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Fault Detection for Industrial Chemical Production Using Siamese Autoencoder

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Abstract: Nowadays, deep learning has emerged as a transformative technology in various domains, including process monitoring. Massive advanced deep learning algorithms, such as autoencoder, recurrent neural network, and convolutional neural network, have been explored in the application of chemical processes to enhance the overall monitoring performance. Nevertheless, deep learning models often imply complex structures and a huge number of parameters, leading to limited generalization ability when they are employed in industrial chemical processes. In this work, the above limitation is addressed by monitoring the representative and discriminative features extracted in the latent space by Siamese autoencoder. The reconstruction ability and discriminative information between a pair of inputs are considered in the extraction of latent features, by which better process monitoring performance can be achieved with much fewer model parameters. Case study on an industrial chemical process is investigated to demonstrate the effectiveness of the proposed method.

Keywords: Process monitoring, deep learning, Siamese neural network, catalytic reforming, heat exchanger.

1. INTRODUCTION

Safe and stable operation has been an important prerequisite for chemical production. With the increasing scale and complexity of modern industrial processes, the various nonideal conditions and random factors during practical process operation can rarely be sufficient described by first-principle models, leading to a poor process monitoring performance.

Relying on the rapid development of measurement techniques, complex industrial systems are equipped with massive sensors, and large amounts of data implying internal process operation information can be stored through the distributed control systems (DCS), which facilitates the emergence of data-driven process monitoring methods(Severson, et al. (2016)).

Multivariate statistical process monitoring (MSPM), represented by principal component analysis (PCA) and partial least square (PLS), has been an effective way to detect abnormal deviations based on process data since 1990s (Kresta, et al. (1991)). Generally, MSPM methods transform data into a lower representative space through liner projection, where monitoring statistics are then established for fault detection(Chiang, et al. (2000)). Qin reviewed the application of traditional MSPM methods in process industry(Qin (2012)). Kano et al. evaluated the performance of different MSPM methods in monitoring Tennessee Eastman (TE) process(Kano, et al. (2002)), which is a well-known benchmark simulation process. Nevertheless, different from simulation processes, chemical industrial processes are far more complex with significant nonlinearity and process dynamics, making it difficult to be captured through statistical feature extraction(Ji and Sun (2022)).

As an alternative, deep learning techniques have attracted significant attentions as a new branch of data-driven process monitoring research(Kong and Ge (2021)). Under this category, autoencoders (AEs) have been widely reported to be employed for fault detection(Wan, et al. (2019)). The AE can be regarded as a special neural network structure containing an encoder layer and a decoder layer. The encoder layer is used for feature extraction and dimensionality reduction, and the decoder layer is adopted for data reconstruction. The overall objective of AEs is to minimize the difference between original data and reconstructed data. Benefitting from the activation functions of neural networks, AEs are able to effectively extract the nonlinear relationships among process variables.

The process dynamics and other complex features of industrial process data can also be considered simultaneously through the integration with different neural network structure, such as recurrent neural network (RNN)(Zhang, et al. (2020)) and convolutional neural network (CNN)(Wu and Zhao (2018)). To further improve fault detection performance, Ma et al considered the model residuals of CNN to amplify the process deviations(Ma, et al. (2022)). Zhang and Qiu integrated the dynamic latent variable model into the CNN to better capture process dynamics(Zhang and Qiu (2022)). Yu et al proposed a long short-term memory (LSTM) AE to extract the long-term time dependency(Yu, et al. (2021)). Ma et al. proposed a three-dimensional convolutional AE for spatial feature extraction in three-dimensional equipment(Ma, et al. (2023)).

One main issue should be concerned is the generalization ability of the deep learning models, as the powerful fitting ability is derived from complex model structure and numerous trainable parameters. Regularization is an effective technique to avoid overfitting by applying certain constraints on the parameters of the model. Lee at al. proposed a variation AE-based process monitoring method to constrain the distribution of latent features(Lee, et al. (2019)). Cheng et al. further combined variation AE with RNN(Cheng, et al. (2019)). Cacciarelli and Kulahci proposed orthogonal AEs to regularize the correlation among latent variables(Cacciarelli and Kulahci (2022)). Although the aforementioned regularization could reduce the risk of overfitting, the feature extraction ability and fault detectability of the model can also be affected.

In this work, a Siamese AE (SAE) with constraints is proposed for monitoring chemical industrial processes. The Siamese neural network (SNN) contains two subnetworks with two different inputs but the same structure and parameters(Bromley, et al. (1993)), implying that the size of the dataset can be extended while the complexity of the model is the same as ordinary neural networks. Moreover, the training objective of the Siamese AE consists of both the reconstruction error and the conditional contrastive loss, by which the global features of variable correlation and local features of sample distance can be considered simultaneously to enhance the process monitoring performance. The effectiveness of the proposed methods is verified through a heat exchanger unit of a catalytic reforming process.

2. PRELIMINARIES

2.1 PCA

PCA is a widely used data analysis method for statistical process monitoring. It can reduce the dimension of data and extract the main information of process variables through examining the variance-covariance of the process variables(Wang and He (2010)). Given a set of normalized historical data $\boldsymbol{X}_{n\times m}$ consisting of n data samples and m process variables, the data can be transformed as follows,

$$\boldsymbol{X}_{n\times m} = \boldsymbol{T}\boldsymbol{P}_{m\times k}{}^{T} + \boldsymbol{E} \tag{1}$$

where $\boldsymbol{T} = \boldsymbol{X}_{n\times m}\boldsymbol{P}_{m\times k}$ is the score matrix, $\boldsymbol{P}_{m\times k}$ denotes the projection matrix, which is solved through the Lagrange multiplier method, k is the number of the principal components, and $\boldsymbol{E}$ represents the residual.

For online monitoring, the real-time sample $\boldsymbol{x}$ is transformed by $\boldsymbol{P}_{m\times k}$ into principal component space (PCS), and the T^2 statistic is adopted to measure the changes in PCS,

$$T^2 = \sum_{i=1}^{k} \frac{(\boldsymbol{p}_i{}^{T}\boldsymbol{x})^2}{\lambda_i} \tag{2}$$

where $\boldsymbol{p}_i$ represents the projection of the i th projection direction and λ_i denotes its corresponding eigenvalue. Relatively, the squared prediction error (SPE) statistic is used to monitor the residual space.

$$SPE = \sum_{i=k+1}^{m} (\boldsymbol{p}_i{}^{T}\boldsymbol{x})^2 \tag{3}$$

Under the assumption that process data follow a multivariate Gaussian distribution, the control limits of T^2 and SPE statistics at certain confidence intervals can be determined(Jackson and Mudholkar (1979)).

2.2 AE, RNN, and LSTM

The AE can be regarded as a nonlinear version of PCA, which adopts neural networks to fit the nonlinear relationship among variables. As shown in Figure 1, the encoder compresses the input data into a lower-dimensional representation, while the decoder works to reconstruct the original input data with the compressed representation. Generally, AEs can be trained using backpropagation to minimize the difference between the original input and the reconstructed output.

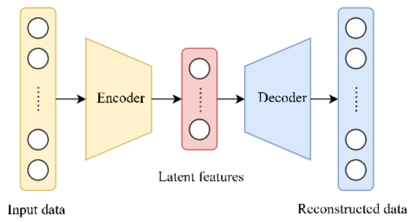

Figure 1. The structure of an ordinary AE.

RNN is a special neural network structure, which can extract dynamic features of the process through the information transfer in latent states h_t, so it is widely applied to time series analysis. The schematic diagram of the RNN model is shown in Figure 2(a), and it can be seen that the latent state h_t of the RNN model at the moment t is related not only to the input x_t at the current moment, but also to the latent state h_{t-1} of the previous moment, and thus the dynamic information in the time series could be captured.

Theoretically, the long-term temporal dependence in the time series can be considered by the iterative calculation of the latent states, but this simple state transfer in RNN does not work well in dealing with the long-term time series because each iteration multiplies the latent states of the past moments by the weight coefficients, which means the weight coefficients of the latent states in distant moments will be very small or even close to zero, and therefore the long-term information is almost forgotten by the RNN.

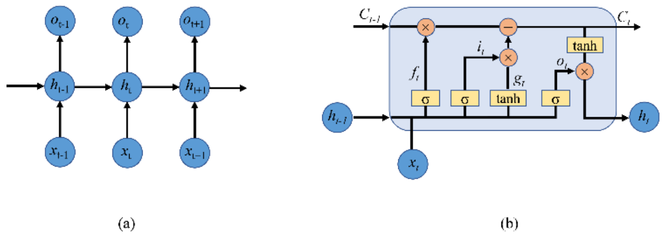

Figure 2. The schematic diagram of (a) RNN, (b) LSTM.

Comparatively, LSTM neural network is proposed as a special RNN and shows good performance in dealing with long-term time dependence of time series, which is widely used in the fields of time series prediction and process monitoring, etc. As shown in Figure 2(b), the LSTM neural network adopts three gate structures and one memory unit to decide the transfer and update of information between latent states. The LSTM neural network introduces the concept of memory through the memory unit C_t, while the transfer and updating of information in the latent state can be controlled through the gate structure calculated as follows,

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i) \tag{4}$$

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f) \tag{5}$$

$$g_t = tanh(W_g \cdot [h_{t-1}, x_t] + b_g) \tag{6}$$

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o) \tag{7}$$

$$C_t = f_t \odot C_{t-1} + i_t \odot g_t \tag{8}$$

$$h_t = o_t \odot tanh(C_t) \tag{9}$$

where i_t, f_t, o_t represent the input gate, forget gate, and output gate, respectively, x_t is the input at the current moment, g_t is the candidate state at the current moment, C_t, C_{t-1} are the memory cells at the current moment and the previous moment, h_t, h_{t-1} denote the latent states at the current and the previous moments, W, b are the weight and bias, and $\sigma, tanh$ are activation functions. Benefiting from these gate structures, irrelevant information from past moments can be forgotten by the LSTM neural network, while useful information can be selectively stored in the memory cells, which makes the LSTM neural network more effective in extracting long-term temporal dependency of time series data. Meanwhile, the complexity and parameters of the model are also significantly increased, making it be vulnerable to overfitting when the dataset is insufficient.

2.3 SNN

SNN is a special type of neural network architecture that contains two inputs. As shown in Figure 3, it is composed of two identical sub-networks that share the same weights and are connected to a loss function that compares the similarity between the two embeddings. The SNN can learn the similarity between pairs of inputs directly from the data without requiring any explicit supervision. It has been widely used in various applications such as face verification and signature verification.

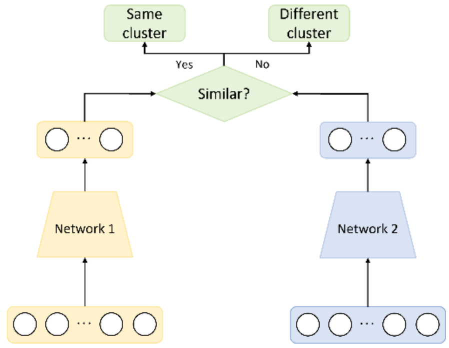

Figure 3. The schematic diagram of SNN.

With the multi-input structure of the SNN, features of each input can be extracted by a sub-network, and the model is trained through learning the similarity of latent features. The sub-networks share the same parameters, which reduces the number of trainable parameters and extend the available training samples, and therefore the generalization ability of the model can be enhanced, making it better capture the data features and effectively avoid the occurrence of overfitting, especially for few-shot learning tasks or even one-shot learning tasks(Zhou, et al. (2021)).

3. SAE-based fault detection method

3.1 Motivation

The SAE model is proposed to improve the generalization and fault detection capability of deep learning models for process monitoring applications. According to the structural design of SNN shown in Figure 3. A single-layer neural network is used as the basis model to extract the latent features of the input data,

$$z_1 = f(w_1 x_{1+} b_1) \tag{10}$$

$$z_2 = f(w_1 x_{2+} b_1) \tag{11}$$

where x_1, x_2 are the two inputs of the SNN, z_1, z_2 are the corresponding latent features extracted by the encoder, w_1, b_1 are weight and bias.

In most cases, only one type of data is considered in industrial process monitoring, i.e., time series data. Since the two inputs of the network have the same data source and are significantly similar, the two LSTM neural networks in the SAE model proposed in this section use the same weights and structure. On the other hand, by introducing the twin neural network structure, the generalization ability of the model trained with the same sample size can be significantly improved. As mentioned earlier, this stems from the multiple-input structure of the SNN. For n training samples, the two-input SNN is able to naturally extend the sample size to $n(n-1)/2$ by data integration. In addition, to further investigate the distribution of latent features extracted by the deep learning model, the conditional contrastive loss is adopted as the loss function to regularize the distribution of latent features,

$$loss = w_1 \frac{\| x_1 - \widetilde{x_1} \|_2^2}{n} + w_2 \frac{\| x_2 - \widetilde{x_2} \|_2^2}{n} + w_3 \| z_1 - z_2 \|, x_1, x_2 \in P \tag{12}$$

$$loss = \widetilde{w_1}\frac{\| x_1 - \widetilde{x_1} \|_2^2}{n} + \widetilde{w_2}(\max(margin - \| z_1 - z_2 \| ,0)), x_1 \in P, x_2 \in N \quad (13)$$

where $\widetilde{x_1}, \widetilde{x_2}$ are the reconstruction of the decoder, $w_1, w_2, w_3, \widetilde{w_1}$, $\widetilde{w_2}$ are weights of each term of the loss function, P represents that the input belongs to normal operating conditions in this fault detection task, N represents that the input belongs to abnormal operating conditions, and $margin$ is a user-defined parameter.

The purpose of the constraints imposed on the feature space by Equation 12 and Equation 13 is to minimize the distance between the normal samples in the feature space and to maximize the distance between the normal and faulty samples in the feature space. Meanwhile, the reconstruction error of the normal input samples remains as one item of the loss function to extract more representative features from the data and ensure the data reconstruction capability of the model. The weights occupied by each item of the loss function in the model training can be adjusted by the weight coefficients, and the conditional contrastive loss is used as the main target in this work, with a weight of 0.8. In summary, with the loss function, the distribution of the normal samples in the feature space in historical data can be compressed to a minimum range, which can effectively improve the fault detection capability of the model.

As for the implementation of fault detection, in most existing AE-based process monitoring studies, the reconstruction error is used as the loss function for model training and fault detection is performed by monitoring the changes in the reconstruction error, without discussing the differences between the features of normal data and fault data extracted in the latent space, resulting in a complete black-box process for process monitoring and poor transparency of fault detection. In fact, feature extraction, as the core part of process monitoring models, makes faults more easily be detected in the feature space by monitoring the changes in the distribution of latent variables. Therefore, the fault detection of the proposed SAE model is performed based on the T^2 statistic in the feature space, which is also consistent with the training objective of the SAE model,

$$T^2 = z_t \Lambda_z^{-1} z_t^T \quad (14)$$

where z_t is the latent feature extracted at t step, and Λ_z is the covariance matrix of the eigenvectors. A control limit can be determined by the kernel density estimation (KDE) method(Silverman (1986)), by which the online process monitoring can be realized

3.2 Process monitoring procedures

The implementation procedures of SAE model in process monitoring modeling and online application are shown in Figure 4, which mainly consists of two parts: offline modeling and online monitoring, and the specific steps of each part are as follows:

Offline modeling:

(1) Data under normal operating conditions are selected from historical data for model training.

(2) Training data are normalized to zero mean and unit variance.

(3) Normalized training data are divided into two parts and input into the SNN.

(4) The SAE-based process monitoring model is determined.

(5) The T^2 statistics of normal samples are calculated by the encoder of the SAE model.

(6) The control limit of the T^2 statistic is determined through KDE method.

Online monitoring:

(1) Test data are normalized with the mean and variance of training data.

(2) Normalized test data are input into the trained encoder of the SAE model.

(3) T^2 statistics of test data are calculated and compared with the control limit.

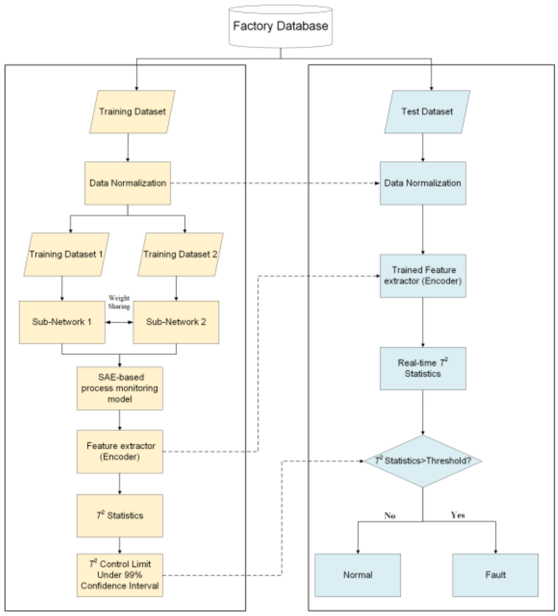

Figure 4. The implementation procedures of the proposed SAE-based process monitoring method.

4. CASE STUDIES

4.1 Description on the heat exchanger unit of the catalytic reforming process and datasets

In this section, the proposed SAE-based process monitoring method is validated through a heat exchanger unit in a catalytic reforming process. The unit consists of four reactors, four heating furnaces and one plate heat exchanger, which is shown in Figure 5. A total of 28 process variables collected from the DCS of the facility are selected for process monitoring, including the pressure, temperature, and flow rate of the process.

The pressure-drop at the hot side of the key equipment heat exchanger could increase abnormally, which would affect its heat exchange efficiency, resulting in increasing fuel gas consumption of the heating furnace. Therefore, it is necessary to monitoring the heat exchanger unit to early detect this type of abnormal deviation. Although there are several fault types in this process, the step fault is easy to be detected and cannot be utilized to verify the strength of the proposed method. Therefore, a slowly changing fault is considered in this case study.

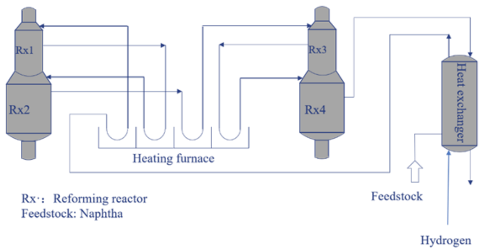

Figure 5. The flow chart of the heat exchange unit of the catalytic reforming process.

In this case study, a dataset consisting of 3,000 samples with a sampling frequency of 1 minute under normal operating conditions is used to train the process monitoring model, 20% of which is used as the validation data. The test dataset contains 1,000 samples with a fault that occurs at the 660th sample. The fault is shown as an abnormal rise of the pressure drop at the hot side of the heat exchanger, which is a slowly changing cumulative process, and hard to be noticed by the operators at its early stage because it does not reach the alarm limit of DCS.

The monitoring performance of the proposed method is evaluated by fault detection delay (FDD) and false alarm rate (FAR), and compared with other related methods including PCA, AE, and LSTM AE.

4.2 Results and discussion

The process monitoring results of different methods are shown in Figure 6. It can be shown that the fault can be detected by the proposed method at the 679th sample, which is at least 22 minutes earlier than other methods.

The evaluation indicators of different methods are summarized in Table 1. According to the results, PCA is able to detect this fault but it takes 65 minutes and the FAR is high. AE performs better than PCA because the nonlinear feature of data can be captured by the neural networks in AE. Although LSTM is effective to extract the long-term time dependency of time series, the process monitoring performance is not enhanced in this case study. The reason could be attributed to the huge number of parameters, which are much more than the number of available training samples. Comparatively, the proposed SAE-based process monitoring method achieve the best performance over different methods. The fault can be detected by the proposed method much earlier with the lowest FAR. The number of parameters of the proposed method is also much less than LSTM AE.

In summary, it can be proved that the SAE-based process monitoring method proposed in this work can effectively improve the generalization performance of the neural network model and significantly enhance the fault detection capability of the model without increasing the complexity of the model structure and the number of parameters, showing good prospects for practical industrial applications.

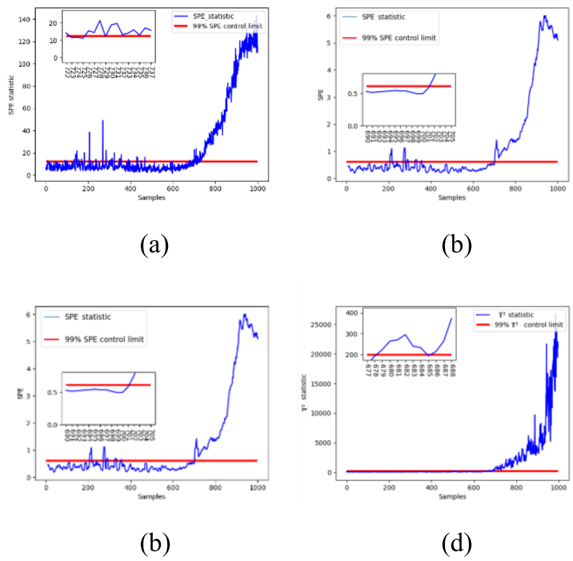

Figure 6. Process monitoring results of different methods: (a) PCA SPE, (b) AE, (c) LSTM AE, (d) SAE.

Table 1. Summary of process monitoring results

Method	FDD	FAR	Parameters
PCA T^2	198	5.76%	/
PCA SPE	65	6.36%	/
AE	41	5.49%	20,252
LSTM AE	42	6.00%	182,448
SAE	19	2.13%	34224

5. CONCLUSIONS

This work presents a SAE-based process monitoring method with a promising generalization performance and fault detectability. With the multi-input structure of the SNN, the sample size of the training dataset can be significantly expanded, and the conditional contrastive loss is adopted to constrain the distance between the two inputs in the feature space, which effectively compresses the distribution range of normal data in the latent space, and therefore fault data can be early and effectively detected through observing changes in the T^2statistic established in the latent space. The application in two industrial chemical processes illustrate that the proposed SAE method significantly improves the generalization and fault detectability of the ordinary neural network model without increasing the complexity of the model structure and the number of parameters, which provides an effective strategy for further research on the practical industrial application of deep learning models in process monitoring.

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