Supplementary Information: An Evaluation of Anomaly Detection and Diagnosis in Multivariate Time Series

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S1 TAXONOMY OF ALGORITHMS EVALUATED

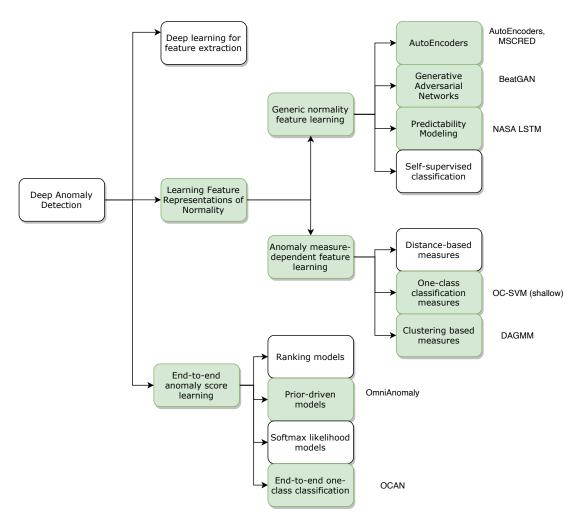


Fig. S1: Anomaly detection algorithms tested in this work (shaded green), based on the taxonomy proposed by [1] for deep anomaly detection. While we do include OC-SVM in the schematic, it is not a deep method. In addition to those shown in the diagram, we also test Raw Signal and PCA, which are not deep methods.

Not all techniques in this taxonomy are suitable for unsupervised or semi-supervised multivariate time-series (MVTS) anomaly detection in a streaming scenario. Based on the discussion on each category in [1]:

Deep learning for feature extraction techniques rely on sophisticated feature extraction techniques which were developed primarily for images, and may not be suitable for MVTS.

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- *Self-supervised classification* techniques rely on data augmentation techniques that have been developed primarily for image data. We are not aware of any existing deep algorithms of this type for MVTS.
- Distance-based measures are computationally intensive at test-time, and hence not suitable for streaming test setting that we work in.
- Ranking models require some form of labelled anomalies which we do not assume.
- Softmax likelihood models have been developed primarily for heterogeneuous data sources or categorical data. We are
 not aware of any existing deep algorithms of this type for MVTS.

S2 DATASETS

The datasets contain data from sensors and actuators which interact with each other and the environment in intelligent and stochastic ways. Due to the dynamic nature of the systems we consider, induced anomalies might only become evident after some delay (sometimes several minutes), and the channel behaviour may not return to normal even after the anomaly inducing mechanism has been withdrawn [2].

S2.1 SWaT

The Secure Water Treatment dataset [2] can be requested on the iTrust website [3]. The dataset has 51 channels, which consist of sensors such as flow meters, level transmitters, conductivity analyzer and actuators such as motorized valves and pumps. The dataset has 14 channels corresponding to signals from various pumps that are constant in train but these are retained as they are allowed to change during testing. The initial 7 days of data consist of normal operation (training set) while 36 attacks were launched in the last 4 days (test set). Each attack compromises one or more channel(s). One of the attacks was much longer (598 mins) than all others (under 30 mins each). This biases the scores of all algorithms depending on whether this event was detected, so we cut this event in the test set to 550 s (the average event length) by discarding anomalous time-points for the rest of the event. Note that since 2 of the attacks were launched right one after the other, we treat it as a single anomalous sequence, and hence consider 35 anomalous events. Of these, root cause labels are available for 33 attacks while the remaining attacks have discrepancies in their root cause labels. For one of the attacks, the start and end points did not match any events listed in the 'List of Attacks' sheet provided on the dataset website [3]. For another attack, the provided root cause does not match any of the available channels.

S2.2 WADI

The Water Distribution testbed [4] is an operational, scaled-down version of a water distribution network in a city. It is connected to the SWaT plant and takes in a portion of its reverse-osmosis output. The distribution network consists of 3 distinct control processes, namely - primary grid, secondary grid and return water grid - each controlled by its own set of Programmable Logic Controllers (PLCs). The dataset, also hosted by iTrust [3] consists of data from 123 sensors and actuators collected over 14 days for normal operation (training set) and 2 days with 15 attacks (test set). Since 2 attacks were launched at the same time, we consider 14 anomalous events in this paper. We use all 14 events for anomaly detection, but for anomaly diagnosis, we have root cause labels for only 12 of the 14 events. For the remaining 2 events, the labels do not specify exactly which component(s) was compromised.

S2.3 DMDS

The DAMADICS (Development and Application of Methods for Actuator Diagnosis in Industrial Control Systems) benchmark [5] consists of real process data from the Lublin Sugar Factory as well as a simulator to generate artificial faults. Here we use only the real dataset with induced faults in the industrial system, available publicly [6]. The dataset consists of data for 25 days of operation, from Oct-29 to Nov-22, 2001 of 3 benchmark actuators - one each located upstream and downstream of evaporator station, and the third controlling flow of water to the steam boiler system. Artificial faults were induced on Oct-30, Nov-9, Nov-17 and Nov-20. Unlike SWaT and WADI, the train and test splits for normal and test operation were not provided. We chose train-test splits such that the test is entirely after train as would be expected in a real scenario, the train is continuous, and the train contains no anomalies. Accordingly, we used the data from Nov-3 to Nov-8 (6 days) as the training set and data from Nov-9, Nov-17 and Nov-20 (3 days) as the test set. From this, the first 10800 points from the training set were dropped as the system appeared much more unstable than the rest of the training set, potentially from the anomaly induced earlier on Oct-30. In addition, the initial part of the test set appears quite unstable across multiple channels even though no anomaly is recorded. Therefore we also drop the first 45000 points from the test set.

S2.4 SKAB

The Skoltech Anomaly Benchmark [7] testbed consists of a water circulation system and its control system, along with a data-processing and storage system. Examples of the type of anomalies induced include partial valve closures, connecting shaft imbalance, reduced motor power, cavitation and flow disturbances. Train and test splits are provided by the authors.

S2.5 MSL and SMAP

These are expert-labeled datasets from real anomalies encountered during the operation of two spacecraft - Soil Moisture Active Passive (SMAP) satellite and the Mars Science Laboratory (MSL) rover, Curiosity [8]. Unlike the other datasets, each entity in MSL and SMAP consists of only 1 sensor, while all the other channels are one-hot-encoded commands given to that entity. We use all channels as input to the model, but the model error of only the sensor channel is used for anomaly detection, as done by [8]. The total number of variables is 1375 and 1485 for SMAP and MSL respectively, making these much larger than the single-entity datasets in terms of number of variables. The data is however divided into 55 and 27 entities respectively. The authors provide train-test splits so that for the first anomaly encountered in test at time t, the training set is from time t-5 days to t-3 days (if available), and the test set goes from t-3 days to t+2 days. The data is sampled each minute, so the training set is much shorter than other datasets.

S2.6 SMD

SMD, or Server Machine Dataset was published by [9] on their Github repository https://github.com/NetManAIOps/OmniAnomaly. The data was collected over 5 weeks from a large internet company. It consists of data from 28 entities regularly sampled every minute. The train-test split is 50% each for train and test, suggested by the authors. An interpretation label is provided for each anomaly which we use for anomaly diagnosis.

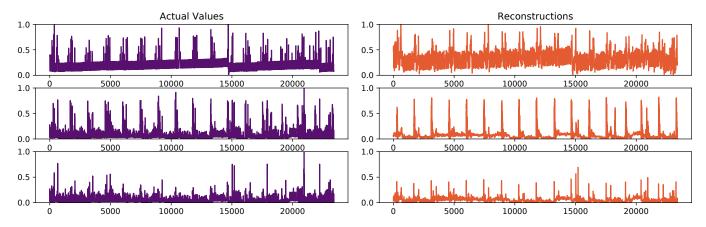


Fig. S2: Left: Signals from three channels from the SMD dataset, showing strong correlations across channels and time. Right: Reconstructions of the three channels by Univariate AutoEncoder, accounting for only temporal correlations.

S3 ADDITIONAL DETAILS ABOUT MODELS

Univariate Fully-Connected Auto-Encoder (UAE): In this method, we train a separate auto-encoder for each channel. Each encoder is a multi-layer perceptron with l_w nodes in the input to p dimensions in the latent space, with the number of dimensions reducing in powers of 2 in each layer, similar to [10]. The decoder is a mirror image of the encoder, and we use tanh activation.

Fully-Connected Auto-Encoder (FC AE): This is similar to UAE, but now we have a single model over all the channels. Thus, the input sample is a flattened subsequence, a vector of size $l_w \times m$.

Long Short Term Memory Auto-Encoder (LSTM AE): We use a single LSTM layer for each of the encoder and decoder. [11] used only the first principal component (PC) of the MVTS as input to LSTM-ED, but since this can result in major information loss, we choose the number of PCs corresponding to 90% explained variance. We set the hidden size to be the same size as the number of PCs.

S4 HYPERPARAMETERS AND IMPLEMENTATION

In some algorithms, we set the architecture size as a function of m to accommodate different datasets, eg. the hidden size. All other hyperparameters are kept constant across datasets, obtained by hyperparameter tuning on the SWaT dataset only. All the deep learning methods except OmniAnomaly and OCAN are trained for a maximum of 100 epochs with early stopping using the reconstruction or prediction error on the 25% held-out validation set and patience = 10.

TABLE S1: Online code references

Model	Adapted from
LSTM VAE	https://github.com/TimyadNyda/Variational-Lstm-Autoencoder
NASA LSTM	https://github.com/khundman/telemanom
DAGMM	https://github.com/danieltan07/dagmm
OmniAnomaly	https://github.com/NetManAIOps/OmniAnomaly
MSCRED	https://github.com/Zhang-Zhi-Jie/Pytorch-MSCRED, https://github.com/SKvtun/MSCRED-Pytorch
OCAN	https://github.com/PanpanZheng/OCAN
BeatGAN	https://github.com/Vniex/BeatGAN

TABLE S2: Hyperparameters are tuned using the minimum validation reconstruction error criterion, based only on the SWaT dataset. We tested 50 random hyperparameter configurations for each of TCN AE, LSTM VAE and OC-SVM, and 20 random configurations for FC AE. The chosen hyperparameter is shown in the 'Value' column. m is the number of channels in each entity of a dataset.

Model	Hyperparameters	Sampling distribution	Value
FC AE	learning rate	\log -unif($\log(10^{-4})$, $\log(10^{-3})$)	10^{-4}
	z-dim	int of $\{\frac{m}{5}, \frac{m}{4}, \frac{m}{3}, \frac{m}{2}, \frac{m}{1}, 2m, 3m, 4m, 5m\}$	$int(\frac{m}{2})$
TCN AE	learning rate	$\log - \text{unif}(\log(10^{-4}), \log(10^{-2}))$	1.5×10^{-4}
	z-dim	$int \in [3, 10]$	8
	dropout rate	unif(0.2, 0.5)	0.42
LSTM VAE	learning rate	\log -unif($\log(10^{-4})$, $\log(10^{-2})$)	9.5×10^{-3}
	(z-dim, hidden-dim)	$\{(3,15),(3,5)\}$	(3, 15)
	λ_{reg}	unif(0,1)	0.55
	$\lambda_{kulback}$	unif(0,1)	0.28
OC-SVM	γ	$\left\{\frac{1}{\#features}, \operatorname{uniform}(10^{-5}, 10^5)\right\}$	1 #features
	ν	unif(0,0.5)	0.489

TABLE S3: Key hyperparameter values used for each models. m is the number of channels in an entity of the dataset, LR is the learning rate, p refers to the hidden size. * Learning rate annealing was used as per [9]

Model	Epochs	LR	Batch size	Design	Framework
PCA	-	-	-	$n_{PCA,0.9}$ =components for explained vari-	Scikit-learn
				ance=0.9	
OC-SVM	-	-	-	$\gamma = 1/m$, $\nu = 0.489$	_
UAE	100	0.001	256	p=5	Pytorch
FC AE	100	0.0001	128	p=int(m/2)	Pytorch
LSTM AE	100	0.001	64	PCA before model with $n_{PCA,0.9}$, hidden-layers=3	Pytorch
TCN AE	100	1.5×10^{-4}	128	dropout=0.42, p=3, hidden-layers=min(10, int(m/6)), kernel-size=5	Pytorch
LSTM VAE	100	9.5×10^{-3}	128	Hidden layers=2, hidden-dim=15, z-dim=3, λ_{reg} =0.55, $\lambda_{kulback}$ =0.28	Tensorflow
BeatGAN	100	10^{-4}	128	λ_{reg} =0.55, $\lambda_{kulback}$ =0.28 z-dim=10, beta1=0.5	Pytorch
MSCRED	100	10^{-4}	128	As in [12]. For WADI, PCA before model	Pytorch
MISCRED	100	10	120	with $n_{PCA,0.9}$	1 ytorch
DAGMM	200	10^{-4}	128	z-dim=m, GMM_k =3, λ_{energy} =0.1,	Pytorch
				λ_{cov} =0.005	-)
NASA LSTM NPT	100	10^{-3}	64	LSTM-units=m, LSTM-layers=2,	Keras
				dropout=0.3, NPT params from [8]	
NASA LSTM	100	10^{-3}	64	LSTM units=m, LSTM layers=2,	Keras
				dropout=0.3	
OmniAnomaly	20	0.001*	50	All params as in [9]: z-dim=3, RNN-	Tensorflow
,				units=500, dense-units=500, NF-layers=20	
OCAN	100	10^{-4}	128	As in [13]	Tensorflow

TABLE S4: Training time for deep learning algorithms in minutes for the single-entity datasets (with early stopping), trained on a single Nvidia GeForce RTX 2080 Ti GPU. UAE, the top performing model in the evaluation, is the third slowest. The slow speed of UAE training is because we trained the channel-wise models sequentially but since each model is independent, it is easily parallelizable. On the other hand, FC AE the second best model, is the fastest to train.

	DAMADICS	SWaT	WADI
BeatGAN	9	10	19
DAGMM	37	45	115
FC AE	6	11	2
LSTM AE	23	116	142
LSTM VAE	98	93	77
MSCRED	221	510	330
NASA LSTM	22	25	14
OCAN	41	42	121
OmniAnomaly	186	165	262
TCN AE	20	20	38
UAE	65	104	268

S5 COMPARISON WITH PUBLISHED RESULTS

TABLE S5: Point-adjusted F_1 score for the MSL, SMAP and SMD datasets with the best-f1 threshold, comparing results reported in the literature against UAE Gauss-D and Random Anomaly Detector (discussed in section 6 in the main text).

Model	MSL	SMAP	SMD
OmniAnoAlgo (reported by authors) [9]	0.9014	0.8535	0.9620
OmniAnoAlgo (reproduced by us)	0.8459	0.8678	0.9424
USAD (reported by authors) [10]	0.9109	0.8186	0.9382
Random Anomaly Detector	0.8512	0.7418	0.7585
UAE Gauss-D	0.9204	0.8961	0.9723

Here we discuss the results in our paper with other published works on the datasets we use.

Comparisons on WADI dataset with the point-wise F_1 score: Recently, [10] propose USAD, an adversarially trained auto-encoder model for MVTS anomaly detection, and tested it on 5 of the 6 datasets that we test here. They report a point-wise F_1 of 0.2328 with the best-F-score threshold on the WADI dataset. [14] report F_1 score of 0.37 on the WADI dataset with the best-F-score threshold using a Generative Adversarial Network, MAD-GAN. We obtain comparable or better scores in this work, shown in Table S10 using the Gauss-D scoring function and Table S11 with the Gauss-D-K scoring function. The best overall algorithm, UAE, attains an F_1 score of 0.4740 (an improvement of 46.5% over MAD-GAN) with the Gauss-D-K scoring function, while the best performing algorithm on WADI in this table is LSTM VAE, with an F_1 score of 0.5025.

Comparison with point-adjusted F_1 results: [9] and [10] report results on SMAP, MSL and SMD datasets with the point-adjusted F_1 score with the OmniAnomaly and USAD algorithms respectively. Based on the experiments discussed in the main text section 6, we do not use this metric to draw comparisons in this paper. However, for the sake of completeness, we show a comparison of the scores of UAE using Gauss-D threshold vs. the results reported by the authors of OmniAnomaly and USAD in Table S5. Once again, UAE is the top performing algorithm.

Aside from the works discussed above, point-wise F_1 score with the best-F-score threshold have been published previously on the SWaT dataset. [14] report a score of 0.77 with the MAD-GAN algorithm, and [10] report a score of 0.79 with the USAD algorithm. However these results are not directly comparable with our results. This is because in our study, we have shortened a long anomaly that biases the results (discussed in section III in the main text) in the SWaT dataset, and as a result our test set is different from these works. We note that some algorithms we tested indeed achieved better F_1 score with the best-F-score threshold than the literature methods on SWaT dataset, but these algorithms were not the top-performing by Fc_1 score.

S6 DEMONSTRATIONS OF METHODS

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Algorithm 1: MVTS anomaly detection with an auto-encoder model, Gauss-S scoring and tail-p threshold.
  input: Anomaly-free time-series: \mathbf{X}_{train} \in \mathbb{R}^{n_1 \times m}
             Test time-series with anomalies: \mathbf{X}_{test} \in \mathbb{R}^{n_2 \times m}
             Window size l_w; step size l_s; tail-probability \epsilon
  output: Predicted binary anomaly labels \hat{y_t} for each time point in n_2
             Channel-wise anomaly scores A^1, ..., A^m each of size n_2
  Step 1: Train FC AE Hidden size p
   for epoch in max epochs do
       \dot{Loss} \leftarrow 0
        for Training sub-sequences \mathbf{S}_{t,train} \leftarrow \mathbf{X}_{train}[t-l_w+1,..,t] \in \mathbb{R}^{l_w \times m} with step size l_s=10 do
            Encode sub-sequence to latent space:
             z^1, ..., z^p \leftarrow Encoder(\mathbf{S}_{t,train})
             Reconstruct original sub-sequence:
             \hat{\mathbf{S}}_{t,train} \leftarrow Decoder(z^1,..,z^p)
             Loss \leftarrow Loss + rms(\mathbf{S}_{t,train} - \hat{\mathbf{S}}_{t,train})
       Update parameters of Encoder and Decoder to minimize Loss
  end
  Step 2: Apply Gauss-S scoring function
   Obtain reconstruction errors from FC AE on train: \mathbf{E}^i_{t,train} = \mathbf{S}^i_{t,train}[t] - \hat{\mathbf{S}}^i_{t,train}[t], for each channel i \in m
   Fit \mathbf{E}^i_{train} \sim N(\mu^i, \sigma^i) for each channel i \in m
   Get the reconstruction errors \mathbf{E}_t^i = \mathbf{S}_{t,test}^i[t] - \hat{\mathbf{S}}_{t,test}^i[t] on test data
   for t \leftarrow 1 to n_2 do
      Get probability scores for each channel
        for each channel i \leftarrow 1 to m do
           \mathbf{A}_t^i \leftarrow \log(1 - \Phi(\frac{\mathbf{E}_t^i - \mu^i}{\sigma^i})), \Phi \text{ is the cdf of } N(0, 1)
      \mathbf{a}_t \leftarrow -\sum_{i=1}^m \mathbf{A}_t^i
  Step 3: Apply tail-p threshold
   th_{tail-p} \leftarrow -m \log(\epsilon)
   \mathbf{prediction} \leftarrow \mathbf{1}_{(x>=th_{tail-p})}(\mathbf{a})
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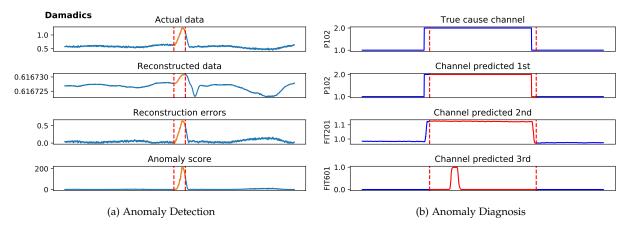


Fig. S3: Examples of (a) anomaly detection on DAMADICS dataset and (b) anomaly diagnosis on SWaT dataset using UAE model and Gauss-S scoring function.

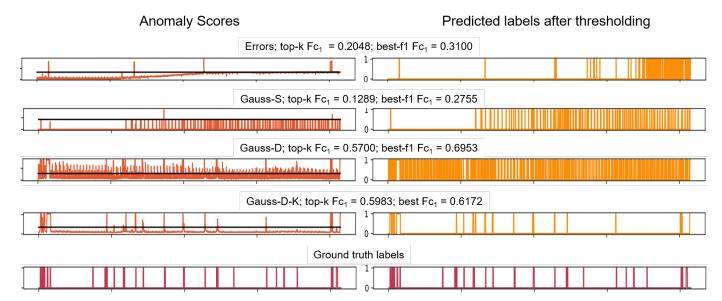


Fig. S4: The effect of scoring function on the anomaly detection performance of UAE for the SWaT dataset. Plots on the left show the scoring function after aggregation across channels, and the solid black line is the top-k threshold. Plots on the right show the anomaly labels for each scoring function. Some anomalies stand out with the Error scoring function but others go undetected. Gauss-D has a much better Fc_1 score, but it appears noisy. The Gauss-D-K scoring function does smoothing across time and channels with a Guassian kernel, so the scoring function appears much less noisy.

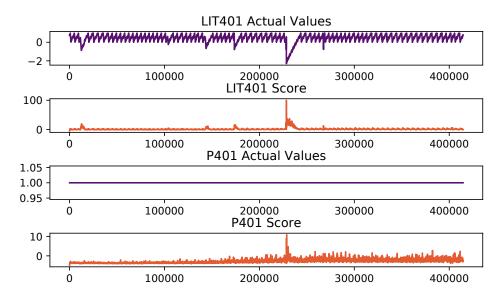


Fig. S5: An example showing spurious correlations learnt by OmniAnomaly on SWaT. Channel P401 does not vary at all during test, but OmniAnomaly's score for channel P401 shows peaks corresponding to an anomaly in LIT 401. The signals are shown from the test set. P401 stays constant in both train and test.

S7 STATISTICAL TESTS

We follow recommendations from [15] for multiple classifier comparisons across multiple datasets. For each comparison, we first use the Friedman test to find whether the overall comparison between k methods on N groups (eg. datasets) is statistically significant. If this comparison is significant, we follow this with post-hoc tests using Hochberg's step-up procedure [16] to compare the best method against all other methods. All tests below are conducted at significance level $\alpha=0.05$.

S7.1 Effect of scoring functions on anomaly detection performance

The null hypothesis for Friedman test is that all scoring functions perform the same over N=70 combinations of datasets and models, and k=4 scoring functions. The Friedman-statistic is 57.13 which is larger than the critical value resulting in a p-value of 2.4e-12, thus we reject the null hypothesis. Post-hoc tests using Hochberg's step-up procedure indicate that the difference between the performance of Gauss-D-K vs. all other methods is statistically significant. Furthermore, the difference between the performance of Gauss-D vs. Gauss-S and Error is statistically significant.

S7.2 Effect of model on anomaly detection performance

The null hypothesis for Friedman test is that all algorithms in Table IV (main text) perform the same with N=7 datasets and k=13 methods. We find that the Friedman statistic 43.53 is greater than the exact tabled critical value 20.23 [17], resulting in p-value 1.83e - 5 and reject the null hypothesis. Next we compare UAE against other models using post-hoc tests [16] and find that only the comparisons between UAE and the bottom 6 algorithms are statistically significant.

S8 ADDITIONAL RESULTS

S8.1 Fc_1 score with top-k threshold

TABLE S6: Fc_1 score mean and standard deviation over 5 seeds, with the top-k threshold using the chosen hyperparameters. The scoring function is Gauss-D for all algorithms except those denoted with *. The overall mean is a mean over all the datasets. The performance of Raw Signal and PCA models is deterministic.

	DM	IDS	M	SL	SK	AB	SM	AP	SN	1D	SW	/aT	WA	ADI	Mean	Rank
Algo	Mean	Std														
Raw Signal	0.4927		0.2453		0.5349	0.0000	0.2707		0.5151		0.3796		0.4094		0.4068	9.3
PCA	0.5339		0.4067		0.5524	0.0000	0.3793		0.5344		0.5314		0.3747		0.4733	5.6
UAE	0.6378	0.008	0.5111	0.0085	0.5550	0.0022	0.4793	0.0074	0.5501	0.0046	0.5713	0.0087	0.5105	0.01	0.5450	1.6
FC AE	0.6047	0.005	0.4514	0.0048	0.5408	0.0040	0.3788	0.0056	0.5395	0.0064	0.4478	0.0528	0.5639	0.0193	0.5038	4.7
LSTM AE	0.5999	0.0141	0.4481	0.0065	0.5418	0.0054	0.4536	0.0109	0.5271	0.0062	0.5163	0.0148	0.4265	0.0057	0.5019	4.7
TCN AE	0.5989	0.0204	0.4354	0.0105	0.5488	0.0041	0.3873	0.0054	0.5800	0.0037	0.4732	0.0114	0.5126	0.0784	0.5052	3.9
LSTM VAE	0.5939	0.0085	0.3910	0.0059	0.5439	0.0022	0.2988	0.004	0.5427	0.0046	0.4456	0.003	0.5758	0.0143	0.4845	6.0
BeatGAN	0.5391	0.1099	0.4531	0.0075	0.5437	0.0063	0.3732	0.0091	0.5479	0.0099	0.4777	0.0061	0.4908	0.0558	0.4894	5.0
MSCRED	0.2906	0.0129	0.3944	0.0045	0.5526	0.0076	0.3724	0.0062	0.4145	0.0057	0.4315	0.0117	0.3253	0.0033	0.3973	8.1
NASA LSTM	0.1284	0.0074	0.4715	0.0124	0.5339	0.0100	0.4280	0.0077	0.3879	0.0036	0.1398	0.0143	0.1058	0.0449	0.3136	8.9
DAGMM*	0.0000	0	0.1360	0.0188	0.0000	0.0000	0.1681	0.0205	0.0187	0.015	0.0000	0	0.0256	0.0573	0.0498	12.9
OmniAnomaly*	0.1425	0.1189	0.4120	0.0108	0.4561	0.0264	0.3767	0.0094	0.5002	0.0121	0.1466	0.0985	0.2443	0.0202	0.3255	9.4
OCAN*	0.2532	0.0925	0.3009	0.0323	0.4369	0.0271	0.2787	0.0177	0.4614	0.0095	0.1547	0.1502	0.0000	0	0.2694	11.0

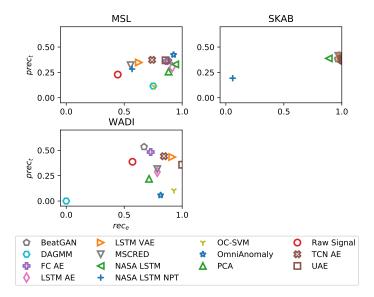


Fig. S6: Plots of $prec_t$ vs. rec_e for algorithms with the top-k threshold and scoring functions as in Table IV in main manuscript. See plots for additional datasets in Fig. 4 in main manuscript.

TABLE S7: Fc_1 score of various models with the *Gauss-D-K* scoring function (except the starred algorithms that specify their own scoring functions) with the *top-k* threshold.

	DN	1DS	M	SL	SK	AB	SM	AP	SN	ИD	SW	/aT	WA	ADI	Mean	Rank
Algo	Mean	Std														
Raw Signal	0.4693		0.2974		0.5405	0.0000	0.3190		0.5591		0.4086		0.4790		0.4390	7.9
PCA	0.5356		0.5217		0.5585	0.0000	0.4585		0.5557		0.4811		0.3068		0.4883	5.4
UAE	0.6199	0.0054	0.5193	0.021	0.5604	0.0034	0.6116	0.0141	0.5805	0.0041	0.6105	0.0158	0.5561	0.0149	0.5798	2.0
FC AE	0.6048	0.0039	0.5060	0.0076	0.5442	0.0042	0.5672	0.0093	0.5651	0.0056	0.4786	0.0475	0.5083	0.011	0.5392	4.0
LSTM AE	0.6029	0.0097	0.5346	0.0103	0.5364	0.0202	0.5605	0.0068	0.5381	0.0032	0.4715	0.0092	0.3505	0.005	0.5135	5.9
TCN AE	0.6035	0.0199	0.5231	0.0057	0.5515	0.0059	0.5615	0.0072	0.6034	0.0053	0.4353	0.0158	0.4685	0.0854	0.5353	4.0
LSTM VAE	0.5924	0.0075	0.4623	0.0035	0.5433	0.0042	0.4975	0.0046	0.5784	0.0045	0.4444	0.001	0.5289	0.0132	0.5210	5.3
BeatGAN	0.5380	0.1129	0.5329	0.0132	0.5391	0.0095	0.5698	0.0097	0.5550	0.0107	0.4760	0.0266	0.4648	0.0723	0.5251	5.3
MSCRED	0.2960	0.0173	0.4096	0.007	0.5502	0.0081	0.4009	0.0073	0.4085	0.0045	0.3769	0.0147	0.2905	0.0216	0.3904	8.7
NASA LSTM	0.1276	0.008	0.5503	0.0098	0.5338	0.0103	0.6410	0.0131	0.3874	0.0042	0.1348	0.0199	0.1958	0.0446	0.3672	8.4
DAGMM*	0.0000	0	0.1360	0.0188	0.0000	0.0000	0.1681	0.0205	0.0187	0.015	0.0000	0	0.0256	0.0573	0.0498	12.9
OmniAnomaly*	0.1425	0.1189	0.4120	0.0108	0.4561	0.0264	0.3767	0.0094	0.5002	0.0121	0.1466	0.0985	0.2443	0.0202	0.3255	10.1
OCAN*	0.2532	0.0925	0.3009	0.0323	0.4369	0.0271	0.2787	0.0177	0.4614	0.0095	0.1547	0.1502	0.0000	0	0.2694	11.1

S8.2 Fc_1 score with best-F-score threshold

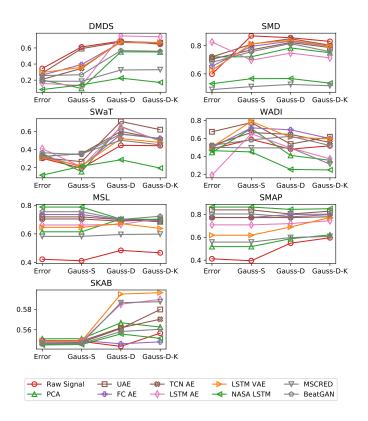


Fig. S7: Effect of scoring functions on the Fc_1 score using the best-F-score (best- Fc_1) threshold.

TABLE S8: Fc_1 score of various models with the *Gauss-D* scoring function (except the starred algorithms that specify their own scoring functions) with the *best-F-score* threshold (best Fc_1 in this case).

	DM	IDS	M	SL	SK	AB	SM	AP	SM	/ID	SW	/aT	WA	ADI	Mean	Rank
Algo	Mean	Std	'													
Raw Signal	0.6856		0.4841		0.5438	0.0000	0.5485		0.8568		0.4469		0.4801		0.5780	8.0
PCA	0.5521		0.7045		0.5668	0.0000	0.5874		0.7840		0.6556		0.4099		0.6086	6.3
UAE	0.6744	0.0083	0.6996	0.0104	0.5612	0.0034	0.8024	0.0154	0.8226	0.0075	0.7112	0.0127	0.5363	0.0185	0.6868	4.0
FC AE	0.6687	0.0173	0.6991	0.0078	0.5463	0.0009	0.7984	0.0111	0.8321	0.0026	0.5703	0.0269	0.6955	0.037	0.6872	5.3
LSTM AE	0.7504	0.0246	0.6661	0.0096	0.5849	0.0244	0.7193	0.0108	0.7472	0.0066	0.6493	0.0048	0.4934	0.047	0.6587	5.4
TCN AE	0.6824	0.0208	0.6890	0.0127	0.5619	0.0103	0.7716	0.0189	0.8495	0.0038	0.6016	0.0293	0.6438	0.1075	0.6857	4.0
LSTM VAE	0.6730	0.0042	0.6718	0.025	0.5948	0.0391	0.6897	0.0207	0.8383	0.0096	0.5215	0.0082	0.6128	0.0089	0.6574	5.0
BeatGAN	0.5673	0.1219	0.7011	0.0189	0.5583	0.0097	0.7778	0.0294	0.8153	0.0078	0.5750	0.0085	0.6230	0.0618	0.6597	5.1
MSCRED	0.3262	0.0053	0.5958	0.0053	0.5864	0.0097	0.5977	0.0068	0.5249	0.0083	0.5030	0.0098	0.4935	0.0666	0.5182	8.0
NASA LSTM	0.2249	0.041	0.7030	0.0118	0.5559	0.0158	0.8431	0.0103	0.5666	0.0047	0.2874	0.0353	0.2535	0.0324	0.4906	8.0
DAGMM*	0.0305	0.0027	0.2601	0.0201	0.5449	0.0049	0.3351	0.0198	0.1066	0.0095	0.0891	0.0004	0.1264	0.0255	0.2132	12.7
OmniAnomaly*	0.2317	0.1833	0.7381	0.0188	0.5491	0.0007	0.6782	0.019	0.7904	0.0174	0.2836	0.1009	0.4192	0.0396	0.5272	8.0
OCAN*	0.2488	0.0988	0.5396	0.0457	0.5482	0.0016	0.4902	0.0173	0.6666	0.0139	0.2541	0.1604	0.1245	0.0117	0.4103	11.1

S8.3 Fc_1 score with tail-p threshold

TABLE S9: Fc_1 score mean and standard deviation over 5 seeds, with the tail-p threshold and Gauss-D scoring function, with the following exceptions - * predefined scoring function and tail-p threshold. † predefined scoring and threshold. NASA LSTM NPT uses Non-Parametric Threshold. OC-SVM scores are thresholded at 0.5. The value of the threshold, $-\log_{10}(\epsilon) \in \{1:5\}$, and the value that gives the best Fc_1 is used here. The mean is calculated over all the datasets.

dataset	DMDS Mean	Std	MSL Mean	Std	SKAB Mean	Std	SMAP Mean	Std	SMD Mean	Std	SWaT Mean	Std	WADI Mean	Std	Mean	Avg Rank
Raw Signal	0.6192		0.2618		0.5340	0.0000	0.2924		0.6952		0.4266		0.4613		0.4701	8.1
PCA	0.2505		0.3527		0.5559	0.0000	0.3638		0.4915		0.5979		0.3349		0.4210	7.0
UAE	0.6429	0.0139	0.4571	0.0221	0.5545	0.0017	0.5135	0.0181	0.5440	0.0064	0.6467	0.011	0.5267	0.0239	0.5551	3.1
FC AE	0.6630	0.0144	0.4514	0.011	0.5429	0.0027	0.4379	0.0123	0.5209	0.007	0.5472	0.0307	0.5802	0.0477	0.5348	4.9
LSTM AE	0.3679	0.0162	0.4004	0.0102	0.5725	0.0303	0.4276	0.0077	0.4386	0.0023	0.5903	0.0133	0.4212	0.0058	0.4598	6.3
TCN AE	0.5569	0.0414	0.4438	0.0089	0.5484	0.0041	0.4469	0.0117	0.5675	0.013	0.5753	0.0346	0.5711	0.115	0.5300	4.7
LSTM VAE	0.6426	0.007	0.3917	0.0232	0.5767	0.0376	0.3700	0.0137	0.6175	0.0138	0.5123	0.0144	0.5878	0.0236	0.5284	4.7
BeatGAN	0.4171	0.141	0.4656	0.0103	0.5469	0.0190	0.3843	0.0063	0.4475	0.0097	0.5446	0.0208	0.5918	0.0659	0.4854	5.4
MSCRED	0.1367	0.0029	0.3629	0.0153	0.5798	0.0105	0.3361	0.0119	0.3085	0.0057	0.4787	0.0088	0.4416	0.1045	0.3778	8.1
NASA LSTM	0.1130	0.0096	0.4495	0.0134	0.5396	0.0198	0.4410	0.0181	0.3336	0.0058	0.2088	0.0299	0.2252	0.0514	0.3301	8.9
DAGMM*	0.0000	0	0.1800	0.0278	0.5430	0.0063	0.2419	0.0103	0.0000	0	0.0000	0	0.0000	0	0.1378	13.0
OmniAnomaly*	0.0557	0.0012	0.5008	0.01	0.5487	0.0006	0.4542	0.006	0.4444	0.0108	0.1497	0.0345	0.1072	0.0008	0.3230	7.7
NASA LSTM NPT [†]	0.1440	0.003	0.3403	0.0442	0.0902	0.0000	0.5869	0.012	0.1957	0.0028	0.0251	0.0057	0.1333	0	0.2165	10.3
OC-SVM [†]	0.0337	0	0.1717	0	0.5380	0.0000	0.1757	0	0.0893	0	0.0765	0	0.1876	0	0.1818	12.7

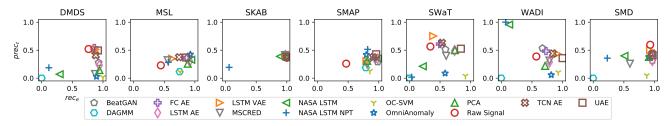


Fig. S8: $prec_t$ vs. rec_e for the tail-p threshold for the algorithms shown in Table S9. For NASA LSTM NPT, we use NPT, i.e. non-parametric threshold, and for OC-SVM we threshold at 0.5, instead of tai-p threshold.

S8.4 Point-wise F_1 score

TABLE S10: Point-wise F_1 score (i.e., the F_1 score) of various models with the *Gauss-D* scoring function (except the starred algorithms that specify their own scoring functions) with the *best-f1* threshold.

Model	DMDS	MSL	SKAB	SMAP	SMD	SWaT	WADI	Mean	Avg Rank
Raw Signal	0.4015	0.3059	0.5369	0.3009	0.4106	0.3068	0.3634	0.3751	9.6
PCA	0.3958	0.3982	0.5377	0.3334	0.4517	0.3954	0.2846	0.3995	6.6
UAE	0.5165	0.4454	0.5375	0.3937	0.4351	0.4544	0.3503	0.4476	3.4
FC AE	0.4902	0.4377	0.5375	0.3692	0.4429	0.3545	0.4056	0.4339	4.5
LSTM AE	0.4844	0.4088	0.5372	0.3752	0.4295	0.3956	0.3319	0.4232	6.1
TCN AE	0.4654	0.4366	0.5374	0.3729	0.4826	0.3931	0.3805	0.4384	4.1
LSTM VAE	0.4724	0.4001	0.5374	0.2998	0.4326	0.3136	0.4081	0.4091	7.1
BeatGAN	0.4023	0.4193	0.5376	0.3413	0.4529	0.3885	0.3629	0.4150	5.3
MSCRED	0.2624	0.4007	0.5411	0.3468	0.4661	0.3558	0.2316	0.3721	6.3
NASA LSTM	0.0971	0.4104	0.5373	0.3838	0.4228	0.1225	0.1284	0.3003	9.1
DAGMM*	0.0305	0.1938	0.5372	0.1964	0.0662	0.0592	0.0968	0.1686	12.8
OmniAnomaly*	0.1321	0.4277	0.5400	0.3699	0.4288	0.1726	0.2659	0.3339	7.4
OCAN*	0.2365	0.3155	0.5439	0.2656	0.4437	0.1307	0.1236	0.2942	8.9

TABLE S11: Point-wise F_1 score (i.e., the F_1 score) of various models with the *Gauss-D-K* scoring function (except the starred algorithms that specify their own scoring functions) with the *best-f1* threshold.

Model	DMDS	MSL	SKAB	SMAP	SMD	SWaT	WADI	Mean	Avg Rank
Raw Signal	0.4119	0.3323	0.5369	0.3593	0.4583	0.3760	0.4132	0.4126	9.0
PCA	0.4090	0.5323	0.5376	0.4481	0.4860	0.4453	0.3054	0.4520	6.4
UAE	0.5205	0.5402	0.5382	0.5755	0.4732	0.5799	0.4740	0.5288	2.9
FC AE	0.4942	0.5205	0.5387	0.5421	0.4828	0.4506	0.4902	0.5027	3.4
LSTM AE	0.4923	0.5355	0.5372	0.5317	0.4551	0.4480	0.3247	0.4749	6.2
TCN AE	0.4714	0.5493	0.5377	0.5453	0.5195	0.4256	0.4348	0.4977	4.1
LSTM VAE	0.4834	0.4897	0.5377	0.4875	0.4673	0.4158	0.5024	0.4834	5.9
BeatGAN	0.4055	0.5373	0.5378	0.5254	0.4826	0.4416	0.4155	0.4780	5.6
MSCRED	0.2650	0.4479	0.5412	0.3852	0.4671	0.3652	0.2664	0.3911	7.7
NASA LSTM	0.0998	0.5481	0.5381	0.5933	0.4412	0.1309	0.2031	0.3649	7.7
DAGMM*	0.0305	0.1938	0.5372	0.1964	0.0662	0.0592	0.0968	0.1686	12.8
OmniAnomaly*	0.1321	0.4277	0.5400	0.3699	0.4288	0.1726	0.2659	0.3339	9.4
OCAN*	0.2365	0.3155	0.5439	0.2656	0.4437	0.1307	0.1236	0.2942	9.9

S8.5 AU-ROC score

TABLE S12: Area under the receiver operator characteristic curve (AU-ROC) of various models with the *Gauss-D* scoring function (except the starred algorithms that specify their own scoring functions).

Model	DMDS	MSL	SKAB	SMAP	SMD	SWaT	WADI	Mean	Avg Rank
Raw Signal	0.7073	0.4379	0.4855	0.4953	0.7475	0.7273	0.7733	0.6249	10.0
PCA	0.7413	0.6175	0.5037	0.5684	0.7900	0.8249	0.6583	0.6720	7.3
UAE	0.8852	0.6712	0.5088	0.6256	0.8298	0.8279	0.7405	0.7270	2.6
FC AE	0.9280	0.6602	0.4914	0.6272	0.8028	0.8085	0.7912	0.7299	4.0
LSTM AE	0.8404	0.6205	0.5040	0.6137	0.8196	0.8164	0.6808	0.6993	5.4
TCN AE	0.8109	0.6184	0.5002	0.6262	0.8282	0.7596	0.7109	0.6935	5.5
LSTM VAE	0.9146	0.5986	0.5002	0.5628	0.7587	0.7570	0.7892	0.6973	7.2
BeatGAN	0.7960	0.6517	0.4941	0.5993	0.8269	0.7889	0.7086	0.6951	6.1
MSCRED	0.6866	0.6436	0.5270	0.6020	0.8157	0.7069	0.6951	0.6681	6.4
NASA LSTM	0.6743	0.6580	0.4885	0.6406	0.7538	0.5489	0.4633	0.6039	9.1
DAGMM*	0.4287	0.4761	0.5080	0.5459	0.4767	0.4663	0.5025	0.4863	11.1
OmniAnomaly*	0.6804	0.6523	0.5075	0.6588	0.7972	0.5900	0.5275	0.6305	6.9
OCAN*	0.6948	0.5803	0.5192	0.5656	0.7736	0.5327	0.4708	0.5910	9.3

TABLE S13: Area under the receiver operator characteristic curve (AU-ROC) of various models with the *Gauss-D-K* scoring function (except the starred algorithms that specify their own scoring functions).

Model	DMDS	MSL	SKAB	SMAP	SMD	SWaT	WADI	Mean	Avg Rank
Raw Signal	0.7159	0.4815	0.4814	0.4878	0.7917	0.7618	0.7704	0.6415	9.7
PCA	0.7486	0.7448	0.4983	0.6483	0.8275	0.8440	0.7084	0.7171	6.4
UAE	0.8890	0.7679	0.5079	0.7643	0.8599	0.8637	0.8178	0.7815	1.9
FC AE	0.9317	0.7594	0.4874	0.7396	0.8375	0.8249	0.8166	0.7710	4.3
LSTM AE	0.8421	0.7548	0.4984	0.7306	0.8410	0.8350	0.7273	0.7470	4.7
TCN AE	0.8117	0.7160	0.4977	0.7239	0.8601	0.7696	0.7514	0.7329	5.4
LSTM VAE	0.9186	0.6812	0.4967	0.6479	0.7961	0.7766	0.8116	0.7327	6.6
BeatGAN	0.7967	0.7591	0.4886	0.7109	0.8523	0.8066	0.7381	0.7360	5.7
MSCRED	0.6898	0.6723	0.5267	0.6374	0.8171	0.7212	0.7233	0.6840	7.7
NASA LSTM	0.6830	0.7670	0.4876	0.7577	0.7690	0.5663	0.5091	0.6485	8.6
DAGMM*	0.4287	0.4761	0.5080	0.5459	0.4767	0.4663	0.5025	0.4863	11.3
OmniAnomaly*	0.6804	0.6523	0.5075	0.6588	0.7972	0.5900	0.5275	0.6305	8.9
OCAN*	0.6948	0.5803	0.5192	0.5656	0.7736	0.5327	0.4708	0.5910	9.9

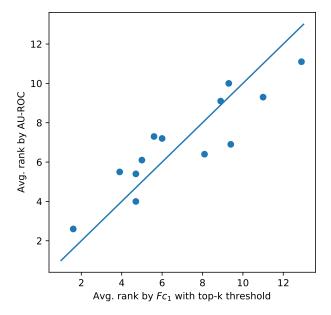


Fig. S9: Comparison of average ranks of algorithms from Fc_1 score (Table S6) vs. AU-ROC score (Table S12). The two metrics are generally in agreement, as evidenced by the closeness of scatter points to the x=y line.

S8.6 AU-PRC score (Average Precision)

TABLE S14: Area under the precision recall curve (AU-PRC), calculated through average precision (AP), of various models with the *Gauss-D* scoring function (except the starred algorithms that specify their own scoring functions).

Model	DMDS	MSL	SKAB	SMAP	SMD	SWaT	WADI	Mean	Avg Rank
Raw Signal	0.2946	0.2092	0.3549	0.2121	0.3492	0.2348	0.2525	0.2725	10.0
PCA	0.3144	0.2659	0.3694	0.2618	0.3859	0.3784	0.1520	0.3040	7.0
UAE	0.4134	0.3459	0.3699	0.3220	0.3835	0.3829	0.2186	0.3480	3.3
FC AE	0.4147	0.3314	0.3535	0.2819	0.3932	0.3298	0.3125	0.3453	4.9
LSTM AE	0.3972	0.3003	0.3683	0.2978	0.3644	0.3704	0.1756	0.3249	6.3
TCN AE	0.3776	0.3228	0.3654	0.2965	0.4285	0.3425	0.2761	0.3442	4.6
LSTM VAE	0.3845	0.3216	0.3666	0.2337	0.3812	0.2843	0.2886	0.3229	6.4
BeatGAN	0.3273	0.3171	0.3628	0.2592	0.4034	0.3388	0.2780	0.3267	6.1
MSCRED	0.1298	0.3182	0.3870	0.2624	0.4104	0.3208	0.1521	0.2830	6.0
NASA LSTM	0.0569	0.3138	0.3616	0.3052	0.3599	0.1011	0.0802	0.2255	9.7
DAGMM*	0.0129	0.1274	0.3709	0.1808	0.0441	0.0434	0.0597	0.1199	11.6
OmniAnomaly*	0.0844	0.3299	0.3724	0.3090	0.3802	0.1118	0.2081	0.2565	6.6
OCAN*	0.2067	0.2224	0.3756	0.2232	0.3958	0.1174	0.0513	0.2275	8.6

TABLE S15: Area under the precision recall curve (AU-PRC), calculated through average precision (AP), of various models with the *Gauss-D-K* scoring function (except the starred algorithms that specify their own scoring functions).

Model	DMDS	MSL	SKAB	SMAP	SMD	SWaT	WADI	Mean	Avg Rank
Raw Signal	0.2968	0.2528	0.3541	0.2874	0.4060	0.2731	0.3519	0.3174	9.1
PCA	0.3167	0.4582	0.3669	0.3855	0.4358	0.3943	0.1665	0.3606	6.0
UAE	0.4130	0.4543	0.3710	0.5323	0.4334	0.4608	0.3814	0.4352	3.3
FC AE	0.4150	0.4422	0.3502	0.4871	0.4451	0.3900	0.4315	0.4230	4.6
LSTM AE	0.3976	0.4568	0.3673	0.4773	0.4037	0.3864	0.2395	0.3898	5.7
TCN AE	0.3778	0.4753	0.3648	0.5009	0.4802	0.3513	0.3439	0.4135	4.3
LSTM VAE	0.3822	0.4226	0.3646	0.4318	0.4278	0.3411	0.4073	0.3968	6.1
BeatGAN	0.3268	0.4595	0.3592	0.4710	0.4478	0.3604	0.3577	0.3975	5.1
MSCRED	0.1314	0.3779	0.3874	0.3288	0.4115	0.3063	0.2514	0.3135	7.3
NASA LSTM	0.0585	0.4682	0.3587	0.5573	0.3839	0.1076	0.1538	0.2983	8.6
DAGMM*	0.0129	0.1274	0.3709	0.1808	0.0441	0.0434	0.0597	0.1199	11.7
OmniAnomaly*	0.0844	0.3299	0.3724	0.3090	0.3802	0.1118	0.2081	0.2565	9.4
OCAN*	0.2067	0.2224	0.3756	0.2232	0.3958	0.1174	0.0513	0.2275	9.7

S8.7 Root cause results

TABLE S16: RC-Top3-all metric for all datasets with root cause labels using the Gauss-D scoring function except starred.

	DMDS		SMD		SWaT		WADI		Overall mean	Avg Rank
Algo	Mean	Std	Mean	Std	Mean	Std	Mean	Std		Ü
Raw Signal	0.7059		0.9635		0.3143		0.5000		0.6209	6.5
PCA	0.8235		0.7831		0.4857		0.5000		0.6481	7.2
UAE	0.9647	0.032	0.9498	0.006	0.6286	0.020	0.5428	0.039	0.7715	1.8
FC AE	0.9412	0.0000	0.9522	0.0053	0.6000	0.0286	0.4428	0.0783	0.7341	3.8
LSTM AE	0.8117	0.0263	0.9360	0.0032	0.5771	0.0128	0.5143	0.0319	0.7098	5.2
TCN AE	0.9177	0.0526	0.9448	0.0064	0.5143	0.0452	0.5286	0.1083	0.7263	4.5
LSTM VAE	0.9177	0.0322	0.9501	0.0019	0.4571	0.0000	0.5000	0.0000	0.7062	4.8
BeatGAN	0.9176	0.0526	0.9424	0.0089	0.5543	0.0256	0.4571	0.0391	0.7178	5.8
MSCRED	0.7765	0.0263	0.8526	0.0101	0.5200	0.0424	0.0714	0	0.5551	8.2
OmniAnomaly*	0.9177	0.0671	0.9272	0.0067	0.3772	0.0619	0.4857	0.0319	0.6770	7.2

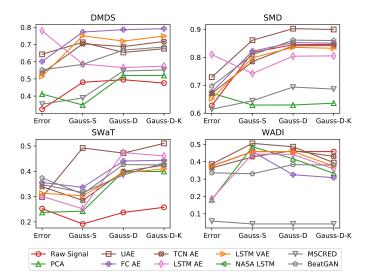


Fig. S10: Effect of scoring functions on the HitRate@150 performance for various algorithms and datasets.

TABLE S17: Hitrate@150 for independent anomaly diagnosis with the Gauss-D scoring function except starred.

	DMDS		SMD		SWaT		WADI		Overall mean	Avg Rank
Algo	Mean	Std	Mean	Std	Mean	Std	Mean	Std		
Raw Signal	0.4951	0.0000	0.8453	0.0000	0.2374	0.0000	0.4583	0.0000	0.5090	6.6
PCA	0.5196	0.0000	0.6291	0.0000	0.3990	0.0000	0.4167	0.0000	0.4911	7.6
UAE	0.6540	0.011	0.9026	0.003	0.4717	0.013	0.4861	0.031	0.6286	2.2
FC AE	0.7863	0.0096	0.8529	0.0025	0.4404	0.0083	0.3250	0.0745	0.6012	4.0
LSTM AE	0.5657	0.0281	0.8039	0.0089	0.4737	0.0206	0.4417	0.0410	0.5712	5.2
TCN AE	0.6883	0.0356	0.8413	0.0031	0.3990	0.0279	0.4639	0.0999	0.5981	3.9
LSTM VAE	0.7226	0.0172	0.8357	0.0009	0.3939	0.0000	0.4583	0.0000	0.6026	4.6
BeatGAN	0.6676	0.05	0.8615	0.0045	0.4263	0.0347	0.3833	0.0712	0.5847	4.2
MSCRED	0.5461	0.0602	0.6934	0.0056	0.3848	0.0263	0.0417	0	0.4165	8.8
OmniAnomaly*	0.6451	0.1127	0.8294	0.0071	0.2232	0.0322	0.3528	0.0076	0.5126	7.8

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