Adaptive Informatics Applications

Chapter 15

Intelligent data engineering

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15.1 Failure management with data analysis

Miki Sirola, Jukka Parviainen, Jaakko Talonen, Golan Lampi, Tuomas Alhonnoro, Risto Hakala, Timo Similä

Early fault detection with data-analysis tools in nuclear power plants is one of the main goals in NoTeS-project (test case 4) in TEKES technology program MASI. The industrial partner in this project is Teollisuuden Voima Oy, Olkiluoto nuclear power plant. Data analysis is carried out with real failure data, training simulator data and design based data, such as data from isolation valve experiments. A control room tool, visualization tools and various visualizations are under development.

A toolbox for data management using PCA (Principal Component Analysis) and WRLS (Weighted Recursive Least Squares) methods has been developed [1]. Visualizations for e.g. trends, transients, and variation index to detect leakages are used. Statistically significant variables of the system are detected and statistical properties and important visualizations are reported. Data mining methods and time series modelling are combined to detect abnormal events.

X-detector tool based on feature subset selection has been developed. The idea is to do real-time monitoring and abnormality detection with efficient subsets. Measuring dependencies and cluster separation methods are used in variable selection in this visualization tool.

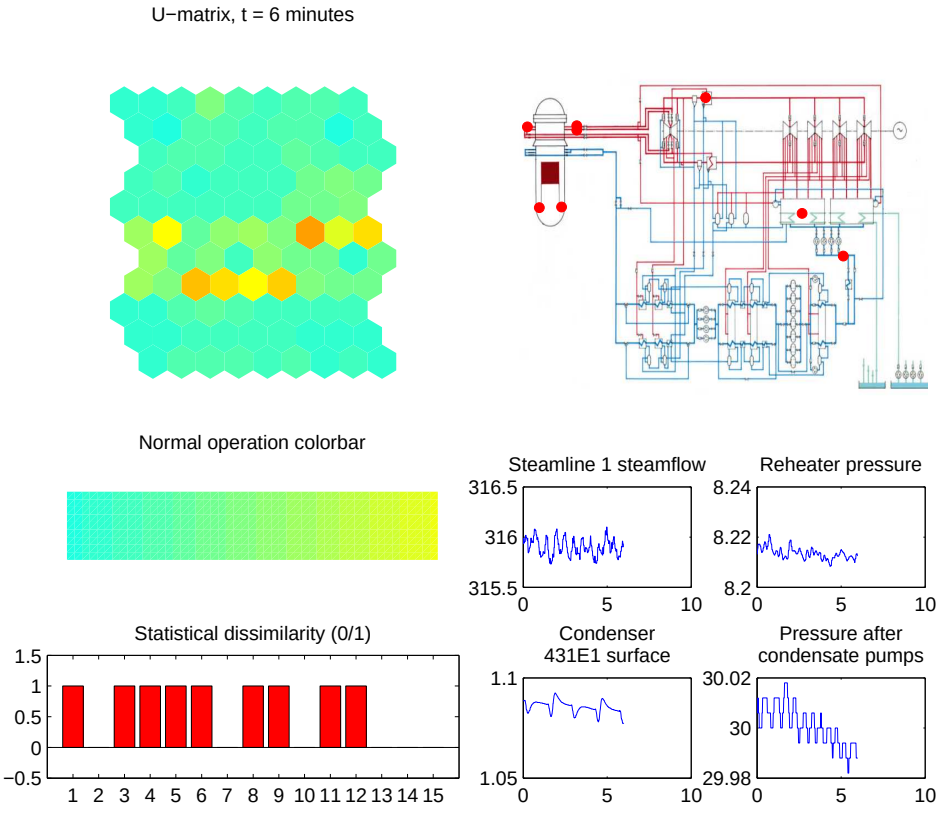

Figure 15.1: X-detector tool user interface: leakage in the main circulation pump. SOM visualization combined with statistical Kolmogorov-Smirnov test, process flow diagram and selected process variable graphs.

Decision support prototype DERSI for failure management in nuclear power plants is under development. It is a control room tool for operator or analysis tool for expert user. It combines neural methods and knowledge-based methods. DERSI utilizes Self-Organizing Map (SOM) method and gives advice by rule-based reasoning. The operator is provided by various informative decision support visualizations, such as SOM maps for normal data and failure data, state U-matrix, quantization error for both component level and state U-matrix, time-series curves and progress visualizations. DERSI tool has been tested in fault detection and separation of simulated data [2].

A separate study of process state and progress visualizations using Self-Organizing Map was also done [3]. All visualizations developed in the project will be collected to make a first proposal for wide monitoring screens.

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15.2 Cellular network performance analysis

Kimmo Raivio, Mikko Multanen, Pasi Lehtimäki

Structure of mobile networks gets more and more complicated when new network technologies are added to the current ones. Thus, advanced analysis methods are needed to find performance bottlenecks in the network. Adaptive methods can be utilized, for example, to perform hierarchical analysis of the networks, detecting anomalous behavior of network elements and to analyse handover performance in groups of mobile cells.

Combination of the Self-Organizing Map and hierarchical clustering methods can be utilized to split the analysis task into smaller subproblems in which detection and visualization of performance degradations is easier. The method consists of successive selection of a set of cellular network performance indicators and hierarchical clustering of them. Initially only a couple of key performance indicators are utilized and later some more specific counters are used. Thus, the root cause of degradation is easier to find [1]. The method can be utilized both in general network perfromance analysis and in more specific subareas like soft handover success rate [3].

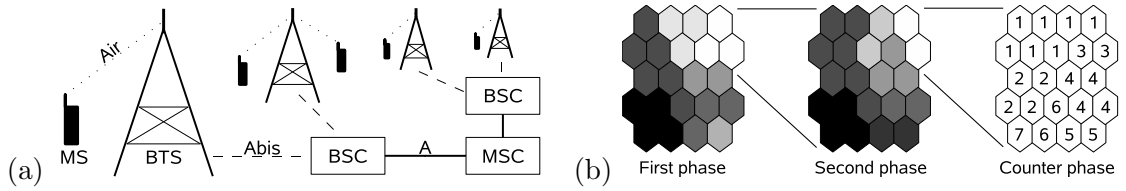

Figure 15.2: Architecture of a cellular network (a) and simple view of the hierarchical analysis algorithm (b).

In outlier detection as well neural as statistical methods can be used to find out network elements with decreased performance or otherwise anomalous traffic profile. Statistical approaches may include both parametric and non-parametric methods. An example of parametric method is Gaussian mixture model. Correspondingly, nearest-neighbor and Parzen windows are non-parametric methods. A neural method called Neural gas is very similar to the statistical approaches and it can be used also in this task [2].

It can be said, that neural and other learning methods can be utilized in the analysis of complicated performance degradation problems in cellular networks. The analysis tools can be built in a way to require only a minimal amount of knowledge of the network itself.

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15.3 Predictive GSM network optimization

Pasi Lehtimäki, Kimmo Raivio

In this study, the focus is on the final step of the mobile network monitoring procedure, that is, on making adjustments to configuration parameters so that the amount of predictable, regularly occurring performance degradations or faults is minimized. In order to automate the configuration parameter optimization, a computational method to evaluate the performance of alternative configurations must be available. In data-rich environments like cellular networks, such predictive models are most efficiently obtained with the use of past data records.

In blocking prediction, the interest is to compute the number of blocked requests at different conditions. This can be based on the use of well known Erlang-B formula. The expected value for the number of blocked requests is obtained by multiplying the number of arriving requests with the blocking probability, leading to $B = \lambda p(N_c|\lambda, \mu, N_c)$. The expected value for the congestion time is $C = p(N_c|\lambda, \mu, N_c)$ and the expected value for the number of channels in use is $M = \sum_{n=0}^{N_c} np(n|\ \lambda, \mu, N_c)$.

In [2], it was shown that the Erlang-B formula does not provide accurate predictions for blocking in GSM networks if low sampling rate measurements of arrival process are used in the model. More traditional regression methods can be used for the same purpose with the assist of knowledge engineering approach in which Erlang-B formula and regression methods are combined. With the use of Erlang-B formula, the dependencies between B, C and M that remain the same in each base station system need not be estimated from data alone. The data can be used to estimate other relevant and additional parameters that are required in prediction. In [2] and [1], a method to use Erlang-B formula and measurement data to predict blocking is presented. The regression techniques are used to estimate the arrival rate distribution describing the arrival process during short time periods. The Erlang-B formula is used to compute the amount of blocking during the short time periods.

Suppose that the time period is divided into N_s segments of equal length. Also, assume that we have a vector $\boldsymbol{\lambda} = [0 \ \ 1\Delta_\lambda \ \ 2\Delta_\lambda \ \ \ldots \ \ (N_\lambda - 1)\Delta_\lambda]$ of N_λ possible arrival rates per segment with discretization step Δ_λ. Let us denote the number of blocked requests during a segment with arrival rate λ_i with $B_i = \lambda_i p(N_c|\lambda_i, \mu, N_c)$, where $p(N_c|\lambda_i, \mu, N_c)$ is the blocking probability given by the Erlang distribution. Also, the congestion time and the average number of busy channels during a segment with arrival rate λ_i are denoted with $C_i = p(N_c|\lambda_i, \mu, N_c)$ and $M_i = \sum_{n=0}^{N_c} np(n|\lambda_i, \mu, N_c)$. In other words, the segment-wise values for blocked requests, congestion time and average number of busy channels are based on the Erlang-B formula.

Now, assume that the number of segments with arrival rate λ_i is θ_i and $\sum_i \theta_i = N_s$. Then, the cumulative values over one hour for the number of requests T, blocked requests B, congestion time C and average number of busy channels M can be computed with

$$\begin{bmatrix} \lambda_1 & \lambda_2 & \ldots & \lambda_{N_\lambda} \\ B_1 & B_2 & \ldots & B_{N_\lambda} \\ \frac{C_1}{N_s} & \frac{C_2}{N_s} & \ldots & \frac{C_{N_\lambda}}{N_s} \\ \frac{M_1}{N_s} & \frac{M_2}{N_s} & \ldots & \frac{M_{N_\lambda}}{N_s} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_{N_\lambda} \end{bmatrix} = \begin{bmatrix} T \\ B \\ C \\ M \end{bmatrix} \tag{15.1}$$

or in matrix notation $\mathbf{X}\boldsymbol{\theta} = \mathbf{Y}$.

Now, the problem is that the vector $\boldsymbol{\theta}$ is unknown and it must be estimated from the data using the observations of $\mathbf{Y}$ and matrix $\mathbf{X}$ which are known a priori. Since the output

vector $\mathbf{Y}$ includes variables that are measured in different scales, it is necessary to include weighting of variables into the cost function. By selecting variable weights according to their variances estimated from the data, the quadratic programming problem

$$\min_{\boldsymbol{\theta}} \quad \left\{ \frac{1}{2} \boldsymbol{\theta}^T \mathbf{H} \boldsymbol{\theta} + \mathbf{f}^T \boldsymbol{\theta} \right\} \tag{15.2}$$

$$w.r.t \quad 0 \leq \theta_i \leq N_s, \ i = 1, 2, ..., N_\lambda, \tag{15.3}$$

$$\sum_{i=1}^{N_\lambda} \theta_i = N_s \tag{15.4}$$

is obtained where $\mathbf{f} = -\mathbf{X}^T \mathbf{W}^T \mathbf{W} \mathbf{Y}$ and $\mathbf{H} = \mathbf{X}^T \mathbf{W}^T \mathbf{W} \mathbf{X}$ include the weighting matrix $\mathbf{W}$. In other words, the goal is to find the vector $\boldsymbol{\theta}$ that provides the smallest prediction errors for variables T, B, C and M.

The optimization problem could be solved for each of the N_d observation vectors separately, leading to N_d solution vectors $\boldsymbol{\theta}$ for hour h. Since we are interested in long-term prediction of blocking, we should somehow combine the solution vectors so that behavior common to all solution vectors are retained and non-regular properties of the demand are given less attention.

Let us denote the ith solution vector for hour h with $\boldsymbol{\theta}_h^{(i)}$ and the jth element of the corresponding solution vector with $\theta_{jh}^{(i)}$. Since $\theta_{jh}^{(i)}$ described the number of segments with arrival rate $\lambda = \lambda_j$ during ith observation vector at hour h, the probability for a random segment during ith observation period to have an arrival rate $\lambda = \lambda_j$ can be computed from $\theta_{jh}^{(i)}$ with $p_{jh}^{(i)} = \theta_{jh}^{(i)} / N_s$, where N_s is the number of segments in a period.

The probability for observing a segment with arrival rate $\lambda = \lambda_j$ at hour h would become

$$p_{jh} = \frac{1}{N_d N_s} \sum_{i=1}^{N_d} \theta_{jh}^{(i)}. \tag{15.5}$$

Now, the arrival rates λ_j and their probabilities p_{jh} for hour h form a probabilistic model. Let us define a column vector

$$\underset{seg \mapsto hour}{\boldsymbol{\theta}_h} = \mathbf{p}_h N_s \tag{15.6}$$

that maps the segment-wise candidate arrival rates λ_j to the total number of arrived requests T in a single one hour time period with

$$T = \boldsymbol{\lambda} \underset{seg \mapsto hour}{\boldsymbol{\theta}_h}. \tag{15.7}$$

Note that the parameter vector $\boldsymbol{\theta}_{h,seg \mapsto hour}$ can also be used to map the vector $\mathbf{B} = [B_1 \ B_2 \ \ldots \ B_{N_\lambda}]$ of segment-wise blocking candidates to the total number of occurrences of blocked requests during one period. Similarly, the cumulative values for the average number of busy channels and the congestion time can be computed.

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15.4 Learning from environmental data

Mika Sulkava, Jaakko Hollmén

Data analysis methods play an important role in increasing our knowledge of the environment as the amount of data measured from the environment increases. Gaining an insight into the condition of the environment and the assessment of the its future development under the present and predicted environmental scenarios requires large data sets from long-term monitoring programs. In this project the development of forests in Finland has been studied using data from various forest monitoring programs. In addition, the global changes and drivers of the CO_2 exchange of forests have been studied based on eddy covariance data from a high number of sites around the world.

The work in this project includes collaboration with a high number of parties. During 2006–2007, there has been cooperation with two research units of the Finnish Forest Research Institute, University of Antwerp, and numerous researchers in the carbon cycling community all around the world. The latest journal contributions are joint work of a team of more than a dozen researchers from nine countries in three continents.

Plant nutrients play an integral role in the physiological and biochemical processes of forest ecosystems. The effects of nitrogen and sulfur depositions on coniferous forests have been studied using the Self-Organizing Map. It was concluded that evidence for deposition-induced changes in needles has clearly decreased during the nineties. The results of the effects of the depositions have been presented in conferences [1, 2].

Various environmental factors and past development affect the growth and nutritional composition of tree needles as they are aging. Different regression models have been compared to find out how these effects could be modeled effectively and accurately during the second year of the needles [3]. We found that sparse regression models are well suited for this kind of analysis. They are better for the task than ordinary least squares single and multiple regression models, because they are both easy to interpret and accurate at the same time.

Good quality of analytical measurements techniques is important to ensure the reliability of analyses in environmental sciences. We have combined foliar nutrition data from Finland and results of multiple measurement quality tests from different sources in order to study the effect of measurement quality on conclusions based on foliar nutrient analysis [4, 5]; see Figure 15.3. In particular, we studied the use of weighted linear regression

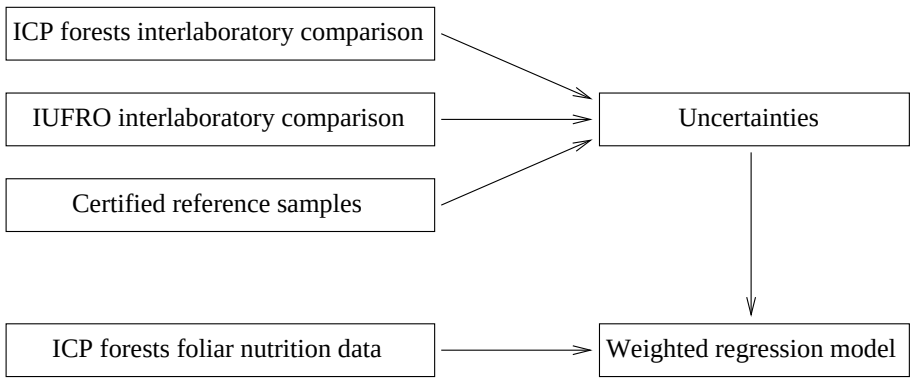

Figure 15.3: Fusion of measurement quality metadata from three different sources and forest nutrition data made it possible to use weighted regression models for trend detection.

models in detecting trends in foliar time series data and showed that good precision of the measurement techniques may decrease the time needed to detect statistically significant trends in environmental time series by several years.

The dependencies between the atmospheric CO_2 exchange of the world's forests and different environmental factors and between the annual radial growth of coniferous trees and environment and properties of the trees have been studied since 2006. First results concerning the significance of photosynthesis in differences between yearly CO_2 exchange have been published lately [6, 7]. Also, the effects of nitrogen deposition on CO_2 exchange in forests have been studied [8].

Finally, the effects of environmental conditions on radial growth of trees has been studied. Methods for automatic detection of the onset and cessation of radial growth [9] and for model selection and estimation based on expert knowledge [10] have been developed.

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15.5 Parsimonious signal representations in data analysis

Jarkko Tikka, Jaakko Hollmén, Timo Similä

The objective in data analysis is to find unsuspected and practical information from large observational data sets and to represent it in a comprehensible way. While utility is a natural starting point for any analysis, understandability often remains a secondary goal. A lot of input variables are available for a model construction in many cases. For instance, in the analysis of microarray data the number of input variables may be tens of thousands. It is impossible to evaluate all the possible combinations of input variables in a reasonable time. In this research, improved understandability of data-analytic models is sought by investigating sparse signal representations that are learned automatically from data. Naturally, the domain expertise is useful in many cases in validation of results, but it may also be biased by established habits and, thus, prevent making novel discoveries.

In a time series context, parsimonious modeling techniques can be used in estimating a sparse set of autoregressive variables for time series prediction [7]. We presented a filter approach to the prediction: first we selected a sparse set of inputs using computationally efficient linear models and then the selected inputs were used in the nonlinear prediction model. Furthermore, we quantified the importance of the individual input variables in the prediction. Based on experiments, our two-phase modeling strategy yielded accurate and parsimonious prediction models giving insight to the original problem.

The problem of estimating sparse regression models in a case of multi-dimensional input and output variables has been investigated in [4]. We proposed a forward-selection algorithm called multiresponse sparse regression (MRSR) that extends the Least Angle Regression algorithm (LARS) [1]. The algorithm was also applied to the task of selecting relevant pixels from images in multidimensional scaling of handwritten digits. The MRSR algorithm was presented in a more general framework in [5]. In addition, experimental comparisons showed the strengths of MRSR against some other input selection methods. The input selection problem for multiple response linear regression was formulated as a

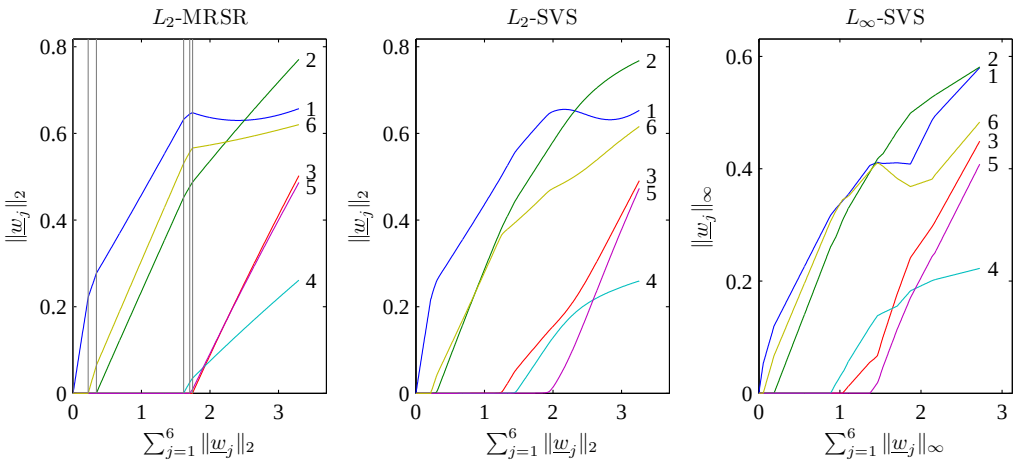

Figure 15.4: Solution paths of the importance factors of input variables. In the subfigure on the left panel, vertical lines indicate the breakpoints of the MRSR algorithm, i.e the points where a new input variable is added to the subset of selected input variables. All the solution paths end to the ordinary least square solution.

convex optimization problem to minimize the error sum of squares subject to a sparsity constraint in [6]. The proposed simultaneous variable selection (L_2-SVS) method is related to L_∞-SVS method [10]. We also reported an efficient algorithm to follow the solution path as a function of the constraint parameter. In Figure 15.4, the solution paths of MRSR, L_2-SVS, and L_∞-SVS are illustrated using a data set, which includes six input variables. The most important inputs are x_2, x_1, and x_6 according to all the three methods. The multiresponse sparse regression is studied further in [2, 3].

The artificial neural networks are an appropriate choice to model dependencies in nonlinear regression problems, since they are capable to approximate a wide class of functions very well. A disadvantage of neural networks is their black-box characteristics. We have developed input selection algorithms for radial basis function (RBF) networks in order to improve their interpretability [8, 9]. A backward selection algorithm (SISAL-RBF), which removes input variables sequentially from the network based on the significance of the individual regressors, was suggested in [9]. The calculation of ranking of inputs is based on partial derivatives of the network. Only 15% of the available inputs were selected by the SISAL-RBF without sacrificing prediction accuracy at all in the case of real world data set [9]. In [8], each input dimension was weighted and a sparsity constraint was imposed on the sum of the weights. The resulting constrained cost function was optimized with respect to the weights and other parameters using alternating optimization approach. The optimum weights describe the relative importance of the input variables. Applications to both simulated and benchmark data produced competitive results.

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Chapter 16

Time series prediction

Amaury Lendasse, Francesco Corona, Antti Sorjamaa, Elia Liitiäinen, Tuomas Kärnä, Yu Qi, Emil Eirola, Yoan Miché, Yongnang Ji, Olli Simula

16.1 Introduction

Amaury Lendasse

What is Time series prediction? Time series prediction (TSP) is a challenge in many fields. In finance, experts forecast stock exchange courses or stock market indices; data processing specialists forecast the flow of information on their networks; producers of electricity forecast the load of the following day. The common point to their problems is the following: how can one analyse and use the past to predict the future? Many techniques exist: linear methods such as ARX, ARMA, etc., and nonlinear ones such as artificial neural networks. In general, these methods try to build a model of the process. The model is then used on the last values of the series to predict the future values. The common difficulty to all the methods is the determination of sufficient and necessary information for an accurate prediction.

A new challenge in the field of time series prediction is the Long-Term Prediction: several steps ahead have to be predicted. Long-Term Prediction has to face growing uncertainties arising from various sources, for instance, accumulation of errors and the lack of information.

Our contributions in TSP research. The TSP group is a new research group. It has been created in 2004. A notable achievement has been the organization of the first European Symposium on Time Series Prediction (ESTSP'07) on February 2007 in Helsinki. (`http://www.estsp.org`, [1]). For this symposium, a time series competition has been organized and a benchmark has been created.

In the reporting period 2006 - 2007, TSP research has been established as a new project in the laboratory. Nevertheless, TSP research has already been extended to a new direction: "Chemoinformatics".

This Chapter starts by introducing some theoretical advances undertaken during the reporting period, including the presentation of the ESTSP´07 competition. Also the problem of input selection for TSP is reported. The applications range includes Chemoinformatics.

16.2 European Symposium on Time Series Prediction

Amaury Lendasse and Antti Sorjamaa

Time series forecasting is a challenge in many fields. In finance, experts forecast stock exchange courses or stock market indices; data processing specialists forecast the flow of information on their networks; producers of electricity forecast the load of the following day. ESTSP 2007 was a unique opportunity for researcher from Statistics, Neural Networks, Machine Learning, Control and Econometrics to share their knowledge in the field of Time Series Prediction.

The common point to their problems is the following: how can one analyse and use the past to predict the future?

Many techniques exist for the approximation of the underlying process of a time series: linear methods such as ARX, ARMA, etc. , and nonlinear ones such as artificial neural networks. In general, these methods try to build a model of the process. The model is then used on the last values of the series to predict the future values. The common difficulty to all the methods is the determination of sufficient and necessary information for an accurate prediction.

A new challenge in the field of time series prediction is the Long-Term Prediction: several steps ahead have to be predicted. Long-Term Prediction has to face growing uncertainties arising from various sources, for instance, accumulation of errors and the lack of information to predict the future values.

Papers were presented orally (single track).

The following is a non-exhaustive list of machine learning, computational intelligence and artificial neural networks topics covered during the ESTSP conferences:

- Short-term prediction
- Long-term prediction
- Econometrics
- Nonlinear models for Time Series Prediction
- Time Series Analysis
- Prediction of non-stationary Time Series
- System Identification
- System Identification for control
- Feature (variable or input) Selection for Time Series
- Selection of Exogenous (external) variables

The goal of the competition is the prediction of the 50 next values (or more) of the time series. The evaluation of the performance was done using the MSE obtained from the prediction of both the 15 and the 50 next values.

So far, there are now 74 values available and the results can be found in http://www.cis.hut.fi/projects/tsp/ESTSP/. In the following figure the predictions of all the competition participants are plotted in blue. In red and in the table below are shown the real values so far.

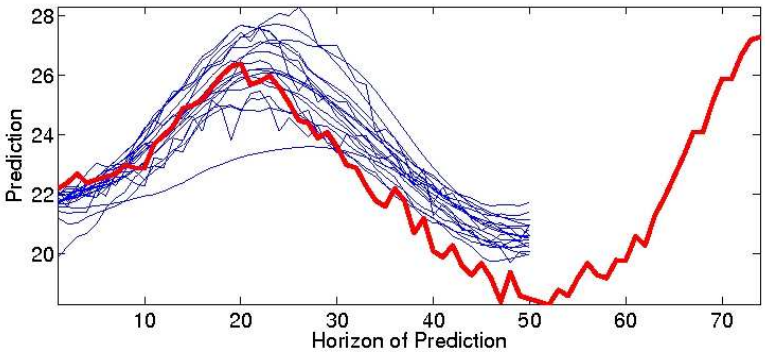

Figure 16.1: The ESTSP Benchmark.

16.3 Methodology for long-term prediction of time series

Amaury Lendasse, Yu Qi, Yoan Miché and Antti Sorjamaa

The time series prediction problem is the prediction of future values based on the previous values and the current value of the time series (see Equation 16.1).

$$\hat{y}_{t+1} = f_1(y_t, y_{t-1}, ..., y_{t-M+1}). \tag{16.1}$$

The previous values and the current value of the time series are used as inputs for the prediction model. One-step ahead prediction is needed in general and is referred as Short-Term Prediction. But when multi-step ahead predictions are needed, it is called Long-Term Prediction problem.

Unlike the Short-Term time series prediction, the Long-Term Prediction is typically faced with growing uncertainties arising from various sources. For instance, the accumulation of errors and the lack of information make the prediction more difficult. In Long-Term Prediction, performing multiple steps ahead prediction, there are several alternatives to build models. Two variants of prediction strategies are studied and compared [2]: the Direct (see Equation 16.2) and the Recursive Prediction Strategies (see Equation 16.1).

$$\hat{y}_{t+k} = f_k(y_t, y_{t-1}, ..., y_{t-M+1}). \tag{16.2}$$

16.4 Nonparametric noise estimation

Elia Liitiäinen, Francesco Corona, Emil Eirola and Amaury Lendasse

The residual variance estimation problem (or Nonparametric noise Estimation) is well-known in machine learning and statistics under various contexts. Residual variance estimation can be viewed as the problem of estimating the variance of the part of the output that cannot be modelled with the given set of input variables. This type of information is valuable and gives elegant methods to do model selection. While there exist numerous applications of residual variance estimators to supervised learning, time series analysis and machine learning, it seems that a rigorous and general framework for analysis is still missing. For example, in some publications the theoretical model assumes additive noise and independent identically distributed (iid) variables. The principal objective of our work is to define such a general framework for residual variance estimation by extending its formulation to the non-iid case. The model is chosen to be realistic from the point of view of supervised learning. Secondly, we view two well-known residual variance estimators, the Delta test and the Gamma test in the general setting and we discuss their convergence properties. Based on the theoretical achievements, our general approach seems to open new directions for future research and it appears of fundamental nature [3]. We have also applied NNE for time series prediction [4].

16.5 Chemoinformatics

Francesco Corona, Elia Liitiäinen, Tuomas Kärnä and Amaury Lendasse

Many analytical problems related to spectrometry require predicting a quantitative variable through a set of measured spectral data. For example, one can try to predict a chemical component concentration in a product through its measured infrared spectrum. In recent years, the importance of such problems in various fields including the pharmaceutical, food and textile industries have grown dramatically. The chemical analysis by spectrophotometry rests on the fast acquisition of a great number of spectral data (several hundred, even several thousands).

In spectrometric problems, one is often faced with databases having more variables (spectra components) than samples; and almost all models use at least as many parameters as the number of input variables. These two problems, colinearity and risk of overfitting, already exist in linear models. However, their effect may be even more dramatic when nonlinear models are used (there are usually more parameters than in linear models, and the risk of overfitting is higher). In such high-dimensional problems, it is thus necessary to use a smaller set of variables than the initial one. We have proposed methods to select spectral variables by using concepts from information theory:

- the measure of mutual information [5].
- the measure of topological relevance on the Self-Organizing Map [6]
- the Functional Data Analysis (FDA) [7]
- Nonparametric Noise Estimation [8]

One particular application has been studied in the field of Oil Production.

In this industrial application, there has been applied process data from Neste Oil Oyj. The aim has been to get new empirical modelling tools, which are based on information technology. The outcome has been emphasized on tools, which are suitable in fast data mining from large data sets. The test cases have included:

- Analysis of instrumental data, on-line monitoring data and quality data
- Non-linear processes
- Identification of delays between stages in industrial processes
- Robust variable selection methods

Analysis of instrumental data, on-line monitoring data and quality data The case has been progressed using a real process data set having 13000 on-line samples (time points) and over a thousand variables. The variables contained different blocks: Z (NIR), X (Process variables) and Y (Quality of end product).

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