Anomaly Detection with Robust Deep Autoencoders

original article by C. Zhou and R. C. Peffenroth

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Deep Autoencoders

- A Deep Autoencoder (DAE) is constituted by two main components: an encoder E and a Decoder D.
- The main objective of a DAE is to learn the identity map so that the reconstruction $\bar{X} = D(E(X))$ is as close as possible to the original input X.
- The encoder and decoder functions E, D can be any kind of mapping between the data space and the coded space. Usually they are Deep Neural Networks e.g. FCNN complex models such as Long Short Term Memory (LSTM).
- The objective is usually to find the minimum reconstruction error w.r.t. some parametrized encoding and decoding functions and a distance (in this case the L_2 norm)

$$\min_{\theta,\phi} \|X - D_\theta(E_\phi(X))\|_2 \tag{1}$$

Principal Component Analysis

- Assume to have a set of N samples of n dimensional data, so that $X \in \mathbb{R}^{N \times n}$ s.t. each column has 0 mean (we can just shift the data to fulfill this request).
- Principal Component Analysis (PCA) is defined as an orthogonal linear transformation such that the new coordinate system of $\mathbb{R}^n$ satisfies: the i-th component of the coordinate system has the i-th greatest data variance if we project all samples on that component.
- Ideally we are trying to fit a n-ellipsoid into the data. The length of an axis of the ellipsoid represents the variance of data along that axis.
- PCA is often used for dimensionality reduction or encoding: we can project the data on the first $k < n$ principal components.

Principal Component Analysis

Mathematically we can define:

$$w_1 = \arg\max_{\|w\|_2=1} \|Xw\|_2^2 = \arg\max_w \frac{w^T X^T X w}{w^T w} \tag{2}$$

for the first component. Then for the k-th component we first subtract the first $k-1$ principal component from X

$$\hat{X}_k = X - \sum_{i=1}^{k-1} X w_i w_i^T \tag{3}$$

and finally solving again the similar problem:

$$w_k = \arg\max_{\|w\|_2=1} \|\hat{X}_k w\|_2^2 = \arg\max_w \frac{w^T \hat{X}_k^T \hat{X}_k w}{w^T w} \tag{4}$$

Robust Principal Component Analysis

- Robust Principal Component Analysis (RPCA) is a generalization of PCA that aims to reduce the sensitivity of PCA to outliers.
- The idea is to find a low-dimensional representation of data cleaned from the sparse outliers that can disturb the PCA process.
- We therefore assume that data X can be represented as $X = L + S$: L has low rank and is the low-dimensional representation of X while S is a sparse matrix consisting of the outlier elements that cannot be captured by the representation.

Robust Principal Component Analysis

- The problem can be addressed as:

$$\min_{L,S} \rho(L) + \lambda \|S\|_0 \tag{5}$$

$$\text{s. t. } \|X - L - S\|_F^2 = 0 \tag{6}$$

where $\rho(\cdot)$ is the rank of a matrix and we used the zero norm.

- This optimization problem is NP-hard and tractable only for small metrices.
- Usually it is substituted by the following problem, which is convex and tractable also for large matrices:

$$\min_{L,S} \|L\|_* + \lambda \|S\|_1 \tag{7}$$

$$\text{s. t. } \|X - L - S\|_F^2 = 0 \tag{8}$$

where $\|\cdot\|_*$ is the nuclear norm i. e. the sum of singular values of a matrix.

Robust Deep Autoencoders

- The main idea behind Robust Deep Autoencoders (RDAE) is to combine the representation learning of DAEs and the anomaly detection capability of RPCA.
- Noise and outliers are incompressible in the lower dimensional space we want to represent our data in.
- The objective is to learn a good low dimensional representation except for few exceptions.
- We will see two RDAE typed, one for l_1 regularization and one for $l_{2,1}$.

RDAE with l_1 regularization

- The RDAE objective is to decompose data $X = L_D + S$ just as in RPCA.
- By removing the noise S the autoencoder can better reconstruct L_D.
- As before, the best choice to obtain a sparse S would be to use a loss of the type $\|S\|_0$ which counts the non-zero entries, solving the problem

$$\min_{\theta} \|L_D - D_\theta(E_\theta(L_D))\|_2 + \lambda\|S\|_0 \tag{9}$$

$$\text{s.t. } X - L_D - S = 0 \tag{10}$$

- The parameter λ controls the sparsity of S and plays an essential role.

The role of λ

- As we said, the role of λ is very important.
- A smaller λ means that the norm of S plays a less important role and much of the loss will come from the DAE.
- The model will reconstruct better but recognize less outliers. This could be helpful if we want a more faithful representation e.g. for supervised tasks.
- A larger λ, instead, gives more importance to the norm of S as a loss.
- This means that the model will recognize more (or even too much) outliers, sacrificing some reconstruction performance.

The true objective

- As for the RPCA the previous loss is non tractable. We then instead focus on the following problem:

$$\min_{\theta} \|L_D - D_\theta(E_\theta(L_D))\|_2 + \lambda\|S\|_1 \tag{11}$$

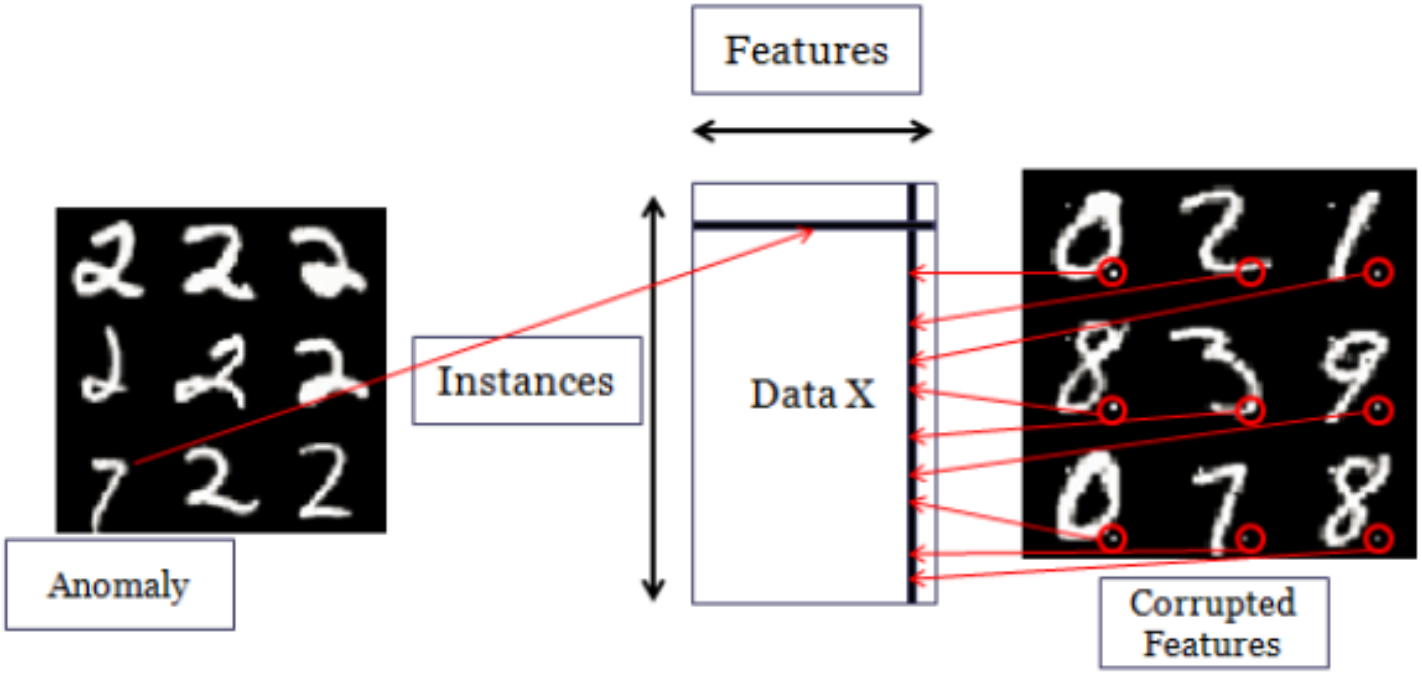
$$\text{s.t. } X - L_D - S = 0 \tag{12}$$

Notice two things:

- The autoencoder is trained with L_D, the part of its decomposition assumed to be outliers and noise free.
- There is no specific requirement about the DAE, in fact D_θ and E_θ are generic decoder, encoder functions.

RDAE with $l_{2,1}$ regularization

- The RDAE with l_1 penalization assumes that outliers and noise are not structured. The l_1 penalty is indeed just a regularization to induce sparsity.
- In general we can have multiple types of errors: an instrument that corrupts an input feature or outliers where the input data is in some way structurally different from normal data.


Features
Instances
Data X
Anomaly
Corrupted
Features

The $l_{2,1}$ norm

- The $l_{2,1}$ norm is defined as ($X \in \mathbb{R}^{N \times n}$):

$$\|X\|_{2,1} = \sum_{j=1}^{n} \|X_j\|_2 = \sum_{j=1}^{n} \left(\sum_{i=1}^{N} |X_{ij}|^2 \right)^{\frac{1}{2}} \tag{13}$$

- The $l_{2,1}$ norm can be seen as introducting a l_2 norm regularization over each feature and then adding a l_1 regularization accross features.
- We can also do the other way around: to recognize data anomalies (by row) just apply the $l_{2,1}$ norm to X^T.

- The final optimization problem for the RDAE with $l_{2,1}$ regularization for data anomalies is then

$$\min_{\theta} \|L_D - D_\theta(E_\theta(L_D))\|_2 + \lambda\|S^T\|_{2,1} \tag{14}$$

$$\text{s.t. } X - L_D - S = 0 \tag{15}$$

- For detecting feature anomalies we just need to change the objective to

$$\min_{\theta} \|L_D - D_\theta(E_\theta(L_D))\|_2 + \lambda\|S\|_{2,1} \tag{16}$$

$$\text{s.t. } X - L_D - S = 0 \tag{17}$$

The proximal operator

- To see in detail the training procedure for the RDAE we first need to consider the proximal operator.
- For general optimization problems of the form $\min f(x) + \lambda g(x)$ where g is convex some of the most used methods require to find

$$\text{prox}_{\lambda,g}(x) = \arg\min_y g(y) + \frac{1}{2\lambda}\|x - y\|_2^2 \tag{18}$$

- In this case we then want to obtain a solution of the problems

$$\text{prox}_{\lambda,l_1}(x) = \arg\min_y l_1(y) + \frac{1}{2\lambda}\|x - y\|_2^2 \tag{19}$$

$$\text{prox}_{\lambda,l_{2,1}}(x) = \arg\min_y l_{2,1}(y) + \frac{1}{2\lambda}\|x - y\|_2^2 \tag{20}$$

- For the l_1 norm, the solution to the proximal problem is

$$\text{prox}_{\lambda,l_1}(x) = \begin{cases} x_i - \lambda, & x_i > \lambda \\ x_i + \lambda, & x_i < -\lambda \\ 0, & x_i \in [-\lambda, \lambda] \end{cases} \tag{21}$$

  which in the case of $S \in \mathbb{R}^{N \times n}$ gets applied element by element.

- For the $l_{2,1}$ norm, we obtain (let $S_{\cdot j}$ be the column vector $S_{ij}, j = 1, \ldots, N$)

$$(\text{prox}_{\lambda,l_{2,1}}(S))_{ij} = \begin{cases} S_{ij} - S_{ij} - \lambda \frac{S_{ij}}{\|S_{\cdot j}\|_2}, & \|S_{\cdot j}\|_2 > \lambda \\ 0, & \|S_{\cdot j}\|_2 \leq \lambda \end{cases} \tag{22}$$

  if we are considering feature wise anomalies, substitute S with S^T for data anomalies.

The main algorithm

- The method used to train the RDAE is the Alternating Direction Method of Multipliers (ADMM).
- The main idea is to optimize the problem

$$\min_{\theta} \|L_D - D_\theta(E_\theta(L_D))\|_2 + \lambda\|S^T\|_{2,1} \tag{23}$$

$$\text{s.t. } X - L_D - S = 0 \tag{24}$$

  by doing it in two steps at each iteration.
- First, we fix S and optimize the DAE loss $\|L_D - D_\theta(E_\theta(L_D))\|_2$ with backpropagation as usual.
- Then, we fix L_D and optimize the regularization term with the proximal method.

The full procedure is the following: given input $X \in \mathbb{R}^{N \times n}$, initialize $L_D \in \mathbb{R}^{N \times n}, S \in \mathbb{R}^{N \times n}$ as zero matrices, $L_S = X$ and initialize the DAE randomly. For each iteration do:

- $L_D = X - S$
- Minimize $\|L_D - D_\theta(E_\theta(L_D))\|_2$ with backpropagation.
- Set $L_D = D(E(L_D))$ as the reconstruction.
- Set $S = X - L_D$.
- Optimize S using a $\text{prox}_{\lambda,l.}$ function of choice.
- If $c_1 = \frac{\|X - L_D - S\|_2}{\|X\|_2} < \epsilon$ or $c_2 = \frac{\|LS - L_D - S\|_2}{\|X\|_2} < \epsilon$ we have early convergence.
- Set $L_S = L_D + S$.

Return L_D and S.

Results

- I tried to reproduce some of the results by the original article.
- For the main article results the database used was the MNIST digits database.
- The train data contains 50000 samples while the test set contins 10000 images.
- Data was flattened from images of shape $(28, 28, 1)$ into vectors of length 784. Train data is then a matrix in $\mathbb{R}^{50000 \times 784}$.
- Pixel walues are converted from integers between 0 and 255 to floats between 0 and 1.

Implementation

- The RDAE and the standard DAEs used in this experimental tries were implemented using Tensorflow 2.9.1 on python 3.8.
- For the random forest classifier and the isolation forest models were taken from SciKit-learn version 1.1.1.
- Full implementation and details can be found on GitHub

l_1 Robust Deep Autoencoder

- To assess the performance of the l_1 RDAE the proposed procedure is the following:
- The training images get corrupted with a percentage of pixel (from 5% to 50%) changed to a random value between 0 and 1.
- Both the RDAE with l_1 regularization and a standard DAE (with same architecture as the DAE from the RDAE) are trained on these corrupted images.
- A random forest classifier is then trained on the feature extracted at the bottomneck layers of the two models.
- We test how these RF classifiers perform on the test set.

- This let us see how well the model is able to extract the important features of the images in a meaningful way.
- In this case the RDAE and DAE need to denoise the images and recognize which charactheristics are improtant.
- Both architectures are simple FCNN with layers of size 784 (input), 200 and 10 (the bottleneck and hidden feature layer).
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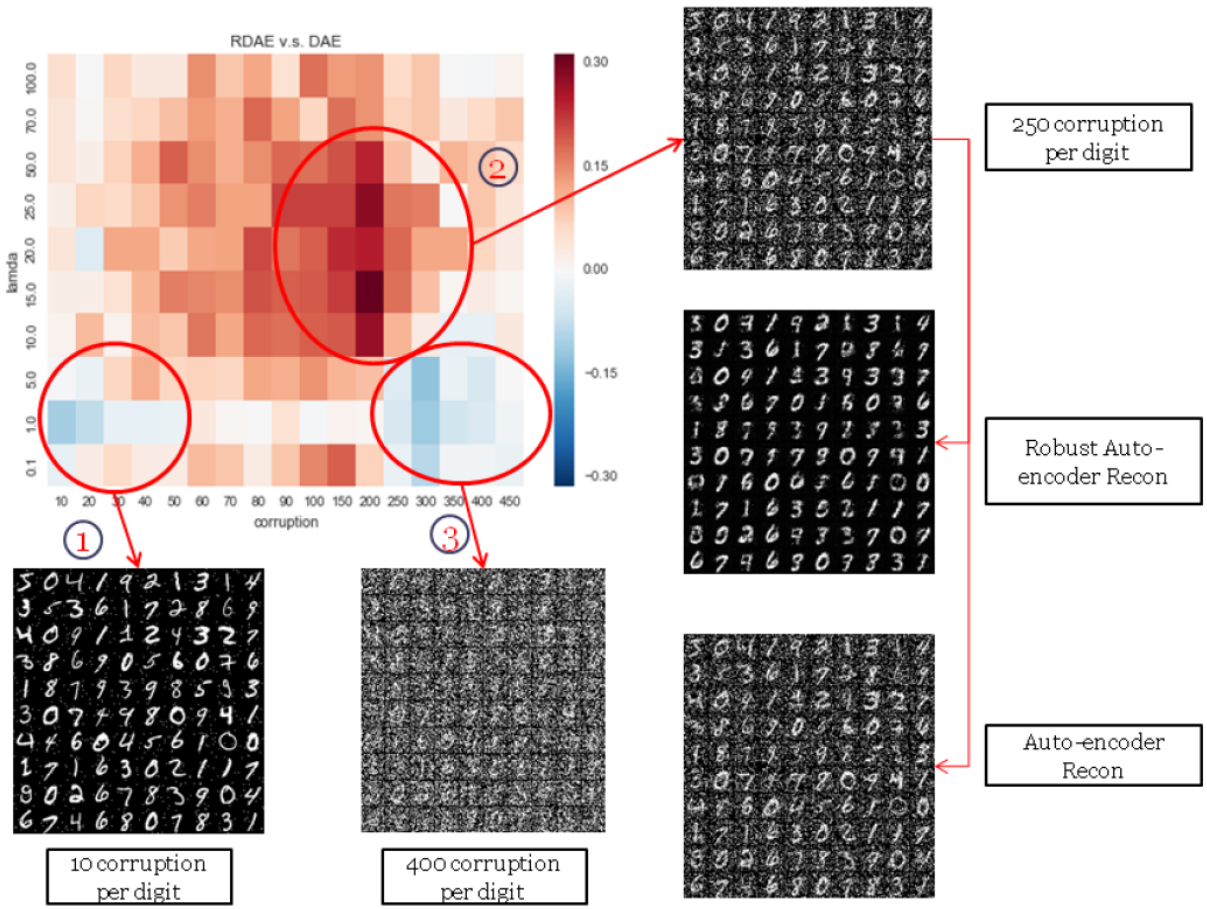
L_1 RDAE analysis

- Unfortunately, I could not replicate the results by the article.
- I tried with different values for the parameters and different setups.
- In any case, the L_1 RDAE performance was really similar to the performance of a simple Deep Autoencoder, in some cases worse.
- This is not to say that the RDAE has a poor performance, as we will see it can have some better reconstructions with corrupted data.
- The simpler approach seems to work better for supervised task with the hidden layer.
- The article was written when Tensorflow and other libraries were still in progress. It could also be that recent improvements benefit the DAE performance.

Original results



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$l_{2,1}$ Robust Deep Autoencoder

- The anomaly detection experiment is based on the recognizing of a specific digit of the MNIST dataset.
- First all the 4 digit images in the training set are collected in our dataset.
- Then, some images are chose at random from all the other digits until they are around 5% of total images in the dataset.
- This will be considered as the outliers of our data.

- The $l_{2,1}$ RDAE is trained on this dataset without any side information.
- Without telling the model which images are 4 digits and which are outliers the model itself must recognize the latters from original data on his own.
- The model architecture is the same as for the l_1 RDAE experiment.
- The only parameter that requires tuning is λ.

- Model performance is assessed by seeing how it is able to recognize the correct "outliers".
- The metrics used are the accuracy, the precision score, the recall score and the F1 score defined down below.

$$ACC = \frac{TP + TN}{P + N} \quad P = \frac{TP}{TP + FP} \tag{25}$$

$$R = \frac{TP}{TP + FN} \quad F1 = 2\frac{P \cdot R}{P + R} \tag{26}$$

- The F1 score, which tries to average in some way precision and recall, is the metrics used to select the λ parameter.
- λ is the only parameter that is fine tuned (in a semi-supervised way).

Original performance

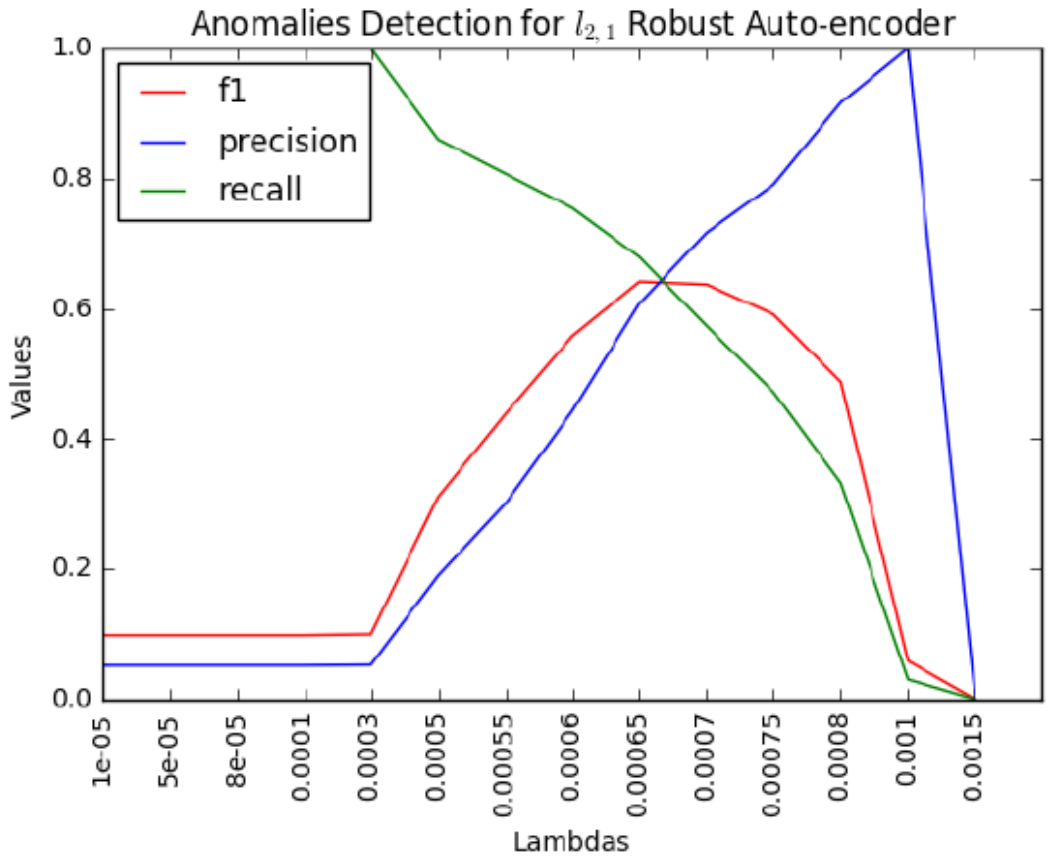


Figure: $L_{2,1}$ RDAE anomaly detection performance from original article

Anomaly detection performance

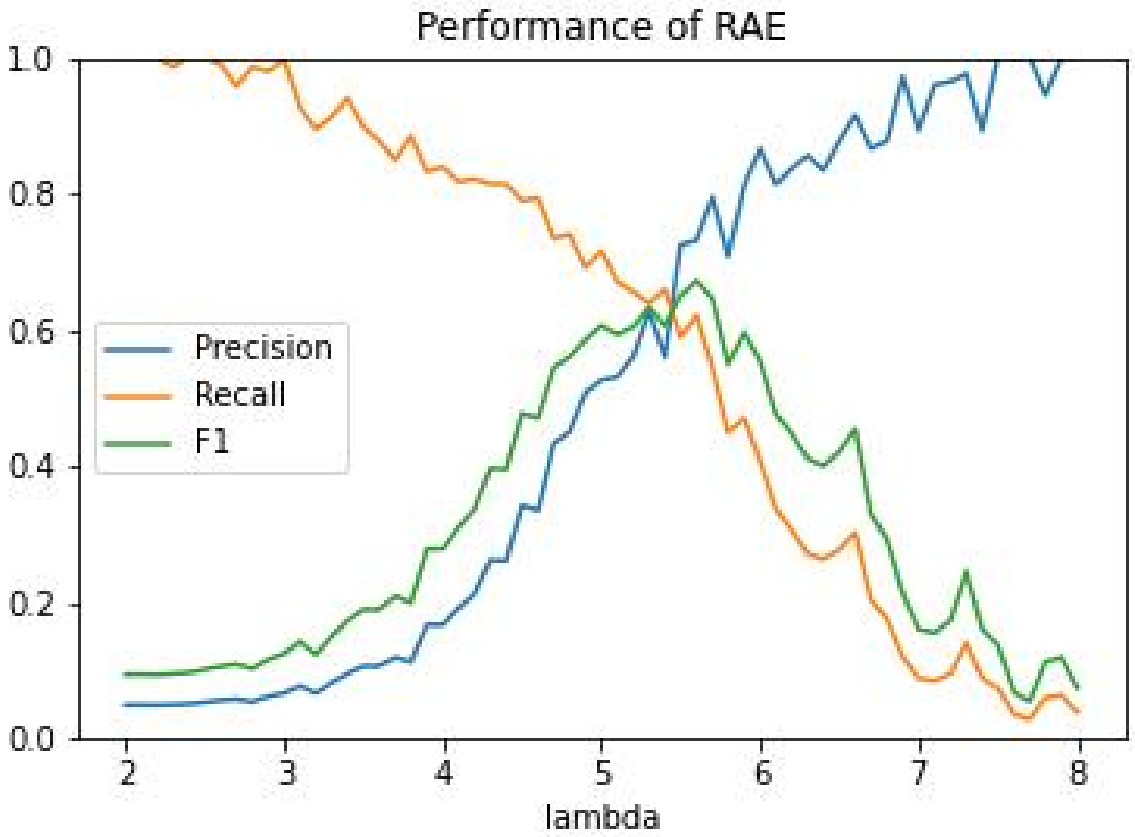


Figure: $L_{2,1}$ RDAE anomaly detection performance. λ from 2 to 8

Anomaly detection performance

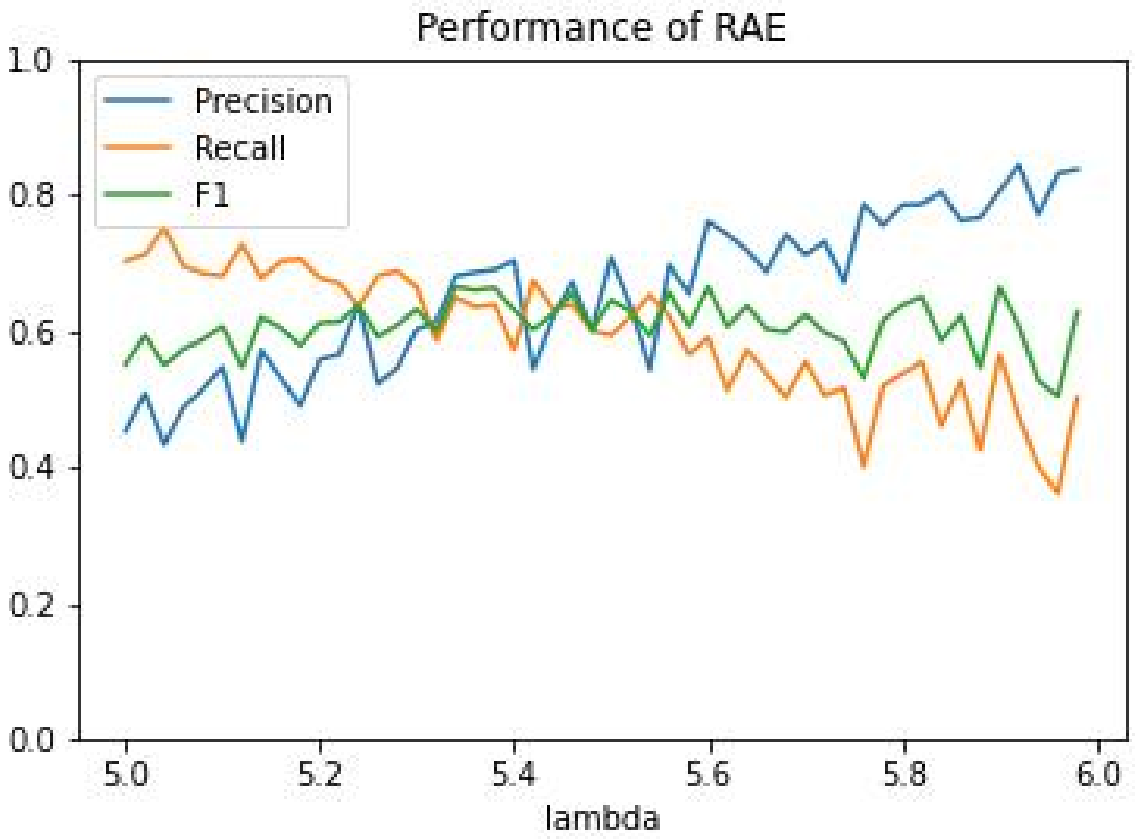


Figure: $L_{2,1}$ RDAE anomaly detection performance. λ from 5 to 6

Anomaly detection performance

Figure: $L_{2,1}$ RDAE anomaly detection performance. λ from 5.4 to 5.6

- The maximum performance is obtained with $\lambda = 5.468$ with an F_1 score of 0.668.
- Focusing on all values from $\lambda = 5$ to $\lambda = 6$ the RDAE has an accuracy of over 95% in recognizing anomalies. The F_1 score in this range is almost everytime above 0.55.
- The F_1 score is almost everytime above 0.6 for λ in the $[5.4, 5.6]$ range.
- Best result obtained by the authors is an F_1 score of 0.64 for $\lambda = 0.00065$. This different value of λ is in my opinion due to the different parameters of the neural network.

- We are now going to have a look at the final and reconstructed images obtained from the RDAE.
- For each value of λ we have 3 main images to look at: the reconstructionof the original images from the DAE in the RDAE, the final L_D image (the "clean" version, in this case it should only contain 4s) and the S image, which should be non empty only for outliers.
- We look 3 different values for λ: the best one identified above, 8.0 which adds too much penalization with few outliers identified and 4.0 which is a low value and a lot of 4s are considered outliers.

Original Images data

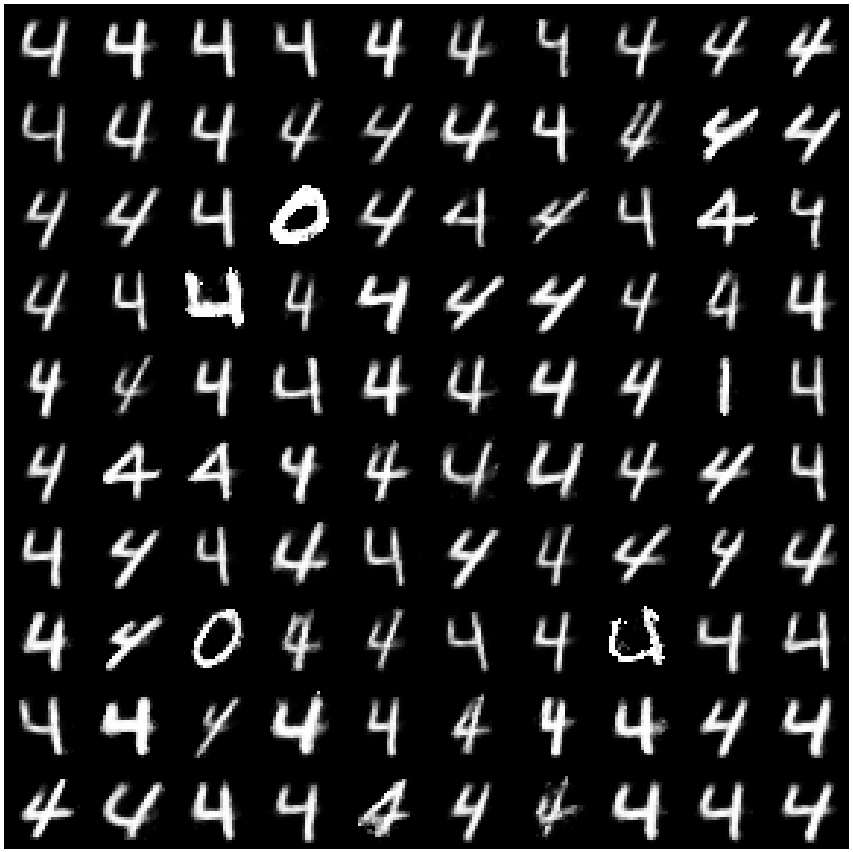
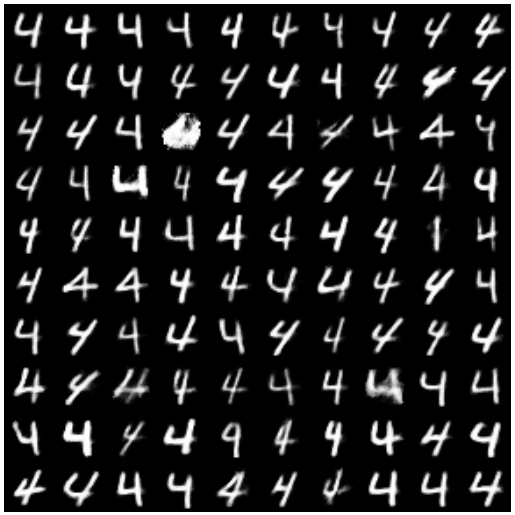
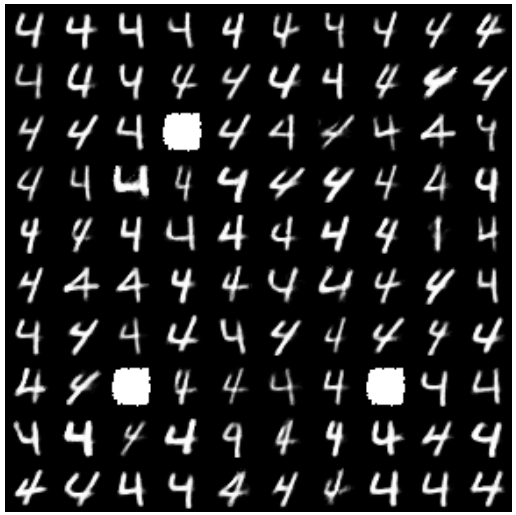


Figure: Original images for the $L_{2,1}$ RDAE

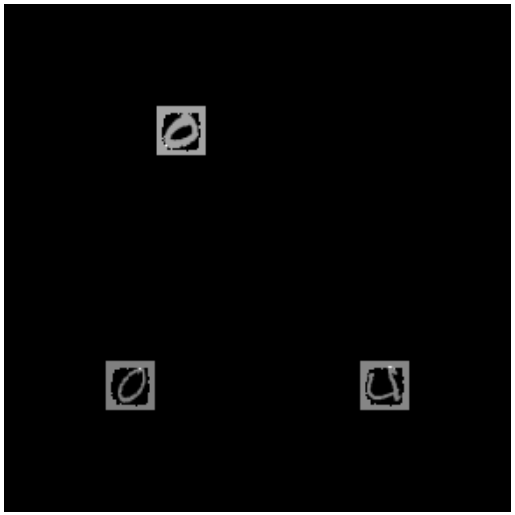
$\lambda = 5.468$



(a) Reconstruction



(b) Cleaned data



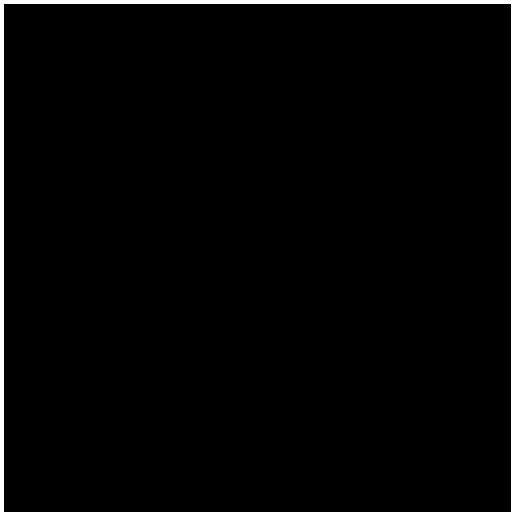
(c) Outliers detection

Figure: Accuracy: 0.970, precision: 0.722, recall: 0.621, F1 score: 0.668

$\lambda = 8.0$

(a) Reconstruction

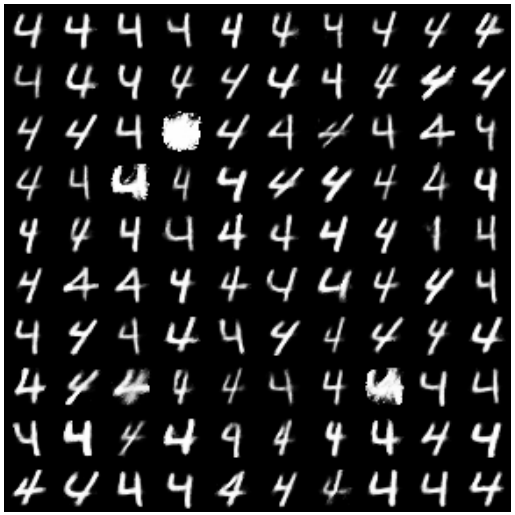
(b) Cleaned data



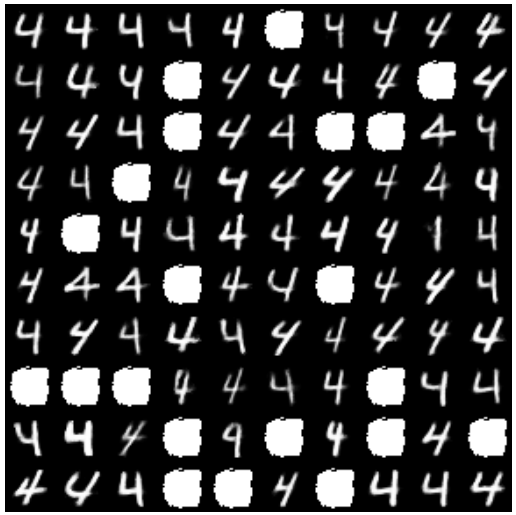
(c) Outliers detection

Figure: Accuracy: 0.953, precision: 1.00, recall: 0.0386, F1 score: 0.0743

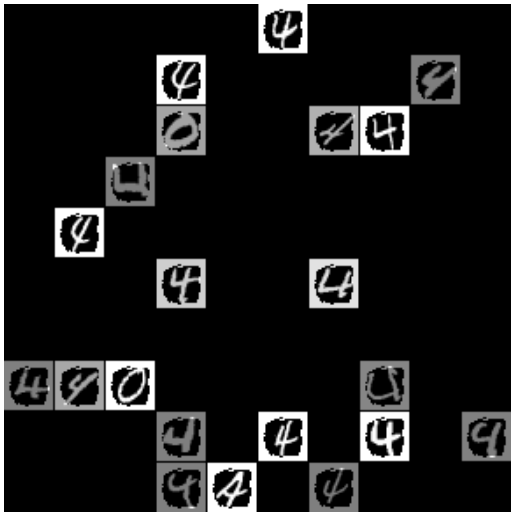
$\lambda = 4.0$



(a) Reconstruction



(b) Cleaned data



(c) Outliers detection

Figure: Accuracy: 0.788, precision: 0.167, recall: 0.839, F1 score: 0.278

- The performance of the RDAE as outlied detector is compared with the one obtained using the isolation forest method.
- The isolation forest method was a SOTA method for outlied detection. It is based on the idea that outliers are few and different and are separated from the rest.
- These outliers gets recognized using isolation trees which try to separate points from others.
- The only parameter which is peculiar to the method and which gets selected with the same metrics is the outlier fraction (from 0 to 0.5)

Isolation forest performance

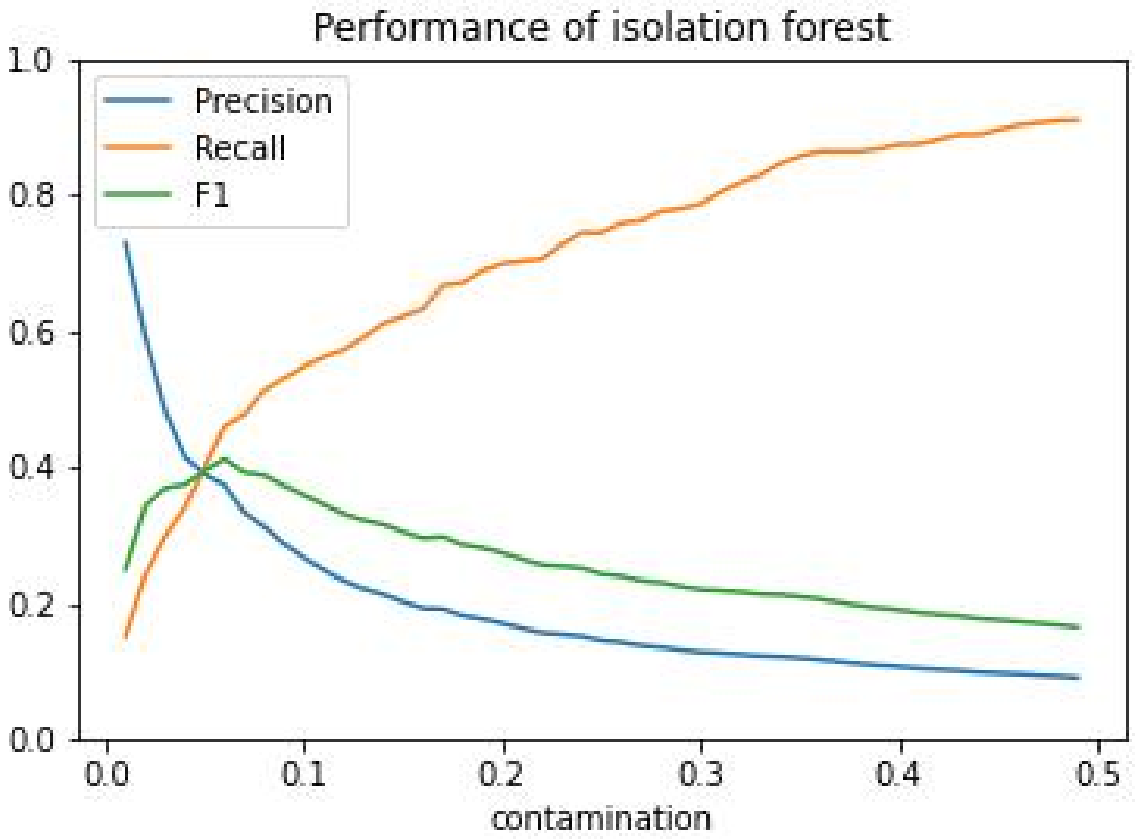


Figure: Isolation forest performance

- The best isolation forest performance is 0.41 with the outlier fraction set to the value of 0.06 (which is really close to the outlier true fraction of 5%).
- This result is really close to the original article. The authors obtained a best F_1 score of 0.37 with 0.11 outlier fraction.
- The little difference is in my opinion related to the different datasets but they are comparable.
- In each case the performance by isolation forest is far worse than the RDAE.

Time series experiment

- I tried to apply this method to time series, on which we focused in this course.
- In this case we are going to use a dataset from the Numenta Anomaly Benchmark (NAB). The database is called machine temperature system failure.
- It is the sensor data of an internal component of a large, industrial mahcine. It should have 3 anomalies: the first anomaly is a planned shutdown of the machine. The second anomaly is difficult to detect and directly led to the third anomaly, a catastrophic failure of the machine.
- Data has 22464 timesteps in total. I chose to consider subsequences of length 144. The final dataset has then 22321 training time series.
- Data is normalized all togheter to be in $(0, 1)$.

RDAE architectures

I tried using two architectures for the autoencoder part in the RDAE.

- The first one is a Dense Neural Network with hidden layers of 60 and 20. It is trained for 20 outer iterations and 50 inner iterations for the autoencoder, a batch size of 256 , $\epsilon = 10^{-8}$.
- The second one is a LSTM with two layers of 32 and 16 units, 10 outer iterations and 25 inner iterations with same batch size as before.

Analysis

- Since data is unlabeled we don't have a clear benchmark for finding the correct value for λ.
- I tried different values for λ until the number of anomalies detected is nor too high nor too low.
- For each architecture I picked some random anomalies and non-anomalies, to show how the RDAE is acting on time series and to have a look at what kind of anomalies it detectes.

Anomalies found

λ	0.1	0.5	0.7	1.0	2.0	3.0	3.2	3.3	3.5
Dense	All	751	250	14	0	0	0	0	0
LSTM	All	7525	4208	2068	306	109	74	9	0

Table: Anomalies found by the two architecures w.r.t. λ

Dense RDAE

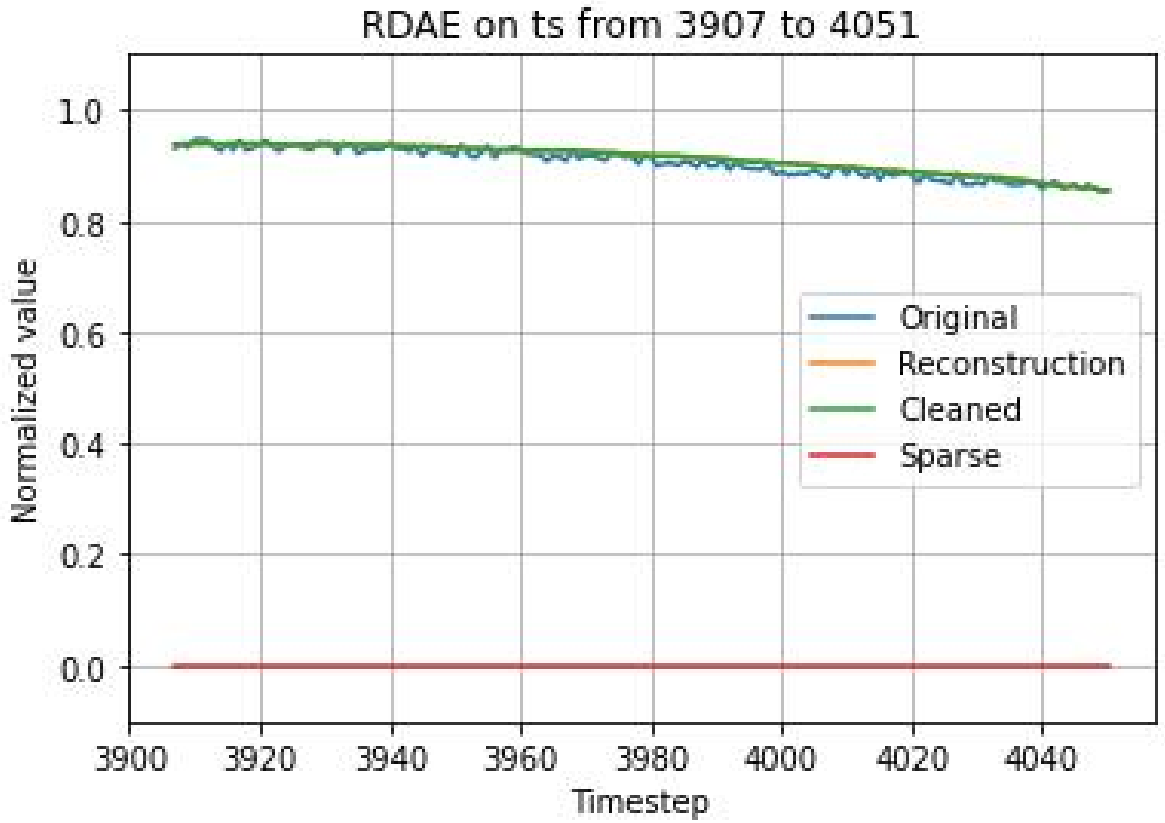
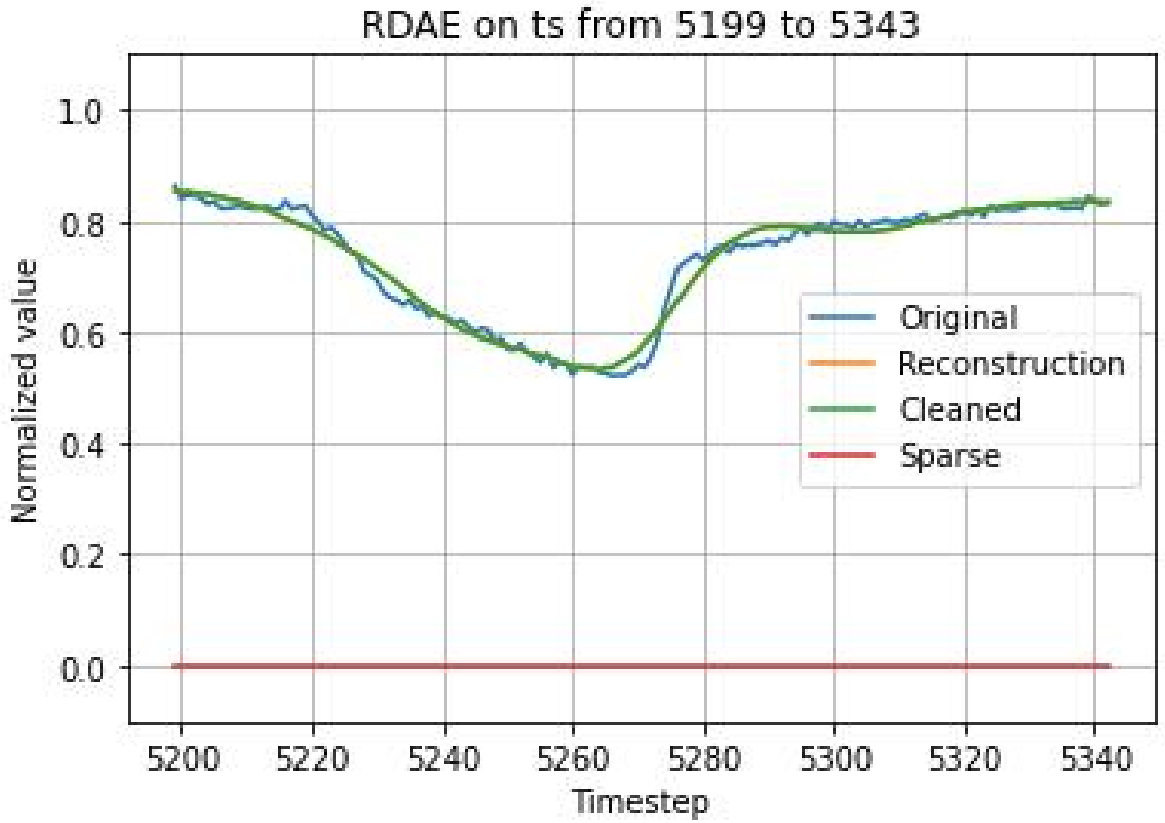


Figure: Example of a non anomaly subsequence for $\lambda = 1.0$

Dense RDAE



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Dense RDAE

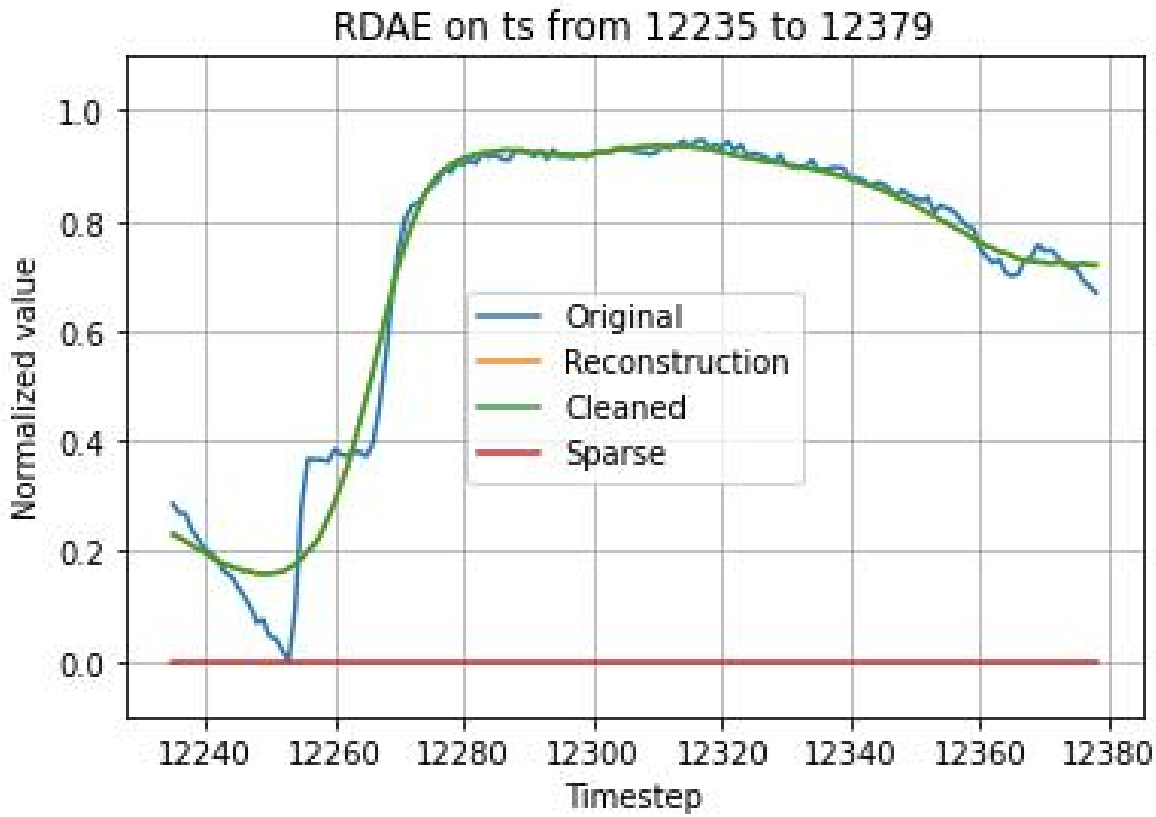

Figure: Example of a non anomaly subsequence for $\lambda = 1.0$

Dense RDAE

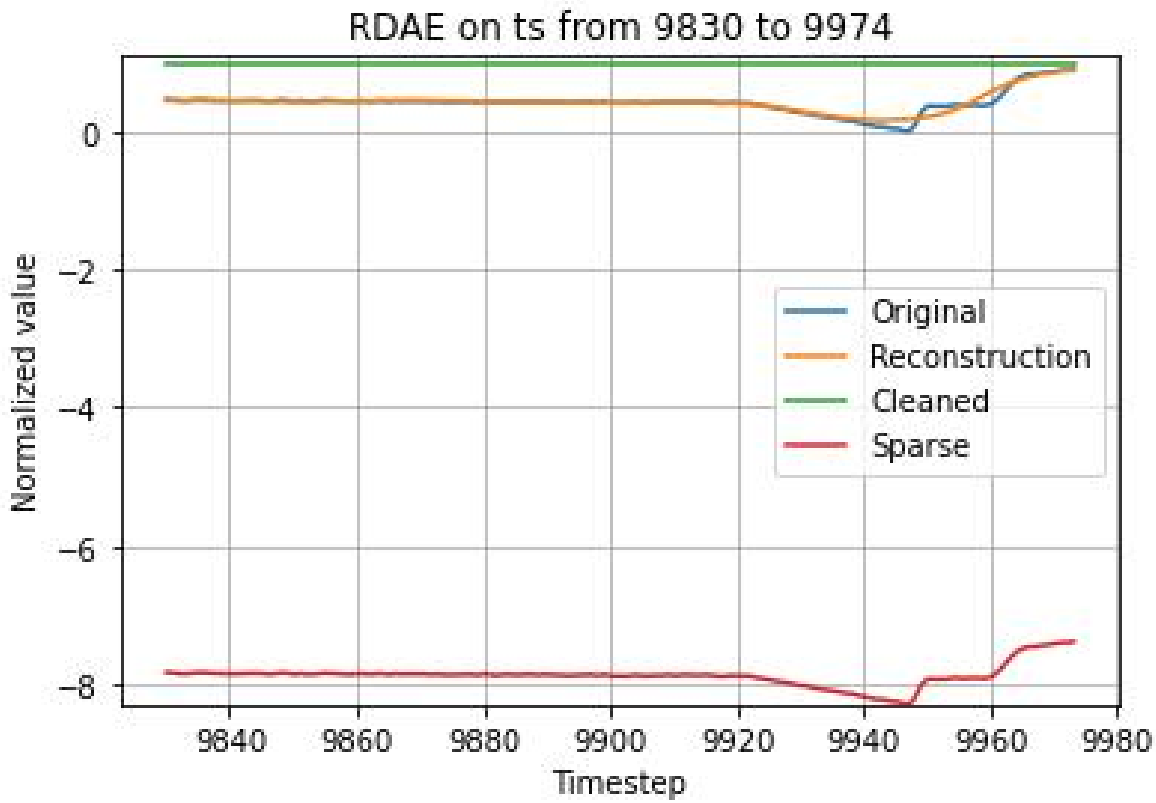

Figure: Example of a anomaly subsequence for $\lambda = 1.0$

Dense RDAE

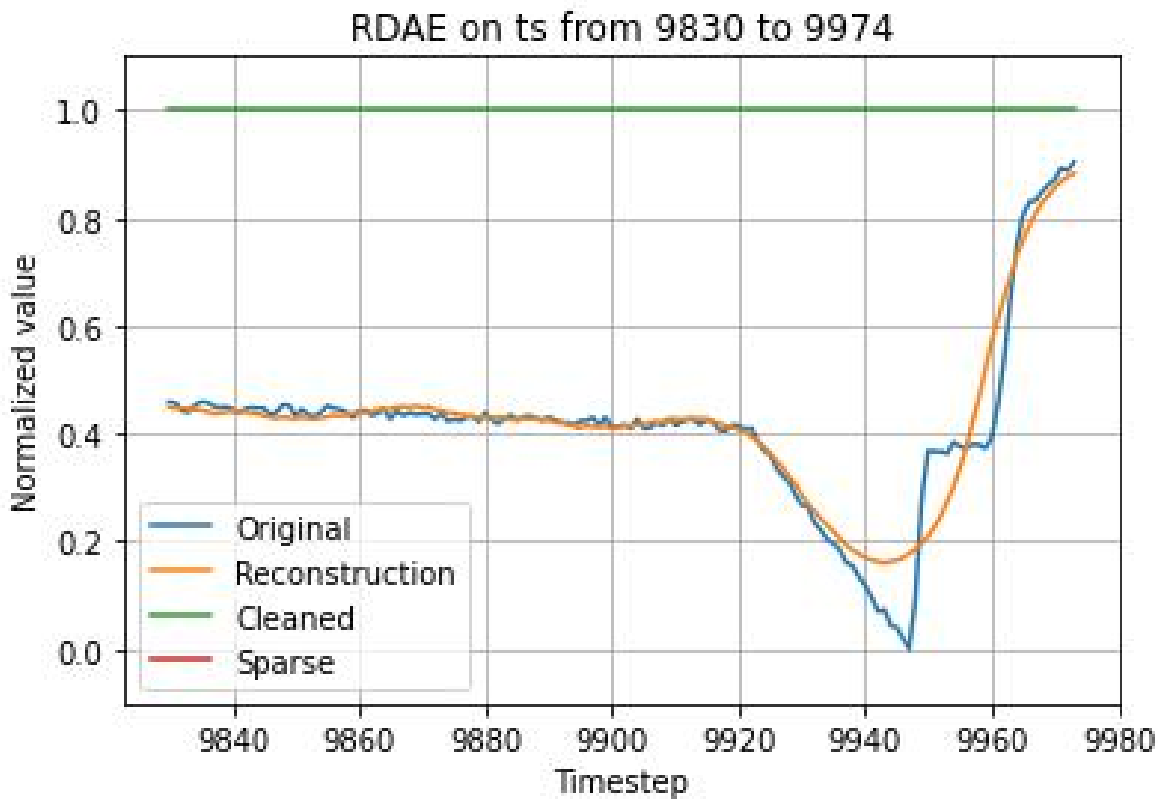

Figure: Example of a anomaly subsequence for $\lambda = 1.0$

Dense RDAE

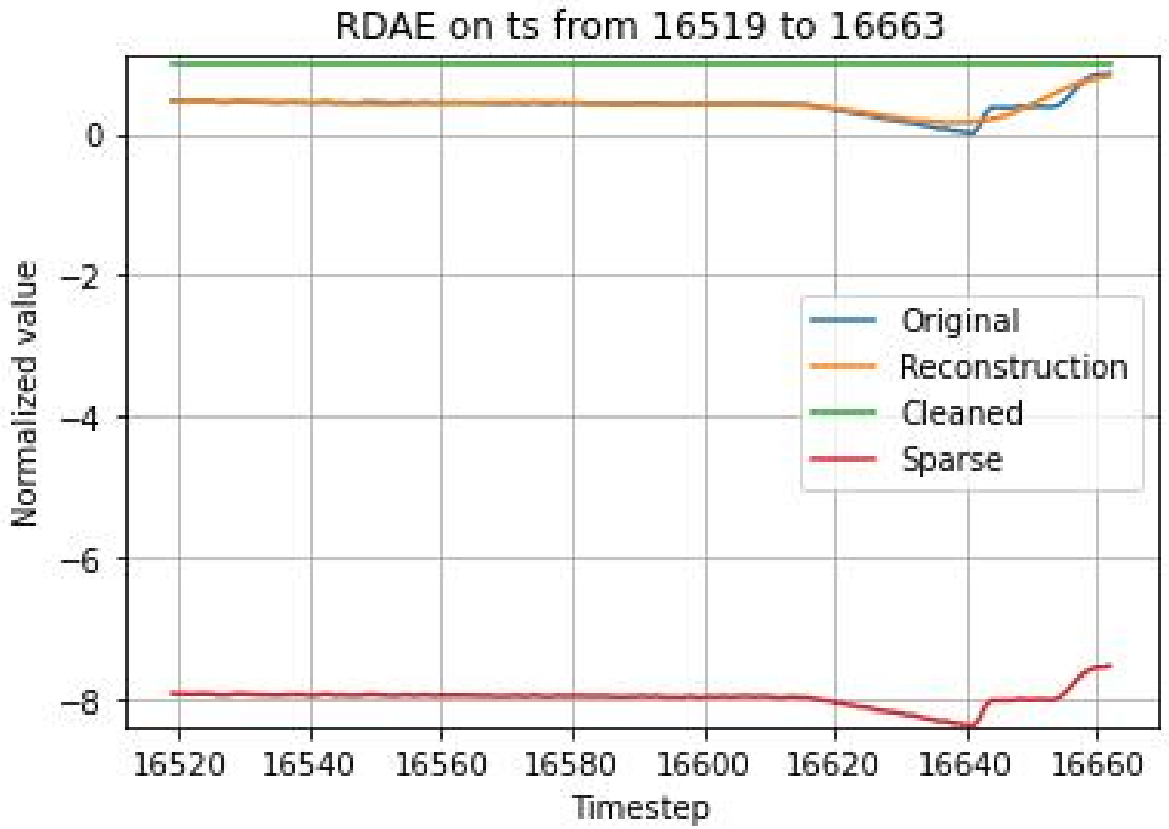

Figure: Example of a anomaly subsequence for $\lambda = 1.0$

Dense RDAE

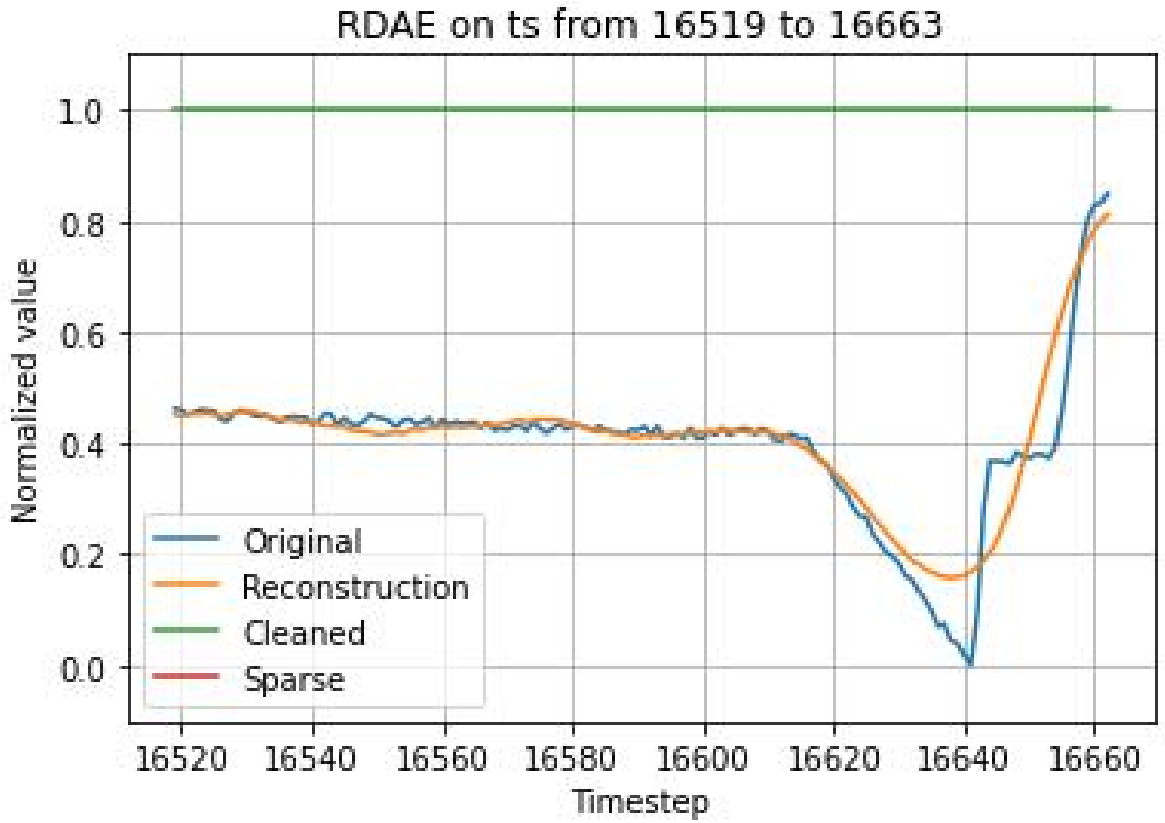

Figure: Example of a anomaly subsequence for $\lambda = 1.0$

Dense RDAE

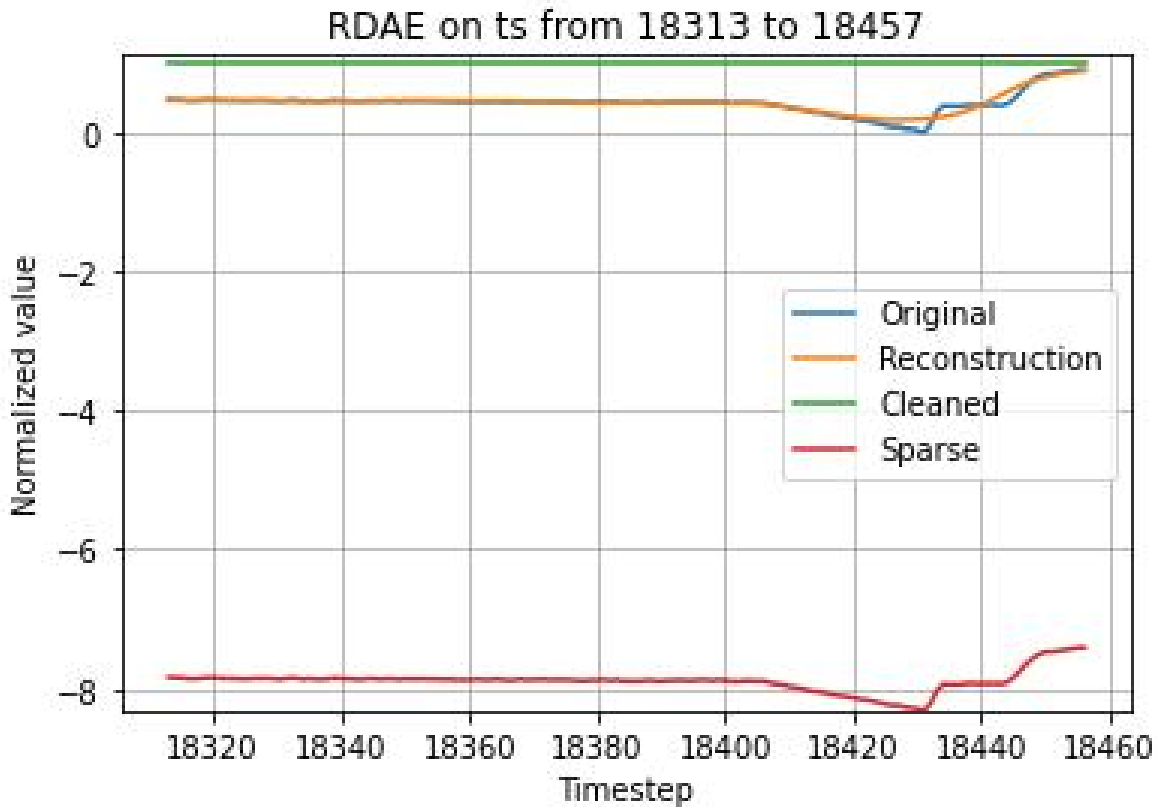

Figure: Example of a anomaly subsequence for $\lambda = 1.0$

Dense RDAE

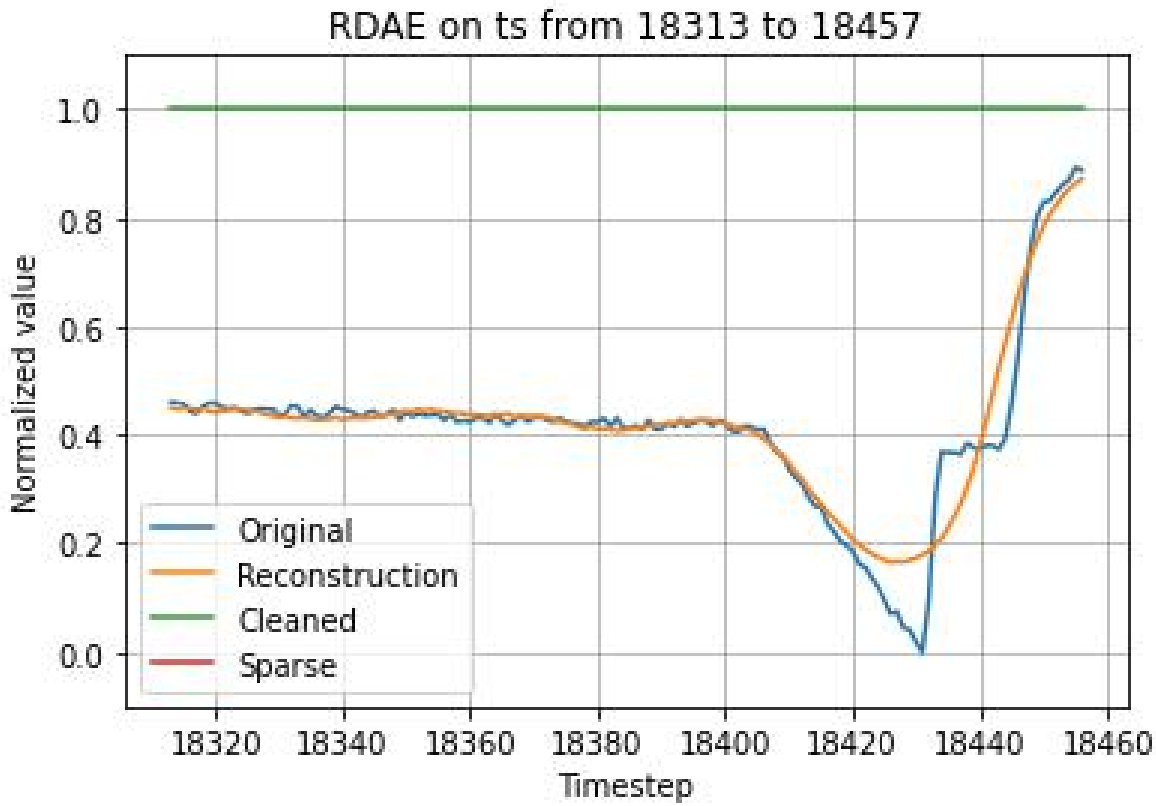

Figure: Example of a anomaly subsequence for $\lambda = 1.0$

Dense RDAE

- All of the anomalies found reach the 0 value (min temperature of all time series).
- Note that the different anomalies found DO NOT overlap. So each of the failures is only recognized once.
- This may also create problems, since as you can see one failure is not recognized as anomaly.
- In general, the reconstruction is a non-noisy version of the signal.

LSTM RDAE

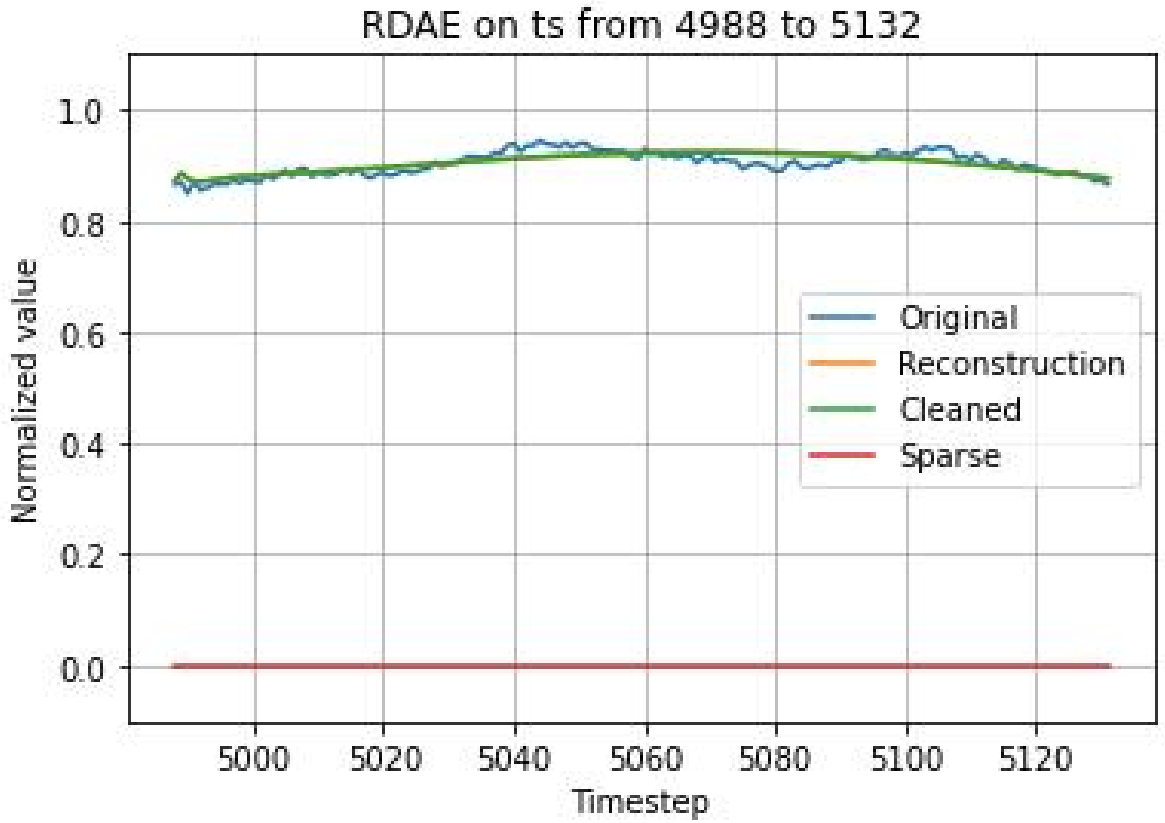

Figure: Example of a non anomaly subsequence for $\lambda = 3.3$

LSTM RDAE

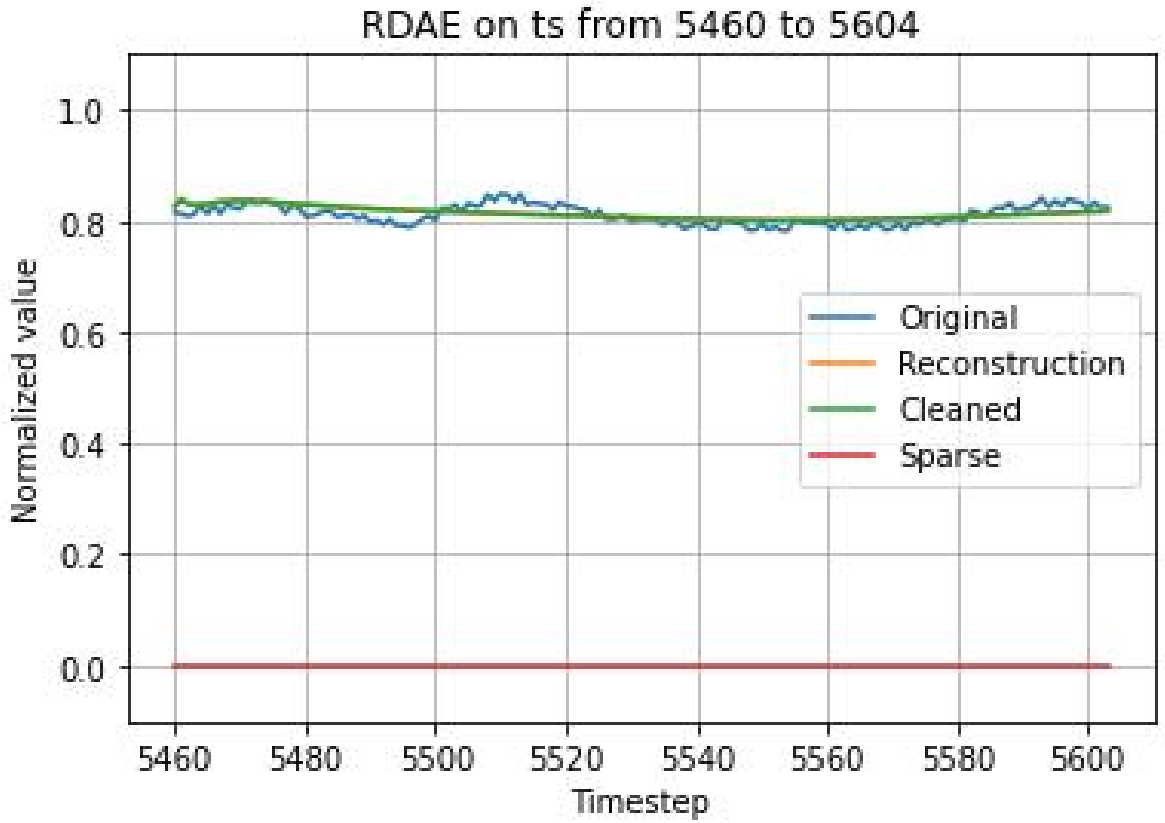

Figure: Example of a non anomaly subsequence for $\lambda = 3.3$

LSTM RDAE

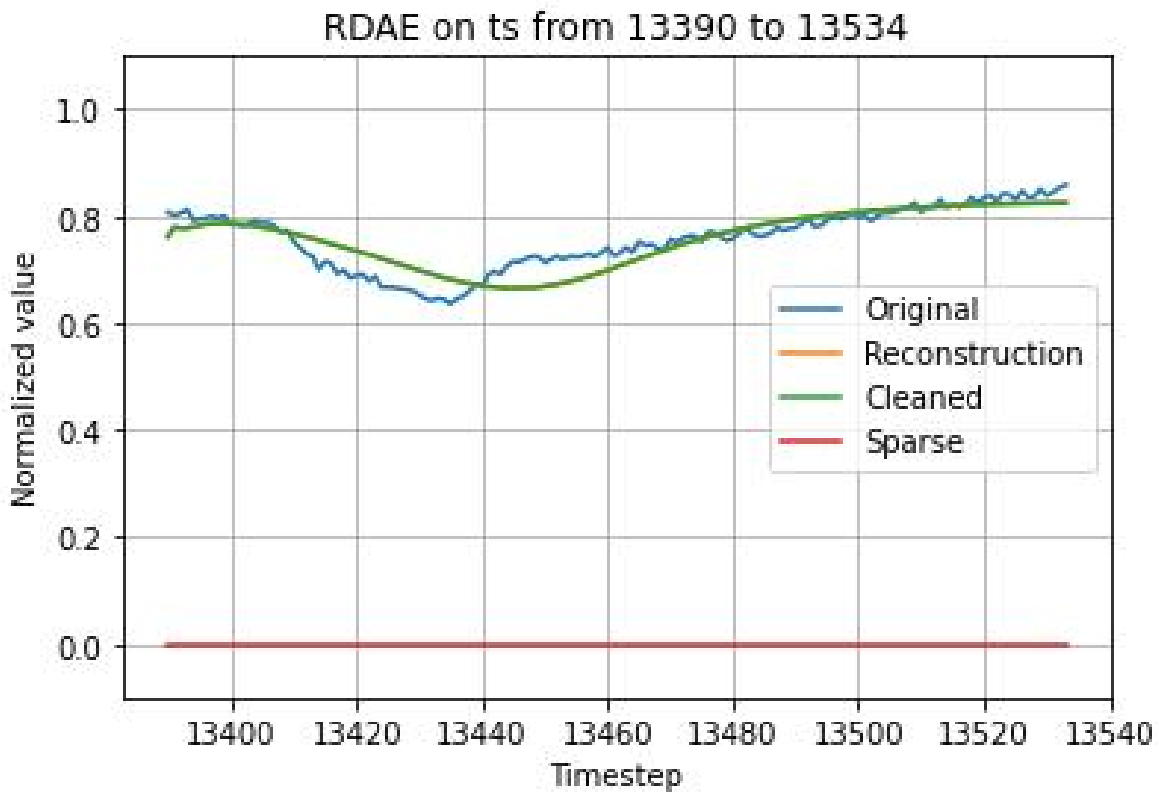

Figure: Example of a non anomaly subsequence for $\lambda = 3.3$

LSTM RDAE

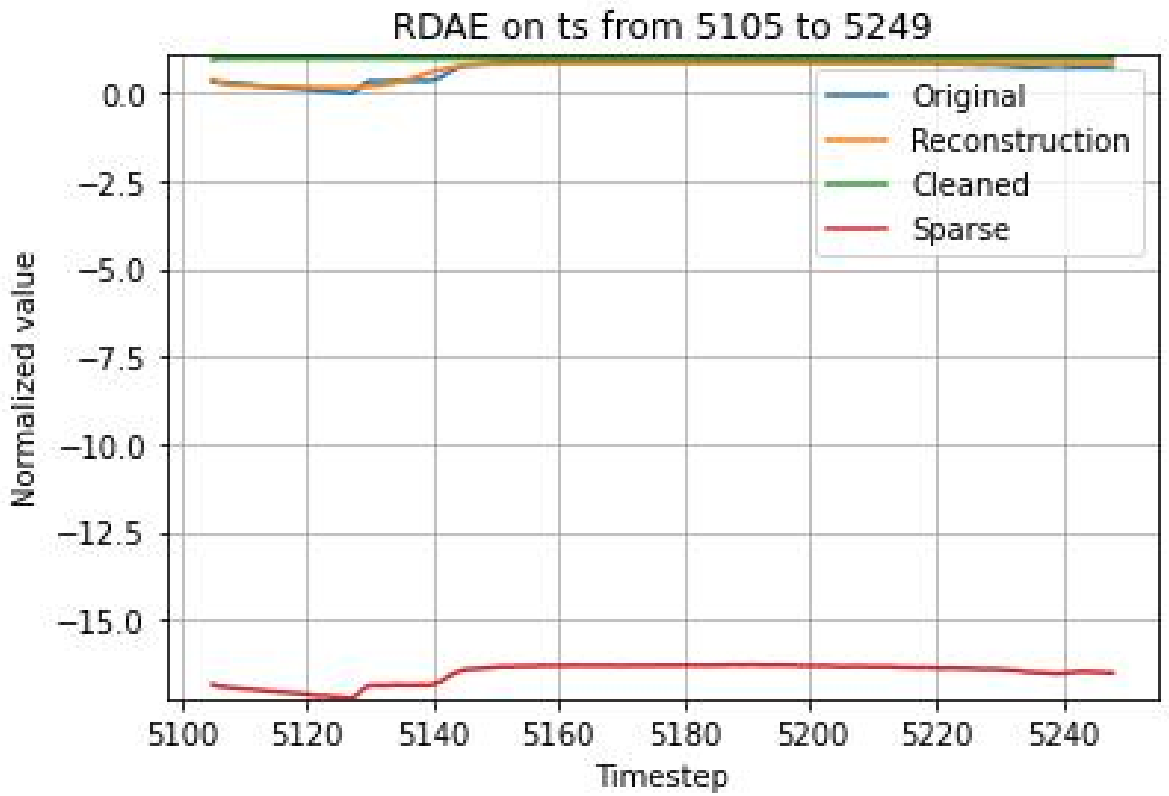

Figure: Example of a anomaly subsequence for $\lambda = 3.3$

LSTM RDAE

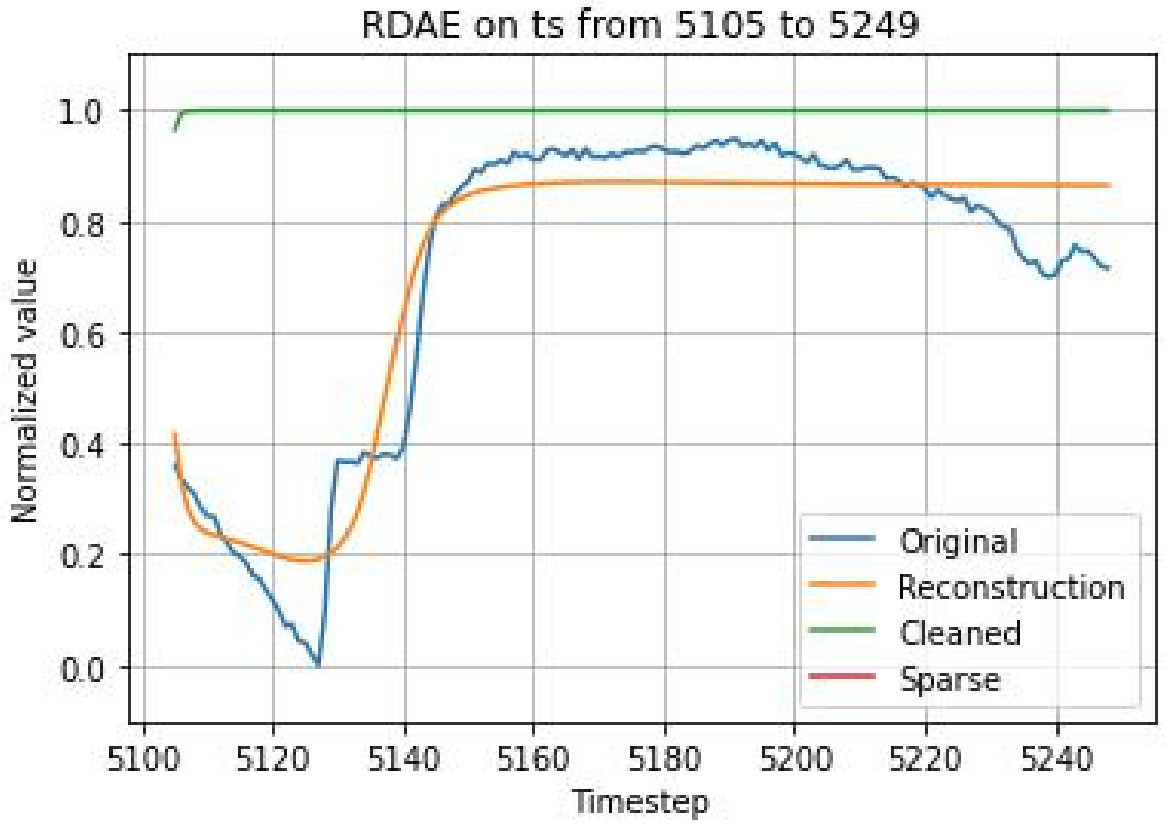

Figure: Example of a anomaly subsequence for $\lambda = 3.3$

LSTM RDAE

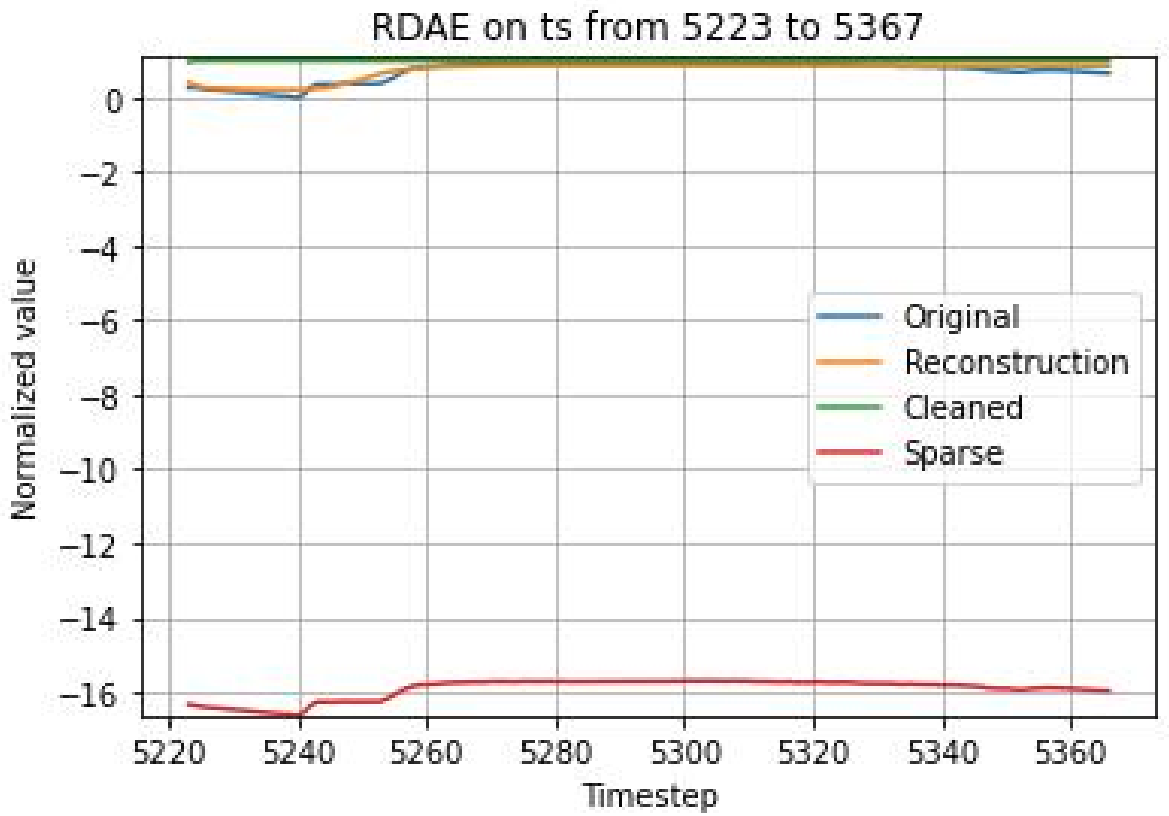

Figure: Example of a anomaly subsequence for $\lambda = 3.3$

LSTM RDAE

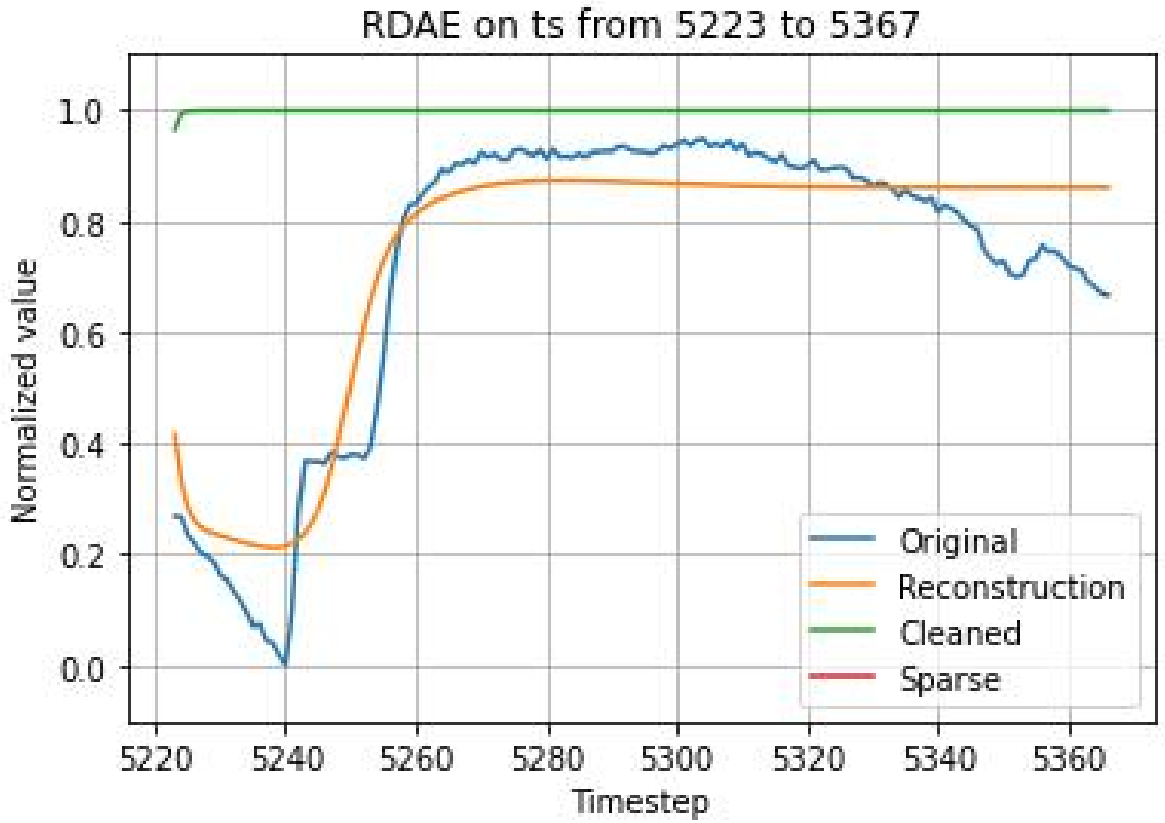

Figure: Example of a anomaly subsequence for $\lambda = 3.3$

LSTM RDAE

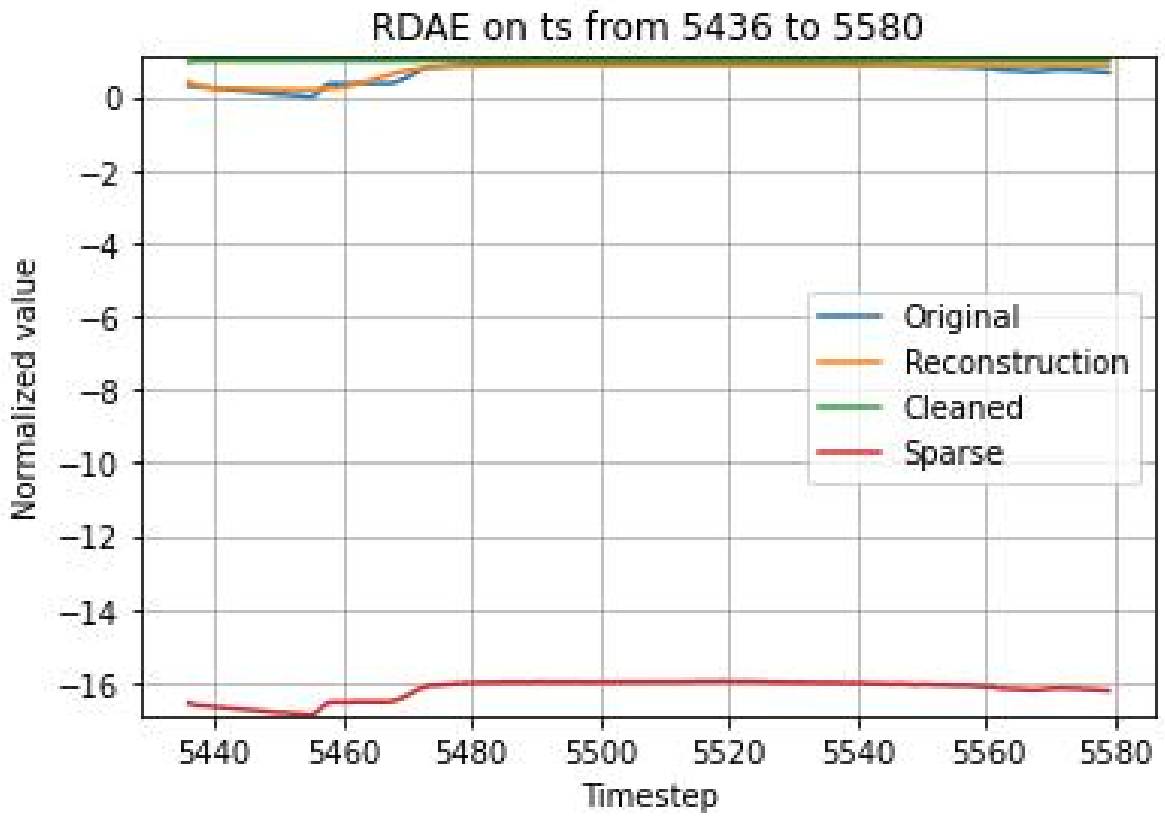

Figure: Example of a anomaly subsequence for $\lambda = 3.3$

LSTM RDAE

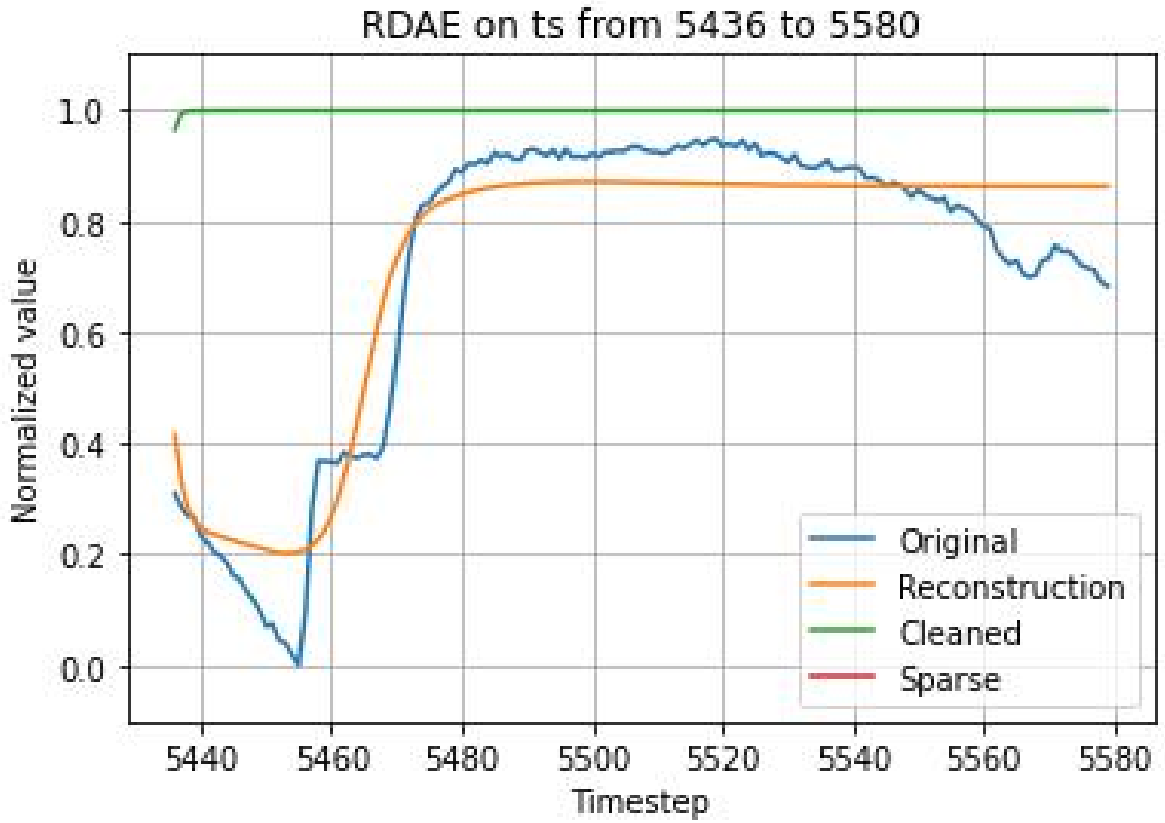

Figure: Example of a anomaly subsequence for $\lambda = 3.3$

Dense RDAE

- All of the anomalies found reach the 0 value (min temperature of all time series).
- Also in this case different anomalies found DO NOT overlap. So each of the failures is only recognized once. In this case this happens at the beginning of the subsequence
- The reconstruction here is far worse than in the dense case.
- Performance could be improved using more parameters in the LSTM case. Note that computation time is much higher (~ 4 minutes for dense, ~ 20 minutes for LSTM, with the help of a RTX3070 laptop).

https://github.com/AlexThirty/SaMLMfTSA

Thank you!


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