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• **Supplementary File** •

A Novel Deep Quality-Supervised Regularized Autoencoder Model for Quality-Relevant Fault Detection

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Appendix A Construction of monitoring statistics

For online sample $\boldsymbol{x}_{new}$, the three statistics are established as follows,

$$\boldsymbol{T}^2_{y,new} = \left(\boldsymbol{h}_{y,new} - \bar{\boldsymbol{h}}_{y,nor}\right)^T \Sigma^{-1}_{H_y,nor} \left(\boldsymbol{h}_{y,new} - \bar{\boldsymbol{h}}_{y,nor}\right) \tag{A1}$$

$$\boldsymbol{T}^2_{o,new} = \left(\boldsymbol{h}_{o,new} - \bar{\boldsymbol{h}}_{o,nor}\right)^T \Sigma^{-1}_{H_o,nor} \left(\boldsymbol{h}_{o,new} - \bar{\boldsymbol{h}}_{o,nor}\right) \tag{A2}$$

$$\boldsymbol{SPE}_{new} = \left(\boldsymbol{res}_{new} - \boldsymbol{r\bar{e}s}_{nor}\right)^T \Sigma^{-1}_{RES,nor} \left(\boldsymbol{res}_{new} - \boldsymbol{r\bar{e}s}_{nor}\right) \tag{A3}$$

where $\boldsymbol{h}_{y,new}$, $\boldsymbol{h}_{o,new}$, and $\boldsymbol{res}_{new}$ are quality-relevant features, quality-irrelevant features, and residuals obtained by $\boldsymbol{x}_{new}$ through deep QS-RAE. $\bar{\boldsymbol{h}}_{y,nor}$ and $\Sigma_{H_y,nor}$ are the mean and covariance in quality-relevant subspace obtained from the training data, respectively. $\bar{\boldsymbol{h}}_{o,nor}$, $\Sigma_{H_o,nor}$, $\boldsymbol{r\bar{e}s}_{nor}$, and $\Sigma_{RES,nor}$ have the same meaning.

Appendix B TE benchmark process

The TE benchmark process provides a test platform that is suitable for academic research such as industrial process control and optimization and fault detection and diagnosis [1]. At present, the TE process is a very important standard test platform to evaluate the monitoring performance of algorithms [2, 3]. The process contains 52 variables, of which there are 33 measured variables (XMEAS (1-22) and XMV (1-12)) and 19 component variables (XMEAS (23-41)). In addition, the TE process set 21 faults to validate the detection effect. For a detailed introduction to the TE process, please refer to [1]. The confidence level for each statistic is set to 0.99.

In this study, we used 33 measured variables as input data and XMEAS (35) as quality variable [4,5]. The training data contains 500 normal samples for establishing offline model. Each fault contains 960 samples, where the abnormal disturbances are introduced into the process since the 161st sample. The structure of deep QS-RAE is set to 33-27-20-14-8-14-20-27-33 in this study.

Table B1 lists the monitoring results of several quality-relevant fault detection methods, including kernel PCR (KPCR), kernel PLS (KPLS), total KPLS (TKPLS) [6], modified KPLS (MKPLS) [4], modified kernel LS (MKLS) [5], and SAE. The results of KPCR originated from [7]; the results of KPLS, TKPLS, MKPLS and MKLS originated from [8]. In order to accurately evaluate the monitoring performance of each method on process quality, this study defines a statistical indicator that describes the actual impact of process quality as follows,

$$Affect_D = \left(\frac{y_{real} - mean(\boldsymbol{y}_{nor})}{std(\boldsymbol{y}_{nor})}\right)^2 \tag{B1}$$

where y_{real} is the actual value of the process quality, $mean(\boldsymbol{y}_{nor})$ is the mean of process quality under normal conditions, and $std(\boldsymbol{y}_{nor})$ is the standard deviation of process quality under normal conditions. Similarly, the control limit of $Affect_D$ under normal conditions is calculated using KDE. Then the actual impact of the process quality in each fault and the fault detection rate (FDR) of each detection method can be calculated according to the following formula,

$$FDR = \frac{Number\ of\ samples\ exceeding\ the\ control\ limit}{Number\ of\ fault\ samples} \tag{B2}$$

The last column of Table B1 lists the extent to which process quality was actually affected when each fault occurs. Because of the action of the control loop, a few faults only cause the process quality to deviate from the normal state at the beginning of the faults, and then gradually return to normal as the control loop acts. Such faults can be considered as partial quality-relevant faults, including faults 1, 5, and 7. For faults 2, 6, 8, 12, 13, 18, and 21, the process quality cannot be restored to normal through the control loop. These faults can be regarded as quality-relevant faults. For the remaining faults, the process quality is not affected and can be considered as quality-irrelevant faults.

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Table B1 The monitoring result (T_y^2) of quality-relevant monitoring methods

Fault NO.	KPCR	KPLS	TKPLS	MKPLS	MKLS	SAE	Deep QS-RAE	Affect Rate
F1	0.5250	0.9962	0.9687	0.9687	0.5377	0.3613	0.2788	0.2500
F2	0.6290	0.9800	0.8950	0.8950	0.8837	0.9788	0.9013	0.8400
F3	0.0120	0.0250	0.0150	0.0150	0.0577	0.0550	0.0400	0.0750
F4	0.0080	0.6662	0.2037	0.2037	0.0602	0.0950	0.0563	0.0600
F5	0.1700	0.2487	0.1075	0.1075	0.3036	0.2088	0.1575	0.1775
F6	0.9780	0.9950	0.9750	0.9750	0.4782	0.9725	0.9675	0.9625
F7	0.2990	0.9900	0.5575	0.5575	0.3949	0.3200	0.3675	0.2175
F8	0.8220	0.9687	0.6487	0.6487	0.7704	0.7475	0.6700	0.6600
F9	0.0080	0.0112	0.0200	0.0200	0.0502	0.0450	0.0338	0.0675
F10	0.2070	0.8237	0.6262	0.6262	0.4886	0.2438	0.1825	0.1175
F11	0.0250	0.5475	0.1937	0.1937	0.0966	0.0763	0.0513	0.0750
F12	0.7950	0.9875	0.6800	0.6800	0.7629	0.7550	0.6675	0.6900
F13	0.8300	0.9462	0.8675	0.8675	0.7942	0.7813	0.7275	0.6775
F14	0.0000	0.9850	0.7050	0.7050	0.0339	0.1488	0.0463	0.0350
F15	0.0430	0.0625	0.0487	0.0487	0.1267	0.0950	0.0513	0.0600
F16	0.1090	0.6337	0.3862	0.3862	0.2008	0.1788	0.1100	0.0800
F17	0.1730	0.8225	0.4875	0.4875	0.1330	0.3175	0.2638	0.1175
F18	0.8790	0.8900	0.8762	0.8762	0.3447	0.8738	0.8688	0.8700
F19	0.0000	0.0275	0.0137	0.0137	0.0103	0.0088	0.0138	0.0625
F20	0.2570	0.3712	0.1612	0.1612	0.2848	0.2425	0.1413	0.1175
F21	0.1920	0.5187	0.5450	0.5450	0.3061	0.2200	0.3375	0.3475
Dis	0.0870	0.3438	0.1876	0.1876	0.1351	0.0768	0.0376	-

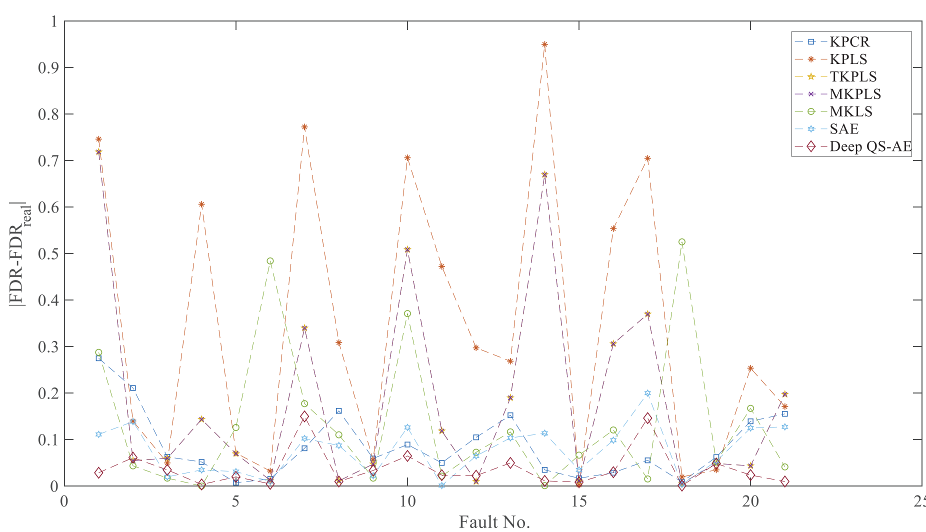

Figure B1 Approximation degree for each fault between the quality-relevant FDRs of each method and the actual affected degree of process quality.

For each fault, in order to measure the approximation degree between the quality-relevant FDRs of each method and the actual affected degree of process quality, we subtract the quality-relevant FDRs of each method from the actual impact of process quality and perform a de-symbolization operation. The result is shown in Figure A1. For the 21 faults in the TE process, the last row of Table B1 lists the average value of the closeness between the quality detection results of each method and the actual impact of process quality. It can be found that the reliability of deep QS-RAE for quality-relevant fault detection is higher than several other methods, because its corresponding quality-relevant statistics T_y^2 are closer to the actual impact of process quality.

The FDRs of each method for the quality-irrelevant spaces are listed in Table B2, including KPLS, TKPLS, MKPLS, SAE, DBN, and neural component analysis (NCA) [9]. The highest FDR for each fault is shown in bold in Table B2. Compared with other fault detection methods, the method based on deep QS-RAE obviously achieves the best monitoring performance. Deep QS-RAE achieves the highest FDR on 14 of 21 faults. Especially for the monitoring results of faults 10, 11, 16, 19, 20 and 21, the FDRs of deep QS-RAE is much higher than the compared methods. Although the maximum FDRs were not achieved on 7 faults, the difference between the FDRs obtained by deep QS-RAE and the maxima is very small. This indicates that the proposed deep QS-RAE not only performs well in the detection of process faults, but also show high reliability in the detection of quality-relevant faults.

Table B2 FDRs of the compared methods for quality-irrelevant spaces

Fault NO.	KPLS		TKPLS		MKPLS	SAE		DBN	NCA		Deep QS-RAE	
	Q	*T2-o*	*T2-r*	*Q*	*T2-o*	*T2-o*	*Q*		*T2*	*Q*	*T2-o*	*Q*
F1	0.9975	0.9962	0.9875	0.9925	0.9975	0.9925	0.9975	**1.0000**	0.9950	0.9930	0.9925	0.9988
F2	0.9800	0.9800	0.9800	0.9700	0.9850	0.9700	0.9863	0.9800	0.9830	0.9850	0.9800	**0.9888**
F3	0.0025	0.0162	0.0012	0.0000	0.0062	0.0075	**0.1875**	0.0300	0.0160	0.0210	0.0388	0.1738
F4	0.6087	0.4875	0.0025	0.1400	0.9975	0.0300	1.0000	0.9800	0.3670	0.9430	0.1600	**1.0000**
F5	0.2162	0.2462	0.0962	0.2200	**1.0000**	0.1563	0.9913	0.9900	0.2560	0.2890	0.2325	**1.0000**
F6	**1.0000**	0.9875	0.9775	**1.0000**	**1.0000**	0.9800	1.0000	**1.0000**	0.9950	0.9910	1.0000	**1.0000**
F7	**1.0000**	0.9725	0.9100	0.9587	**1.0000**	0.2850	1.0000	**1.0000**	**1.0000**	**1.0000**	0.8550	**1.0000**
F8	0.9712	0.9437	0.8162	0.9500	0.9762	0.8663	**0.9900**	0.9800	0.9730	0.9750	0.9538	0.9888
F9	0.0012	0.0087	0.0037	0.0000	0.0037	0.0125	**0.1763**	0.0300	0.0210	0.0600	0.0375	0.1388
F10	0.3562	0.7937	0.0237	0.3287	0.6937	0.1075	0.8663	0.5500	0.3370	0.2720	0.3725	**0.9013**
F11	0.4825	0.5225	0.0212	0.3662	0.6712	0.0463	0.8050	0.6500	0.4800	0.6990	0.2763	**0.8250**
F12	0.9787	0.9725	0.7437	0.9700	0.9937	0.8100	0.9963	0.9900	0.9900	0.9450	0.9600	**0.9988**
F13	0.9375	0.9450	0.7075	0.9425	0.9512	0.8800	**0.9563**	0.9400	0.9490	0.9510	0.9375	0.9550
F14	0.9987	0.9862	0.3312	0.9987	**1.0000**	0.5050	1.0000	**1.0000**	0.9960	**1.0000**	0.8763	**1.0000**
F15	0.0012	0.0375	0.0000	0.0100	0.0250	0.0125	**0.2288**	0.0400	0.0250	0.0910	0.0400	0.2263
F16	0.1500	0.5100	0.0025	0.1637	0.6525	0.0225	0.9250	0.0600	0.1440	0.2340	0.2713	**0.9413**
F17	0.8475	0.7975	0.3700	0.8050	0.9425	0.5763	0.9650	0.9400	0.8460	0.4670	0.7550	**0.9700**
F18	0.8937	0.8862	0.8737	0.8912	0.8975	0.8713	**0.9163**	0.9000	0.9010	0.8790	0.8863	0.9100
F19	0.0250	0.0162	0.0125	0.0000	0.3050	0.0113	0.7875	0.4500	0.0000	0.0060	0.0263	**0.9375**
F20	0.3850	0.3325	0.0275	0.3600	0.5787	0.0750	0.8188	0.5600	0.3090	0.4800	0.3788	**0.9125**
F21	0.3400	0.3762	0.0612	0.3225	0.4537	0.0225	0.5088	0.4800	0.3520	0.2800	0.4025	**0.6163**

Appendix C Ablation Study

The ablation study consists of the following four cases: $\alpha = \gamma = 1$, $\beta = 0$ (Case 1); $\beta = \gamma = 1$, $\alpha = 0$ (Case 2);$\alpha = \beta = 1$, $\gamma = 0$ (Case 3);$\alpha = \beta = \gamma = 1$ (Case 4). The quality-relevant fault detection results are shown in Table C1. This study takes $|FDR_{quality-relevant,i} - AffectRate_i|$ as the evaluation index. $FDR_{quality-relevant,i}$ is the quality-relevant FDR for the ith fault. $AffectRate_i$ is the actual affected degree of process quality for ith fault. The smaller the index is, the closer the quality-relevant fault detection for the ith fault is to the actual situation. The Friedman test is used to evaluate the quality-relevant fault detection performance of the four cases, and the results are shown in Table C2. Table C2 shows that Case 4 in which three regularization terms are considered comprehensively ranks first, and achieves the most reliable quality-relevant monitoring performance. The lack of any of the three regularization terms will have an impact on the reliability of quality-relevant fault detection.

Table C1 Quality-relevant fault detection results of ablation study

Fault NO.	Case 1	Case 2	Case 3	Case 4	Affect Rate
F1	0.3725	0.5625	0.2163	0.4613	0.2500
F2	0.9125	0.8713	0.9513	0.8500	0.8400
F3	0.0650	0.0650	0.0450	0.0400	0.0750
F4	0.0450	0.0738	0.0450	0.0163	0.0600
F5	0.1838	0.1788	0.1675	0.1738	0.1775
F6	0.9838	0.9763	0.9688	0.9725	0.9625
F7	0.3613	0.3338	0.2963	0.3038	0.2175
F8	0.6838	0.8000	0.7150	0.7438	0.6600
F9	0.0563	0.0363	0.0388	0.0438	0.0675
F10	0.2188	0.2125	0.1975	0.1800	0.1175
F11	0.0700	0.0700	0.0500	0.0650	0.0750
F12	0.6888	0.7438	0.6913	0.6913	0.6900
F13	0.7288	0.7888	0.7950	0.7600	0.6775
F14	0.1550	0.0913	0.0600	0.1100	0.0350
F15	0.0488	0.0650	0.0675	0.0625	0.0600
F16	0.1425	0.1638	0.1088	0.1238	0.0800
F17	0.3288	0.2775	0.1475	0.2950	0.1175
F18	0.8763	0.8738	0.8875	0.8563	0.8700
F19	0.0163	0.0338	0.0075	0.0475	0.0625
F20	0.2088	0.1975	0.3275	0.2438	0.1175
F21	0.2300	0.4025	0.3513	0.3425	0.3475

Table C2 Friedman test result of ablation study

	Case 1	Case 2	Case 3	Case 4
Ranking	2.64	2.48	2.52	2.36

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