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An Unsupervised Method for Anomaly Detection in Multi-Stage Production Systems Based on LSTM Autoencoders

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In multi-stage production systems, products are manufactured on a lot-basis through several processing steps, possibly involving various machines in parallel. In case of production of defective items, it is needed to identify the production step responsible of the problem so as to be able to take the proper countermeasures. In this context, the objective of the present work is to develop a model for the detection of anomalies in the operation of a machine of a multistage production system. The main difficulties to be addressed are the lack of labeled data collected while anomalies are occurring in the considered production stage, and the large number of monitored signals in the system, that can be considered for the detection. We, then, formulate the anomaly detection problem as unsupervised classification of multi-dimensional time series and we propose an approach which consists of: *a*) a model for the reconstruction of time-series, utilizing Deep Long Short Term Memory (DLSTM) autoencoders, for catching the highly non-linear dynamics of the signals. *b*) the definition of an abnormality indicator based on the residuals, i.e., the differences between the measured and the reconstructed signal values. The proposed method is verified considering benchmark data from a plasma etching machine used in the semiconductor manufacturing industry.

Keywords: Semiconductor industry, Multi-stage production systems, Anomaly detection, Multi-dimensional time series, Unlabelled data, Long short term memory, Autoencoder,

1. Introduction

The capability of detecting anomalies in the production processes is fundamental for manufacturing companies, such as those producing semiconductors, electronics, medical devices, pharmaceuticals and chemicals, which are characterized by several complex stages

which can take several days to complete (Yang et al. (2021).

Anomaly detection deals with the analysis of time-series data collected by sensors for monitoring the system behavior during production. According to (Lindemann et al. (2021)), anomalies can be of three categories: point, context and collective. Point anomalies abruptly projects the process outside the expected trend. They are typically identified by setting lower and upper thresholds for the values of the individual variables of the time series. Context anomalies involve short time intervals, whereas collective anomalies cause a gradual drift of the process. The identification of context and collective anomalies is a more challenging task than the identification of point anomalies, since they require to consider the values of several data points in the multi-dimensional time series of the monitored variables.

Several approaches based on model-based or data-driven methods have been proposed for detecting anomalies in semiconductor manufacturing, where multivariate time-series signals are measured in the different stages of the production process (Moyne et al. 2017). Azamfar et al. 2020 developed a framework based on Support Vector Machines (SVM), K-Nearest Neighbors (KNN), Linear Discriminant Analysis, Decision Tree and Deep Convolutional Neural Network classifiers. The training of these supervised models need labelled examples of patterns collected both in normal process conditions and during the presence of anomalies. Fan et al. 2020a developed a model based on the use of autoencoders for detecting defective wafers using production data. The encoder produces as output feature a high-level latent representation of the normal condition data, whereas the decoder reconstructs the expected values of the signals in normal condition. Then, the reconstruction error can be interpreted as an index of abnormality of the production process. In (Fan et al. 2020), several machine learning approaches, such as random forest, k-means, ensemble learning classifier, and t-SNE are used to detect anomalies in the production processes. These methods are typically suitable for detecting point anomalies and require the availability of labelled data to do that, but they are not tailored to the analysis of time series.

The present work addresses the following major challenges:

- unlabelled data are, i.e., the groundtruth state of the production machine when the data were collected is not known;
- large number of monitoring signals;
- highly non-linear dynamics of the monitored signals, with the previous values of the time series directly impacting the next values.

To properly address these challenges we exploit the recent advancements of deep learning, which have allowed the development of methods for obtaining high-level representations of unlabelled time series data (Längkvist et al. (2014)). Specifically, we consider the use of Long Short-Term Memory (LSTM) recurrent neural networks, which are emerging due to their capability of learning cyclic patterns in sequential time-series data (Tchatchoua et al. (2021).

The proposed method is made of: a) a model for the reconstruction of the expected normal condition behaviour of the measured signals; the model is based on the use of stacked LSTM autoencoders, which allow learning the signal dynamics and building a low-dimensional, high-level, latent representation of the normal condition data; b) an abnormality indicator, which elaborates the residuals, i.e. the differences between measured and reconstructed signals; c) a threshold for triggering the detection of the anomaly.

The proposed method is applied to multi-dimensional time-series signals monitored on a plasma etching machine of a semiconductor manufacturing industry. The data are taken from the benchmark proposed in (Wise et al. (1999)).

The remaining part of the work is organised as follows. Section 2 illustrates the problem statement. Section 3 describes the proposed methodology. Section 4 introduces the case study and discusses the obtained results. In Section 5, conclusions are drawn.

2. Problem formulation

In the semiconductor manufacturing industry devices are produced on a lot-basis. Each lot consists of several wafers whose production is performed passing through several machines, each one dedicated to a specific function.

Considering a single machine, the matrix $\boldsymbol{X}(k) \in R^{T(k)\times n}$ contains the time series of the measurements of n signals in the period of time T(k), during which the generic k-th wafer has been processed:

$$\boldsymbol{X}(k) = \begin{bmatrix} \boldsymbol{x_1}(k) \\ \boldsymbol{x_2}(k) \\ \vdots \\ \boldsymbol{x_{T_k}}(k) \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{T_k1} & x_{T_k2} & \dots & x_{T_kn} \end{bmatrix} \quad (1)$$

where $x_{t,j}$, $t = 1,\cdots,T(k), j = 1,\cdots,n$ indicates the measurements of signal j at time t. For simplicity of notation, we assume that the processing of the k-th. wafer starts at time 0 and ends at time $T(k)$, and that all measurements are synchronously acquired every one arbitrary unit of time. A training set $D_{train} = [\boldsymbol{X}(k)]_{\ k=1:N_{train}}$, collected during the production of N_{train} wafers is available. Notice that since the state of the machine during the production of the wafers is unknown, the training set may contain wafers produced while the machine was experiencing an abnormal condition.

In this context, the objective of the present work is to develop a method to detect an anomaly of a machine during the production of a test wafer.

3. Proposed method

The problem outlined in section 2 is addressed by (Figure 1):

- developing an unsupervised signal reconstruction model, which reproduces the machine expected behavior in normal conditions through the reconstruction, $\widehat{\boldsymbol{X}}_{test}$, of the data, $\boldsymbol{X}_{test}$ collected during the production of the test wafer;
- defining an abnormality indicator in terms of residuals, i.e. $\boldsymbol{r} = \boldsymbol{X}_{test} - \widehat{\boldsymbol{X}}_{test}$;
- setting a proper threshold for the abnormality indicator, to detect anomalies.

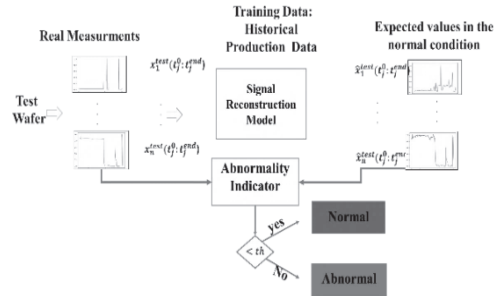

Fig.1. Representation of the conceptual steps of the proposed method for anomaly detection

3.1.1 Signal Reconstruction Model

The signal reconstruction model developed in this work is based on the use of autoencoders (AE), i.e. unsupervised neural networks that learn a high-level lumped representation of the data. It is built by minimizing the reconstruction error of the input patterns using as loss function the mean square error (MSE).

An Autoencoder consists of two parts, an encoder and a decoder. The encoder receives in input l consecutive signals values, $x(t-l+1),\dots,x(t)$, and maps them into a latent space of a dimensionality lower than the dimensionality n of the input space. Then, the decoder receives in input the latent features and reconstructs the original input patterns (Hsieh et al. (2019). Different types of autoencoders have been proposed such as Vanilla autoencoders (Cheng et al. (2021)), Convolutional autoencoders (Lee et al. (2020)), Regularized autoencoders (Vu et al. (2020)) and LSTM autoencoders (Ahmed et al. (2019)). These latters are considered in this work, due to their ability of catching the dynamic behaviour of multidimensional time series and long-term dependencies. Figure 2 shows a stacked LSTM Autoencoder built by stacking layers of encoders and decoders, each one formed by LSTM cells.

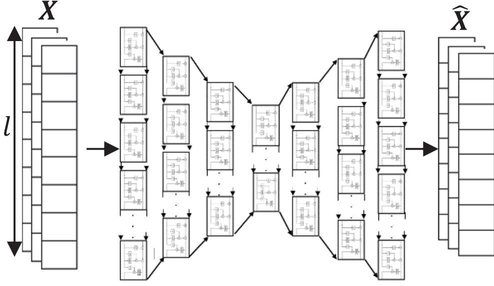

Fig. 2. Reconstruction model based on a stacked LSTM Autoencoder (Ahmed et al.2019)

Figure 3 shows a typical LSTM cell, which consists of input, forget and output gates. These gates control the information flow within a cell. The function of the forget gate is to keep the information from the previous time step (Provotar et al. (2019)). It receives in input the hidden state of the cell at the previous time step, h_{t-1}, and the input vector at the present time, x_t, and provides in output (Hochreiter et.al (1997)):

$$f_t = \sigma\left(W_f[h_{t-1}, x_t] + b_f\right) \quad (2)$$

where W_f is the weight matrix, b_f is the bias vector and σ is a sigmoid function which provides a number between 0 and 1. Notice that when $f_t = 0$, the information about the system state at the previous time step is completely forgot, whereas when $f_t = 1$, it is kept.

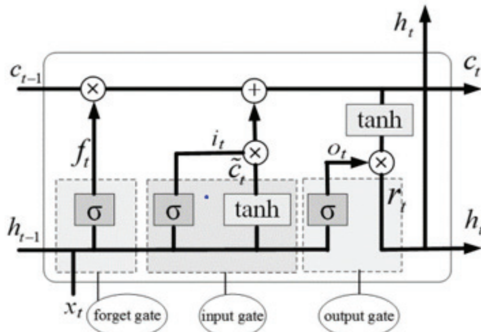

Fig. 3. LSTM cell (Gong et al. 2019)

The function of the input gate is to quantify the importance of the new information. It combines the outcomes of the two functions:

$$i_t = \sigma(W_i[h_{t-1}, x_t] + b_i) \quad (3)$$

$$\tilde{C}_t = \tanh(W_c[h_{t-1}, x_t] + b_c) \quad (4)$$

where $\tilde{C}_t$ is the cell activation vector at time t. Notice that the use of the tanh activation function, which produces an outcome in the range $[-1,1]$, allows deciding if the new information is going to be added $[\tau_t > 0]$ or subtracted $[\tau_t < 0]$.

The outcome gate is used for updating the hidden cell at the next time step:

$$o_t = \sigma(W_o[h_{t-1}, x_t] + b_o) \quad (5)$$

where h_{t-1}, W_o and b_o indicate the past hidden state vector, and the weight matrix and the bias vector associated to the output gate, respectively. Notice that due to the use of the sigmoid function, the gate output o_t is between 0 and 1.

Finally, using the information of the above gates, the hidden cell and the memory cell are updated:

$$C_t = f_t C_{t-1} + i_t \tilde{C}_t \quad (6)$$

$$h_t = o_t \tanh(C_t)$$

3.1.2 Abnormality indicator

Let $\widehat{\boldsymbol{X}}^{test}$ be the reconstruction provided by the stacked LSTM autoencoder of the time series data $\boldsymbol{X}^{test}$ measured during the production of a test wafer; the abnormality indicator (AI) is defined by:

$$AI(test\,wafer) = \sum_{t=1}^{T(k)} \boldsymbol{r}_t^{test}(\boldsymbol{r}_t^{test})^T \quad (7)$$

where $\boldsymbol{r}^{test} = \boldsymbol{X}^{test} - \widehat{\boldsymbol{X}}^{test}$ is the residual between the measured and reconstructed signals at time t. An anomaly is detected when $AI(test\,wafer)$ is larger than a properly set threshold.

In this work, the threshold is set equal to the 95-th percentile of the distribution of the residuals estimated considering a set of validation data.

4. Case study

To evaluate the performance of the proposed method, the benchmark dataset presented in (Wise et. al 1991) is considered. It contains data collected from a semiconductor plasma etching machine, Lam 9600 plasma etch tool, performing the etching process on semiconductor devices. The dataset contains the measurements of 21 signals, such as radio frequency (RF) power, RF load, chamber pressure, endpoint detector, BIC3 flow. They have been collected during the production of 107 healthy and 21 defective wafers.

To effectively demonstrate the performance of the proposed unsupervised fault detection method, 80% of the data containing healthy and defective wafers are randomly selected and used as training and validation sets, for developing the model and setting the hyperparameters, respectively. The remaining 20% of the data are used to evaluate the performance of the proposed method. Specifically, the training and validation sets contain 17 defective wafers and 85 healthy wafers, whereas the test set is made of 22 healthy and 4 defective wafers.

Three stacked autoencoders made by 64, 32 and 16 LSTM cells, have been stacked in the inner layers, creating a reconstruction model with an architecture of 64-32-16-32-64 cells.

Figure 4 shows the convergence of the loss function on the training and validation sets during the model training. As mentioned earlier, The threshold used to identify the defective wafers is the 95-th percentile of the empirical distribution of the abnormality indicator values on the validation set.

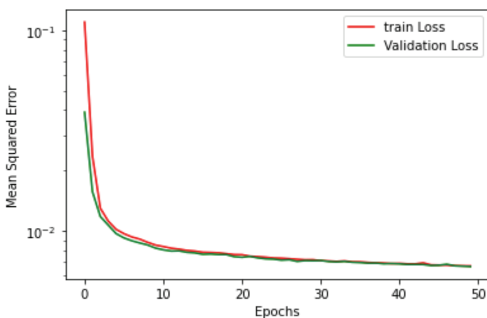

Fig. 4. Evolution of the error in the training and validation sets during the model training

Figure 5 shows the obtained results and Table 1 reports the corresponding confusion matrix. It can been seen that the proposed method is able to correctly predict the state of all the healthy wafers and only of one of the four defective wafers. It is, however, interesting to observe that the abnormality indicator of the defective wafers tends to be larger than that of the healthy wafers.

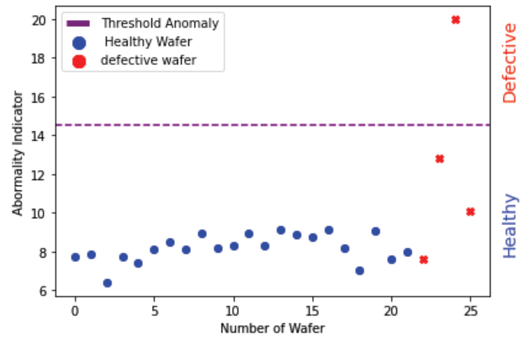

Fig. 5. Abnormality indicator of test datasets without cross-validation

Table 1. Confusion matrix of the model on the test set

<table>
<tr><td colspan="2" rowspan="2">Confusion Matrix
Accuracy: 88.5%</td><td colspan="2">Proposed method</td></tr>
<tr><td>Defective</td><td>Healthy</td></tr>
<tr><td rowspan="2">Groundtruth</td><td>Defective</td><td>1</td><td>3</td></tr>
<tr><td>Healthy</td><td>0</td><td>22</td></tr>
</table>

To reduce the missing alarm rate, i.e. the fraction of defective wafers classified as healthy, we have developed an ad-hoc method to identify and eliminate the defective wafers from the training set. To this purpose, we have divided the training set in 10 folds and applied a 10-Fold cross validation approach. Specifically, the wafers of the test fold with abnormality indicator value larger than the threshold are eliminated: among the 102 wafers of the training set, 10 are recognized as defective. Then, the Stacked LSTM autoencoder is retrained on the remaining 92 wafers. Table 2 reports the new confusion matrix. It can be observed that the performance is significantly more satisfactory with only one false alarm, i.e. one healthy wafer recognized as defective.

Table 2. Confusion matrix after the elimination of the defective wafer from the training set

Confusion Matrix Accuracy: 96.2%		Proposed method	
		Defective	Healthy
Groundtruth	Defective	4	0
	Healthy	1	21

5. Conclusion

An unsupervised anomaly detection method based on stacked LSTM autoencoders has been proposed for the analysis of multi-dimensional time series detection from multi-stage production systems. The obtained signal reconstructions are used to compute a properly defined abnormality indicator that allows identifying the occurrence of anomalies during production. The proposed method has been applied to multi-dimensional time-series signals monitored on a plasma etching machine of a semiconductor manufacturing industry. The obtained results shows the capability of the LSTM cells to deal with the dynamics of the signals and of the stacked architecture of the autoencoders to properly reconstruct the expected behaviour of signals in normal condition.

Future work will devoted to the development of a systematic procedure to eliminate the abnormal condition data from the training set.

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