Deep Learning Approach for Sustainable WWTP Operation: A Case study on Data-Driven Influent Conditions Monitoring

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Abstract

Wastewater treatment plants (WWTPs) are sustainable solutions to water scarcity. As initial conditions offered to WWTPs, influent conditions (ICs) affect treatment units states, ongoing processes mechanisms, and product qualities. Anomalies in ICs, often raised by abnormal events, need to be monitored and detected promptly to improve system resilience and provide smart environments. This paper proposed and verified data-driven anomaly detection approaches based on deep learning methods and clustering algorithms. Combining both the ability to capture temporal auto-correlation features among multivariate time series from recurrent neural networks (RNNs), and the function to delineate complex distributions from restricted Boltzmann machines (RBM), RNN-RBM models were employed and connected with various classifiers for anomaly detection. The effectiveness of RNN based, RBM based, RNN-RBM based, or standalone individual detectors, including expectation maximization clustering, K-means clustering, mean-shift clustering, one-class support vector machine (OCSVM), spectral clustering, and agglomerative clustering algorithms were evaluated by importing seven years ICs data from a coastal municipal WWTP where more than 150 abnormal events occurred. Results demonstrated that RNN-RBM-based OCSVM approach outperformed all other scenarios with an area under the curve value up to 0.98, which validated the superiority in feature extraction by RNN-RBM, and the robustness in

multivariate nonlinear kernels by OCSVM. The model was flexible for not requiring assumptions on data distribution, and could be shared and transferred among environmental data scientists.

Keywords: Wastewater treatment plant, Influent conditions monitoring, Machine learning, Unsupervised deep learning

1. Introduction

For decades, the Kingdom of Saudi Arabia (KSA) has experienced a significant rise in both urbanization and population levels (Khan et al., 2017). The high living standards in KSA, a leading country from the Middle East, have exerted considerable pressure on energy service, water supply, and wastewater treatment. The annual gap between water supply and demand in KSA, which was around 11.5 billion m³, may not be eliminated by only enhancing energy-intensive desalination processes (da Silva et al., 2018; Lefers et al., 2016; Torregrossa et al., 2019). Therefore, wastewater treatment plants (WWTPs) that contributed to water resource reclamation have been given vital importance and are regarded as promising sustainable solutions to the water scarcity in KSA.

Resilient WWTPs have to sustain long-term qualified performance, despite temporally volatile volumes or qualities of the incoming wastewater (Haimi et al., 2013; Zhu and Anderson, 2017). Stringent discharge limits and rising operational costs, as well as intrinsic process nonstationarity and nonlinearity, posed challenges to operators (Corominas et al., 2017; Sweeney and Kabouris, 2014). As initial conditions offered to WWTPs, influent conditions (ICs) affect treatment units states, ongoing processes mechanisms, and product qualities. ICs accordingly were primary in operation thus emphasized, recorded, and monitored in KSA (Cheng et al., 2019). Anomalies or faults in ICs, often raised by abnormal events, need to be detected and diagnosed promptly to avoid facility failure, maintain effluent quality, support downstream operations, improve system resilience, reduce labor costs, and provide smart environments (Li et al., 2017; Lorimer et al., 2018).

All over the years, methods were developed for prediction as well as fault detection and diagnosis, including mechanistic model-based (or analytical methods), and model-free (or data-driven methods) (Venkatasubramanian et al., 2003). Analytical models, based on ideal hypotheses, utilizing first principles, could theoretically explain system behavior, reveal process mechanism, but request prior hyperparameters for calibration and would be questioned by costly high-dimensional

computation and ill-conditioned problems (Haimi et al., 2013). Data-driven methods may perform systematic and objective exploration, visualization, and interpretation of data, identify essential factors, features or patterns, and endorse then optimize data-supported decision-making (Gibert et al., 2018a). Validated data-driven monitoring methods could be transferred and shared conveniently among domain experts, due to the versatile nature of data science models (Gibert et al., 2018b). Though we have stronger computation power nowadays, due to the limited investments in instrumentation, control, and automation in WWTPs, and the lack of data science background for WWTP professionals, it could be demanding to make the best of the data (Newhart et al., 2019; Yuan et al., 2019). Today, data-driven methods have been more common in the environmental field, even though not as widespread as, for example, in petrochemical industry where soft-sensors have been extensively utilized since billions of dollars were once wasted annually due to abnormal events (Venkatasubramanian et al., 2003). Environmental data have been adopted by data-driven methods for anomaly detection in meteorological signals (Hill and Minsker, 2010), prediction of downstream pollutants concentration in river networks (Álvarez-Cabria et al., 2016), and sludge bulking monitoring in WWTPs (Capodaglio et al., 1991).

Traditionally in data-driven modeling, time series analyses have widely been developed to model WWTPs (Kazor et al., 2016). Boyd et al. (2019) validated autoregressive integrated moving average (ARIMA) models in daily influent flow forecasting for five stations across North America. Li et al. (2019) improved autoregressive with exogenous inputs models to predict inflows at sewage pumping stations with different hydraulic characteristics and climatic conditions. Man et al. (2019) proposed an approach to forecast COD load in municipal sewage based on ARIMA and vector AR algorithms. Xiao et al. (2017) applied multistep ARMA model to monitor and diagnose ICs.

Machine learning is a remarkable multidisciplinary field, where methods could be implemented for fault detection. A traditional artificial neural network (ANN) simulation for the monitoring and control of an anaerobic WWTP was reported (Wilcox et al., 1995). Neural fuzzy models together with ANN were applied for monitoring and predicting WWTPs (Dias et al., 2007). ANN models have also been researched to monitor multiple key parameters including oxidation-reduction potential and UV light intensity in WWTPs (Lin et al., 2012). K-nearest neighbor methods were tested to predict influent conditions (Kim et al., 2016). Hybrid approaches combining ANN with multiple linear regression were researched to forecast biochemical oxygen demand of the influent, which was expensive and

difficult to measure with traditional hard sensors (Zhu et al., 2018).

Deep learning methods have gained much attention from researchers recently for their power to extract knowledge from large and complex datasets (Deutsch and He, 2018; Oneto et al., 2017; Wang et al., 2016; Yang et al., 2018). In the literature, numerous deep learning architectures have been employed to address practical problems. Among them, one consensus was that recurrent neural networks (RNNs) can capture long-term dependencies (Boulanger-Lewandowski et al., 2012; Martens and Sutskever, 2011). Their outputs were based on the actual and past sequential information of inputs (Czuszynski et al., 2018). Therefore, algorithms based on RNNs were proven to be effective in numerous applications including motion tracking of robot manipulators (Xiao et al., 2018), polyphonic music generation and transcription (Boulanger-Lewandowski et al., 2012), predicting stock market trends (Yoshihara et al., 2014), intrusion detection (Sheikhan et al., 2012), and gesture recognition (Czuszynski et al., 2018). RNN-based approaches have also been employed to improve sustainable WWTP operations. For instance, Qiao et al. (2012) designed an RNN-based approach to control the dissolved oxygen concentration, nitrate-nitrogen concentration and mixed liquor suspended solids concentration in a WWTP. Baruch et al. (2005) applied RNN in modeling and adaptive control of WWTP processes.

Recently, an improved extension of RNN has been developed by integrating RNN with the restricted Boltzmann machine (RBM). The RNN-RBM permitted freedom to delineate the temporal correlations involved and merged desirable properties of both RNNs and RBMs to handle dependencies in time series (Boulanger-Lewandowski et al., 2012). Specifically, the RNN-RBM model would employ the capability of the RBMs to describe complicated distributions and the efficiency of RNNs to model long-term dependencies. The RNN-RBM model was initially introduced by Boulanger-Lewandowski et al. (2012) to discover temporal dependencies in high-dimensional sequences from polyphonic music generation and transcription. RNN-RBM has also successfully predicted the evolution of traffic congestion in large-scale transportation networks (Ma et al., 2015). Till now, RNN-RBM models, however, have not been employed to monitor ICs from WWTPs.

In this study, in order to monitor and detect abnormal influent conditions for sustainable and resilient wastewater treatment plant operations, we developed data-driven unsupervised anomaly detection approaches based on deep learning methods and clustering algorithms. The coupled RNN-RBM methodology may potentially carry both flexibility and feature extraction capacity, that could de-

scribe temporal dependencies in multivariate time series, and therefore would improve detection performance of following classification models such as agglomerative clustering (AGC), expectation maximization (EM) clustering, k-means (KM), mean-shift (MS), one-class support vector machine (OCSVM), and spectral clustering (SC). Real ICs dataset collected from a coastal municipal WWTP located in Saudi Arabia is adopted to evaluate suggested algorithms. To the best of our knowledge, this is the first investigation case in anomaly detection using RNN-RBM with OCSVM on ICs of WWTPs.

The deep Boltzmann machines (DBM), RNN-RBM methods were introduced in Section 2. The proposed monitoring schemes were described in Section 3. The performance of the recommended approaches were evaluated via real data in Section 4, and conclusions were drawn in Section 5.

2. Preliminaries

This section provided an overview of the DBM, recurrent temporal RBM and coupled RNN-RBM models.

2.1. Deep Boltzmann machine (DBM)

Deep Boltzmann machine was initially introduced as an extension of restricted Boltzmann machine with multiple hidden layers (Salakhutdinov and Hinton, 2009). DBM was categorized as Markov random field and generative model, since it could be represented by an undirected graph in which deep layers of hidden variables were undirectly connected (illustrated in Figure 1). Generally speaking, with deepen architectures, DBM acquired the enhanced ability to discover and learn well complex statistical structures (representations) of the inputs.

The DBM was trained in an unsupervised manner with unlabeled data. Salakhutdinov and Hinton (2009) investigated a greedy, layer-by-layer pre-training approach, which began by learning a stack of RBMs using the modified *Contrastive divergence* algorithm. The DBM was constructed to offer a richer model than an RBM for discovering relevant features in complex data by incorporating more layers of hidden units. Probability distributions could be defined by energy functions in energy-based probabilistic models. The DBM energy function of the state $\{v, h^{(1)}, h^{(2)}\}$ was:

$$E(v, h^{(1)}, h^{(2)}; \theta) = -v^T W^{(1)} h^{(1)} - h^{(1)} W^{(2)} h^{(2)} \quad (1)$$

Figure 1: Diagram of a deep Boltzmann machine (DBM).

where θ defined the model parameters as $\theta = \{W^{(1)}, W^{(2)}\}$, the vector of visible units was $v \in \{0, 1\}^D$ and the vectors of hidden units were $h^{(1)}, h^{(2)} \in \{0, 1\}^P$. The joint probability distribution assigned by the model to v was:

$$p(v; \theta) = \frac{1}{Z(\theta)} \sum_{h^{(1)}, h^{(2)}} \exp(-E(v, h^{(1)}, h^{(2)}; \theta)) \quad (2)$$

The learning process of an DBM was achieved by minimization of the negative log-likelihood, where its derivative with respect to the model parameters was expressed in the following form:

$$\frac{\partial \log P(v; \theta)}{\partial W^{(1)}} = \mathbb{E}_{P_{data}}[vh^{(1)T}] - \mathbb{E}_{P_{model}}[vh^{(1)T}] \quad (3)$$

where $\mathbb{E}_{P_{model}}[\cdot]$ denoted an expectation with respect to the distribution defined by the model, and $\mathbb{E}_{P_{data}}[\cdot]$ was an expectation with respect to the completed data distribution.

2.2. Recurrent temporal RBM

Traditional neural networks started processing the input assuming the absence of dependencies, neither between the observed data nor the outputs. However, in real practices, temporal dependence on historical data existed in time series data. In other words, the generated output from the network at time instant $t - 1$ would impact the decision at time instant t . To cope with the limitations, recurrent neural networks were introduced (Williams and Zipser, 1989) and had become powerful

tools for time-dependent modeling. RNNs permitted discovery and learning of temporal dependences by incorporating the previous output as inputs. This algorithm was incorporating not only current inputs but also recent past inputs, to produce new outputs (Figure 2).

The topology of RNN was based on nonlinear stacked units, where at connections between units formed a directed cycle (Figure 2). RNN was deep in time steps when unrolled (unfolded over time). This structure enhanced feature discovering and learning of long-term dependencies from sequential time-series data, which made RNNs appropriate for dynamic system modeling.

Figure 2: Diagram of a recurrent neural network (RNN).

The recurrent temporal RBM (RTRBM) (Sutskever et al., 2009) was a succession of conventional RBMs (Figure 3). The parameters of RTRBM models were time-dependent, where their dependencies were on the sequential history at time t . We denoted the RTRBM parameters respectively as b_v , b_h , $W^{(t)}$, and

$$\mathcal{M}^{(t)} \equiv \{v^{(\tau)}, \hat{h}^{(\tau)} | \tau < t\} \quad (4)$$

where $\hat{h}^{(t)}$ was the mean-field value of $h^{(t)}$, and the biases depended on $\hat{h}^{(t-1)}$. The joint probability distribution of RTRBM was defined by (Sutskever et al., 2009):

$$P(v^{(t)}, h^{(t)}) = \prod_{t=1}^T P(v^{(t)}, h^{(t)} | \mathcal{M}^{(t)}) \quad (5)$$

Figure 3: Diagram of a recurrent temporal RBM.

In Eq.5, $P(v^{(t)}, h^{(t)} | \mathcal{M}^{(t)})$ was the joint probability of the t^{th} -RBM, with Eq.6, 7 defining its parameters.

$$b_h = b_h + W' \hat{h}^{(t-1)} \quad (6)$$

$$b_v = b_v + W'' \hat{h}^{(t-1)} \quad (7)$$

In summary, RTRBM had six parameters: $W, b_v, b_h, W', W'', \hat{h}^{(0)}$. Note that the Eq.8 defined a single-layer RNN, with hidden units $\hat{h}^{(0)}$

$$\hat{h}^{(t)} = \sigma(Wv^{(t)} + b_h) = \sigma(Wv^{(t)} + W' \hat{h}^{(t-1)} + b_h) \quad (8)$$

2.3. Coupled RNN-RBM approach

Coupled RNN-RBM model, as an extension of the recurrent temporal RBM, was integrating both models in order to capture and predict temporal dependencies in high-dimensional data (Boulanger-Lewandowski et al., 2012). Generally speaking, as an energy-based model, the RNN-RBM augmented the RNN model by including an RBM at every time step (Boulanger-Lewandowski et al., 2012). The configuration was constructed based on an RBM, whose model parameters were determined from an RNN (Figure 4).

The hidden unit $\hat{h}^{(t)}$ of the RNN layer at time instant t was directly linked to its predecessor $\hat{h}^{(t-1)}$ and to V^t as shown in the Eq. 9:

$$\hat{h}^{(t)} = \sigma(W_2 v^{(t)} + W_3 \hat{h}^{(t-1)} + b_{\hat{h}}) \quad (9)$$

where the parameters of a single-layer RNN-RBM were: $W, b_v, b_h, W', W'', \hat{h}^{(0)}, W_2, W_3$ and $b_{\hat{h}}$. The joint probability distribution of RNN-RBM was obtained

Figure 4: Diagram of a single-layer RNN-RBM.

by placing $\hat{h}^{(t)}$ in Equation (5). In fact, RTRBM was constrained by the hidden units needed to represent the conditional distributions and to transmit temporal information. Combining a complete RNN with distinct hidden units $\hat{h}^{(t)}$ would overcome this constraint.

3. RNN-RBM-based OCSVM anomaly detection approach

In this section, the outline and the training procedure of the RNN-RBM model were presented. The principles of connecting OCSVM with RNN-RBM models to efficiently detect anomalies in multivariate time-series data were illustrated.

Aiming at describing dynamics and autocorrelation in multivariate time series such as ICs data of WWTP, we adopted the data-driven RNN-RBM modeling approach. This method could employ RNN-conditioned RBM as the powerful data distribution estimator to depict local and long-term dependences contained in the dataset (Boulanger-Lewandowski et al., 2012).

In the training step of the RNN-RBM model, anomaly-free data were inputted in an unsupervised manner, to obtain a feature space that may reconstruct the input with limited error via encoding and decoding tasks. The designed and trained RNN-RBM model could thereafter be applied to predict the evolution of inflow conditions of WWTPs. During the training phase, cross-entropy error was set as the cost function to minimize (Vincent et al., 2010). This cost function could quantify the accuracy of the model when representing inputs in the training set, by calculating the dissimilarity between the probability distributions of input and reconstruction from the RNN-RBM model. The cross-entropy was given as:

$$\mathcal{C}(X, \hat{X}) = - \sum_i^n (\hat{X}_i \log(X_i) + (1 - \hat{X}_i) \log(1 - X_i)) \quad (10)$$

where X was the distribution of input data and $\hat{X}$ was the distribution of reconstructed data from the fitted model. The initialization of parameters played a vital role in reaching the global minimum of the cost function. Here, the initial values of deep learning parameters have been tuned in manual manner in the training stage.

Then the designed RNN-RBM model together with clustering algorithms (i.e., EM, KM, MS, OCSVM, SC, and AGC) were adopted to detect abnormalities in multivariate IC time series data (see Figure 5). Here, the output features from the RNN-RBM model were used by the classifiers to differentiate or discriminate between normal and abnormal patterns.

In summary, the proposed RNN-RBM-based anomaly detection approach consisted of three stages: 1) Unsupervised RNN-RBM model construction using time-series training dataset composed of normal observation (with no anomaly). 2) Unsupervised classifiers (i.e., EM, KM, MS, OCSVM, SC, and AGC) training using features discovered by the RNN-RBM model. 3) Anomaly detection on testing dataset using the constructed models. Key steps of the proposed procedure are outlined in Table 1.

Figure 5: RNN-RBM-based OCSVM approach for anomaly detection.

4. Results and discussion

4.1. Data description

To test the proposed schemes for IC monitoring with real dataset, historical ICs from the WWTTP based in King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia (Figure 6) were engaged. This plant had a sustainability mission to provide all treated effluents for irrigation reuse among

Table 1: Main steps in building recurrent probabilistic feature extractors of the proposed system.

Phase 1: Offline modeling	
Step 1	Data (Time series) acquisition and normalization. Abnormal events were reported from operators and labeled as anomalies.
Step 2	Discovering learning model parameters time dependency via unsupervised training of the RNN-RBM, where only one RBM was used at each time-step.
Step 3	Computing the corresponding initialization of different weights and bias for RNN-RBM.
Step 4	Generating new data representation through learned features from the trained RNN-RBM model.
Step 5	Training classifiers with the dataset obtained in the previous step.
Step 6	Defining the hyperplane that separated inliers from outliers, which functioned as the anomaly detector.
Phase 2: Anomaly detection	
Step 1	Collection of new observation $\mathcal{X}$.
Step 2	Normalization of the $\mathcal{X}$ to $\hat{\mathcal{X}}$.
Step 3	Mapping $\hat{\mathcal{X}}$ into feature space $\mathcal{F}_{\hat{\mathcal{X}}}$ using trained RNN-RBM model.
Step 4	Classification of $\mathcal{F}_{\hat{\mathcal{X}}}$ as inlier (normal) or outlier (abnormal) based on each hyperplanes or detectors.

266 the campus, which greatly reduced potable water demand of the university. How- 266
267 ever, more than 150 real abnormal events occurred, such as intensive rainfalls, 267
268 seawater intrusion into the lift station, discharge from construction area over the 268
269 limit, and hypochlorite dosage (see Table 2). All of them caused effects on the 269
270 WWTP operation (downstream processes compared to the inflow) therefore are 270
271 identified and reported by operators. Abnormal events reported from operators, 271
272 as marked in their daily log, when they were examining historical data after the 272
273 event, were recognized and labeled as anomalies, by which binary classification 273
274 scenarios (anomaly detection) were formed. By involving data-driven machine 274
275 learning based monitoring techniques, we hoped to recognize faults in the influ- 275
276 ent, make decisions and take action before they flow into the process, and upgrade 276
277 sustainability of the plant. 277

278 Operators maintained daily sampling of the inflow from headwork, on which 278
279 physical, chemical analysis, and recording are performed. The recorded dataframe 279
280 contains seven years (from Sep. 1st, 2010 to Sep. 1st, 2017) of daily measure- 280

281 ments over twenty-one variables (Table 3) with few not available entry (within 1%, 281
 282 132 out of 63950). Variables were measured by at-line sensors, and recorded daily 282
 283 by operators. Sensors produced by YSI, Xylem Analytics Co. were maintained 283
 284 and calibrated daily to achieve reliable performance. The Pearson's correlation co- 284
 285 efficients from the standard curve of measurements from sensors versus ones from 285
 286 traditional methods were inspected bimonthly to be over 0.90, as reported from 286
 287 the local technician. This study proposed a monitoring method for influent con- 287
 288 ditions, which was at the very beginning of the whole process and may give early 288
 289 warning to operators and facilitate control in downstream processes. Typically, 289
 290 the hydraulic retention time (or reaction time in the whole facility, from headwork 290
 291 to discharge) in a WWTP was long, in comparison with the time required to mea- 291
 292 sure, compute, raise alarm, and take action, which validated the monitoring of 292
 293 influent and its potential for proper control in this industry. To cope with the miss- 293
 294 ingness, and to avoid dropping all partially observed events from the analysis that 294
 295 would result in biases, inefficiencies, and uncertainty, we adopted the R package 295
 296 Amelia for imputation, in which multiple imputations were performed (Honaker 296
 297 et al., 2011). It has been shown that, as an alternative to listwise deletion, multiple 297
 298 imputations could reduce bias and increase efficiency. The algorithms employed 298
 299 both bootstrapping and expectation maximization, whose details are delineated 299
 300 by Honaker and King (2010). In this case study, 100 groups of computations were 300
 301 carried in parallel, and averaged to yield final values. 301

Figure 6: a) The pipeline from the campus, b) the grit chamber and grit classifier inside the headwork, c) the neutralization pit.

302 The training dataset from September 1st, 2010 to May 14, 2011, were used 302
 303 to construct the RNN-RBM model. Instead of displaying all observations of a 303
 304 dataset or only mean with standard deviation, the Table 4 presented summary val- 304
 305 ues of the training dataset: the minimum, the first quartile, the median, the third 305

Table 2: Anomalies in the testing dataframe.

Fault types	Counts
Discharge from construction area	3
InFlow-Total (Rainfall)	5
Internal circulation	3
Lift station maintenance/flushing	2
Lime dumping from RO plant	9
NaOCl dumping from RO plant	26
Others	6
pH over limit	9
Seawater Intrusion	45
TDS over limit	11
Total alkalinity over limit	36
Water supply shutdown	2
Total	157

Table 3: Monitored influent conditions.

No.	Variable name	Measurement scopes
1	InFlow-LS1	Wastewater inflow, from the whole campus area, in m ³ /day
2	InFlow-LS8	Wastewater inflow, from a desalination plant, in m ³ /day
3	InFlow-DP	Wastewater inflow, recycled from WTTP itself, in m ³ /day
4	InFlow-Total	Wastewater inflow, from the whole university, in m ³ /day
5	Temp	Temperature, in Celsius
6	pH	Potential of hydrogen, unitless
7	Conductivity	Conductivity, in μ S/cm
8	TDS	Total dissolved solid, in mg/L
9	TSS	Total suspended solid, in mg/L
10	CaHardness	Calcium hardness, in mg/L
11	MgHardness	Magnesium hardness, in mg/L
12	TotalAlkalinity	Total alkalinity, in mg/L
13	BOD ₅	5-day biochemical oxygen demand, in mg/L
14	COD	Chemical oxygen demand, in mg/L
15	FOG	Fat, oils and grease, in mg/L
16	TKN	Total Kjeldahl nitrogen, in mg/L
17	NH ₃ N	Ammonia, in mg/L
18	NO ₃ N	Nitrate, in mg/L
19	PO ₄ P	Phosphate, in mg/L
20	Cl	Chloride, in mg/L
21	Boron	Boron, in mg/L

quartile, the maximum, kurtosis, and skewness. Skewness and kurtosis were calculated to show the symmetry and shape of the studied time series distributions. From Table 4, we may conclude that several IC variables were positively skewed with strong kurtosis. The training set was normalized after smoothing with the exponentially weighted moving average method to reduce noise effects. Parameters of the constructed RNN-RBM and OCSVM were presented in Table 5.

Table 4: Descriptive statistics of the training dataframe.

	mean	std	min	0.25	0.5	0.75	max	skewness	kurtosis
InFlow-LS1	3021.61	535.45	2228.00	2660.00	2851.00	3244.00	5249.00	1.33	1.89
InFlow-LS8	279.31	156.08	64.00	156.00	228.00	366.00	867.00	1.13	0.92
InFlow-DP	47.43	95.79	0.00	9.00	10.00	36.00	749.00	3.80	18.67
InFlow-Total	3512.92	611.00	2558.00	3036.00	3389.00	3853.00	5642.00	0.86	0.34
Temp	29.31	1.59	25.99	28.10	29.20	30.60	32.50	0.27	-0.85
pH	7.40	0.25	6.59	7.25	7.36	7.52	8.56	0.91	3.20
Conductivity	669.37	284.69	264.00	537.00	625.00	719.00	2466.00	3.19	15.37
TDS	459.48	209.08	174.00	363.00	429.00	492.00	1809.00	3.37	16.69
TSS	68.66	27.29	12.00	49.00	64.00	82.00	187.00	1.14	2.10
CaHardness	72.75	30.78	20.00	52.00	72.00	94.00	176.00	0.49	0.17
MgHardness	41.91	27.46	6.00	24.00	36.00	48.00	156.00	1.81	3.59
TotalAlkalinity	120.88	24.98	68.00	100.00	120.00	136.00	196.00	0.22	-0.33
BOD ₅	99.03	36.95	27.00	71.00	92.00	123.00	224.00	0.58	0.10
COD	152.99	61.83	42.00	102.00	157.00	189.00	329.00	0.50	-0.25
FOG	54.36	53.05	2.90	14.30	37.10	77.10	351.40	1.86	5.25
TKN	17.91	6.18	2.10	13.80	17.30	21.90	37.90	0.30	0.45
NH ₃ N	11.84	4.10	0.94	9.30	12.00	14.50	23.60	-0.06	0.47
NO ₃ N	4.17	1.68	0.10	2.90	4.20	5.10	9.80	0.49	0.47
PO ₄ P	8.25	2.86	1.30	6.40	8.10	10.00	23.50	1.41	6.59
Cl	126.09	75.62	45.00	91.00	107.00	137.00	654.00	4.29	23.37
Boron	1.15	0.33	0.50	0.90	1.10	1.30	2.50	1.40	2.63

The cross-entropy measure was involved in analyzing the accuracy of the constructed model. The stopping rule of training phase would be reached when reconstructions were adequately approximating original inputs. Calculated cross-entropy values along epochs during the training stage displayed that the reconstructed error shrank rapidly with increasing iterations, and converged successfully within 50 steps, validating sufficient learning under the current configurations, for each hyperparameter set.

The testing dataset, with faults, covered the period from May 15, 2011, to September 1st, 2017. Detection performance of developed approaches was cal-

Table 5: Parameters in RNN-RBM and OCSVM.

Models	Parameter	Value
RNN-RBM	batch size	10
	learning rate	0.001
	loss function	cross-entropy
	number of hidden units by layer	40
	number of recurrent hidden units	20
	number of visible units by layer	20
	optimizer	Adam
	training epochs	200
OCSVM	gamma	2
	kernel	radial basis function
	nu	0.001

culated upon the testing dataset. Aside from the OCSVM above, comparisons from the RNN-RBN-based expectation maximization clustering (Dempster et al., 1977), K-means clustering (Arthur and Vassilvitskii, 2007), mean-shift clustering, spectral clustering, and agglomerative clustering algorithms were also computed and displayed. In the expectation maximization clustering algorithm, the fitting between given data and Gaussian mixture models was optimized (Dempster et al., 1977). In such cases, binary clustering algorithms were applied to the features extracted by the RNN-RBN model for anomaly detection. They were trained with only anomaly-free data, but without involving their labels in learning. Most of the clustering algorithms here were parametric, on which two clusters were imposed in the training period, during which normal observations would regroup into a dominant cluster automatically since they share similar features. Besides, for the clustering methods that we can not specify the number of clusters, the same rule was applied by considering only the dominant cluster since it regroups the major elements of the observations. A self-evident assumption is that, unsupervised algorithms would capture the most representative dominant features of the majority observations, which should be the 'most' normal conditions. In other words, we are assuming normal conditions consisted most of the observations, and would exhibit prevalence in clustering, without prior labeling judgment. Thereafter, in the testing phase, easily via existing clusters they could cluster and classify the test data as inlier (normal observation) or outlier (anomaly).

Parameters of the studied algorithms were presented in Table 6. Here, the values of the clustering algorithm parameters are determined via grid search in the training phase. Moreover, performances of detection procedures were quantita-

345 tively evaluated using following metrics: true positive rate (TPR), false positive 345
 346 rate (FPR or recall), accuracy, precision, F1 score (the weighted average of preci- 346
 347 sion and recall), and area under the curve (AUC). 347

Table 6: Parameters in other clustering algorithms.

Models	Parameter	Value
RBM	Learning rate	0.001
	Training epochs	200
	batch size	10
	loss function	cross-entropy
	number of hidden units by layer	40
	number of visible units by layer	20
	optimizer	SGD
DBM	Layers	03
	Learning rate	0.001
	Training epochs	200
	loss function	cross-entropy
	number of hidden units by layer	40
	number of visible units by layer	20
	optimizer	SGD
AGC	Affinity	Euclidean
	Linkage	Ward
EM	Covar	1e-06
	Covariance type	Full
	Iteration	100
KMeans	Init	10
	Iteration	300
Mean-Shift	Bandwidth	0.44
Spectral Clustering	Affinity	RBF
	Gamma	1.0

348 Monitoring results of the studied approaches were displayed in Figure 7, while 348
 349 detection performances were summarized in Table 7. As clearly shown, the detec- 349
 350 tion efficiency and accuracy were greatly enhanced by using the proposed RNN- 350
 351 RBM-based OCSVM approach. Indeed, OCSVM outperformed the other meth- 351
 352 ods (Table 7) by achieving an AUC up to 0.98, which flagged its ability to detect 352
 353 the vast majority of abnormal events reported by the operator, while avoiding 353
 354 raising false alarms at the same time. This fact was attributed to the flexibility 354
 355 of RNN-RBM models and the sensitivity of OCSVM algorithms, that could iden- 355
 356 tify deviation from normal situations both sensitively and accurately in the feature 356
 357 spaces. 357

Figure 7: Monitoring results of RNN-RBM-based (a) one-class support vector machine, (b) expectation maximization clustering, (c) K-means clustering, (d) spectral clustering, and (e) agglomerative clustering.

Other deep probabilistic methods, such as RBM, DBM and RNN were implemented individually for comparison. In these RBM, DBM and RNN-based approaches, binary clustering schemes (i.e., AGC, EM, KM, MS, OCSVM, SC) were applied to the output features of RBM, DBM and RNN models individually only. A summary of the performance of RBM-based, DBM-based and RNN-based anomaly detection schemes were presented in Tables 7. Furthermore, AUC values between RNN-RBM, RNN, RBM and DBM-based anomaly detection approaches, and Standalone clustering algorithms were displayed in Figure 8 to facilitate interpretation of the obtained results.

The results from Table 7 demonstrated that the RNN-RBM-based OCSVM monitoring algorithms clearly outperformed RBM, DBM and RNN-based techniques. Indeed, RBM and DBM models omitted the presence of time dependence

Table 7: Anomaly detection performances.

Scenario	Classifier	TPR	FPR	Accuracy	Precision	F1Score	AUC
DBM	AGC	0.90	0.98	0.31	0.32	0.47	0.46
DBM	EM	0.99	0.87	0.69	0.68	0.81	0.56
DBM	KM	0.99	0.87	0.68	0.66	0.80	0.56
DBM	MS	0.99	0.39	0.96	0.97	0.98	0.79
DBM	OCSVM	0.99	0.25	0.97	0.98	0.98	0.86
DBM	SC	0.97	0.94	0.45	0.44	0.60	0.51
RBM	AGC	0.98	0.92	0.56	0.55	0.71	0.53
RBM	EM	0.96	0.71	0.94	0.97	0.97	0.62
RBM	KM	0.99	0.91	0.54	0.52	0.68	0.54
RBM	MS	0.99	0.90	0.57	0.55	0.71	0.54
RBM	OCSVM	0.99	0.22	0.98	0.98	0.99	0.88
RBM	SC	0.96	0.94	0.51	0.50	0.66	0.51
RNN	AGC	0.94	0.96	0.53	0.55	0.69	0.49
RNN	EM	0.99	0.71	0.90	0.90	0.94	0.64
RNN	KM	0.99	0.77	0.85	0.85	0.92	0.60
RNN	MS	0.99	0.68	0.65	0.91	0.95	0.65
RNN	OCSVM	1.00	0.47	0.95	0.95	0.97	0.76
RNN	SC	0.98	0.92	0.53	0.52	0.68	0.52
RNN-RBM	AGC	0.97	0.93	0.51	0.50	0.66	0.52
RNN-RBM	EM	0.97	0.51	0.95	0.97	0.97	0.72
RNN-RBM	KM	0.99	0.85	0.74	0.73	0.84	0.57
RNN-RBM	MS	0.99	0.29	0.97	0.98	0.98	0.84
RNN-RBM	OCSVM	0.99	0.03	0.99	0.99	0.99	0.98
RNN-RBM	SC	0.96	0.94	0.49	0.49	0.65	0.51
Standalone	AGC	0.93	0.97	0.41	0.42	0.57	0.47
Standalone	EM	0.98	0.94	0.29	0.27	0.42	0.52
Standalone	KM	0.83	0.99	0.22	0.23	0.36	0.41
Standalone	MS	0.99	0.73	0.87	0.87	0.93	0.63
Standalone	OCSVM	1.00	0.38	0.97	0.97	0.98	0.80
Standalone	SC	0.99	0.91	0.53	0.51	0.67	0.54

in modeling time-series data. In other words, they were not designed to model temporal dependency in data. Accordingly, important features and pattern in the data were lost when these feature extractors (RBM and DBM). Also, it can be highlighted that the RNN-RBM-based approach exhibited superior detection performance compared to its counterpart RNN-based approach (Table 7). Amalgamating the desirable proprieties of RNN and RBM was helpful since this would take account for the time dependencies in the multivariate data and thus lead to a more representative model. Here, results also validated that the RNN-RBM-

Figure 8: Area under the curve (AUC) values of proposed algorithms.

based approach, which was describing temporal dependencies, could also support monitoring ICs of WWTPs. We believed this is related to the functionality that RNN-RBM models approximated a complicated distribution for each time step.

Furthermore, as expected, the detection results from the standalone clustering techniques showed unsuitable performance for monitoring multivariate ICs data (Table 7 and Figure 8). The performed experiments confirmed the superiority of recurrent neural networks combined with robust deep probabilistic features extractor, RBM, against standalone machine learning techniques. Moreover, the results from RNN-RBM-based OCSVM showed that the RNN-RBM model is proficient in improving the detection of baseline approaches.

To monitor and detect abnormal influent conditions for sustainable and resilient wastewater treatment plant operations, we developed data-driven unsupervised anomaly detection approaches based on deep learning methods and clustering algorithms. From the results presented, the following opinions were given. First, methods integrating both RNN-RBM and clustering were more efficient and accurate than the standalone clustering techniques. Second, the proposed algorithms outperformed RBM and DBM-based clustering ones, which justified the superior feature extraction quality of RNN-RBM models. It was presented that

396 statistical one-class classifier trained in an unsupervised way (namely OCSVM) 396
397 achieved higher accuracy compared to other adapted binary detectors (cluster- 397
398 ing algorithms). The robustness of OCSVM resided in its nonlinear kernel (e.g., 398
399 radial basis function or Gaussian function) was able to define hyperplane that sep- 399
400 arated normal observation from anomalies via the projection in different dimen- 400
401 sions or features space. Another crucial characteristic of OCSVM was its ability to 401
402 deal with high dimensionality which was the main bottleneck of many classifiers 402
403 (Schölkopf et al., 2001). The OCSVM proved its domination by outperforming 403
404 other methods in all scenarios. 404

405 5. Conclusion 405

406 Data-driven unsupervised anomaly detection approaches based on deep learn- 406
407 ing methods and clustering algorithms were developed in this study, in order to 407
408 monitor and detect influent conditions for sustainable and resilient wastewater 408
409 treatment plant operations. The ability to discover and delineate temporal depen- 409
410 dencies in multivariate time series from RNN-RBM, and the sensitivity to identify 410
411 abnormal features from OCSVM were introduced and merged in this proposed 411
412 strategy. The efficiency of the proposed method were evaluated by real ICs data 412
413 from a coastal municipal WWTP in KSA. The approach involving recurrent neu- 413
414 ral network-restricted Boltzmann machine coupled with one-class support vector 414
415 machine produced the best efficiency and accuracy, compared to RBM or DBM- 415
416 based, or standalone clustering techniques. The RNN-RBM OCSVM detector 416
417 was flexible for not requiring verification of assumptions on data distribution, and 417
418 could be transferred straightforwardly and shared conveniently among various do- 418
419 main experts. 419

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