Anomaly Detection with Robust Deep Autoencoders

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Introduction

- Anomaly detection is a fundamental problem when dealing with large amounts of data.
- e.g. Detect outliers in large datasets that may have bad influence influence our data pipeline.
- e.g. We want to know if a battery is in good state and to detect strange behaviours by looking at its historical data.
- The main challenge is related to the fact that anomalies are sparse points hidden in a large amount of normal data.
- This presentation is about the Robust Deep Autoencoder models [ZP17] and its applications focusing on anomaly detection.

Deep Autoencoders

- A Deep Autoencoder (DAE) has two main components: an encoder E and a Decoder D. It produces a low dimensional representation of data $Z = E(X)$.
- E, D can be any mapping between the data space and the coded space. Usually we use FCNN or more complex models (e.g. LSTM or GRU).
- The DAE learns the identity map so that the reconstruction $\bar{X} = D(E(X))$ is as close as possible to the original input X

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

Principal Component Analysis (PCA)

- Assume following data shape: N samples of d dimensional data $X \in \mathbb{R}^{N \times d}$ and w.l.o.g. each feature has 0 mean.
- Mathematically, PCA is an orthogonal linear transformation U s.t. in the new coordinate system the i-th component has the i-th greatest data variance.
- PCA can be used for dimensionality reduction: project the data on the first $k < d$ principal components.
- How to find the new basis:

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

Robust Principal Component Analysis

- Robust Principal Component Analysis (RPCA) is a generalization of PCA that aims to reduce the sensitivity of PCA to outliers and noise.
- Idea: separate noise and outliers, then learn a low dimensional representation of cleaned data.
- 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 containing outliers and anomalous data.

Robust Principal Component Analysis

- The problem can be addressed as:

$$\min_{L,S} \rho(L) + \lambda \|S\|_0 \tag{3}$$

$$\text{s. t. } X = L + S \tag{4}$$

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

- This optimization problem is NP-hard and tractable only for small metrices.
- New objective:

$$\min_{L,S} \|L\|_* + \lambda \|S\|_1 \tag{5}$$

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

Robust Deep Autoencoders

- Robust Deep Autoencoders (RDAE) idea: combine the representation learning of DAEs and the anomaly detection capability of RPCA.
- Leave out the sparse part S and learn a low-dimensional representation of L.
- There are two kinds of RDAE, one for l_1 regularization and one for $l_{2,1}$.

RDAE and regularization

- We try to decompose data as $X = L_D + S$ as in RPCA and combine the losses in this optimization problem:

$$\min_{\theta} \|L_D - D_\theta(E_\theta(L_D))\|_2 + \lambda \|S\|_1 \tag{6}$$

$$\text{s.t. } X = L_D + S \tag{7}$$

- The parameter λ controls the sparsity of S. A smaller λ means that the norm of S is less important w.r.t. DAE loss (better reconstruction, less outliers) and viceversa.
- Finding the best value for λ is the main challenge.

Regularization and anomalies

- The RDAE with l_1 penalization assumes that outliers and noise are not structured. The l_1 penalty just induces sparsity. We could have different kind of anomalies:
- Feature (column) wise: a feature is corrupted in many samples e.g. a broken pixel in a sensor.
- Data (row) wise: a particular sample is anomalous and very different from the majority of them.

The $l_{2,1}$ norm

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

$$\|X\|_{2,1} = \sum_{j=1}^{d} \|X_j\|_2 = \sum_{j=1}^{d} \left(\sum_{i=1}^{N} |X_{ij}|^2 \right)^{\frac{1}{2}} \tag{8}$$

- 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

$$\min_{\theta} \|L_D - D_\theta(E_\theta(L_D))\|_2 + \lambda \|S^T\|_{2,1} \tag{9}$$

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

The proximal operator

- To see in detail the training procedure for the RDAE we first need to consider the proximal operator.
- General framework: find the solution to $\min f(x) + \lambda g(x)$ where g is convex. Consider

$$\text{prox}_{\lambda,g}(x) = \arg\min_y g(y) + \frac{1}{2\lambda}\|x - y\|_2^2 \qquad (11)$$

- In the case of proximal gradient optimization the iterative step is defined as:

$$x^{k+1} = \text{prox}_{\lambda,g}(x^k - \alpha\nabla f(x^k)) \qquad (12)$$

- For $g(x) = \|x\|_1$, the solution to the proximal problem is

$$\operatorname{prox}_{\lambda,l_1}(x) = \begin{cases} x_i - \lambda, & x_i > \lambda \\ x_i + \lambda, & x_i < -\lambda \\ 0, & x_i \in [-\lambda, \lambda] \end{cases} \tag{13}$$

  for $S \in \mathbb{R}^{N \times d}$ it gets applied element by element.
- $g(x) = \|x\|_{2,1}$: for feature anomalies we obtain (letting $S_{\cdot j}$ be the column vector $S_{ij}, j = 1, \dots, N$)

$$(\operatorname{prox}_{\lambda,l_{2,1}}(S))_{ij} = \begin{cases} S_{ij} - \lambda \frac{S_{ij}}{\|S_{\cdot j}\|_2}, & \|S_{\cdot j}\|_2 > \lambda \\ 0, & \|S_{\cdot j}\|_2 \leq \lambda \end{cases} \tag{14}$$

The proposed optimization method is a two step iterative process (ADMM).
Given input $X \in \mathbb{R}^{N \times d}$, initialize $L_D \in \mathbb{R}^{N \times d}, S \in \mathbb{R}^{N \times d}$ 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 (DAE).
- 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 $c_2 = \frac{\|L_S - L_D - S\|_2}{\|X\|_2} < \epsilon$ we have early convergence.
- Set $L_S = L_D + S$.

Return L_D and S.

Results

- We now have a look at how the model performs on some tasks.
- We will initially use the MNIST digit dataset, using the 50000 training images available.
- 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.

l_1 Robust Deep Autoencoder

- We take a RDAE with a FCNN architecture with layers of size 784 (input), 200 and 10 (the bottleneck and hidden feature layer). 10 outer iterations and 100 inner iterations.
- The training images get corrupted with a percentage of pixel (from 5% to 50%) changed to a random value between 0 and 1. These are used to train the RDAE.
- Implemented using python 3.8 and Tensorflow 2.9.

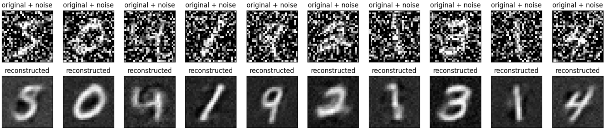


Figure: RAE cleaned data, corruption 50%

$l_{2,1}$ Robust Deep Autoencoder

- To assess the performance of RDAE in anomaly detection we start by using a synthetic labeled dataset.
- All the 4 digit images for training are collected in our dataset.
- Then, some images are chosen at random from all the other digits until they reach 5% of total images in the dataset.
- These will be considered as the outliers of our data.
- Example application: given a pool of batteries find those with problems and/or defects.

- The $l_{2,1}$ RDAE is trained on this dataset without any side information. Same architecture as before.
- The only parameter that requires tuning is λ. We assess performance with the accuracy, precision, recall and $F_1 = 2\frac{PR}{P+R}$ metrics.
- We consider an instance anomalous whenever the S matrix has non-zero entries on its row.

Anomaly detection performance

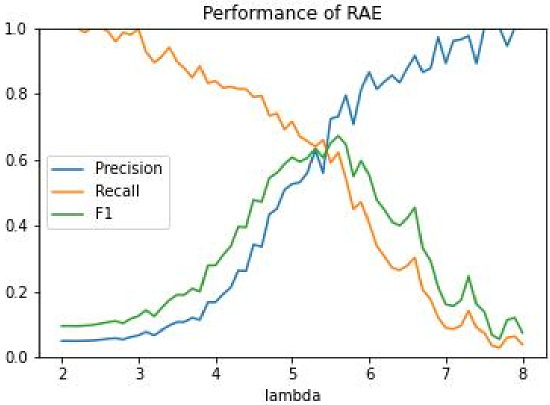


Figure: $L_{2,1}$ RDAE anomaly detection performance. λ from 2 to 8

- The maximum performance is obtained with $\lambda = 5.468$ with an F_1 score of 0.668.
- From $\lambda = 5$ to $\lambda = 6$ the RDAE has a F_1 score almost everytime above 0.55.
- Precision and recall are both in the range $[0.6, 0.7]$ for λ close to the optimal.
- Let's look at the reconstructions by the DAE of the RDAE $D(E(X))$, the cleaned images L_D and the sparse image S from 3 different values of λ: low, optimal and high.

Original Images data

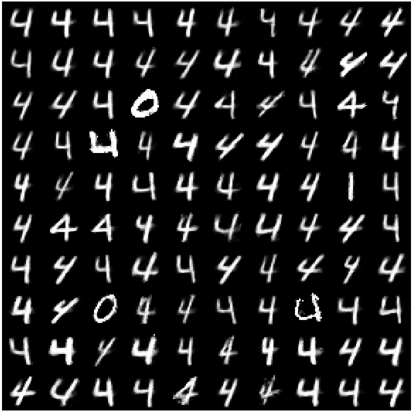
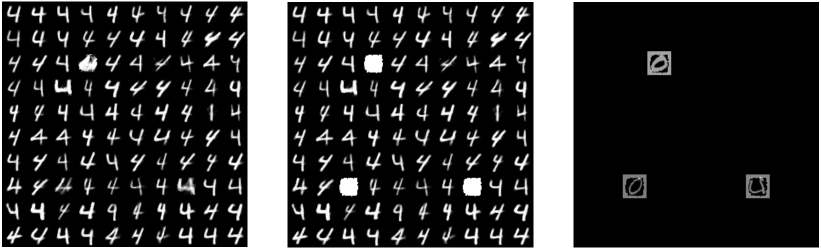


Figure: Original images for the $L_{2,1}$ RDAE

$\lambda = 5.468$



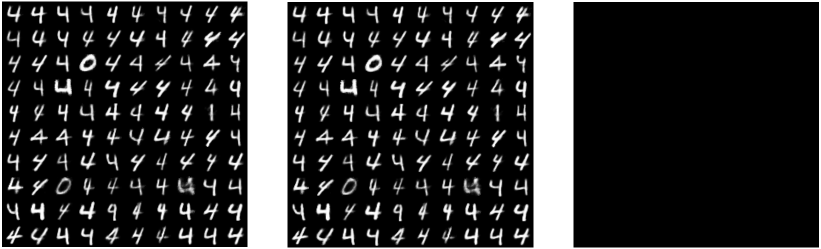
(a) $\bar{X}$, reconstruction

(b) L_D, cleaned data

(c) S, outliers

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

$\lambda = 8.0$



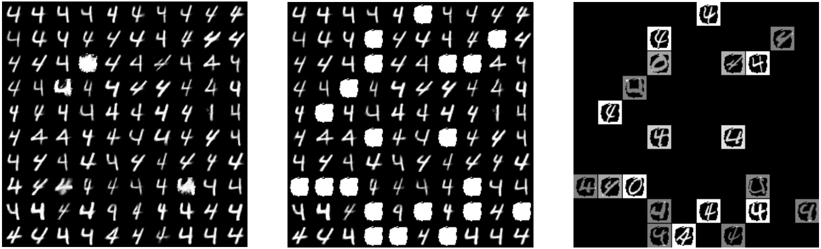
(a) $\bar{X}$, reconstruction

(b) L_D, cleaned data

(c) S, outliers

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

$\lambda = 4.0$



(a) $\bar{X}$, reconstruction (b) L_D, cleaned data (c) S, outliers

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 it is based on the idea that outliers are few and very different from the rest.
- These outliers gets recognized using isolation trees which try to separate points from others.
- The only parameter to be optimized is the outlier fraction (from 0 to 0.5).

Isolation forest performance

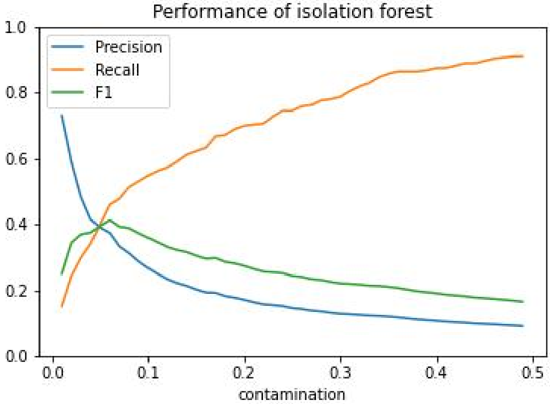


Figure: The performance is far worse than RDAE.

Real World Experiment

- Now we have assessed the performance on a synthetic dataset we want to see how to apply this model to real world challenges.
- Data is in general UNLABELED. Specially with loads of data, we can't do hand labeling of anomalies.
- We want to see if the model still works for time series.

Time series experiment

- In this case we are going to use a dataset similar to our interest.
- It is taken 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 kinds of anomalies: mainly planned shutdowns of the machine, then the second kind should be difficult to detect and directly led to the third anomaly, a catastrophic failure of the machine.
- Example application: Electra Vehicles' EVE-AI analytics. Find strange patterns in driving styles or battery problems through sensors' historical data.

Data processing pipeline

- Data has 22464 timesteps in total. Data signals are taken every 5 minutes.
- I chose to consider subsequences of length 144: this corresponds of windows of 12 hours. The final dataset has then 22321 training time series.
- Data is normalized all togheter to be in $(0, 1)$.

RDAE architectures and analysis

I tried using 3 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, batch size 256 , $\epsilon = 10^{-8}$.
- The second and the third one are a LSTM and a GRU with two layers of 32 and 16 units, 10 outer iterations and 25 inner iterations with same batch size as before.
- Since data is unlabeled we don't have a clear benchmark for the valie of λ. I tried different values to see how the number of outliers scales.

Anomalies found

λ	0.1	0.5	0.7	1.0	2.0	3.0	3.2	3.3	4
Dense	All	751	250	14	0	0	0	0	0
LSTM	All	7525	4208	2068	306	109	74	9	0
GRU	All	7277	4505	2454	331	139	103	80	0

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

Dense RDAE

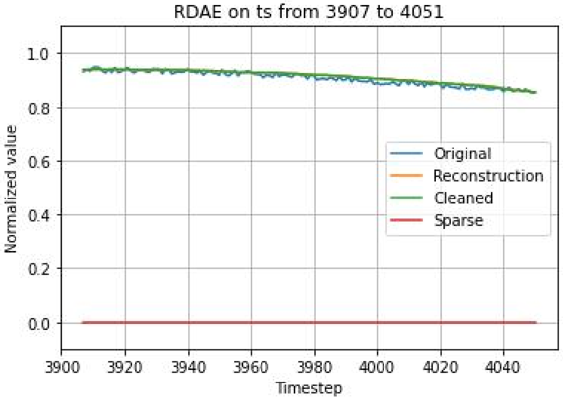


Figure: Example of a non anomaly subsequence for $\lambda = 1.0$

Dense RDAE

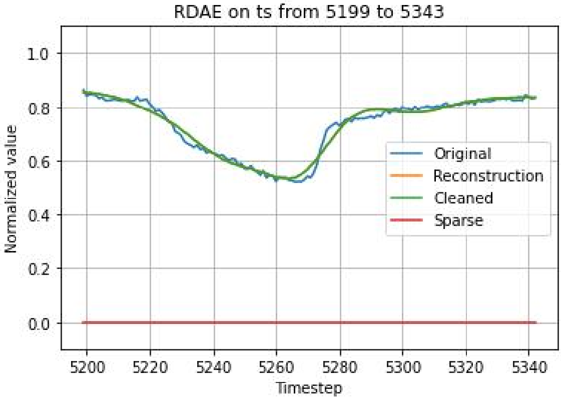


Figure: Example of a non anomaly subsequence for $\lambda = 1.0$

Dense RDAE

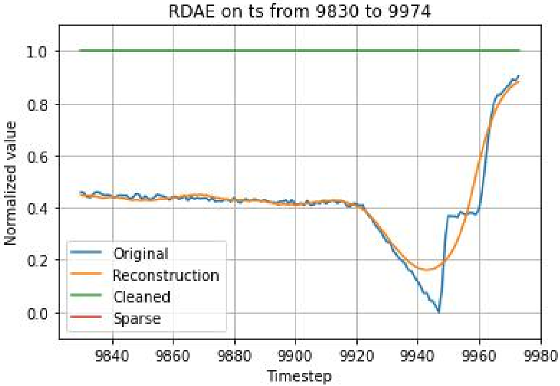


Figure: Example of a anomaly subsequence for $\lambda = 1.0$

Dense RDAE

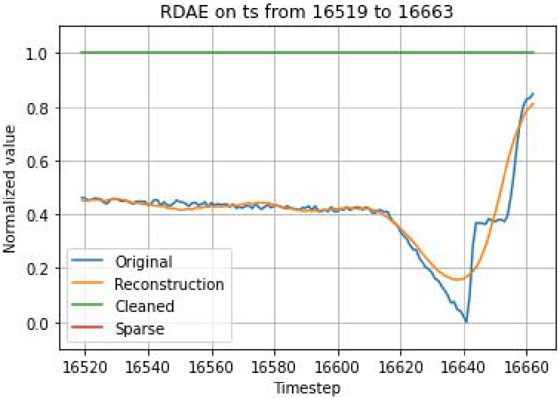


Figure: Example of a anomaly subsequence for $\lambda = 1.0$

Dense RDAE

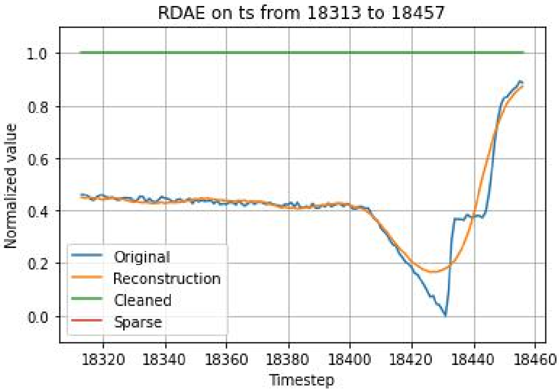


Figure: Example of a anomaly subsequence for $\lambda = 1.0$

Dense RDAE

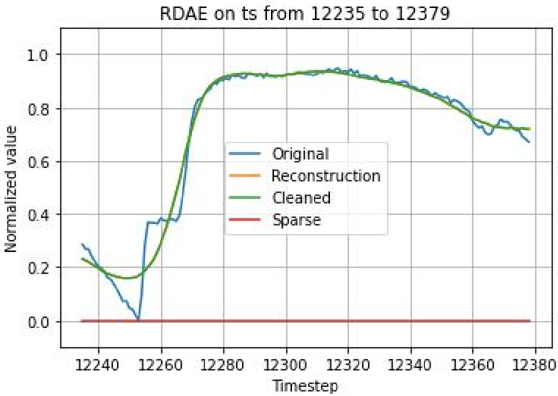


Figure: Example of a non anomaly subsequence for $\lambda = 1.0$

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

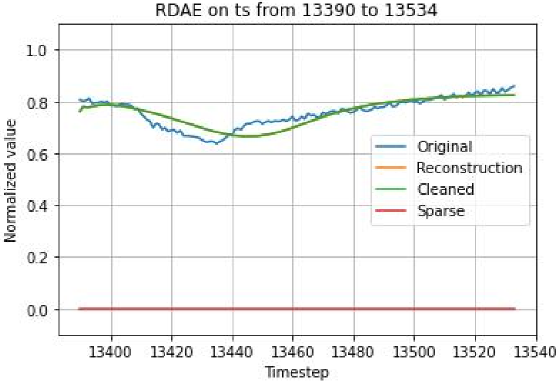


Figure: Example of a non anomaly subsequence for $\lambda = 3.3$

LSTM RDAE

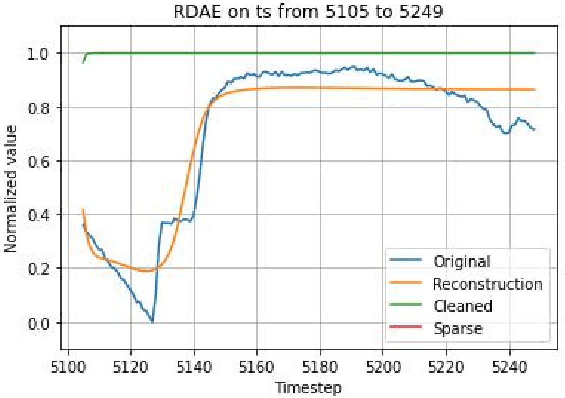


Figure: Example of a anomaly subsequence for $\lambda = 3.3$

Isolation Forest

- I tried to fit an isolation forest on the same data, to see if we get the same kind of outliers.
- With all outlier fraction values tested $(0.0001, 0.0005, 0.001, 0.01)$, non of them showed significant results.
- On the contrary, almost all the anomalies detected I saw were normal time series, almost flat.

Isolation forest anomaly example

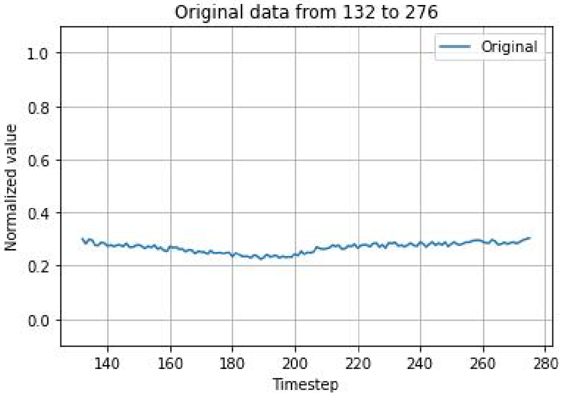


Figure: Example of an anomaly found by the isolation forest with outlier fraction of 0.001

Final comments

- The RDAE is a powerful tool for denoising and anomaly detection with many application both for images, time series and can detect different kinds of anomalies in a general setting.
- Unfortunately the main quest is to find the correct λ value. With unlabeled data this could be very difficult.
- In that case, a possible way out is to know the approximate anomaly rate and to hope the anomalies found match the true ones.

- Note an important thing: after we train the model where is no way to find anomalies on new given data.
- The L_D and S matrices are produced only in the training procedure.
- We can still denoise images with the Autoencoder part.
- It could be tried to add new data after some iteration, without re-initializing. This requires training again the autoencoder, which is the high computational part.

https://github.com/AlexThirty/SaMLMfTSA

Thank you!

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