Prediction Models and Sensitivity Analysis of Industrial Production Process Parameters by Using the Self-Organizing Map

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Abstract

The Self-Organizing Map (SOM) has been applied in monitoring and modeling of technical devices and processes. In this paper, we show how the SOM can be used for building a model of an industrial production process. Such models can then be used in process optimization and control. The model constructed by the SOM is a non-linear regression model of the training data, which consists of measurements from individual end products of the production process. This model can be used for predicting any subset of parameters without the committment to which are dependent and which are independent variables. In addition, this model enables sensitivity analysis of the process parameters. We show also how local linear models can be fitted to the data in order to achieve greater accuracy in the regression. We perform Total Least Squares (TLS) type of regresion using Principal Component Analysis (PCA) in model fitting.

1. INTRODUCTION

The Self-Organizing Map [3] is one of the most popular neural network models. It has been succesfully applied, for instance, in various engineering applications [4]. It is a non-linear, topology preserving mapping from the high-dimensional input space to a network of neurons, or map units. These map units usually form a regular, two-dimensional lattice. The SOM is based on unsupervised training, which means that little or no *a priori* information about data is needed before training. Modeling and monitoring applications of the SOM include data analysis and visualization, process control and fault diagnosis [7] [8] [9].

In this paper, a SOM based method to model an industrial production process is considered. The measurements used in modeling include the incoming raw material characteristics, process parameter settings during the production and the quality characteristics of the end product. This model can be used in predicting the quality parameters of the end product as well as in investigating the sensitivity of the system to parameter changes. To enable higher accuracy, local linear regression models are fitted to the data belonging to one of the Voronoi tesselations. We perform Total Least Squares (TLS) type of regression by using Principal Component Analysis (PCA) in model fitting [5] [6].

As an industrial application, we use these methods in modeling a cold rolling and batch annealing process in steel industry. These methods enable the prediction of end product quality in terms of incoming raw material characteristics and process parameter settings. Performance comparison of these methods is also presented.

2. NON-LINEAR REGRESSION USING THE SOM

2.1. Prediction of Process Parameters

The SOM can be seen as a non-linear regression model of the underlying data. This representation can be used for predicting, for example, the values of quality parameters with given raw material characteristics and process parameter settings. However, no commitment is made to which parameters are independent and which are dependent variables. For example, we could also make predictions of process parameter settings with the knowledge of the characteristics of raw material and the quality of the end product. In an industrial setting, however, one is usually interested in estimating the quality of products with known incoming raw material characteristics and process parameters settings.

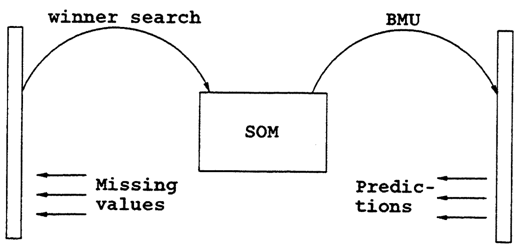

Figure 1. *Prediction of missing components of the input vector*

First, a SOM is trained with measurement data from the process. Regression is accomplished by searching for a best-matching unit (BMU) with the formula (1), where the set S is the set of known vector components.

$$c = \arg\min_i \sum_{k \in S} (x_k - m_{i_k})^2 \tag{1}$$

These components belonging to the set S form the independent variables. The components of the BMU, which are not members of S are given as answers and thus form the dependent variables of the regression model. x_k denotes the kth component of the vector x and the m_{i_k} denotes the kth component of the ith map unit in the SOM. This procedure is depicted in Figure 1 above.

The SOM representation of the process is a generalisation of the input data. The scale of the model, or the size of the smallest detail is determined by the number of map units in the SOM. A SOM with a small number of map units quantizes the input space sparsely, whereas a SOM with a large number of codebook vectors builds a dense lattice of units in the input space. The size of the SOM thus determines the accuracy of the model.

2.2. SOM and Local Linear Models

The accuracy of the SOM model can be increased by building local models for the data in one of the Voronoi tesselations of the SOM. This compensates for the effects of quantization. Voronoi tesselation is a set of points, for which a given codebook vector is a best matching unit. If the system's behavior constrains the values of measurements, one may expect that the data is located in a limited subset of the measurement space, or a low-dimensional manifold. These manifolds could be modeled locally using, for example, linear models. Similar approaches have appeared in [1] and [2].

While the SOM codebook vectors are local averages of the input data, the Principal Component Analysis (PCA) [5] modeling also represents the second order statistics. If the data is concentrated in a subspace that can be approximated with a linear model, PCA can be used for finding a low-dimensional linear approximation of the original data. Total Least Squares (TLS) type of linear regresion is performed by using PCA in model fitting. This approach allows us to have measurement errors also in inputs while the usual Least Squares (LS) approach assumes that the input variables are accurate and there is error in the output variables only [6]. These two modeling methods combined take advantage of the non-linear elasticity of the SOM as well as the local efficiency of the PCA.

Figure 2 illustrates the idea behind this modeling approach. In Figure 2(a) artificial created data cloud is depicted. It is worth noting that the dimension of the manifold is smaller than the dimension of the measurement space. Figure 2(b) shows a trained, one-dimensional SOM with ten codebook vectors. The small circles denote the codebook vectors and the lines denote the topological relations between them. In Figure 2(c) small points are data points belonging to one of the Voronoi tesselations of the SOM. Finally, in 2(d) one of the local linear models is depicted.

3. SENSITIVITY ANALYSIS

It is often desirable to know the behavior of a system under small changes made in the system parameters. This is especially the case in industrial environment, where noise is present both in measurements and in the operating conditions. Firstly, the operation point needs to be stable: small random fluctuations in input parameters

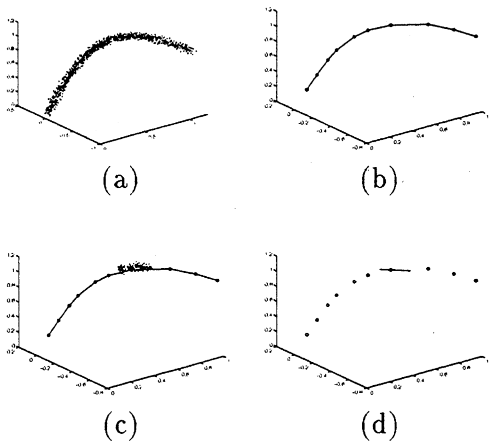

Figure 2. *(a) The artificially created training data, (b) the one-dimensional SOM with ten codebook vectors fitted to the data , (c) data belonging to one of the Voronoi tesselation and (d) a local linear model fitted to the data in vicinity of a neuron*

must not cause large fluctuations in output parameters. Secondly, we would like to move the state of the process in such a direction that better quality is achieved. The model described above can be used for investigating the leverage effects of small changes made in one of the process parameters. This is possible because the system can not reach all the possible values in the space defined by the measurements, but is usually limited to low-dimensional manifold. One could say that the state-space, or the space of possible values is constrained by the characteristic behavior of the system.

This is illustrated in Figure 3, which depicts a two-dimensional SOM trained with data originating from a three-dimensional measurement space. As we impose a small change along one of the axes defined by the measurements, the BMU changes to another map unit. By tracking the change of the best-matching unit caused by the change of the parameters, we can reveal the mutual non-linear dependence of the parameters. Also, we can say that we are "surfing" on a low-dimensional manifold defined by the SOM projection.

A software tool facilitating analysis has also been implemented. With the tool, one can inter-

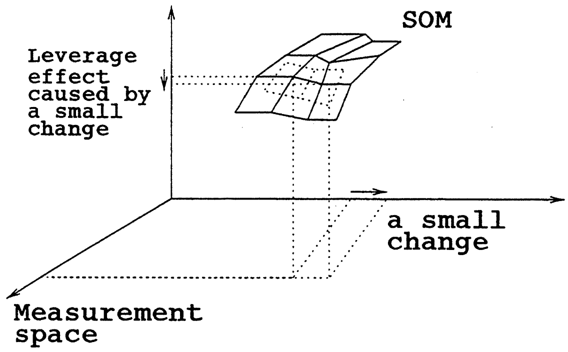

Figure 3. *The small change along one of the measurement axes causes a change in other process parameters*

actively change one of the measurement values and instantly see the effects of that change. This serves as a helpful tool for the process specialist, who can use it in decision making.

4. RESULTS

To validate the modeling approach, we used data originating from an industrial production process. The data vector used in creating the models had 26 components, describing the raw material characteristics in terms of element concentrations, the process settings during the production and the output quality characteristics.

The models created were tested with a testing set, which was not used in the training phase. The training set had 2306 training vectors and the testing set consisted of 906 similar vectors. The output quality was predicted using measurements of the incoming raw material and the process parameter settings during the production. The output of the model was compared with the real value to give an idea of the performance of our model.

In Table 1 we can see some performance measures for our methods for comparison. Both linear and non-linear methods are considered. We can see that the use of local linear models improves the accuarcy of the model with a given number of codebook vectors. By increasing the number of codebook vectors we can also improve the accuracy of the model.

Method	MSE
Global PCA	1.8858
SOM (8 x 6 map units)	0.8098
SOM (14 x 10 map units)	0.6059
SOM (20 x 14 map units)	0.5668
SOM (8 x 6 map units) and local PCA	0.6785

Table 1. *The prediction errors for an independent testing set*

5. SUMMARY

The Self-Organizing Map is used in modeling an industrial production process. The model is constructed in an unsupervised way using various measurements and process parameters. In a practical case study, this model has been successfully used in predicting the quality parameters of the end product of a steel production process.

Using the model, the sensitivity of the production process to changes in the parameter values can also be investigated. The software tool based on the SOM can be used in an interactive way to investigate the leverage effects of various parameters. With the aid of this tool the process specialist can efficiently learn the essential characteristics of the process from large amounts of measurement data.

In complex process environments, analytical modeling of the system is difficult or even impossible. However, mapping the measurement space onto the SOM clusters the process states efficiently. Now, linear modeling of the process behavior locally within these clusters may be possible provided that the measurement data corresponds to local subspaces.

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