MULTIVARIATE STATISTICAL METHODS FOR INDUSTRIAL PROCESS PROGNOSTICS

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Abstract: The paper deals with multivariate statistical methods used for failure prognostics in industrial processes. Modern on-line process monitoring system should support classic fault detection, isolation and diagnosis (FDI) sub-systems to avoid process down-time, increase production, optimize parameters of the production line, etc. However faults usually demand immediate intervention by operator, therefore by using reliable prognostic system, risks can be avoided, maintenance intervals can be scheduled, operation and production strategy can be updated, etc. Presented methods are intended for operator's visual detection of process deviation (along with automated FDI systems) while process monitoring, diagnosis and data analysis tasks are running. By understanding nominal process operation, a hardly detectable small faults and drifts can be used to predict failure scenarios in process prognostics.

Keywords: Fault detection and isolation, prognostics, principal component analysis, multivariate statistical analysis.

1 INTRODUCTION

Failure prognostics is emerging as the next logical step towards improved system condition based maintenance, beside classic fault detection and diagnostics techniques (FDID). These methods form system health management (HMS) platforms which contribute to longer and reliable operation of systems enable them forecasted maintenance intervals, remaining useful life of system components, system reconfiguration, optimisation, etc. In the Artificial Intelligence community prognostics is yet becoming popular as a discipline and differentiates from fault detection and isolation objective, as it detects precursor of failures and predicts remaining time to failure to occur. From technical or production point of view such information are important for operator to prevent un-necessary process down-time, therefore reduces considerable money loss (customer penalty, safety violation, reduced production plan).

Technique for prediction of the system can be developed using raw measurement data or suitable models of processes, upon which the prognostics is realized. Each type has its own advantage (transparency, implementation) therefore various methods can be combined. Most of them come from the field of artificial intelligence and soft computing. In survey paper (Schwabacher, Goebel, 2008) many developed algorithms are divided into two groups; model-based and data-based algorithms, similar to FDID concepts. Other authors sometimes have different classification depending on the field and discipline their work relies on. Very popular are multivariate statistical methods, derivations of Monte Carlo method, support vector machine learning algorithms, Kalman filters, neural networks, fuzzy logic, etc. More about development and various prognostic techniques in use today and classification can be found in literature (references).

In the paper multivariate statistical method are used (principal components (PCA), nonlinear principal components), to achieve very precise detection and prediction of sensor degradation. Algorithm is developed Matlab/Simulink which is thru connected to real time laboratory

hydraulic model. Scenario of level sensor degradation in the tank and pipe clogging due to mineral coating on pipe's wall were tested on the laboratory model, where prognostic system had to operate in small tolerances and under close-loop condition.

2 MULTIVARIATE STATISTICAL METHOD FOR PROGNOSTICS

Process industry demands reliable operation therefore un-necessary process interruptions and changes are usually avoided. However the trend of modern SCADA platforms is integration of various advanced and modern control and FDID algorithms which as a stand-alone system provide information to the operator. Today these platforms usually include basic statistical methods with simple pre-processing algorithms to obtain system health information or small insight into the process behaviour. A classic sensor degradation (due to aging) can bring the system into unstable operation, so detection of sensor fault, prediction if it will lead to a failure (when?) and what effect this has to the process operation (output quality) is very important. Imagine a batch in a pharmacy plant where the growing process of test cells takes a few months. Thru the whole process cells have to be maintained in a certain environment conditions (temperature, pressure...) to comply to world regulations and standards. By implementing prognostic methods, prediction, FDI, and online batch monitoring unwanted process variables deviations can be monitored and analysed in-line before the batch is finished. In case of unpredicted behaviour a prediction potential scenarios can be analysed, or time to solve the faults can determined before the batch will have to be rejected, etc. Similar scenario can be introduced also to other industrial processes.

Multivariate statistical methods proved to be easy to implement and satisfactory for basic industrial tasks, however many of them are linear and not give accurate information. So to improve prognostic system nonlinear techniques should be taken into consideration. Since modern SCADA systems have implemented data acquisition services, statistical model of the process can be obtained upon these large process history datasets by using linear principal component analysis, partial least squares, etc. The linear PCA method does not require much of a processing power and is simple to implement, therefore has been widely used for image compression, fault detection, dimensionality reduction of data (gene expression, meteorology, medicine), etc. It can handle high dimensional and correlated process variables, provides a natural solution to the errors-in-variables problem and includes disturbance decoupling. However, main drawback lies in linearity of this technique therefore a lot of research was invested to nonlinearity and fitting to the nonlinear processes.

Principal component analysis is very popular statistical method for extracting information from measured data, and can also serve as visual information of process (component) changes that needs attention. Rotation and bias of principal components regarding the state of the process is observed and interpreted to obtain system behaviour information. In mathematical term, PCA is performed from aigenvalue decomposition of the covariance matrix from the original measurements. Data matrix X containing n rows with observation of p correlated variables is transformed to independent variables in score matrix T:

$$\frac{X \cdot X}{n-1} = P \cdot D \cdot P \qquad T = XP \tag{1}$$

If sufficient variation is explained in *k* dimensions with $k \le p$ some columns loading matrix *P* can be eliminated. The PCA estimate of *X* is then estimated with residual error *E*:

$$X_{est} = T_k P_k + E_k$$
(2)

Subscript *k* denotes the number of retained principal components.

For purpose of fault detection and diagnosis a statistical measures e.g. Hottteling T^2 or Q-norm is used to define residual bounds for detection of potential faults. However complementary to such distance-based measure a quantitative analysis can be used to visually monitor and predict reduced process performance. For this task the Euclidean concept of distance remains useful (Raich and Cinar, 1995) when considering angles in more than 2 or 3 dimensions. Building on distance between points, the Euclidian angle between points u and v with vertex at the origin, can similarly be defined for higher dimensions using vector products:

$$\cos\left(\theta_{E}\right) = \frac{(u' \cdot v)}{\left(\left\|u\right\| \cdot \left\|v\right\|\right)}$$
(3)

The angle definition is adjusted as weighted distance and the Mahalanobis angle between u and v through the origin can be defined:

$$\cos\left(\theta_{M}\right) = \frac{\left(u \cdot D^{-1} \cdot v\right)}{\left(d\left(u,0\right), d\left(v,0\right)\right)} \tag{4}$$

by using the Mahalanobis distance for points *u* and *v*:

$$d(u,v) = \sqrt{(u-v)' \cdot D^{-1} \cdot (u-v)}$$
(5)

where D is a dispersion. A constant Mahalanobis angle around the line joining point u with the origin is a hyperconical surface, with distortion D. In such way a simple interpretation of the angle is possible through PCA. Rescaling the scores in T so each has equal variance is done by the Mahalanobis distance measure, distorting the ellipsoid described by the scatter of data observations into a sphere. Fig.1 shows first three principal components presented in 3D space, where position (centre) and direction of PC are changed according to different operation regimes of the process. The picture on the right shows possible visual inspection of batch monitoring and prediction of batch quality by using small portion of measurements, that enables and rejection before the batch is finished.



Figure 1: Different PCA models for different process operating regimes(left), and batch prediction (right); rejected batch (red) and accepted batch (blue).

PCA enables quick bat rough results, where process deviation needs to be quite large before reliable results can be obtained. To improve statistical model of the process thus enable better prognostics results nonlinear extension of PCA model is used. NLPCA can be achieved by advanced soft computing algorithms (neural networks, fuzzy logic, genetic algorithm, etc) where auto-associative neural network enables extraction of nonlinear principal components that can be monitored for process deviations.

Despite the fact that the neural network was developed back in 1943 its practical value became important in the 80's as they are very successful at solving different types of problems,

learning, nonlinearity description, etc. Development of neural networks has delivered a special case of a network - an auto-associated structure, which found its use in many different areas (dimensionality reduction, signal processing, compression, etc).

Kramer presented a feed-forward neural network to perform identity mapping, where network inputs are reproduced at the output layer. Kramer's NLPCA is a generalization of a classic PCA, however the fundamental difference between NLPCA and PCA is that NLPCA allows nonlinear mappings from whereas PCA only allows linear mappings. To perform NLPCA, the neural network in Fig. 2 contains three hidden layers of variables between the input and output layers of variables.



Figure 2: Auto-associative artificial neural network structure.

Next to the input layer there is the encoding layer, followed by the bottleneck layer. The network layers are mirrored to the output so next layer is the decoding layer followed by the output of the network. A nonlinear functions maps from the higher dimension input space to the lower dimension bottleneck space, followed by an inverse transform mapping from the bottleneck space back to the original space represented by the outputs, which are to be close to the inputs as possible by minimizing the cost function.

As described in other research papers, a transfer function f_l maps from x, the input column vector of length l, to the encoding layer, represented by $h^{(x)}$, a column vector of length m, with elements,

$$h_{k}^{(x)} = f_{1}\left(\left(W^{(x)}x + b^{(x)}\right)_{k}\right)$$
(6)

where, $b^{(x)}$ is a column vector of length *m* containing the bias parameters, $W^{(x)}$ is an $m \times l$ weight matrix.

A transfer function f_2 maps from the encoding layer to the bottleneck layer containing a reduced number of neurons, which represents the nonlinear principal component u,

$$u = f_2 \left(W^{(x)} h^{(x)} + \overline{b}^{(x)} \right)$$
(7)

The transfer function f_1 is generally nonlinear, while f_2 can also be the identity function. The transfer function f_3 maps from u to the final hidden layer $h^{(u)}$,

$$h_{k}^{(u)} = f_{3}\left(\left(W^{(u)}u + b^{(u)}\right)_{k}\right)$$
(8)

followed by f_4 mapping from $h^{(u)}$ to x', the output column vector of length l, with

$$x_{i} = f_{4} \left(\left(W^{(u)} h^{(u)} + \overline{b}^{(u)} \right)_{i} \right)$$
(9)

The cost function $J = \langle ||x-x'||^2 \rangle$ is minimized to solve the weights and offset parameters of the ANN, meaning finding the optimal values of $W^{(x)}$, $b^{(x)}$, $w^{(x)}$, $\overline{b}^{(x)}$, $w^{(u)}$, $b^{(u)}$, $W^{(u)}$ and $\overline{b}^{(u)}$. Desired minimum square error between the neural network output and the original data is thus minimized. The choice of the number of hidden neurons in an encoding and decoding layer follows a general principle of parsimony. To optimally select the number of mapping nodes Kramer in his paper recommends using final prediction error (FPE) and information theoretic criterion (AIC). In case of a small number of mapping nodes accuracy might be low due to limited representational capacity of the network. On the other hand, if there are too many nodes, the network will be over-fitted. The algorithms and neural network design can be made in Matlab/Simulink by using neural network toolbox. Extraction of nonlinear components is possible from bottle-neck layer, where Fig. 3 shows an extracted nonlinear principal component.



Figure 3: Extracted nonlinear principal component

3 VIRTUAL SENSOR

Instead of just observing changes in the process by nonlinear components, a virtual sensor can be used to reconstruct sensor data measurement from statistical or neural network model. Output(s) of the network and sensor output(s) can be compared to detect deviation or the trend of deviation can be analysed to predict time to fault and failure of the component or process operation.



Figure 4: Virtual sensor scheme with FDID and prognosis algorithm

In case of highly dynamic processes (measurements) a dynamic or even recurrent neural network structure is suggested.



Figure 5: Reconstructed outputs are fed back to the input layer (left) and sensor degradation (right).

4 STUDY CASE: LABORATORY HYDRAULIC MODEL

Principal components analysis, nonlinear principal components analysis and virtual AANN sensor were developed and realized in Matlab/Simulink, and tested on laboratory hydraulic plant as mentioned in the introduction. The process flowsheet of the three-tank laboratory model is depicted in Fig. 6. The upright tanks T_1 and T_2 are mounted above the tank T_3 , hence, the inlet to the tanks also depends on the level (hydrostatic pressure) in the tanks T_1 and T_2 , respectively (the pumps P_1 and P_2 are not an ideal generators to the system). Also, the outlet pipes are mounted at the bottom of the tanks T_1 and T_2 . The nonlinear model was derived from the mass balance equations considering the Torricelli's rule and can be conveniently represented as:

$$A_{1}\frac{dh_{1}}{dt} = q_{1} - q_{21} - q_{11}; \quad A_{2}\frac{dh_{2}}{dt} = q_{2} + q_{21} - q_{22}; \quad A_{3}\frac{dh_{3}}{dt} = q_{22} + q_{11} - q_{1} - q_{2}$$
(10)

where A_i denotes cross-section of the tank, h_i level in the tank and q_{ij} tank volume inflow or outflow, respectively. The medium in the tanks is fluid, which is taken as an ideal and uncompressible, therefore the specific density of the medium can be neglected (V denotes volume, g denotes gravity constant). For one tank a mass balance equation and the outlet of the tank can be described as:

$$q_{in} - q_{out} = \frac{dV}{dt} = A \frac{dh}{dt}; \qquad q_{ij} = S_{Vi} \cdot sign(h_i - h_j) \cdot \sqrt{2 \cdot g \cdot |h_i - h_j|}$$
(11)

where S_{Vi} denotes cross-section of the outlet openness (the valve), h_i and h_j level in the tanks, respectively.



Figure 6: Reconstructed outputs are fed back to the input layer (left) and sensor degradation (right).

Several malfunctions were introduced to the laboratory plant: f_{h1} and f_{h2} – displacement of the level sensors in the tank T_1 and T_2 , respectively (they were separately displaced for approximately 2%), and f_{P1} and f_{P2} – pipeline of the pumps P_1 and P_2 were partially clogged (closing the inlet valves). All test faults were abruptly brought about and no multiple faults were predicted or tested. Obtained data model highly depends on quality of data acquisition

and data extraction from the noise correlated signals. In order to set up as much as modern real industrial environment an OPC standard together with TCP/IP protocol was used. The laboratory model was controlled locally by a PLC and touch-screen display, while the process variables (inputs and outputs of the model) were processed in Matlab/Simulink (Fig. 7).

First, PCA batch prognosis was tested, where Fig. 8 acceptable (blue) and rejected (red)sets of data measurements of the process regime. Level sensor degradation is obvious however small sensor degradation was hard to forecast. Fig. 9 shows forecast upon data measurements of pump, while pipe clogging.



Figure 7: Matlab/Simulink realization



Figure 8: PCA batch process prediction (level sensor degradation; small – left, large – right).



Figure 9: PCA batch process prediction (pipe clogging; small - left, large - right).

Realization of nonlinear principal components by auto-associative neural network was in Matlab/Simulink. Dynamic neural network was trained back-propagation thru time gradient calculations. The Fig. 10 shows first extracted nonlinear component behaviour when small sensor degradation was introduced. The shape and rotation of the curve is changing upon

process regime changes (sensor degradation level). The nonlinear principal component more accurately describes the behaviour of the process regime therefore also smaller process deviations can be predicted and avoided.



Figure 10: Auto-associative neural network structure in Matlab/Simulink (left) and extracted first NLPC.

By using data reconciliation scheme a joint process or each component of the process can be modelled upon history data of the process, with on-line prognosis. In the Fig. 11 an artificial degradation of level sensor is shown. Scheme was realized in Matlab/Simulink and tested for very small deviations (2-4% of measured signal).



Figure 11: Virtual sensor for sensor data reconciliation (left) and level sensor degradation prediction (right)

5. CONCLUSION

In the paper most common multivariate statistical method is used to achieve visual analysis and prediction of potential process failures. Scheme with nonlinear principal components and virtual sensors can improve resolution and robustness to normal process deviation and disturbances, however these methods are merely at the doorstep of true prognostic algorithms emerging every day (remaining useful life prediction, time to failure, etc).

According to surveys prognostics of complex engineered systems remains an area in which much more research is needed. Artificial intelligence and soft computing methods can offer great results, especially if combined into hybrid platforms. Also after detection of failure precursor further action needs to be formulated. Our research will continue in direction of advanced algorithms for prognostics that can be easily implemented into commercial process industry equipment or software that enables advanced mathematical computations to achieve desired results.

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