A RETRAINING PROCEDURE APPLICATION FOR DATA PREDICTION

I. NASTAC¹, A. COSTEA²

This paper describes a special feedforward neural network architecture and an application of retraining algorithm, in order to forecast relevant process variables representative for an industrial application. The artificial neural networks (ANNs) ability to extract significant information provides valuable framework for the representation of relationships present in the structure of the data. The main purpose is to establish an optimum feedforward neural architecture and a well suited delay vector for data forecasting. The evaluation of the output error after the retraining of an ANN shows us that this procedure can substantially improve the achieved results.

Keywords: artificial neural networks, forecasting, retraining procedure, delay vector.

1. Introduction

Artificial Neural Networks (ANNs) are modelling tools having the ability to adapt to and learn complex topologies of inter-correlated multidimensional data. Constructing reliable time series models for data forecasting is challenging due to nonstationarities and nonlinear effects [7]. In this report, we present our feedforward ANN model which is useful in the case where there is a huge amount of data that imply the presence of correlations across time.

The goal of our research was to find a mathematical model describing the relationship between 29 input and 5 output variables of a glass manufacturing system (Fig. 1) [2].

¹ Lecturer, Dept. of Electronics, Telecommunications and Information Technology, University POLITEHNICA of Bucharest, Romania
² Researcher, Turku Centre for Computer Science, Finland
I. Nastac, A. Costea

Fig. 1. Multi-input-multi-output system for glass quality

All inputs and outputs vary dynamically, and there might occur large time-delays. Changing an input variable may result in an output change starting only a couple of hours later and going on for up to several days [2].

The raw data consists of 9408 rows (time steps) – one data set every 15 minutes during 14 weeks. For the first 12 weeks (8064 rows) both input and output data were given and used during training process. During the last 2 weeks (1344 rows) only input data were provided and, finally, we predicted the corresponding 1344 rows of outputs.

The structure of this paper is as follows. Section 1 presents the problem concerning model structure and data preprocessing. In next section we introduce the retraining technique and explain our approach. The main features of our experimental results are given in Section 3, where we discuss specific aspects. Our conclusions are formulated in the final section of the report.

2. Model structure and data preprocessing

A good choice of the training data set is not a trivial task when one wants to make a good prediction. Data preprocessing and data selection remain essential steps in the knowledge discovery process for real world applications and greatly improve the network’s ability to capture valuable information when correctly carried out [6] [7].

In Fig. 2 we present our idea in training a feedforward ANN to be a predictor. Delayed rows of the input data are used to construct representations of the current states. For learning purposes, the network inputs consist of many blocks with delayed values of the glass manufacturing system inputs and one block with delayed system outputs. The ANN target outputs consist of the current values of the glass manufacturing system outputs. Therefore, the network tries to match the current values by adjusting a function of their past values.
At moment $t$, one output, $\text{output}_i(t)$, is affected by the inputs from different past time steps. For example at moment $t$ the output $\text{output}_i(t)$ is affected by all inputs ($\text{input}_1$, ..., $\text{input}_{29}$) at different past time steps: $t-v_1$, $t-v_2$, $t-v_3$, etc. We denote by delay vector, $\text{Vect}_\text{In}$, a vector that includes the delays taken into account for the model:

$$\text{Vect}_\text{In} = [v_1, v_2, ..., v_n]$$ \hspace{1cm} (1)

We used different delay vectors with $n = 7$, $8$ or $9$ elements, whose values belong to intervals that can cover one to three days. The distribution of the elements was approximately similar to Gamma distribution. The elements of each vector were ascendingly ordered. Consequently the maximum value of any vector is $v_n$.

Beside the inputs from different past time steps, the outputs at moment $t$ are affected, in our model, by the outputs from the previous time step $t-1$.

We designed a feedforward ANN with one hidden layer. The ANN model depicted in Fig. 1 restricts the total possible set of training (for model adaptation) to $8064-v_n$ input-output pairs.

Once we have decided all the influences on the output at moment $t$, we have applied Principal Component Analysis (PCA) [4] [9] to reduce the dimensionality of the input space and to un-correlate the inputs. Before applying PCA we have preprocessed the inputs and outputs using normalization. We have
applied the reverse process of normalization in order to denormalize the simulated outputs.

3. Training Procedure

As basic training algorithm we have used the Scale Conjugate Gradient (SCG) algorithm [5] [9]. In order to avoid the over-fitting phenomenon we have applied the early stopping method (validation stop) during the training process [9].

The accuracy of the result was improved applying, in a special way, the retraining technique [6] [8], which is a practical information extracting mechanism directly from the weights of a reference ANN, which was already trained and is perfectly functional at the present time. Briefly, the retraining procedure reduces the reference network weights by a scaling factor \( \gamma \), \( 0 < \gamma < 1 \). These reduced weights are used as initial weights for a new training sequence, with the expectation for a better error as we can see in the following:

- Training an Artificial Neural Network in a natural way, with validation stop starting, with the weights initialized to small uniformly distributed values.
- Reduction of the first network weights with a scaling factor \( \gamma \) (\( 0 < \gamma < 1 \)).
- Retraining the network with the new initial weights.
- Compare the validation error (or training error) in both cases.

The data, that we used for our model, consist of 8064-v input-output pairs. As splitting criterion we have randomly chosen approximately 85% of the data for training set and the remaining for validation.

Next we describe the three steps performed to refine our model:

1. First step was performed in order to decide the proper number of hidden neurons (\( N_h \)). Each of the trainings started with the weights initialized to small uniformly distributed values [3] [6]. We chose the best model according to the smallest error between the desired and simulated outputs. This error was calculated for 8064-v data that include both training and validation sets. We have tested several ANN architecture with \( N_h \) around the geometric mean [1] of input neuron number (\( N_i \)) and output neuron number (\( N_o \)):

\[
\sqrt{N_i \cdot N_o} - 5 \leq N_h \leq \sqrt{N_i \cdot N_o} + 5
\]  

(2)
2. Secondly, we have applied the retraining technique using the ANN architecture (with its associate training and validation sets) obtained in the previous step. We have applied this technique for each value of $\gamma$ ($\gamma = 0.3, 0.4, \ldots, 0.9$), keeping the neural networks that performed the minimum error as the reference network. We repeated this step three times.

3. In this step we have also applied the retraining technique, the only difference from the previous step being that we randomly reconstructed the training and validation sets before each retraining sequence.

The rule used to choose the best model during each step was the mean square error of the differences between real and simulated outputs of 8064-$v_n$ data that include both training and validation sets.

At each of these 3 steps we obtained a new model. Consequently for one single delay vector we had 3 models. We have applied iteratively the 3 steps above for different delay vectors. In total we have used 12 different delay vectors obtaining 36 models.

We have discovered that for the 4-th output (Fig. 3) there are three anomalous extreme values (during timesteps 5490, 5491 and 5492) that could negatively influence the training process.

![Fig. 3. The provided data for the 4-th output](image)
Consequently, for half of our models we have decided to level these values by having them decreased from output_4(5489) to output_4(5493), in order to improve the forecast precision (see Tab. 1).

<table>
<thead>
<tr>
<th>Changing abnormal initial values with level values</th>
<th>Initial values</th>
<th>Level values</th>
</tr>
</thead>
<tbody>
<tr>
<td>output_4(5489)</td>
<td>1471.94130808653</td>
<td>1471.94130808653</td>
</tr>
<tr>
<td>output_4(5490)</td>
<td>1754.4285996792</td>
<td>1467.8</td>
</tr>
<tr>
<td>output_4(5491)</td>
<td>1754.4285996792</td>
<td>1463.7</td>
</tr>
<tr>
<td>output_4(5492)</td>
<td>1754.4285996792</td>
<td>1459.6</td>
</tr>
<tr>
<td>output_4(5493)</td>
<td>1455.63110951847</td>
<td>1455.63110951847</td>
</tr>
</tbody>
</table>

The criterion to choose one of these 36 models was the minimum value of the error ERR (see next section), but used for five intervals in which we had the real values of the outputs.

4. Forecasting Model

In our model, the outputs at moment $t$ are affected by the outputs from the previous time step $t-1$. During the training phases we always used the real data at the input.

In the last part, we tried to predict the 1344 values of outputs in a sequential mode. Therefore (see Fig. 4), in order to produce the outputs at the timestep ($t$) the neural network used as input, beside the real inputs of the glass manufacturing system from different past time steps, the estimated outputs ($t-1$), which was calculated at the previous step ($t-1$) using the outputs ($t-2$), and so on. Applying this iterative process, a forecast may be extended as many steps as required, but in this case, each step may increase the forecasting error.

In order to choose the best model among the 36, we have split the output data corresponding to timestep ($v_{n+1}$) till 8064 in five distinct intervals. The testing intervals are as follows: 400 - 1800; 1850 – 3250; 3300 – 4700; 4750 - 6150 and 6200 - 7600.
We have computed for each interval the error ERR (according to [2]):

$$ERR = \frac{1}{5} \sum_{i=1}^{5} \sum_{n=1}^{N} \frac{|O_{Rni} - O_{Fni}|}{|O_{Rni}|} \cdot f(n)$$

where $N = 1344$ (number of timesteps)

$O_{Rni}$ = real output timestep $n$ of output $i$

$O_{Fni}$ = forecasted output timestep $n$ of output $i$

and $f(n) = \frac{500}{500 + n}$ a weight function decreasing with the number of timestep $n$.

As a measure of model quality we calculated ERR_M as the mean of 5 ERR errors. Then for each of the 36 models we have one ERR_M value. All the 36 models were tested against each other in terms of ERR_M. We have chosen the model with the smallest ERR_M.

The parameters of a model that met our expectations (derived from the step 2) were:

- $\text{Vect. In} = [10 \ 20 \ 35 \ 55 \ 80 \ 120 \ 185 \ 290]$
- Number of hidden neurons = 35
- ERR_M = 0.3602 and ERR_test = 0.4
We noticed that the previous model was among the ones that did not use the level values between output_4(5489) and output_4(5493). Even if the fact was a little bit surprising, we decided to present its characteristics. Applying an iterative process (depicted in Fig. 4), starting with time step 8065, we finally obtained the desired outputs that correspond to time steps 8065-9408.

The outputs of the previously described model are presented in the following figures (5 and 6).

In Fig. 5 the real data (thin lines that correspond to time steps 1-8064) and neural network values (thick lines that correspond to timesteps 291-8064) after training process. Thick lines cover very well the thin lines, excepting first 290 values since the simulated outputs start with this delay imposed by the maximum value of the delay vector Vect_In.
Fig. 6 presents the real outputs (solid lines) and predicted outputs (dotted lines) that correspond to the test set (timesteps 8065-9408).

Among all 36 models that were studied, we discovered other three models better than the one previously presented (see Table 2). All of them used during the training process the level values between output_4(5489) and output_4(5493).

### Table 2

<table>
<thead>
<tr>
<th>Parameters of the better models</th>
<th>3_PCA_II</th>
<th>5_PCA_II</th>
<th>5_PCA_III</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Hidden neurons</strong></td>
<td>39</td>
<td>42</td>
<td>42</td>
</tr>
<tr>
<td><strong>Vect_In</strong></td>
<td>[10 20 30 45 65 95 145 210 330]</td>
<td>[12 22 31 39 47 55 66 79 98]</td>
<td>[12 22 31 39 47 55 66 79 98]</td>
</tr>
<tr>
<td>Result of:</td>
<td>Step 2</td>
<td>Step 2</td>
<td>Step 3</td>
</tr>
<tr>
<td>ERR_test</td>
<td>0.3629</td>
<td>0.3707</td>
<td>0.3788</td>
</tr>
<tr>
<td>err_1</td>
<td>0.4159</td>
<td>0.4361</td>
<td>0.4586</td>
</tr>
<tr>
<td>err_2</td>
<td>0.2593</td>
<td>0.2994</td>
<td>0.3059</td>
</tr>
<tr>
<td>err_3</td>
<td>0.4294</td>
<td>0.3729</td>
<td>0.4991</td>
</tr>
<tr>
<td>err_4</td>
<td>0.3902</td>
<td>0.2904</td>
<td>0.2639</td>
</tr>
<tr>
<td>err_5</td>
<td>0.3196</td>
<td>0.4549</td>
<td>0.3663</td>
</tr>
<tr>
<td>Standard dev. of errs</td>
<td>0.0718</td>
<td>0.0757</td>
<td>0.0994</td>
</tr>
</tbody>
</table>
5. Conclusions

In this paper, we have designed a neural network tool for data prediction. Our method exploits the input-output dependence across time using a delay vector. We employed the PCA procedure in order to reduce the dimensionality of the input space and to un-correlate the inputs. The learning process was refined applying the retraining procedure.

It is important to study the shapes of the graphs before training in order to level some unnatural values. Choosing the best model is not an easy task. It should be improved using more data that cover all potential situations as much as possible. More than five distinct intervals used to compute ERR should also enhance the criterion of the selection.

We were limited by the memory and speed of our computer (512 Mb of RAM and Pentium 4 CPU 1.7 GHz). We are definitely convinced that using vectors with more than 9 elements we can increase the performance of our tool. At the same time there are other efficient algorithms like Levenberg-Marquardt or Bayesian regularization that also necessitate a powerful machine to solve the problem. It is very easy to change in our tool the SCG algorithm with one of these because at the basic level the architecture and the retraining procedure are independent of the training algorithm.

We noticed that the retraining technique significantly improved the achieved result.

REFERENCES