping into the subspace.

Given a set of data $\mathbf{X}$ with dimension n and mean vector $m = E[\mathbf{X}] = 0$. We can compute the covariance matrix $\mathbf{C} = E[\mathbf{X}^{\mathrm{T}}\mathbf{X}]$. Through singular value decomposition (SVD) processing as follows:

$$\underset{nxn}{\left[\mathbf{C}\right]} = \underset{nxn}{\left[\mathbf{V}\right]} \underset{nxn}{\begin{bmatrix} \lambda_1^2 & & \\ & \lambda_2^2 & \\ & & \lambda_n^2 \end{bmatrix}} \underset{nxn}{\left[\mathbf{V}^{\mathrm{T}}\right]}$$

Eigenvalues in order: $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$

Figure 2.4 Singular value decomposition of covariance matrix

Final, selecting the p ($p \leqq n$) largest eigenvalues corresponding eigenvectors construct matrix $\mathbf{V}^*$ and discarding other eigenvectors in data representation. In regression, we shall add the LS phase after K-L transformation to estimate the curve fit. The regressive procedure is representable as:

$$\hat{\mathbf{X}} = \mathbf{X}\mathbf{V}^* \tag{2-6}$$

Using LS method can acquire the weights.

$$\mathbf{B} = \frac{\hat{\mathbf{X}}^{\mathrm{T}}\mathbf{Y}}{\hat{\mathbf{X}}^{\mathrm{T}}\hat{\mathbf{X}}} \tag{2-7}$$

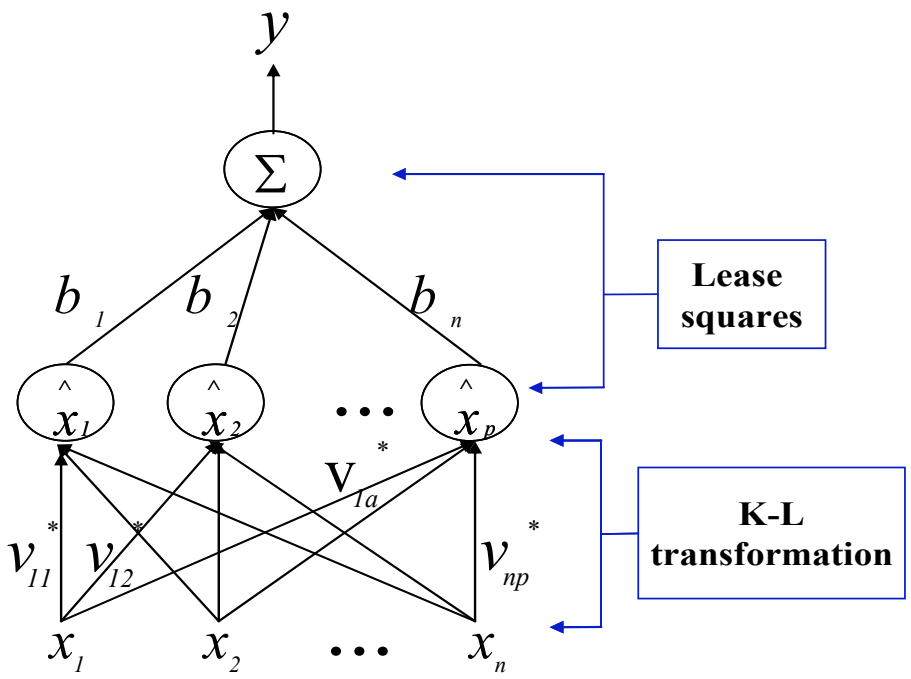


Figure 2.5 Three layer PCA architecture

2.3. Partial Least Squares (PLS)

PLS is one of the most general analysis methods in regression. Here we will show PLS mathematic decomposition, regression algorithm and architecture of three layer multivariate system.

The independent variable matrix $\mathbf{X}_{nxm}$ decomposed into matrix $\mathbf{U}_{nxa}$ with corresponding weighting matrix $\mathbf{P}_{mxa}$ and dependent variable matrix $\mathbf{Y}_{nx1}$ can be decomposed into matrix $\mathbf{V}_{nxa}$ with corresponding weighting matrix $\mathbf{Q}_{ax1}$. The mathematic form is represented as follows:

$$\begin{aligned}\mathbf{X}_{nxm} &= \mathbf{X}^{(1)} + \mathbf{X}^{(2)} + \ldots + \mathbf{X}^{(a)} + E \\ &= \hat{u}_1 \hat{p}_1^{\mathrm{T}} + \hat{u}_2 \hat{p}_2^{\mathrm{T}} + \cdots \hat{u}_a \hat{p}_a^{\mathrm{T}} + E \\ &= \mathbf{U}_{nxa}\mathbf{P}_{axm}^{\mathrm{T}} + E\end{aligned} \tag{2-8}$$

$$\begin{aligned}\mathbf{Y}_{nx1} &= \mathbf{Y}^{(1)} + \mathbf{Y}^{(2)} + \ldots + \mathbf{Y}^{(a)} + F \\ &= \hat{v}_1 \hat{q}_1 + \hat{v}_2 \hat{q}_2 + \ldots + \hat{v}_a \hat{q}_a + F \\ &= \mathbf{V}_{nxa}\mathbf{Q}_{ax1} + F\end{aligned} \tag{2-9}$$

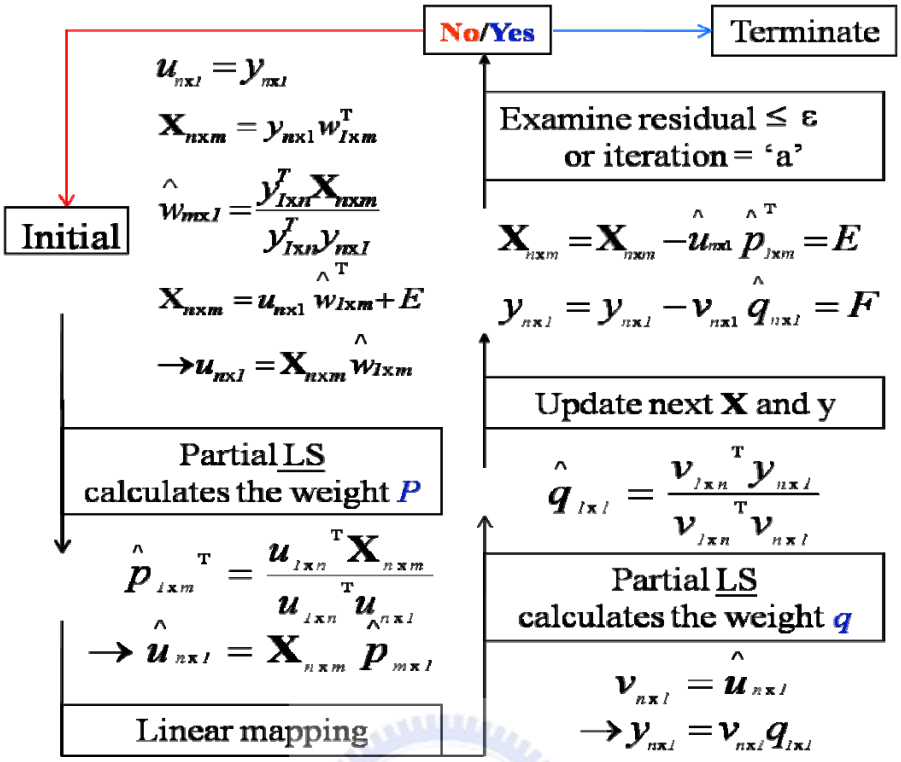


Figure 2.6 PLS algorithm flow chart

After derivative, we exactly find out the residual matrix $\|E_{nxm}\|$ and $\|F_{nx1}\|$ are minimized through the course of decomposing the matrix **X** and **Y** .When computational iteration equation to a ($a \leqq n$) or the residual small than a minimum, PLS would terminate.

Ham [18] and Hsiao [9] bring up an idea which regards PLS as one kind of artificial neural networks. In the purpose, transformation between independent and dependent variables can be represented as three layer network architecture.

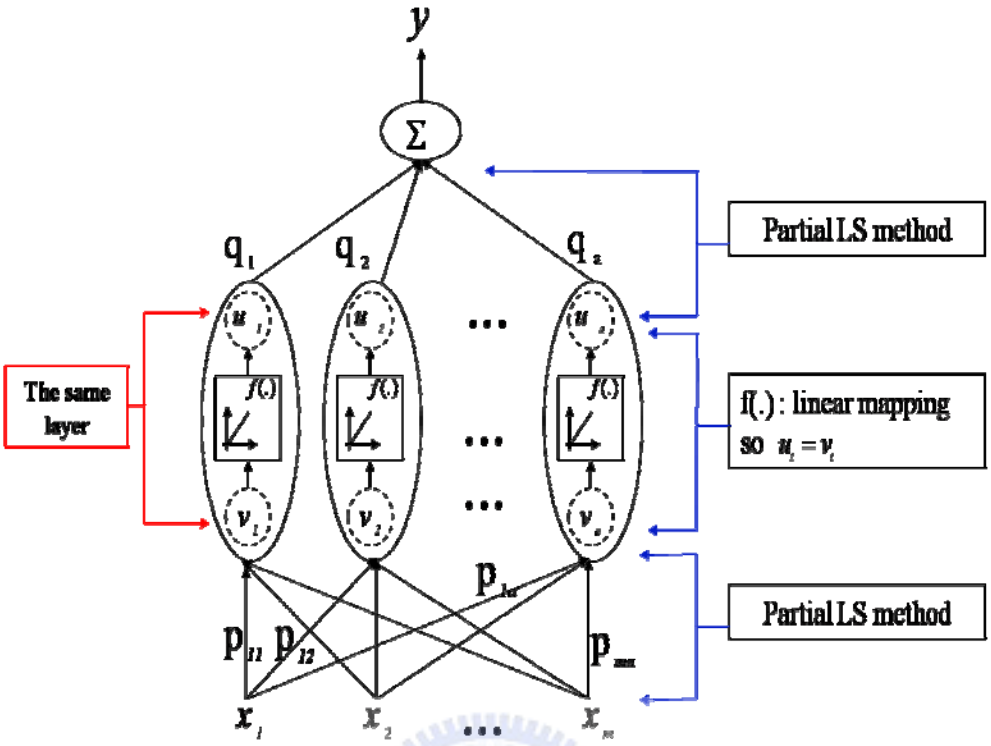


Figure 2.7 Three layer PLS architecture

2.4. Orthogonal Least Squares (OLS)

In this section, we describe OLS structure in the application for radial basis function networks (RBFN) to select adequate centers. This rational approach provides an efficient learning algorithm for fitting appropriate RBFN. Let $\mathbf{X}=[x_1,...,x_n]$ be independent matrix and $y=[y_1,...,y_n]^{\mathrm{T}}$ be dependent matrix then the transformation can be written as:

$$y=\mathbf{P}\boldsymbol{\theta}+E \tag{2-10}$$

where

$\mathbf{P}=[p_1,...,p_n]^{\mathrm{T}}$, $p_i=[\phi(\|x_i-x_j\|)]$, $\phi(.)$ is Gaussian function, with $1 \leqq i$, $j \leqq n$

$\boldsymbol{\theta}=[\theta_1,...,\theta_n]^{\mathrm{T}}$

$E=[e_1,...,e_n]^{\mathrm{T}}$

To make sense of the procedure clearly, we show the computational processing can be represented as:

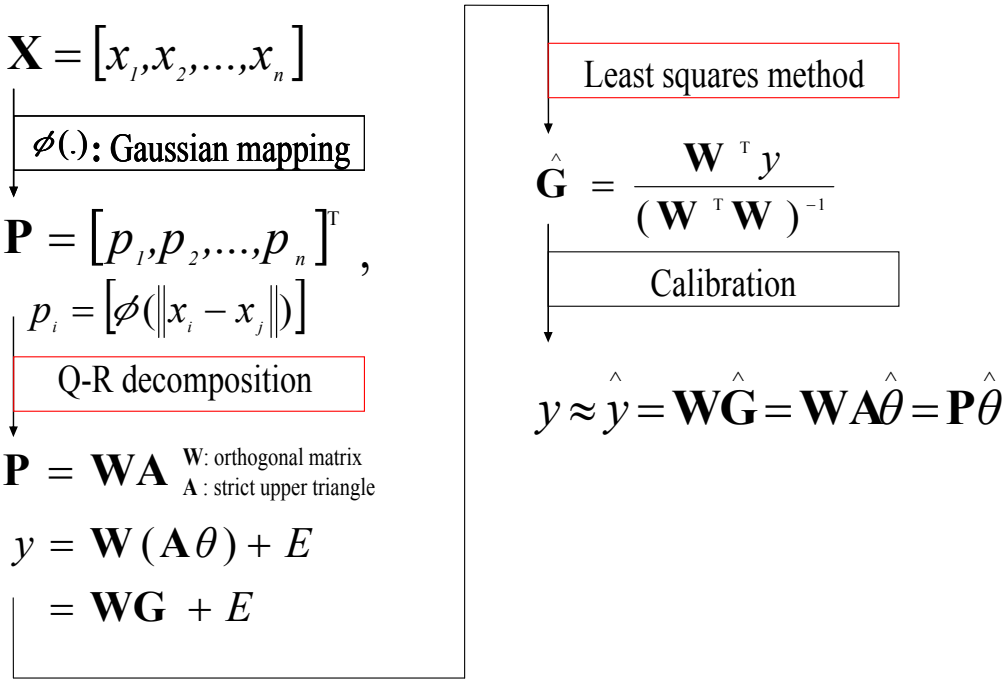


Figure 2.8 OLS based on RBFN flow chart

Simplifying the OLS computational flow, we replace Q-R decomposition with orthogonal processing. Orthogonal decomposition of **P** can be obtained using Gram-Schmidt orthogonal processing computes a column of **A** and selects an adequate regressor vector w_i at a time. OLS makes a criterion to select the regressor vector and minimize the residual each iteration. The error criterion can be written:

$$y^T y = \sum_{i=1}^{n} g_i^2 w_i^T w_i + E^T E \qquad (2\text{-}11)$$

Normalize (2-13) then we can acquire w_i due to error ratio (2-12)

$$\frac{\sum_{i=1}^{n} g_i^2 w_i^T w_i}{y^T y} = \frac{y^T y - E^T E}{y^T y} = \frac{calibration}{desired\ output} \qquad (2\text{-}12)$$

According to (2-14), OLS can pick out an appropriate regressor vector w_i with the error ratio mostly approximates to one each iteration.

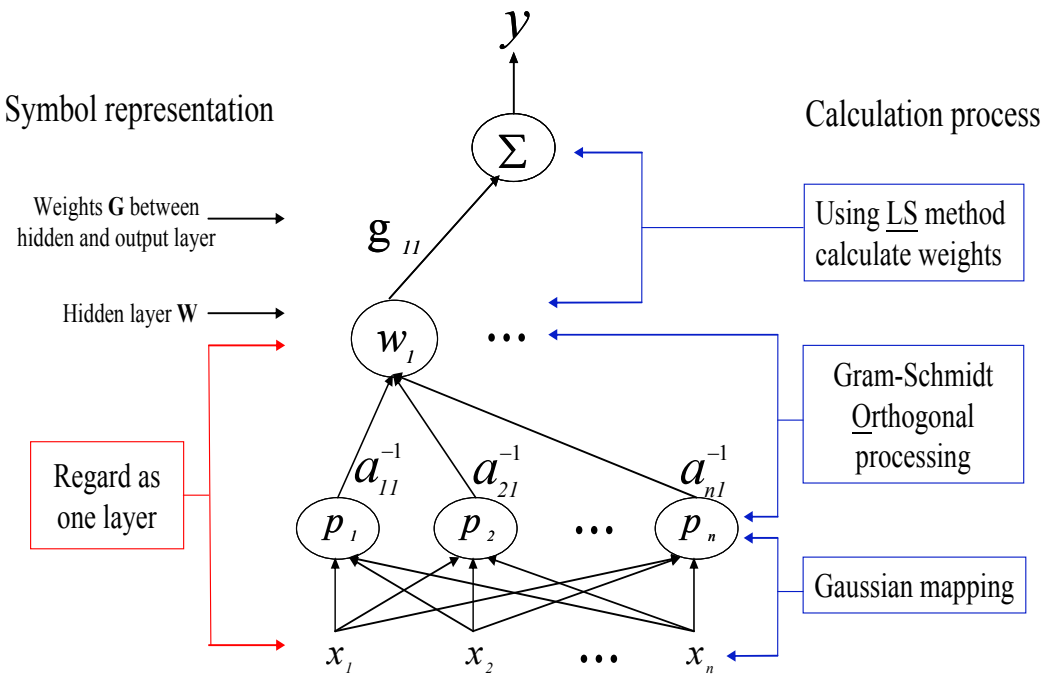


Figure 2.9 Three layer OLS architecture

There is no transformation mapping during Gram-Schmidt orthogonal processing so we shall regard two computational phases in front as one layer in Figure 2.9.

2.5. Regularization

Regularization techniques have been used in the past to avoid overfit [12], [16] and error function of residual is minimized which depends on the network weights as well as the fit error [15]. Essentially it involves adding some multiple of a positive definite matrix to an ill-conditioned matrix so that the sum is no longer ill-conditioned and is equivalent to simple weight-decay in gradient descent methods.

Let's define symbols to illustrate, $A[u]>0$ and $B[u]>0$ are two positive functions of u, so we can try to determine u by either

Minimize: $A[u]$ or $B[u]$ (2-13)

In summary, regularization is Lagrange multiplier equation combines with quadratic constraint to minimize the weighted sum $A[u]+\lambda B[u]$ and lead to a adequate solution for u.

2.6. Regularized Orthogonal Least Squares (ROLS)

ROLS algorithm combines the advantages of both the orthogonal regression and regularization methods to provide an efficient and powerful procedure for constructing models [12].

As mentioned earlier, the error criterion used in deriving the OLS algorithm is the total squared error $E^{\mathrm{T}}E$. But the criterion in certain circumstances is prone to overfitting. To prevent overfitting, regularization method can be applied. Using (2-11), we define the residual squares error over the training set is

$$E_D = \left\| y^{\mathrm{T}} y - \sum_{i=1}^{n} g_i^2 w_i^{\mathrm{T}} w_i \right\| \tag{2-14}$$

And regularized term

$$E_R = \left\| \sum_{i=1}^{n} g_i^2 \right\| \tag{2-15}$$

According to the regularization technique, it can be shown that the regularized error criterion can be expressed as

$$E_e = E_D + \lambda E_R = \left\| y^{\mathrm{T}} y - \sum_{i=1}^{n} g_i^2 w_i^{\mathrm{T}} w_i \right\| + \lambda \left\| \sum_{i=1}^{n} g_i^2 \right\|, \text{ with } \lambda \geq 0. \tag{2-16}$$

Minimizing the equation E_e, we can get the appropriate term w_i.

Finally, we will show diagram of ROLS architecture to understand which computational phase is modified in Figure 2.10.

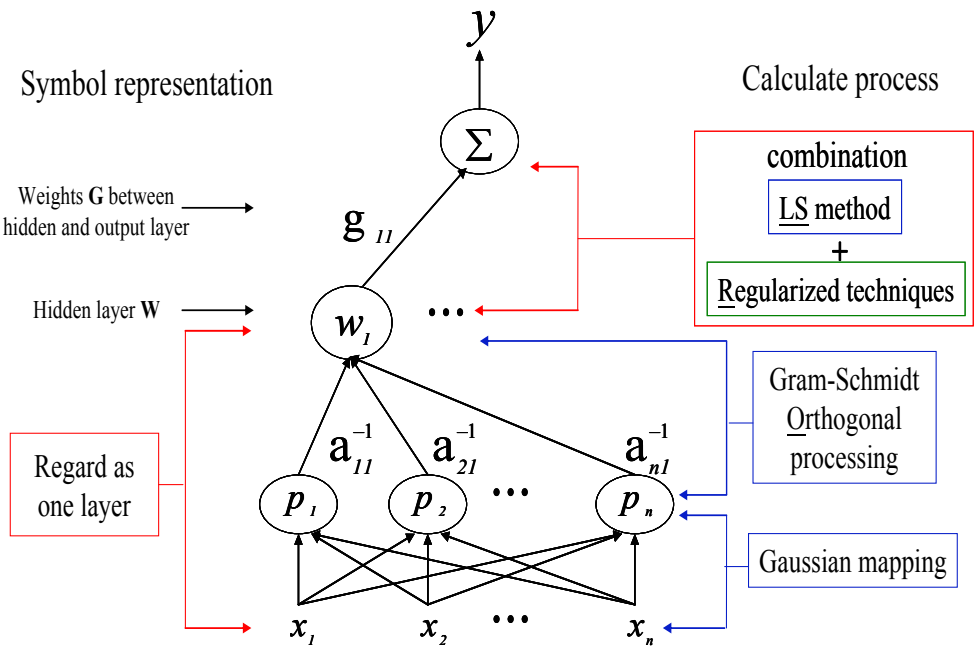


Figure 2.10 Three layer ROLS architecture

Chapter 3. A novel method - Partial Regularized Least Squares (PRLS)

3.1. Relation between PLS and regularization

In this chapter, we will modify PLS architecture to reconstruct a novel calibration method, named as PRLS, to avoid overfitting which occurs when there is noise in the training data and the calibration system is flexible enough to fit to it. Here using the same symbols in section 2.3.

Original PLS calibrates during the processing of decomposing independent and dependent matrix, we only minimized the residual matrix $\|E_{nxm}\|$ and $\|F_{nx1}\|$. In the ideal situation, the calibration will approximate the desired output as minimum as it can be. But real data always goes along with hidden information that we have no idea whether it will interference the prediction or not. In this circumstance, PLS calibration may fit the noisy data and the outcome will lapse from our desire. We shall use the property of regularization and apply it to original architecture to solve this problem.

As mentioned earlier, we exploit the concept of regularization techniques and rewrite the error criterion of PLS as:

$$E_e = E_D + \lambda E_R = E^{\mathrm{T}}E + \lambda q^{\mathrm{T}}q\,, \quad \lambda \geq 0 \tag{3-1}$$

Where q is weighting vector which inferences the output directly. In order to interpret equation E_e and regularized parameter λ, we will illustrate using trade off curve as below

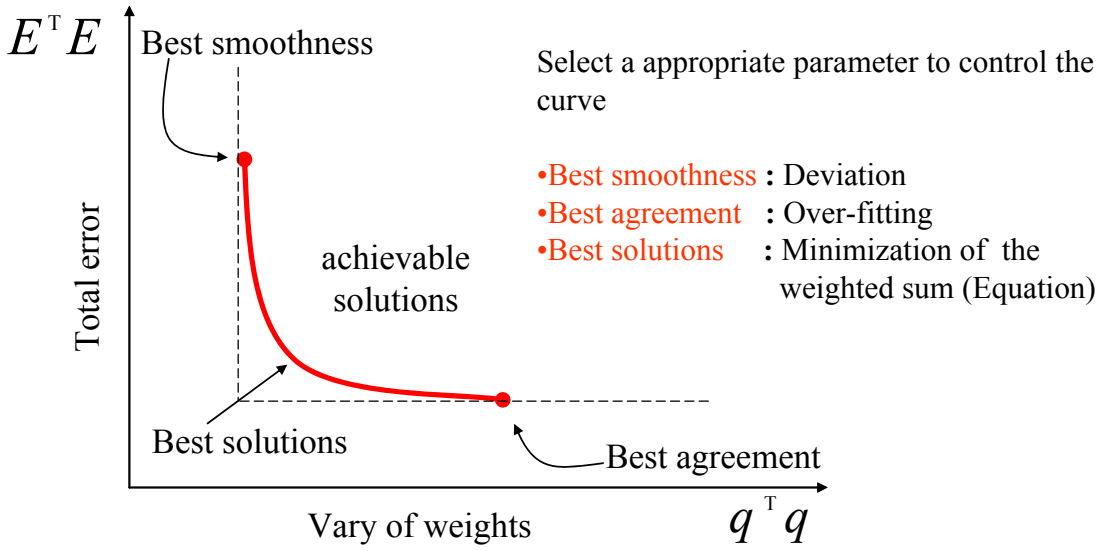


Figure 3.1 Trade off curve

Figure 3.1 illustrates that all achievable solutions are above the trade off curve but some of them conform our desire. Original PLS calibration reduces the total error as far as possible but if there is noise in training data, prediction may also fit the noisy data. Vary of weighting coefficients $q^T q$ controls the curve motion and we add the term multiplies regularized parameter λ to error criterion to make the calibration curve smooth without oscillating. In conclusion, PRLS keeps the calibration's balance between smoothness of curve and accuracy.

3.2. PRLS algorithm

In the following, we will describe the modeling algorithm. Figure 3.2 points out the modulation to PLS. Although there are two computational phases using partial LS method, we only modify the later half because only the second half among two computational phases affects the executed output directly. Next, to understand the architecture obviously, we regard PRLS as a three layer neural network in Figure 3.3.

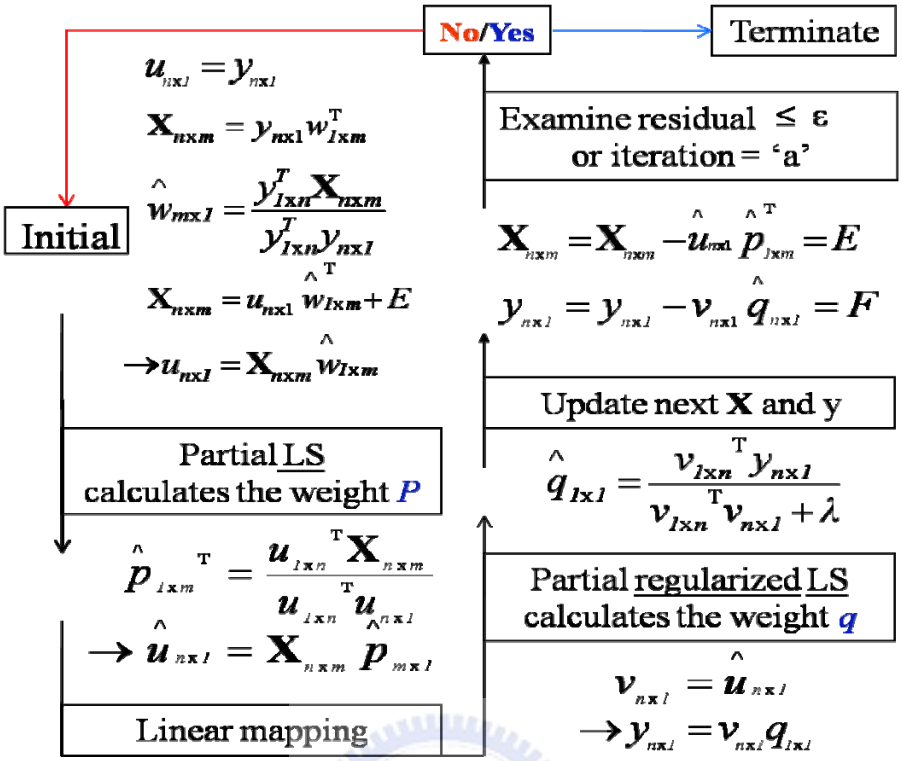


Figure 3.2 PRLS algorithm flow chart

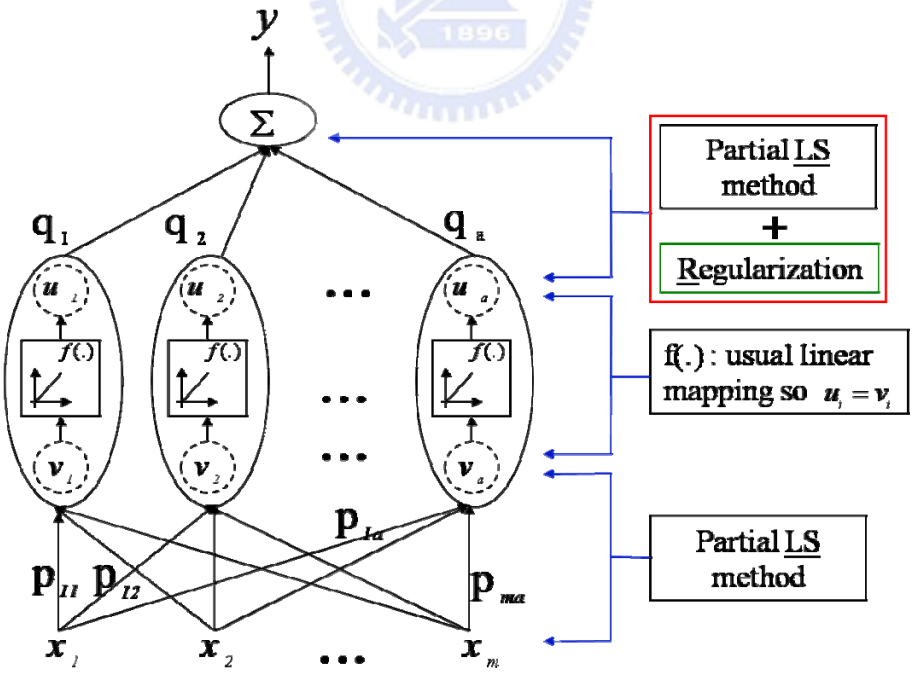


Figure 3.3 Three layer PRLS architecture

Chapter 4. Experiments and discussion

This chapter will demonstrate our simulation experiment results including simulation data and real data from 1D to 2D data and sound files. In the simulation data experiments, results show that PRLS has better performance than PLS and keep calibration stable with noise data. In the real data experiments, we apply our method to analyze environment sound measurement [19] and spectrum of blood glucose measurement [20].

4.1. Illustration

4.1.1. Synthesized simulation data

In simulation data calculation, we use synthesize three kinds of testing data with noise to examine the efficiency of PRLS method. We add the noise generated by Gaussian probability density function with zero mean and set the value of standard deviation, so as to alter the level of noise. The noise to signal (N/S) ratio is also used to set up a standard of the variation. Given a signal data set $signal_i$ and Gaussian noise data set $noise_i$ with zero mean, $1 \le i \le n$. The mean of signal and noise data set are:

$$\mu = \frac{\sum_{\forall n} signal_i}{n}$$

$$\mu_N = \frac{\sum_{\forall n} noise_i}{n} \qquad (4\text{-}1)$$

The variance of a signal and noise data set are

$$Var(signal) = \frac{\sum_{\forall n} (signal_i - \mu)^2}{n}$$

$$Var(noise) = \frac{\sum_{\forall n} (noise_i - \mu_N)^2}{n} \qquad (4\text{-}2)$$

The noise to signal (N/S) ratio is

$$N/S \text{ ratio} = \frac{\sqrt{Var(noise)}}{\sqrt{Var(signal)}} \qquad (4\text{-}3)$$

4.1.2. Criterion of estimation

Two kinds of familiar standards are used to verify the performance of PRLS. It is also used to show the improvement of PLS when calibrating training data with outlier, prediction may overfit to noise. One of them is correlation coefficient indicates the strength and direction of a linear relationship between two variables. It refers to the departure of two variables from independence. The other is root mean square error (RMSE). RMSE is one of many ways to quantify the amount by which an estimator differs from the true value of the quantity being estimated like as a loss function. Following, we will illustrate with simple graphs.

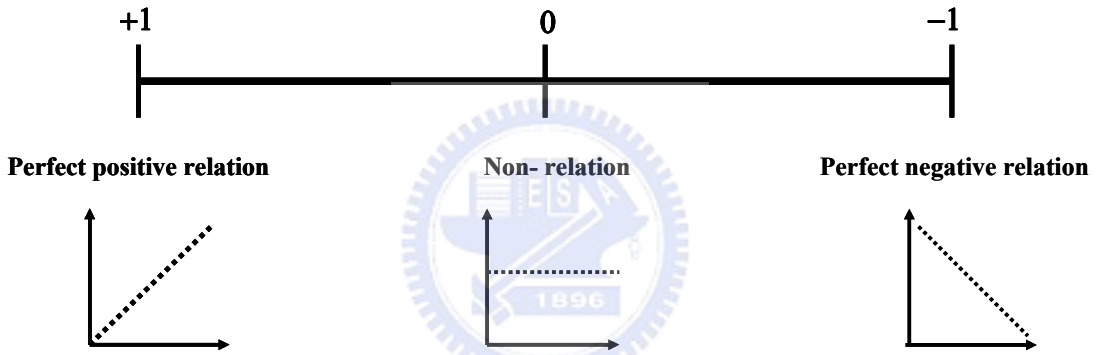


Figure 4.2 A sketch map of correlation coefficient

Several data sets of (x,y) points, with the correlation coefficient of x and y for each set. More approaching positive one more keeping consistency of direction between variables and distributing linearly. On the contrary, closing negative one indicates that the direction is opposite but distribution is also linear.

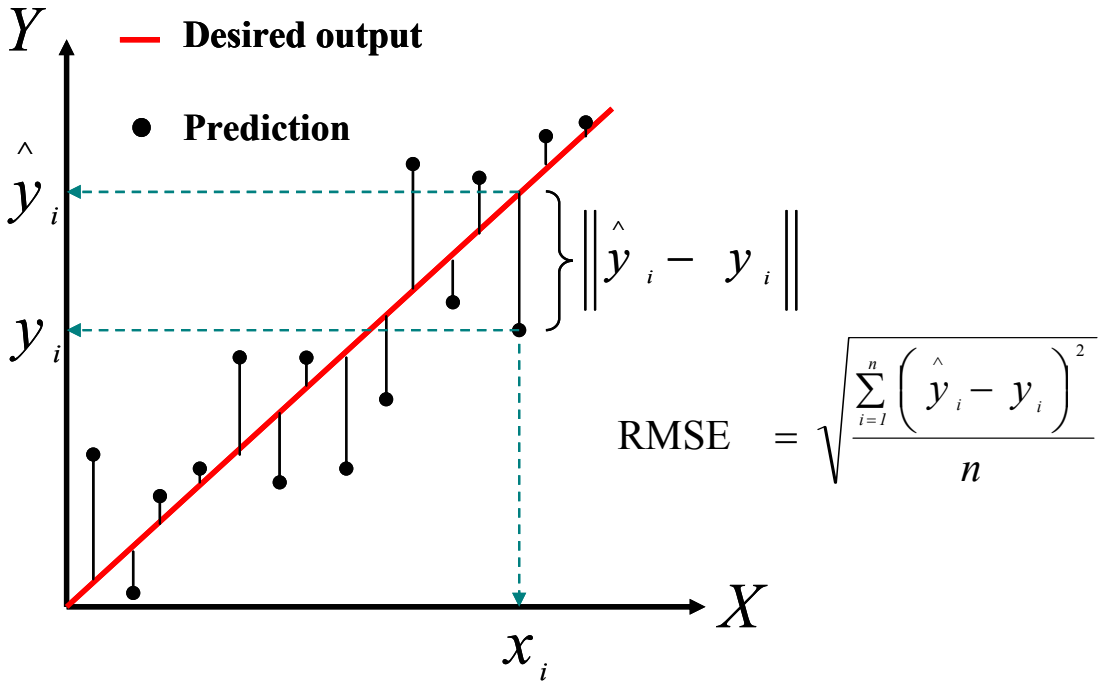


Figure 4.3 Root mean square error

Figure 4.3 shows that the main concept of RMSE is to calculate the average of the distance between prediction and desired output data. To acquire accurate prediction, we hope that RMSE minimizes as far as possible.

4.1.2. Conditional training

Here we also calibrate the training data in different conditions — (1) self-calibration & self-prediction (SCSP) and (2) cross validation (CV). In order to understand easily what is difference between SCSP and CV. We use diagrams to illustrate. Figure 4.4 shows the principle of SCSP and Figure 4.5 shows CV.

SCSP is a traditional training mode and the training data set is also prediction data set. Usually the result of SCSP is ideal if there is no noise hidden in the source data. However data usually goes along with noise and SCSP would be influenced by hidden information so that results may not necessarily meet to desire.

CV is also called leave one out (LOO) method because we select a validation data from original training data set and repeat until each observation in the set is used as validation data. The method also has the property of avoiding overfitting but costs heavy computation. Next, we will compare regularization technique and CV in simulation and real data experiments.

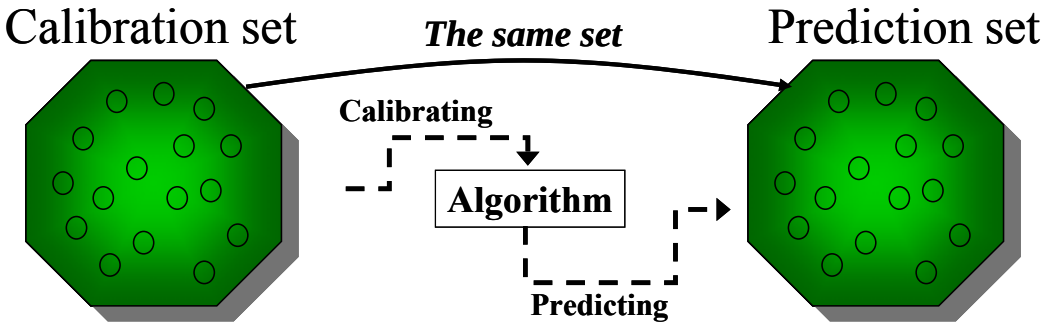


Figure 4.4 Self-calibration & self-prediction (SCSP)

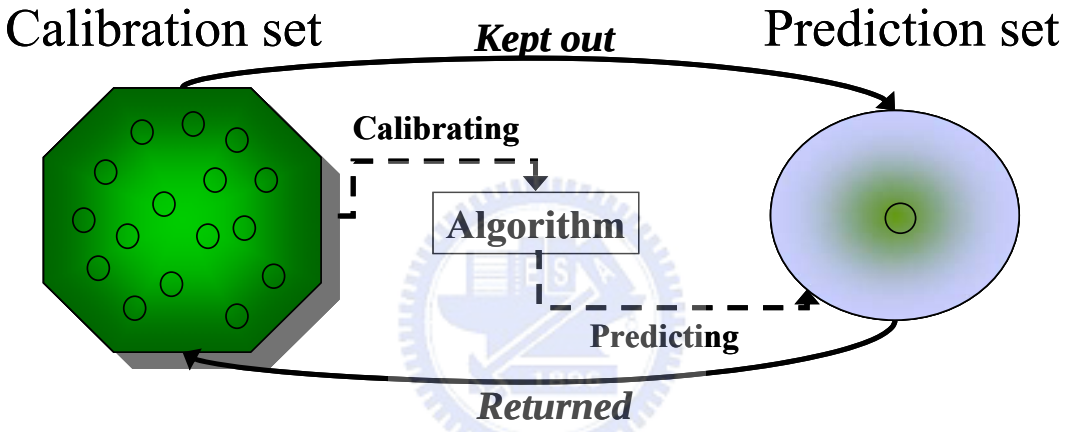


Figure 4.5 Cross validation (CV)

4.2. Simulation data

In this section, PRLS and PLS will calibrate sigmoid and polynomial function and imitative spectrum data under SCSP and CV. After predicting, we apply the criterion of estimation to examine which one is better among two methods and a brief discussion would be written down after experiments.

4.2.1. Sigmoid function

PRLS and PLS are used to approximate to the sigmoid function.

$$f(x_i) = \cos(x_i),\ 0 \leqq x \leqq 2\pi \qquad (4\text{-}4)$$

One hundred training data were generated from $f(x_i)+\varepsilon_i$, where x_i has take from the uniform distribution in $(0,2\pi)$ and the noise ε had a Gaussian distribution with zero mean. The training data and the sigmoid function $f(x_i)$ are plotted in Figure 4.6. The

training data is highly ill-conditioned. Figure 4.7 depicts the correlation coefficient as a function of noise to signal ratio under SCSP and Figure 4.8 depicts the RMSE as a function of noise to signal ratio under SCSP. Figure 4.9 shows the network mapping constructed by PRLS and PLS algorithm with noise to signal ratio is 0.55.

Under CV condition, we set N/S ratio = 0.55 and calibrate sigmoid function again. Figure 4.10 depicts correlation coefficient as a function of iteration. Figure 4.11 depicts RMSE as a function of iteration. Figure 4.12 shows that network mapping constructed by PRLS and PLS with noise to signal ratio is 0.55 under CV.

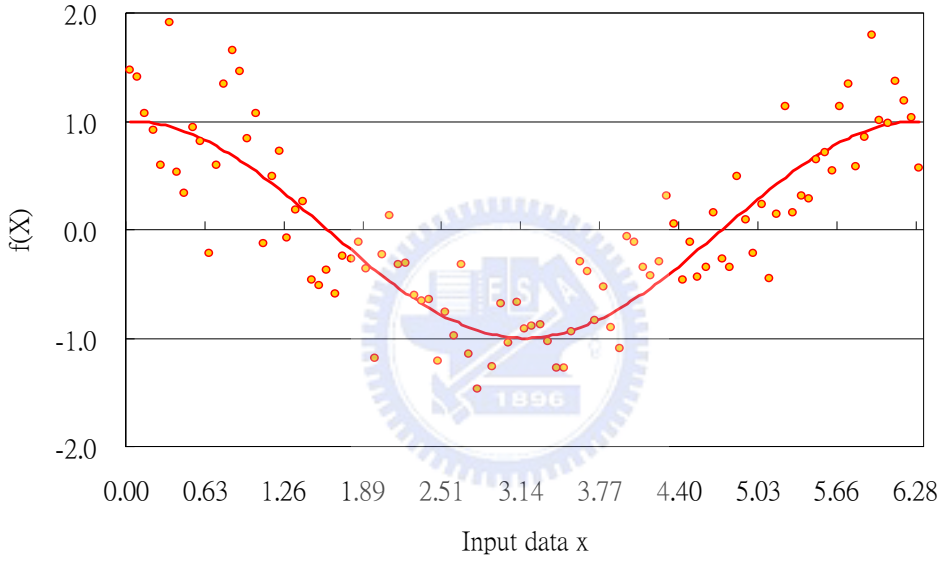


Figure 4.6 Noisy training data (points) and sigmoid function (curve) with N/S ratio = 0.55

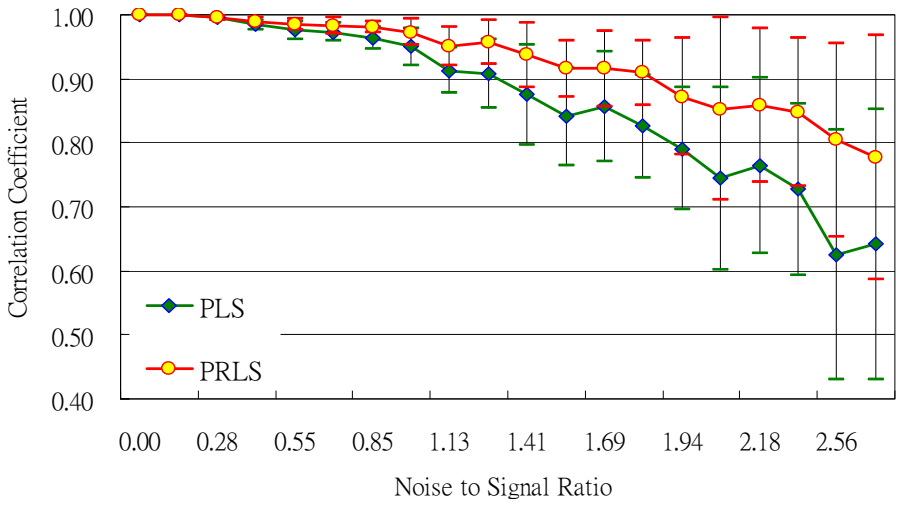


Figure 4.7 Correlation coefficient as a function of N/S ratio under SCSP

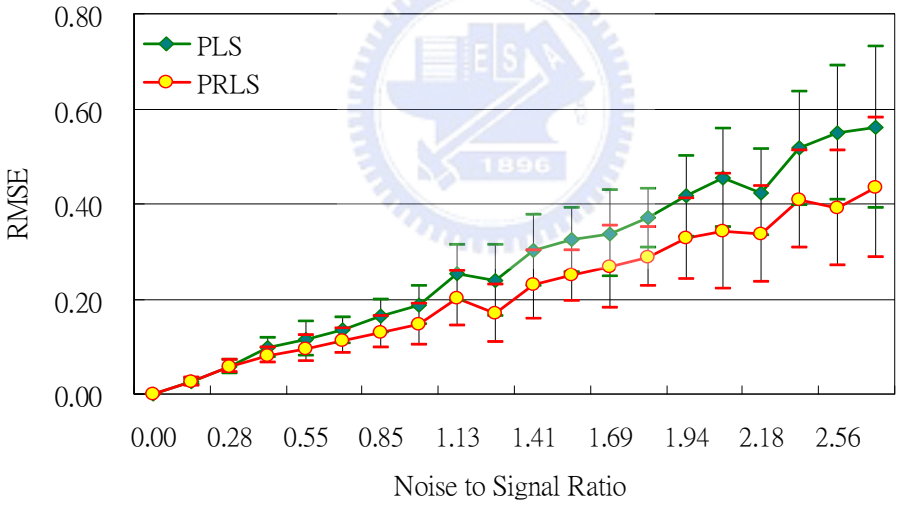


Figure 4.8 RMSE as a function of N/S ratio under SCSP

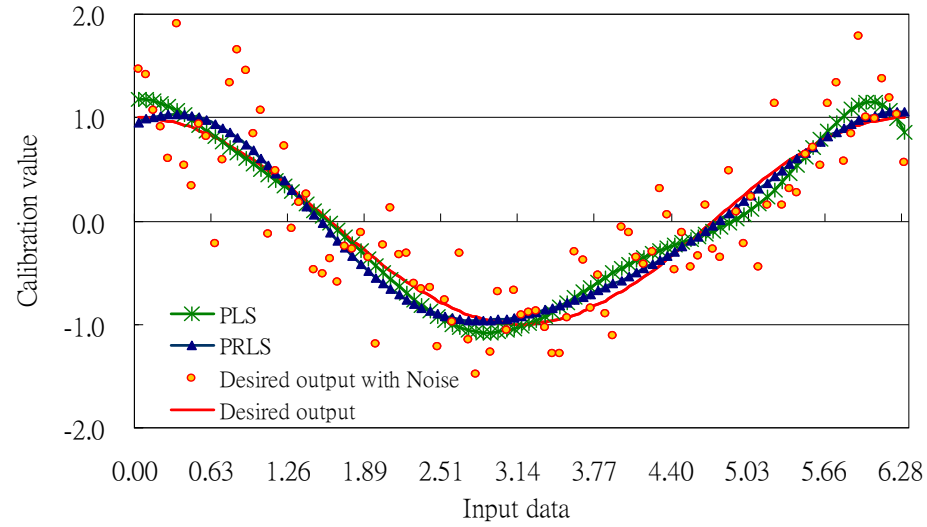


Figure 4.9 Network mapping constructed by PRLS and PLS algorithm under SCSP with N/S ratio = 0.55

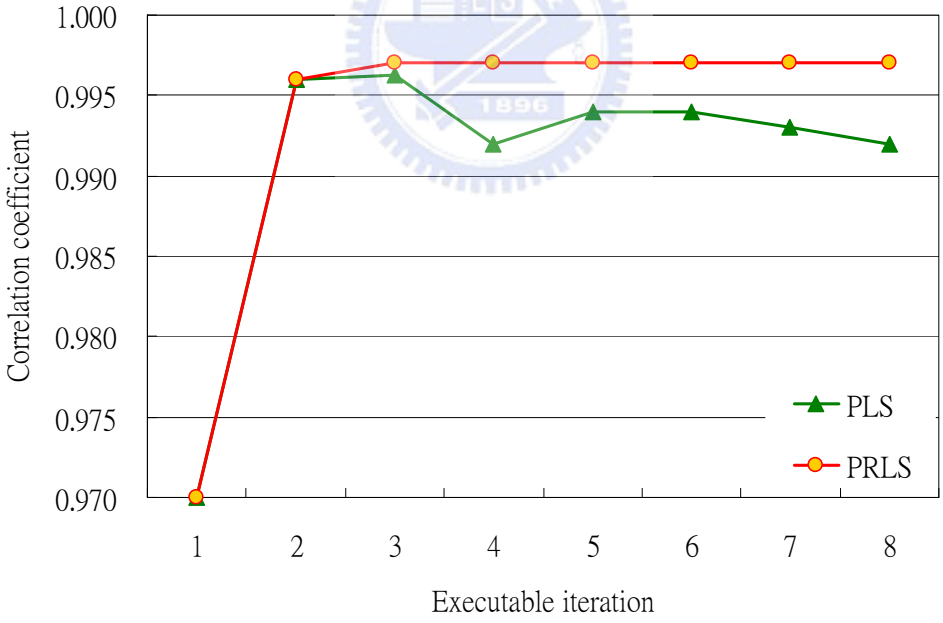


Figure 4.10 Correlation coefficient as a function of iteration under CV

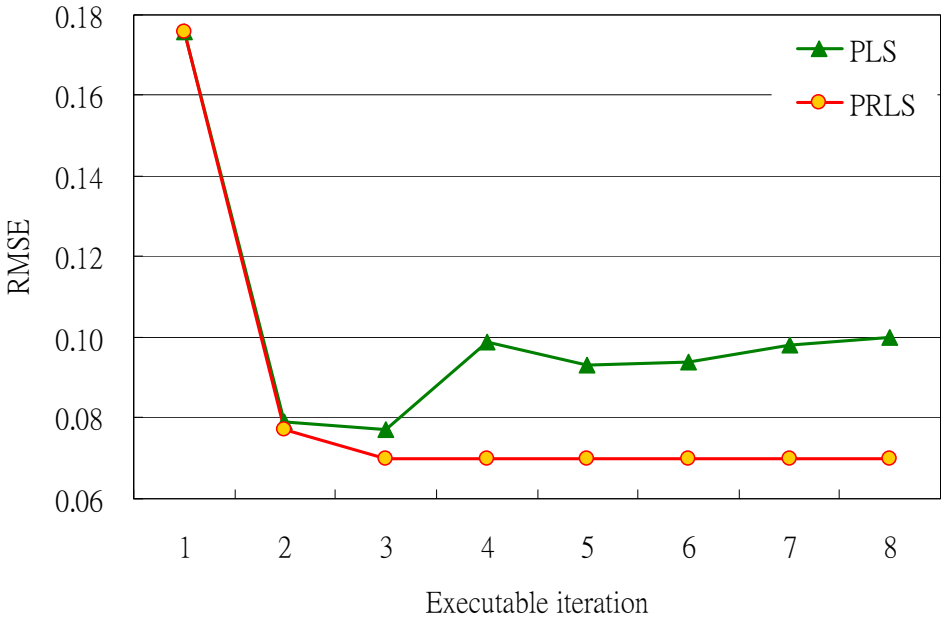


Figure 4.11 RMSE as a function of iteration under CV

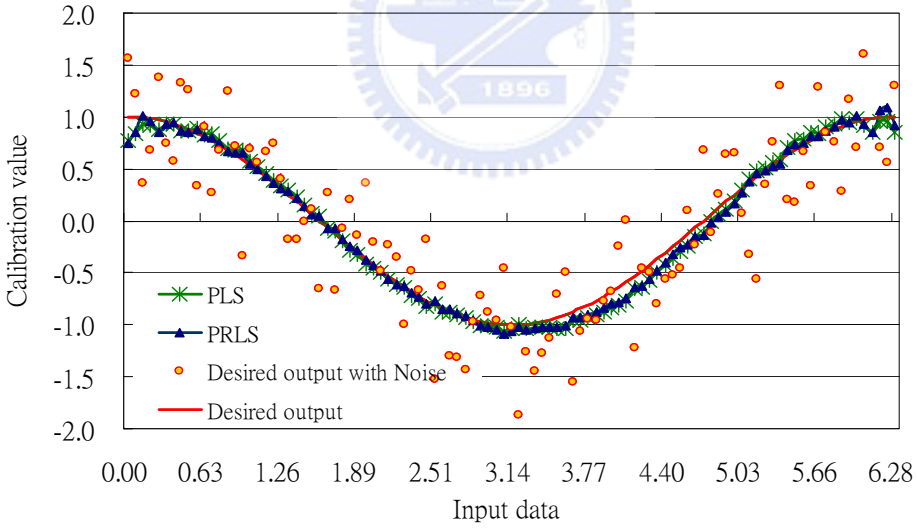


Figure 4.12 Network mapping constructed by PRLS and PLS algorithm under CV with N/S ratio = 0.55

Table 4.1 Optimal CV results for sigmoid function data

	PLS	PRLS
Correlation coefficient	0.9963	0.9971

RMSE	0.0772	0.0694
Adequate iteration	3	3

The results shown in above diagrams and table clearly demonstrate that the PRLS algorithm has better generalization properties

4.2.2 Polynomial function

In this experiment, we use polynomial function to examine.

$$f(x) = 8^{th} \text{ polynomial}, -1 \leqq x \leqq 1 \qquad (4\text{-}5)$$

We divide the range [-1,1] into one hundred parts and the training data were generated in the same way as 4.2.1. The noisy training data set and polynomial function were display in Figure 4.13. In the following, we will still estimate methods under SCSP and CV. Figure 4.14 depicts correlation coefficient as a function of noise to signal ratio and Figure 4.15 depicts RMSE as a function of noise to signal ratio under SCSP. PRLS and PLS prediction with noise to signal ratio is 0.55 under SCSP were plotted in Figure 4.16.

After examining under SCSP, we set constant noise to signal ratio to calibrate under CV and the records of correlation coefficient, RMSE and prediction were expressed in Figure 4.17, Figure 4.18 and Figure 4.19.

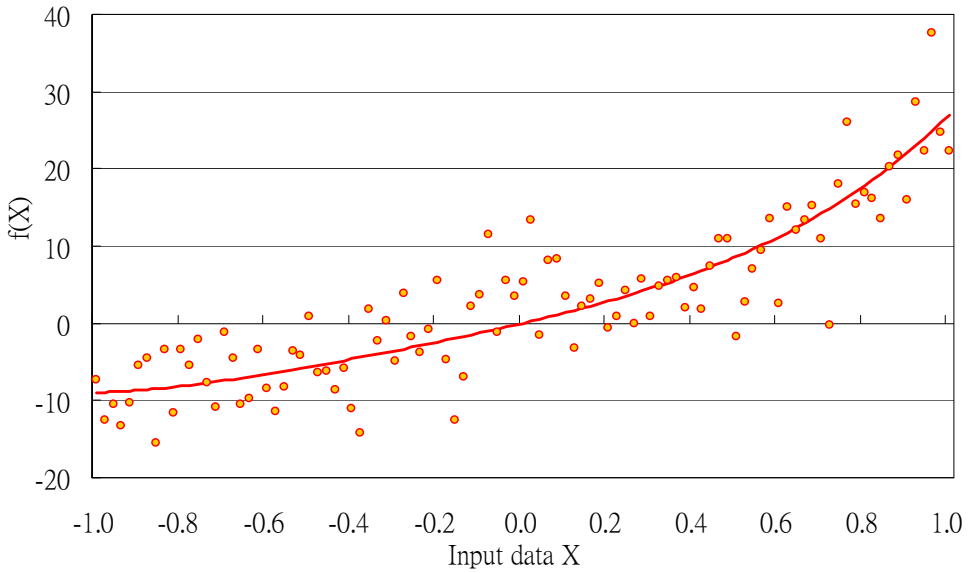


Figure 4.13 Noisy training data (points) and polynomial function (curve) with N/S

ratio = 0.55

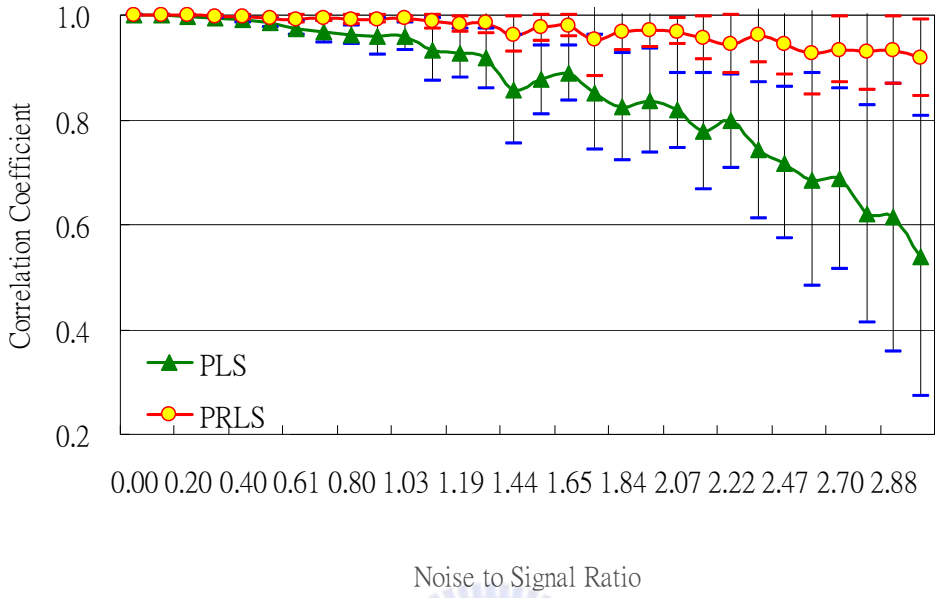


Figure 4.14 Correlation coefficient as a function of N/S ratio under SCSP

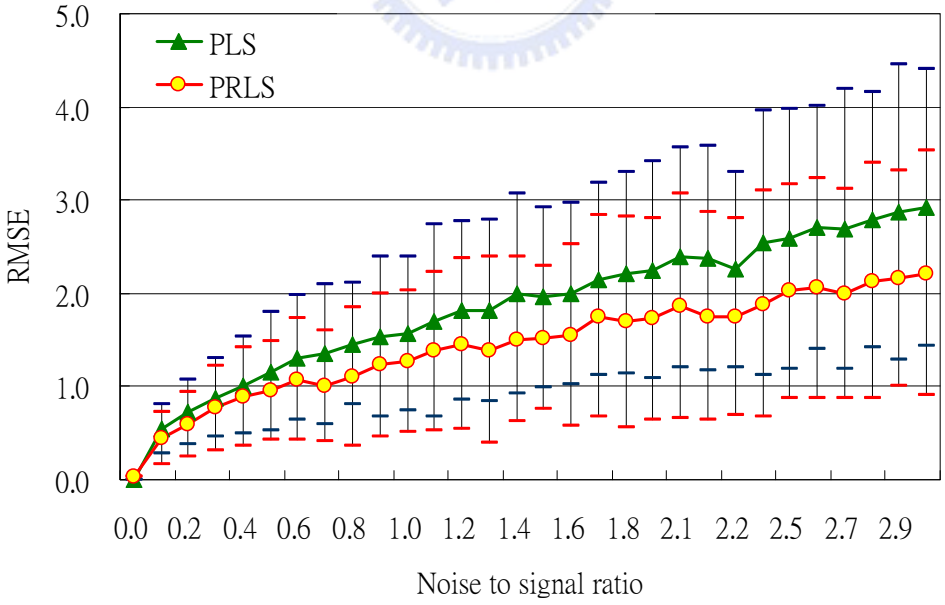


Figure 4.15 RMSE as a function of N/S ratio under SCSP

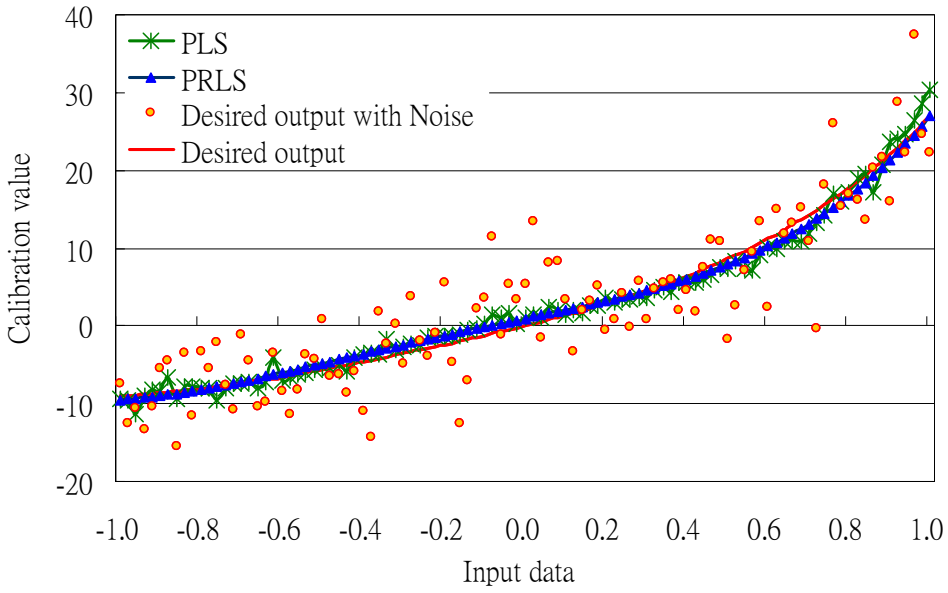


Figure 4.16 Network mapping constructed by PRLS and PLS algorithm under SCSP with N/S ratio = 0.55

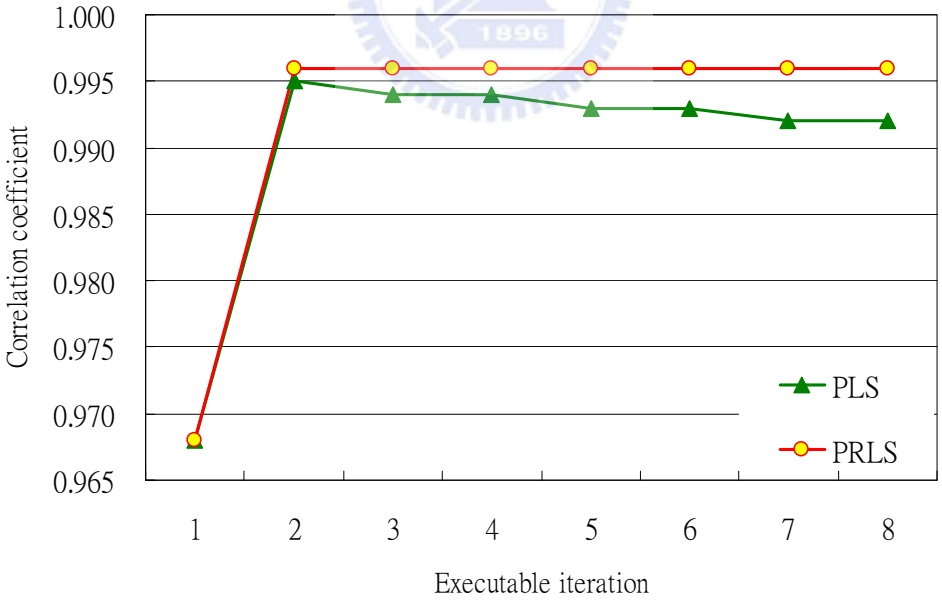


Figure 4.17 Correlation coefficient as a function of N/S ratio under CV

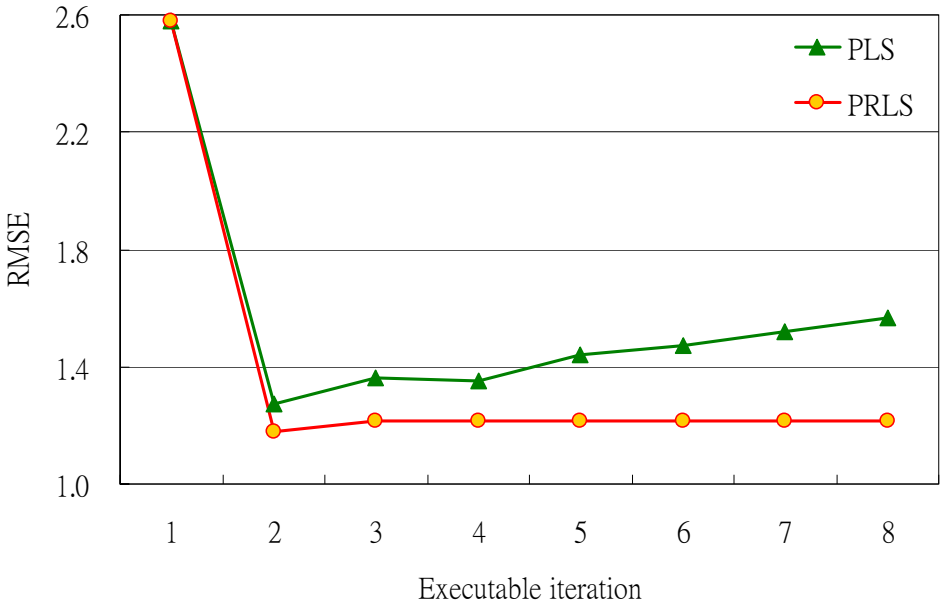


Figure 4.18 RMSE a function of N/S ratio under CV

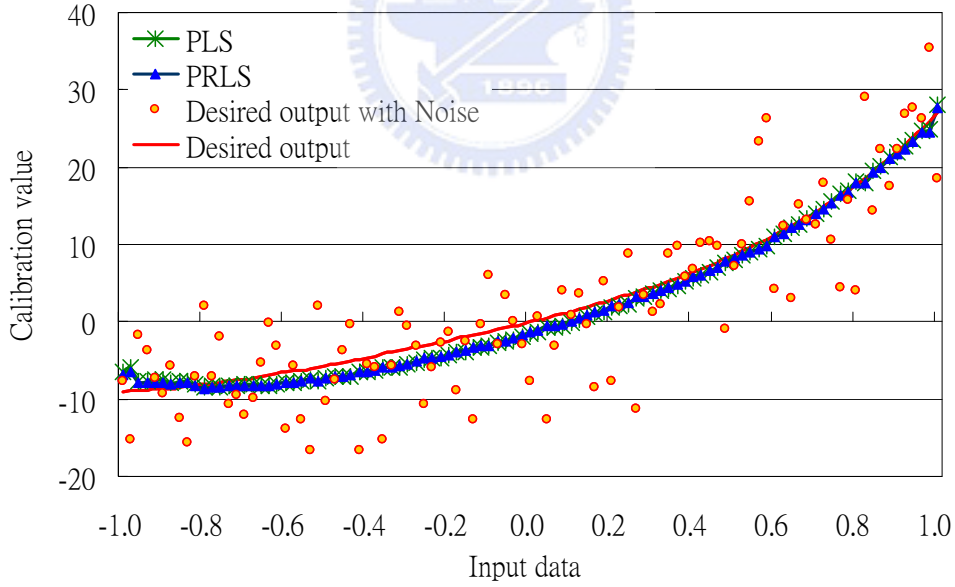


Figure 4.19 Network mapping constructed by PRLS and PLS algorithm under CV with N/S ratio = 0.55

Table 4.2 Optimal CV results for polynomial prediction data

	PLS	PRLS

Correlation coefficient	0.9959	0.9967
RMSE	1.2738	1.1796
Adequate iteration	2	2

From experimental result, we can find out PRLS also has better performance than PLS whether the prediction is under SCSP or CV.

4.2.3 Imitative spectrum

We would like to generate two Gaussian functions g(x) with mean = 400 and standard deviation = 20, h(x) with mean = 420 and standard deviation = 15. f(x) is the linear combination of g(x) and h(x) plotted in Figure 4.20.

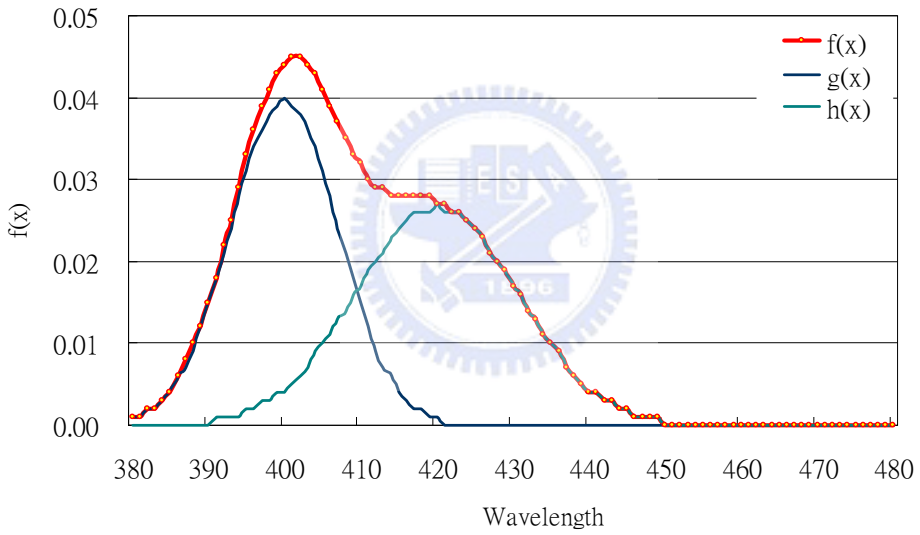


Figure 4.20 Linear combination of two Gaussian functions with different mean and standard deviation

The training data set $X_i + \varepsilon$ can be created by linear combination of g(x) and h(x) with noise where x is the wavelength divided into one hundred identical parts. Desired output Y is the set of weighting coefficients. Figure 4.21 exhibits the training data.

$f(x)\_i = Xi + \varepsilon = w_i \cdot g(x) + (1/w_i) \cdot h(x) + \varepsilon$, $1 \leqq i \leqq 10$

$Y = [w_1, w_2, \ldots, w_{10}] = [1, 1.5, 2, \ldots, 5.5]$ (4-6)

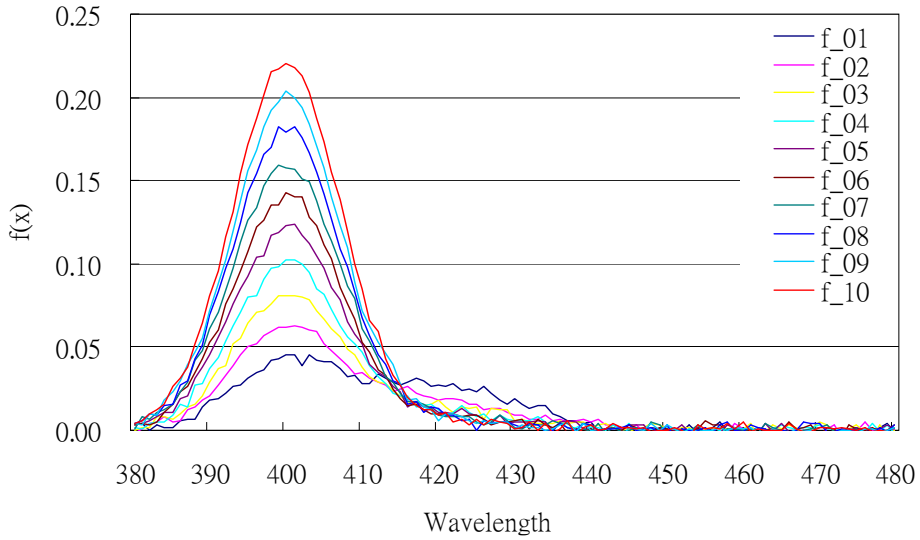


Figure 4.21 Training data sets of imitative spectrum

Next, we show the results of calibration, also divided into two conditions. The first result is under SCSP (Figure 4.22 – Figure 4.24) and the second result is under CV (Figure 4.25 – Figure 4.27) . All of them are shown as below:

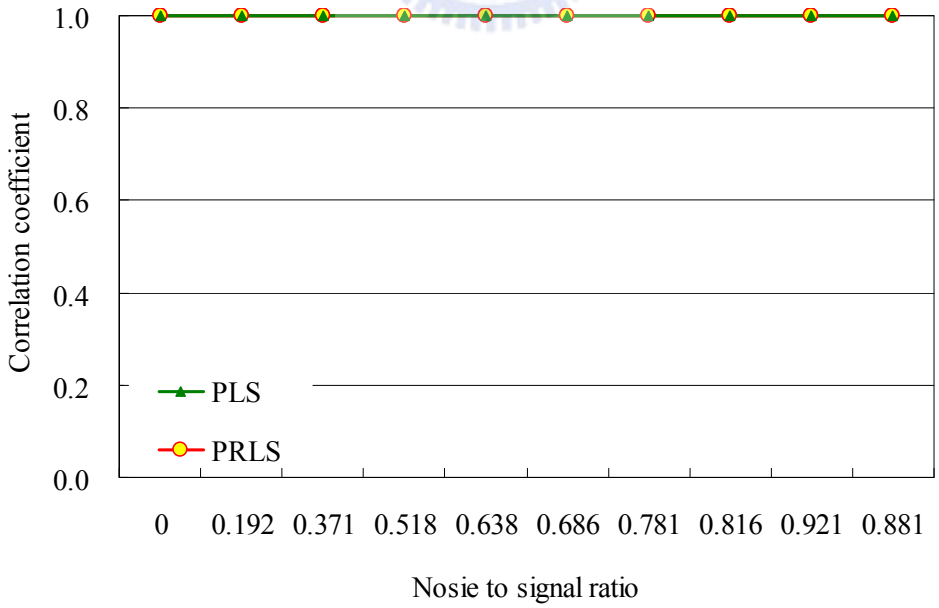


Figure 4.22 Correlation coefficient as a function of executable iteration under SCSP

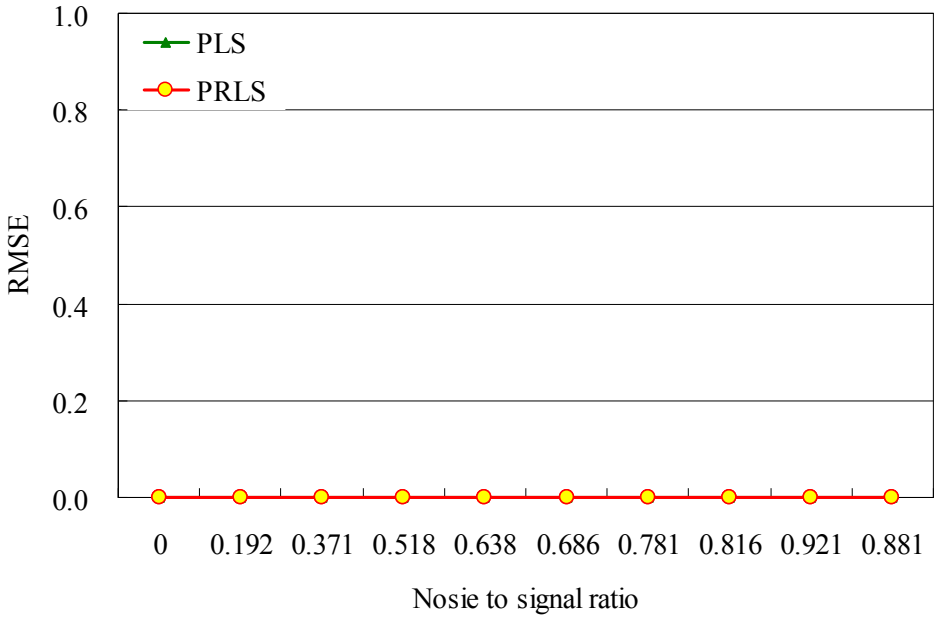


Figure 4.23 RMSE as a function of executable iteration under SCSP

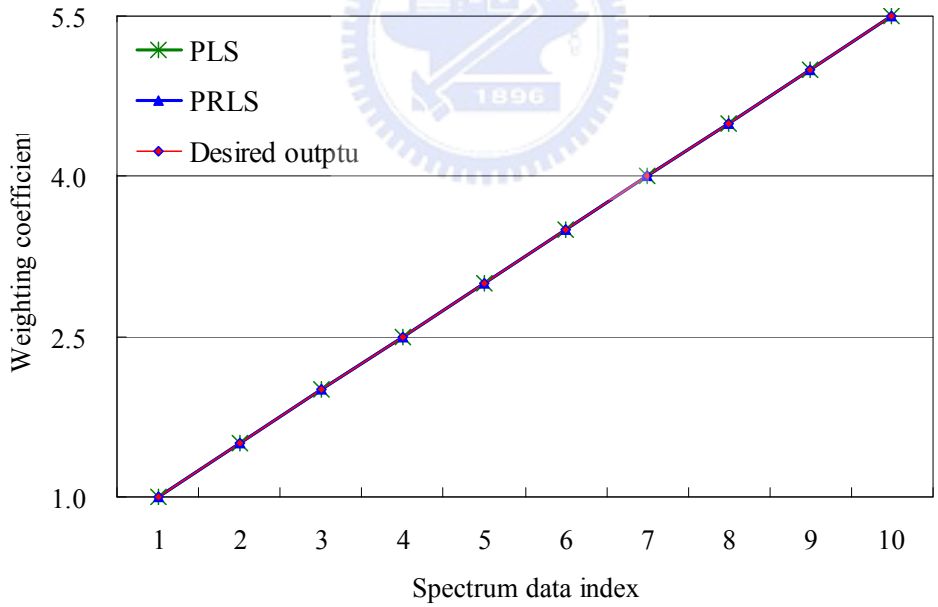


Figure 4.24 Network mapping constructed by PRLS and PLS algorithm under CV with N/S ratio = 0.55

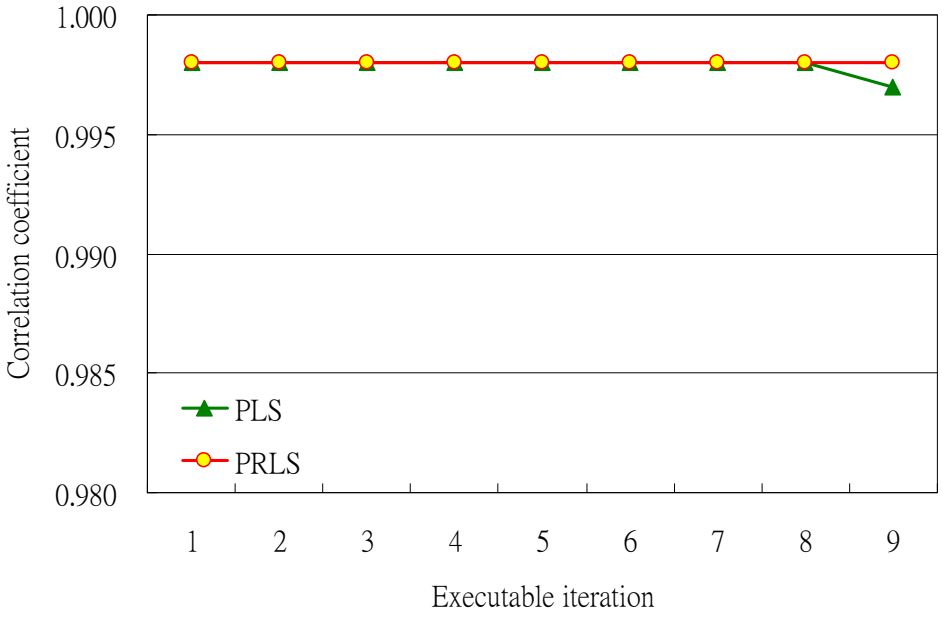


Figure 4.25 Correlation coefficient as a function of executable iteration under CV

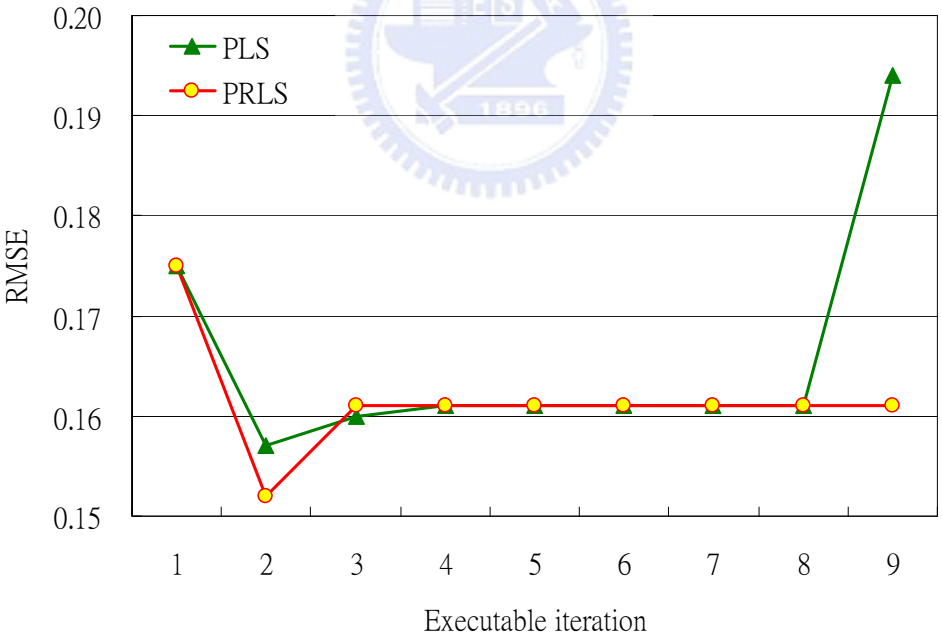


Figure 4.26 RMSE as a function of executable iteration under CV

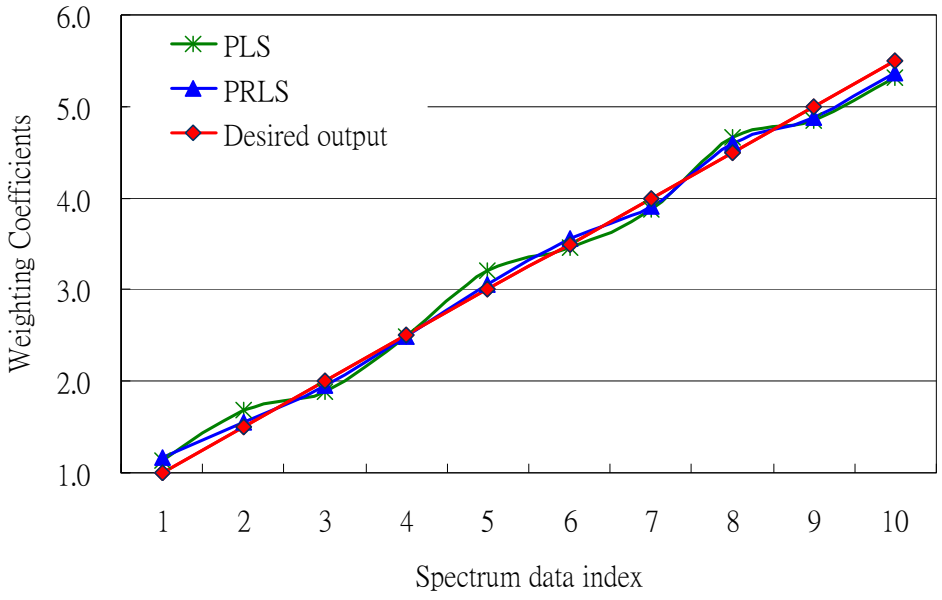


Figure 4.27 Network mapping constructed by PRLS and PLS algorithm under CV with N/S ratio = 0.55

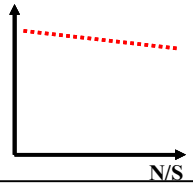
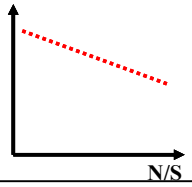
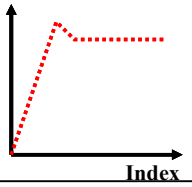
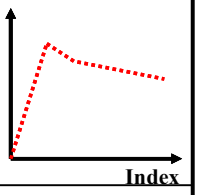
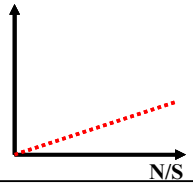
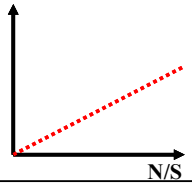
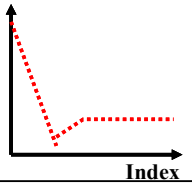
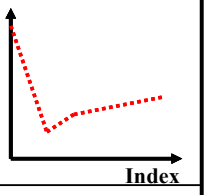
Table 4.3 Optimal CV results for imitative spectrum prediction data

	PLS	PRLS
Correlation coefficient	0.9980	0.9980
RMSE	0.1570	0.1520
Adequate iteration	2	2

4.2.4. Discussion

According to above diagrams and table, we can find out PRLS is improving and keeping prediction stable under noisy training data. Before applying our method to examine real data set, we have a brief discussion first.

Table 4.4 Compilation of simulated experimental results

Condition / Criterion	SCSP		CV	
	PRLS	PLS	PRLS	PLS
Correlation Coefficient				
RMSE				
Time complexity	O(n)		$O(n^2)$	

By observing results of simulation experiments, we made up table 4.4. Idealistically, we hope that result of prediction is high correlation coefficient, small RMSE and consumes light computation. Therefore we wish the height of correlation coefficient always keeps high and slop of RMSE is not abrupt and time complexity is as low as possible. From the table, we can clearly make out PRLS is advantageous among two methods in simulation data experiments.

4.3. Real data

4.3.1. Sound file

In the experiments, we would use ex-100 data to predict the 100th data with two kinds of noisy sound files: (a) Power-station-ambience and (b) Transformer hum. We select 100 data sets to calibrate. Following, we would show the results of experiments.

(a) Power-station ambience

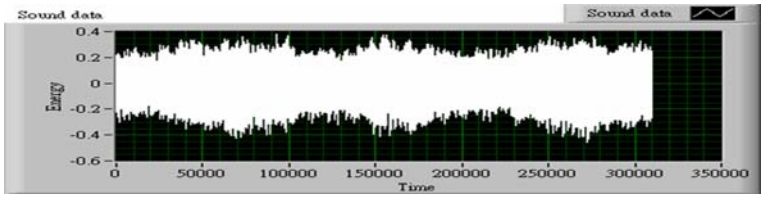


Figure 4.28 Power station ambience source data

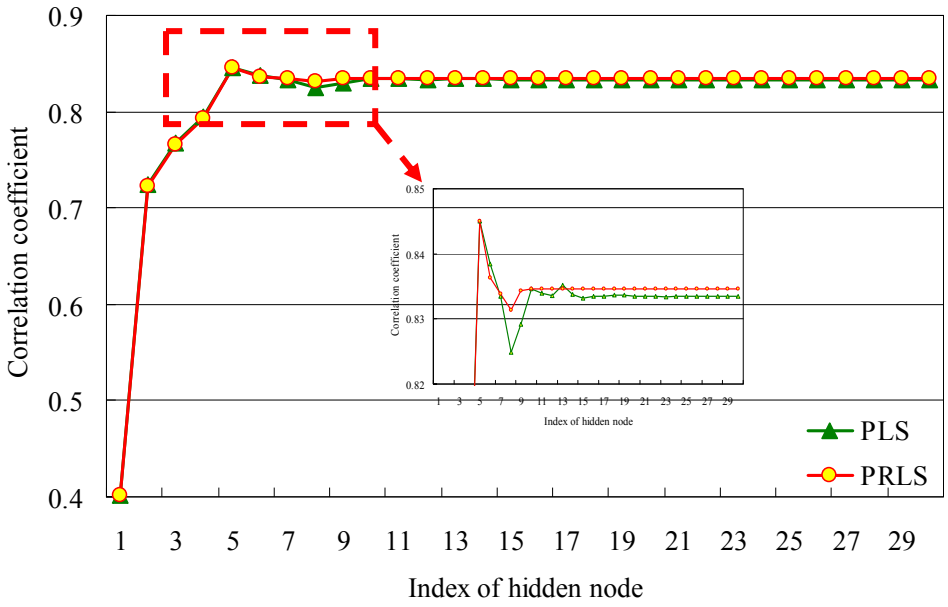


Figure 4.29 Correlation coefficient as a function of index of hidden node under SCSP

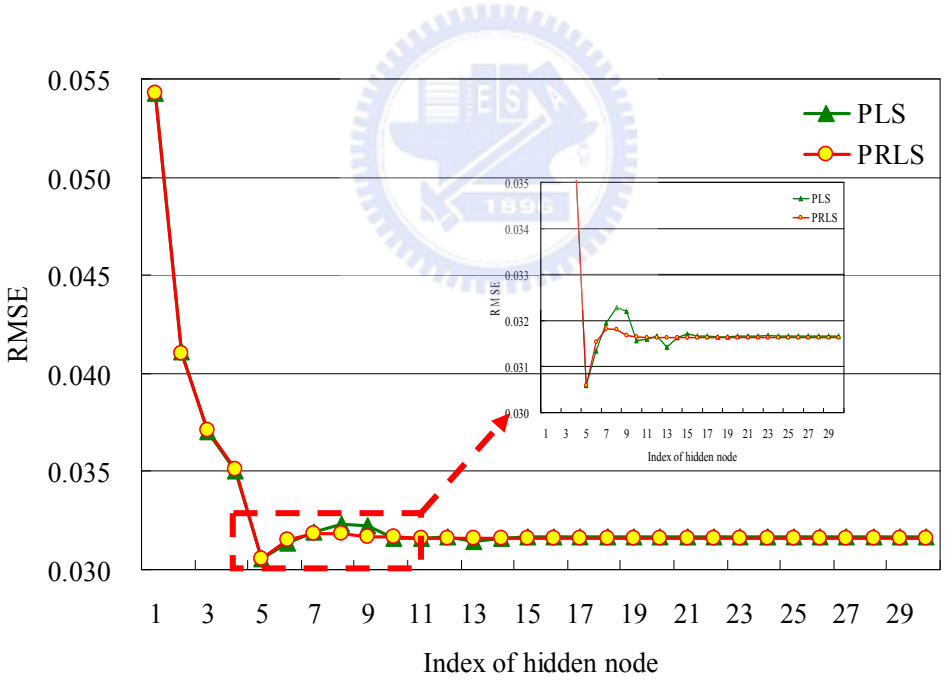


Figure 4.30 RMSE as a function of index of hidden node under SCSP

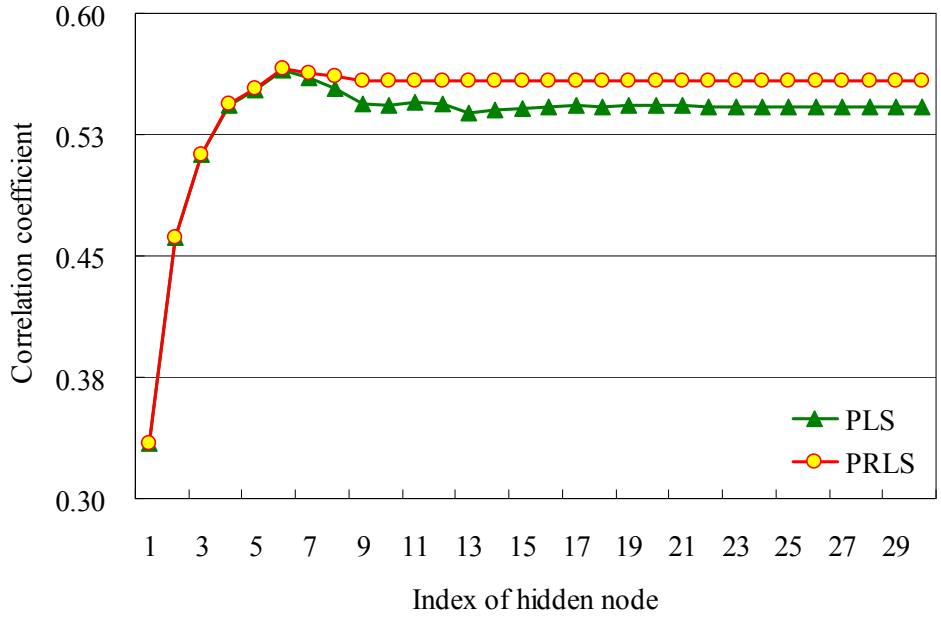


Figure 4.31 Correlation coefficient as a function of index of hidden node under CV

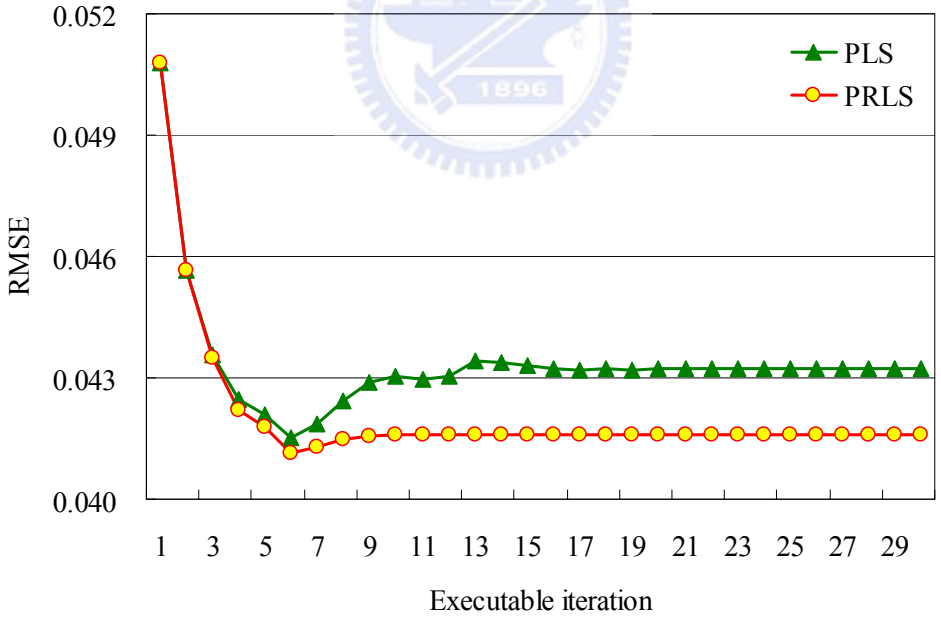


Figure 4.32 RMSE as a function of index of hidden node under CV

Table 4.5 Optimal CV results for power station ambience prediction data

	PLS	PRLS
Correlation coefficient	0.5646	0.5658

RMSE	0.0415	0.0411
Adequate iteration	6	6

(b) Transformer hum

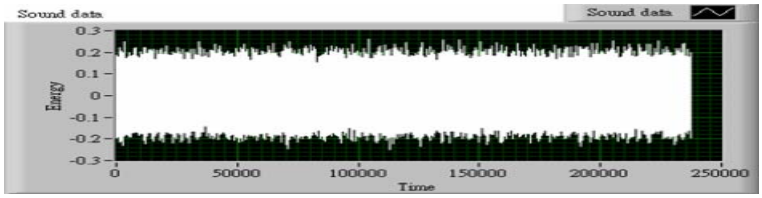


Figure 4.33 Transformer hum source data

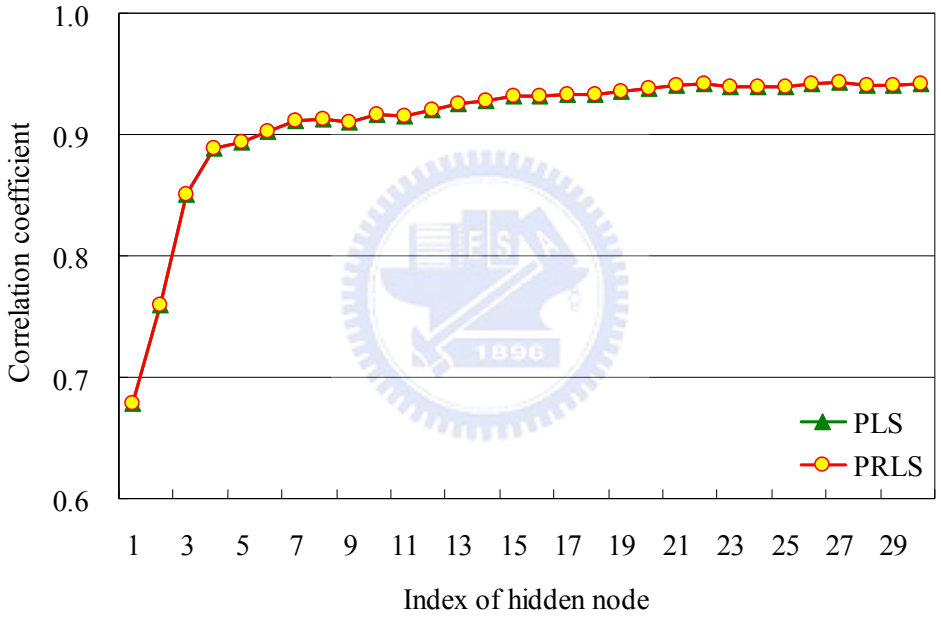


Figure 4.34 Correlation coefficient as a function of index of hidden node under SCSP

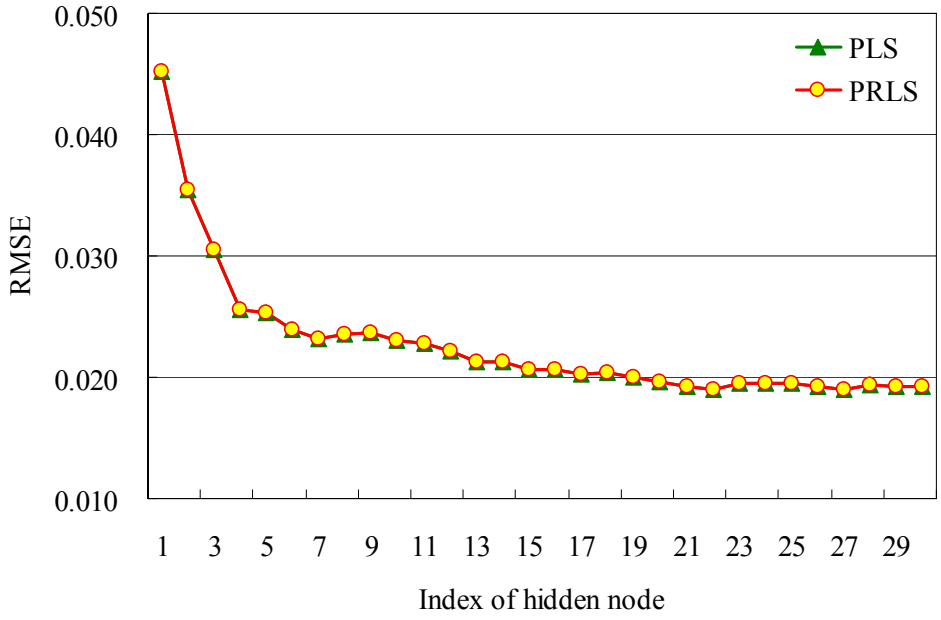


Figure 4.35 RMSE as a function of index of hidden node under SCSP

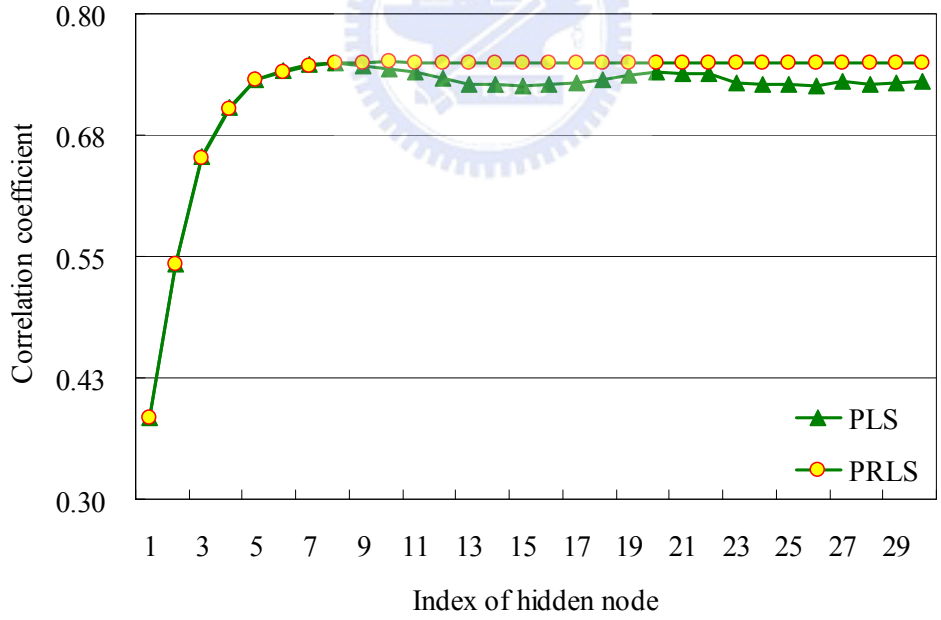


Figure 4.36 Correlation coefficient as a function of index of hidden node under CV

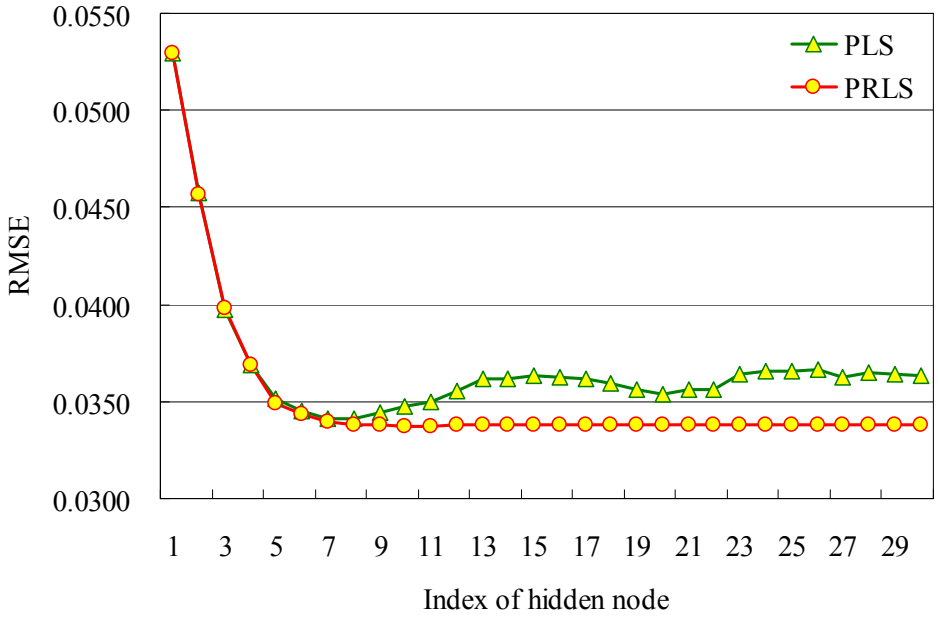


Figure 4.37 RMSE as a function of index of hidden node under CV

Table 4.6 Optimal CV results for transformer hum prediction data

	PLS	PRLS
Correlation coefficient	0.7490	0.7490
RMSE	0.0340	0.0330
Adequate iteration	6	6

4.3.2. Blood glucose data

Diabetes mellitus is one of the most common diseases in the present day, we can analysis the blood glucose data and further control when the density is irregular. In the experiment, we select 37 data sets to evidence our purpose. Figure 4.28 shows blood glucose data with noise. In the following, we would show the results of calibration under SCSP and CV. Figure 4.29 shows that

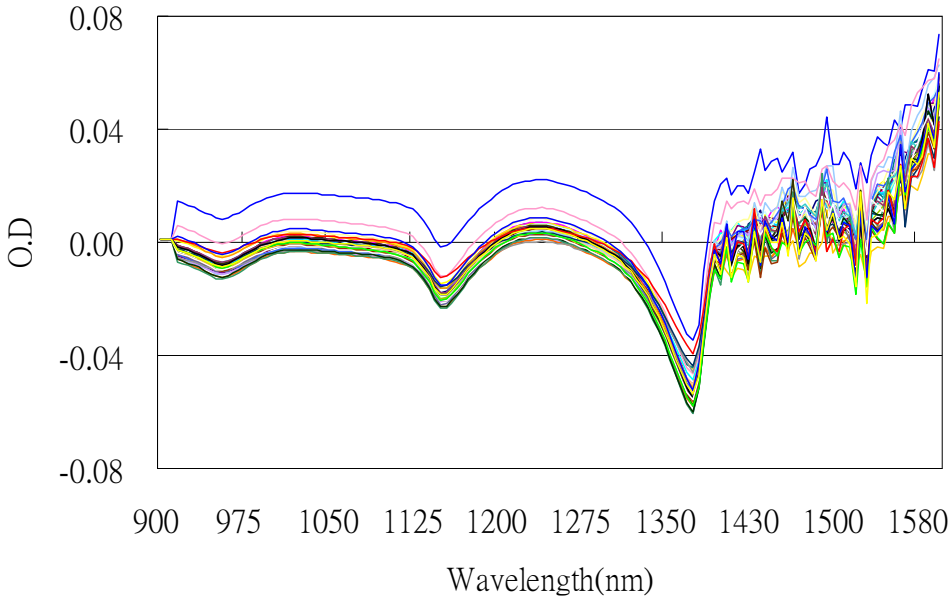


Figure 4.38 Blood glucose data with noise

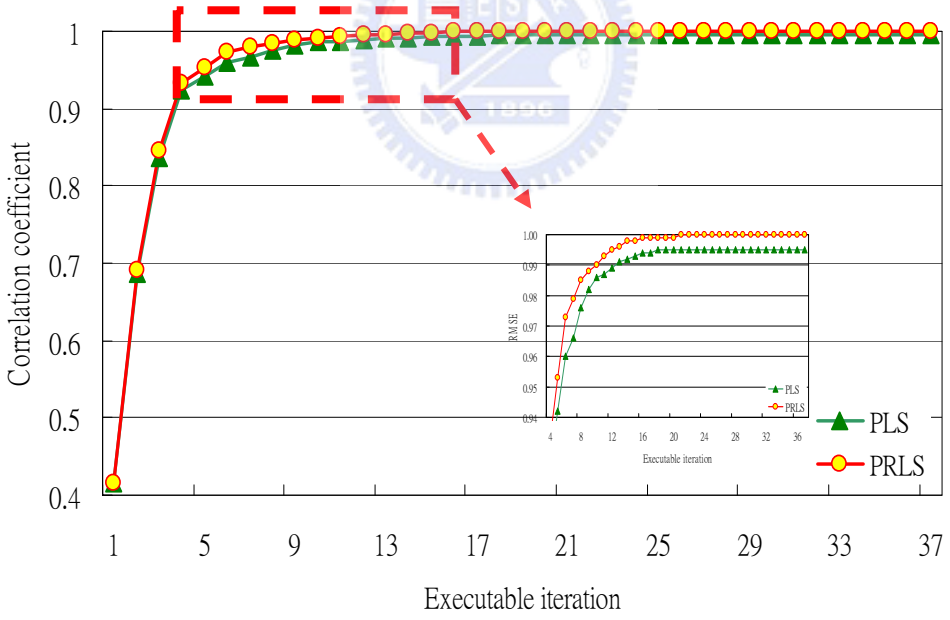


Figure 4.39 Correlation coefficient as a function of executable iteration under SCSP

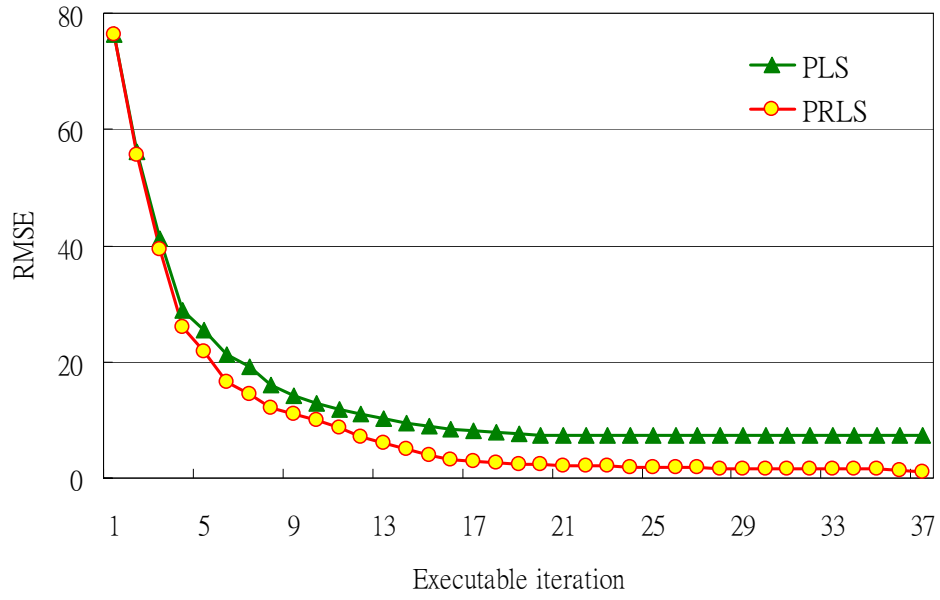


Figure 4.40 RMSE as a function of executable iteration under SCSP

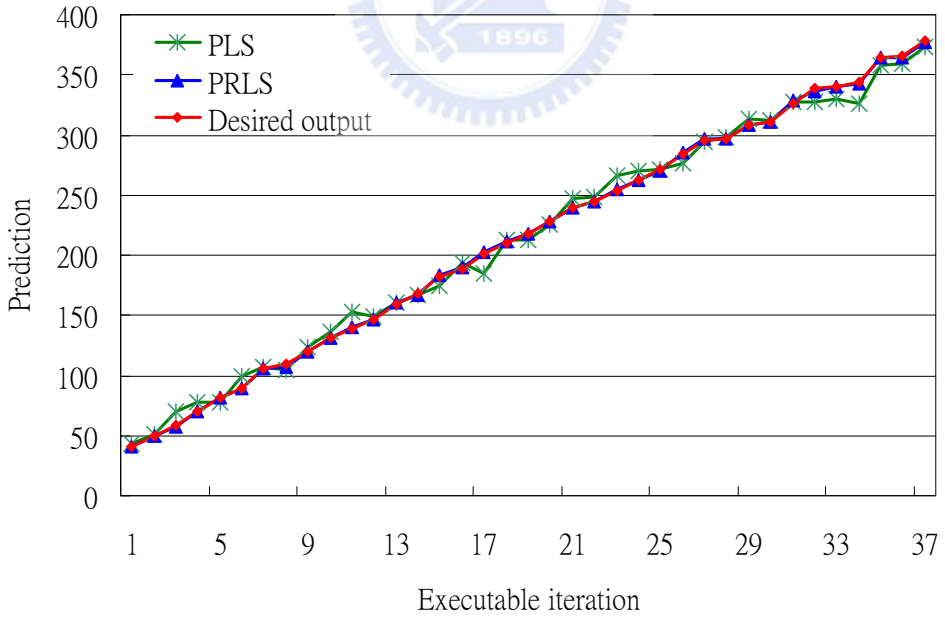


Figure 4.41 Network mapping constructed by PRLS and PLS algorithm under SCSP

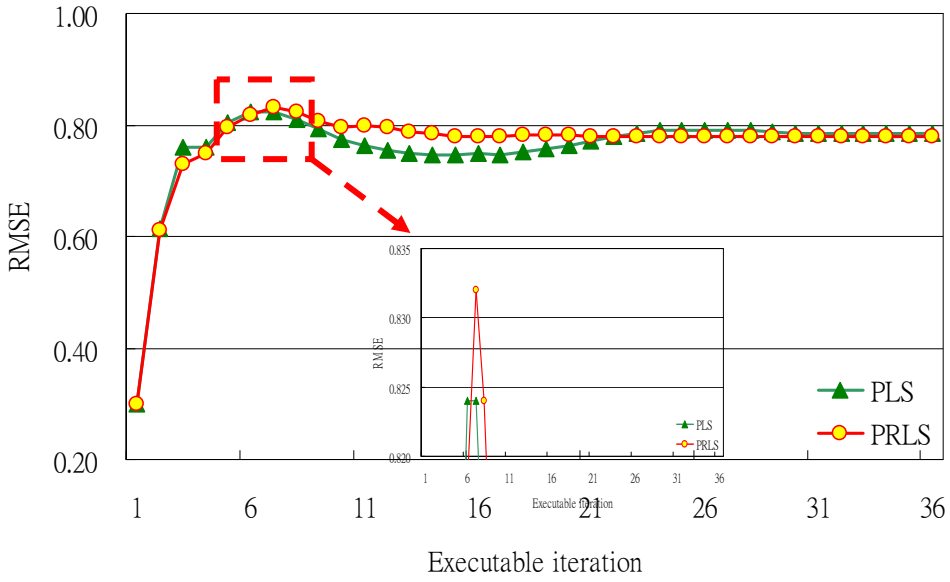


Figure 4.42 Correlation coefficient as a function of executable iteration under CV

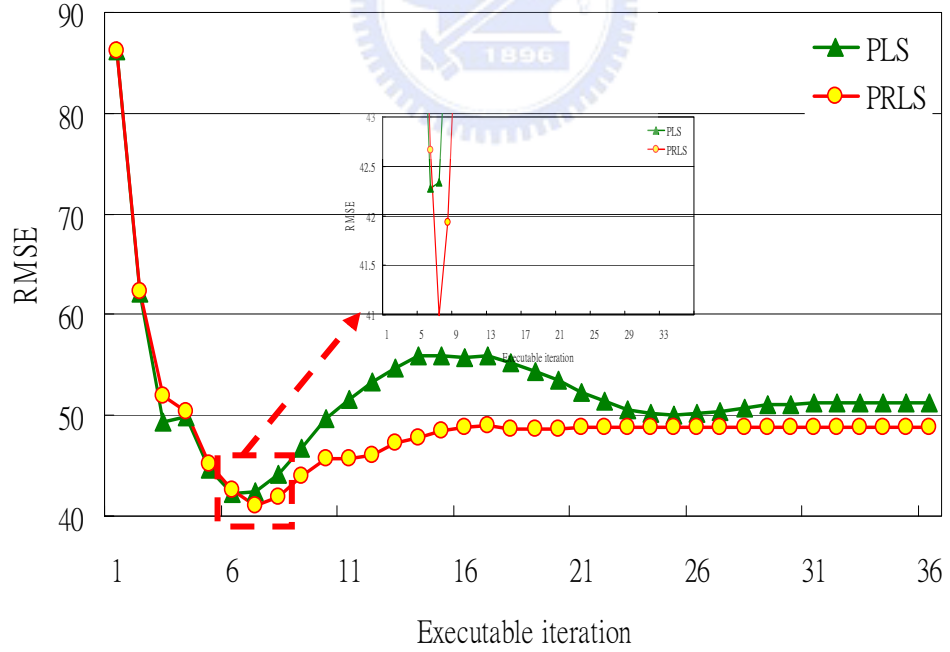


Figure 4.43 RMSE as a function of executable iteration under CV

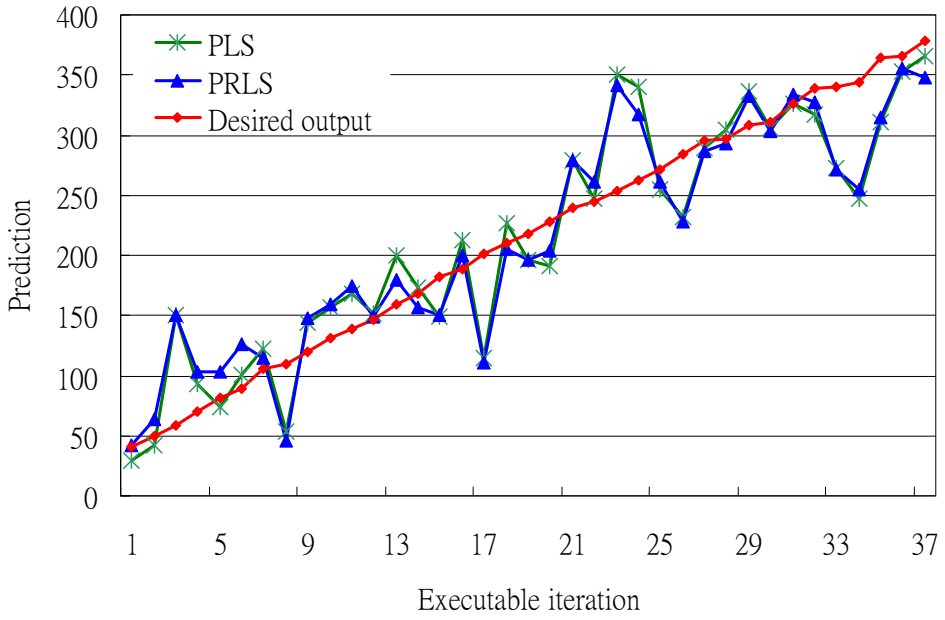


Figure 4.44 Network mapping constructed by PRLS and PLS algorithm under CV

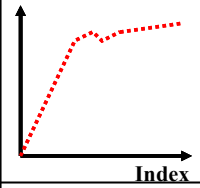
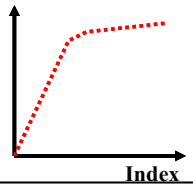
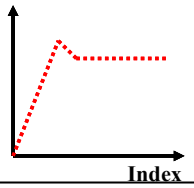
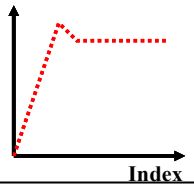
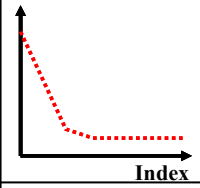
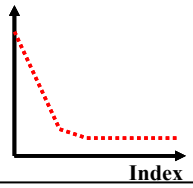
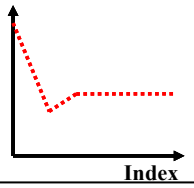
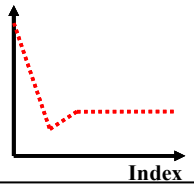
Table 4.7 Optimal CV results for blood glucose data

	PLS	PRLS
Correlation coefficient	0.8240	0.8320
RMSE	42.280	40.993
Adequate iteration	6	7

4.3.3. Discussion

The same as the above section, we also draw a discussion. Due to the viewing results of real experiments, we made up table 4.7 to show which one has better performance in real data experiments. We hope that result of prediction is high correlation coefficient, small RMSE and consumes light computation. Therefore we wish the height of correlation coefficient always keeps high and slop of RMSE is not abrupt and time complexity is as low as possible. From the table, we can clearly make out PRLS is advantageous among two methods in simulation data experiments.

Table 4.7 Compilation of real experimental results

Condition / Criterion	SCSP		CV	
	PLS	PRLS	PLS	PRLS
Correlation Coefficient				
RMSE				
Time complexity	O(n)		$O(n^2)$	

Chapter 5. Conclusion and future works

5.1. Conclusion

The purposed PRLS method is able to handle Gaussian noise under reasonable condition dataset. Although applying CV technique to calibration also has the same property. But we usually have no idea when prediction must terminate under CV in real data set. However our system can find out a value approximated to optimum in the end. Beside the time complexity of calculating under CV is $\mathbf{O}(N^2)$, PRLS just consumes $\mathbf{O}(N)$. If we have a large amount of training data must calibrate, PLS is unsuitable.

From results of simulated experiments, the proposed scheme shows the robustness against the random noise generated by the Gaussian probability density function. In the real data experimental results, system also has better performance than original PLS method when calibrating training data with noise.

5.2. Future works

One of the most important properties of online system is that the response time must minimize as far as it can be. Therefore we consider to apply PRLS to online calibrated system. Although it would cost additional computational time, the amount is not worth mentioning. For the application of neural network, we can combine PRLS with backpropagation networks (BPN). PRLS can be used to initialize the weighting coefficients of BPN to keep BPN stable under noisy training data.

We only use linear transformation inside our scheme. In order to improve the efficiency of learning, developing the nonlinear model is necessary. For a high accuracy of calibration result, we can apply optimization algorithm to our purposed system to calculate the initial value of regularized parameter.

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