Background Robust Deep Autoencoders RDAE training Results

Anomaly Detection with Robust Deep Autoencoders original article by C. Zhou and R. C. Peffenroth

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- Background
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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).
- 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.
- 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 loss function: it is 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 following data shape: N samples of d dimensional data $X \in \mathbb{R}^{N \times d}$ and assume each feature has 0 mean.
- Principal Component Analysis (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 is often used for dimensionality reduction or encoding: we can project the data on the first k < d principal components.

Principal Component Analysis

Mathematically we can define:

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

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

$$\hat{X}_{k} = X - \sum_{i=1}^{k-1} X w_{i} w_{i}^{T}$$
(3)

and finally solving again the similar problem:

$$w_{k} = \underset{\|w\|_{2}=1}{\arg \max} \|\hat{X}_{k}w\|_{2}^{2} = \underset{w}{\arg \max} \frac{w^{T}\hat{X}_{k}^{T}\hat{X}_{k}w}{w^{T}w}$$
(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.
- 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:

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

s. t.
$$||X - L - S||_F^2 = 0$$
 (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.
- The used objective is instead:

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

s. t.
$$||X - L - S||_F^2 = 0$$
 (8)

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

Robust Deep Autoencoders

- Robust Deep Autoencoders (RDAE) 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.
- We want to exclude anomalies and learn a low dimensional representation of data.
- There are two kinds of RDAE, one for I_1 regularization and one for $I_{2,1}$.

RDAE with I_1 regularization

- We try to decompose data as $X = L_D + S$ as in RPCA.
- By removing the noise S the autoencoder can better reconstruct L_D .
- We then combine the two losses in the following minimization problem

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

s.t.
$$X - L_D - S = 0$$
 (10)

• The parameter λ controls the sparsity of S.



The role of λ

- A smaller λ means that the norm of S is less important w.r.t. the DAE loss.
- The model will reconstruct better but recognize less outliers. Helpful if we want a more faithful representation.
- 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.
- Finding the right value for λ is the main challenge for this model.

The true objective

 The previous loss is higly non tractable. We focus on the following problem:

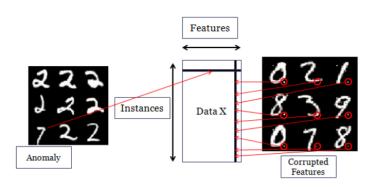
$$\min_{\theta} \|L_D - D_{\theta}(E_{\theta}(L_D))\|_2 + \lambda \|S\|_1 \tag{11}$$

s.t.
$$X - L_D - S = 0$$
 (12)

- The autoencoder is trained with L_D , the supposedly cleaned part.
- There is no specific requirement about the DAE mappings.

Regularization

- The RDAE with I₁ penalization assumes that outliers and noise are not structured. The I₁ 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.



The $I_{2,1}$ norm

• The $I_{2,1}$ norm is defined as $(X \in \mathbb{R}^{N \times d})$:

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

- The $I_{2,1}$ norm can be seen as introducting a I_2 norm regularization over data for each feature and then adding a I_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 $I_{2,1}$ regularization for data anomalies is then

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

s.t.
$$X - L_D - S = 0$$
 (15)

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

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

s.t.
$$X - L_D - S = 0$$
 (17)

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

$$prox_{\lambda,g}(x) = \arg\min_{y} g(y) + \frac{1}{2\lambda} ||x - y||_{2}^{2}$$
 (18)

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

$$x^{k+1} = \operatorname{prox}_{\lambda, g}(x^k - \alpha \nabla f(x^k)) \tag{19}$$



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

$$\operatorname{prox}_{\lambda, l_1}(x) = \arg \min_{y} l_1(y) + \frac{1}{2\lambda} ||x - y||_2^2$$
 (20)

$$\operatorname{prox}_{\lambda, l_{2,1}}(x) = \arg\min_{y} l_{2,1}(y) + \frac{1}{2\lambda} \|x - y\|_{2}^{2}$$
 (21)

• For the I_1 norm, the solution to the proximal problem is

$$\operatorname{prox}_{\lambda,l_{1}}(x) = \begin{cases} x_{i} - \lambda, & x_{i} > \lambda \\ x_{i} + \lambda, & x_{i} < -\lambda \\ 0, & x_{i} \in [-\lambda, \lambda] \end{cases}$$
 (22)

for $S \in \mathbb{R}^{N \times d}$ it gets applied element by element.

• $I_{2,1}$ norm: for feature anomalies we obtain (letting S_{ij} be the column vector $S_{ij}, j=1,\ldots,N$)

$$(\operatorname{prox}_{\lambda, l_{2,1}}(S))_{ij} = \begin{cases} S_{ij} - \lambda \frac{S_{ij}}{\|S_{.j}\|_{2}}, & \|S_{.j}\|_{2} > \lambda \\ 0, & \|S_{.j}\|_{2} \le \lambda \end{cases}$$
(23)

• 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).
- It is a two-step iterative process to solve the problem

$$\min_{\theta} \|L_D - D_{\theta}(E_{\theta}(L_D))\|_2 + \lambda \|S^T\|_{2,1}$$
 (24)

s.t.
$$X - L_D - S = 0$$
 (25)

- First, we fix S and optimize the DAE loss $||L_D D_\theta(E_\theta(L_D))||_2$ with backpropagation.
- 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 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.



```
def prox l1(lam, x):
    return (x > lam) * (x - lam) + (x < -lam) * (x + lam)
    e = np.linalg.norm(x, axis=0, keepdims=False)
    for i in range(len(e)):
            x[:,i] = x[:,i] - lam*e[i]
            x[:,i] = np.zeros(len(x[:,i]))
def get Dense encoder(input size, dense units):
    encoder - tf.keras.Sequential()
    encoder.add(layers.Input(shape=(input size)))
    for i in range(len(dense units)):
        encoder.add(layers.Dense(units=dense units[i], activation='relu'))
    return encoder
def get Dense decoder(input size, dense units):
    decoder = tf.keras.Sequential()
    decoder.add(layers.Input(shape-(dense units[-1])))
    for i in reversed(range(len(dense units)-1)):
        decoder.add(layers.Dense(units=dense units[i], activation='relu'))
    decoder.add(layers.Dense(units=input size, activation='sigmoid'))
    return decoder
```

```
self.encoder = get_Dense_encoder(input_size, dense_units)
    self.decoder = get Dense decoder(input size, dense units)
    encoded - self.encoder(x, training-training)
    decoded - self.decoder(encoded, training-training)
   return decoded
    encoded = self.encoder(x, training=training)
    return encoded
def decode(self, x, training=False):
def train step(self, x):
        x encoded - self.encode(x, training-True)
        x recon = self.decode(x encoded, training=True)
        loss = self.compiled loss(x, x recon)
    gradients = tape.gradient(loss, trainable_vars)
    self.optimizer.apply gradients(zip(gradients, trainable vars))
    self.compiled_metrics.update_state(x, x_recon)
    return {m.name: m.result() for m in self.metrics}
```

```
def __init__(self, AE_type: str, prox_type: str, input_size=784, dense_units=[200, 10], lr=3e-4, timesteps=24, features=1,
   super(RobustAutoencoder, self). init ()
   assert AE type--'Dense' or AE type--'LSTM', 'AE type has to be either Dense or LSTM'
   self AE_type - AE_type
       self.AE = DAE Dense(input size, dense units)
       self.AE.compile(
           optimizer-tf.keras.optimizers.Adam(learning rate-lr),
       self.AE.compile(
           optimizer=tf.keras.optimizers.Adam(learning rate=lr).
```

```
self.default shape = (X.shape[0], X.shape[1])
    self.utils shape = (X.shape[0], X.shape[1])
    self.default_shape = (X.shape[0], X.shape[1], 1)
    self.utils shape = (X.shape[0], X.shape[1])
X = X.reshape(self.default shape)
self.L = np.zeros(self.default_shape)
self.S = np.zeros(self.default shape)
self.LD = np.zeros(self.default shape)
for i in range(train iter):
    self.AE.fit(x-self.LD, batch size-batch size, epochs-AE train iter, verbose-verbose)
    self.LD = self.AE(self.LD).numpy()
    self.S = self.S.reshape(self.utils shape)
    self.S - self.prox_fn(lam-lam, x-self.S.T).T
    self.S - self.S.reshape(self.default shape)
    c1 = tf.linalg.norm(X - self.LD - self.S) / tf.linalg.norm(X)
   c2 = tf.linalg.norm(self.LS - self.LD - self.S) / tf.linalg.norm(X)
return self.LD, self.S
```

Results

- We will initially use the MNIST digit dataset, which consists of 50000 train samples amd 10000 test images.
- Data was flattened from images of shape (28, 28, 1) into vectors of length 784. Train data is then a matrix in $\mathbb{R}^{50000\times784}$.
- Pixel walues are converted from integers between 0 and 255 to floats between 0 and 1.

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.
- From the RDAE obtain the two matrices L_D , the cleaned data, and S, the sparse and anomalous part.

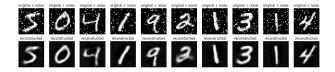


Figure: RAE cleaned data, corruption 10%

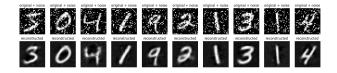


Figure: RAE cleaned data, corruption 20%

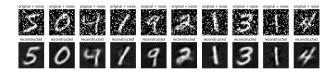


Figure: RAE cleaned data, corruption 30%

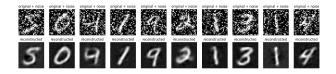


Figure: RAE cleaned data, corruption 40%

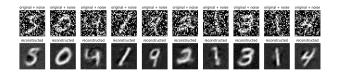


Figure: RAE cleaned data, corruption 50%

1_{2,1} Robust Deep Autoencoder

- The data anomaly detection experiment aims to separeate a specific digit of the MNIST dataset from others.
- All the 4 digit images in the training set 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.

- The I_{2,1} RDAE is trained on this dataset without any side information. It has to recognize outliers completely on its own.
 Same architecture as before.
- The only parameter that requires tuning is λ . We assess performance with the accuracy, precision, recall and $F1 = 2 \frac{PR}{D+R}$ metrics.
- We consider an instance anomalous whenever the S matrix has non-zero entries on its row.

Anomaly detection performance

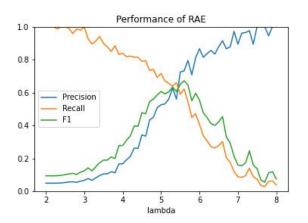


Figure: $L_{2,1}$ RDAE anomaly detection performance. λ from 2 to 8



Anomaly detection performance

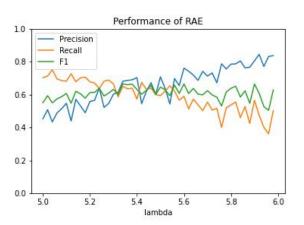


Figure: $L_{2,1}$ RDAE anomaly detection performance. λ from 5 to 6

Anomaly detection performance

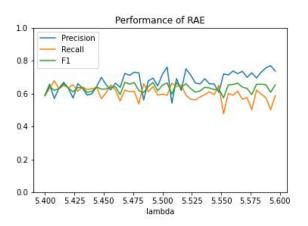


Figure: $L_{2,1}$ RDAE anomaly detection performance. λ from 5.4 to 5.6

- 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.

For each value of λ we analyze 3 images:

- The reconstruction of the original images from the DAE in the RDAE $\bar{X} = D(E(X))$.
- The final L_D image (the "clean" version, in this case it should only contain 4s)
- 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

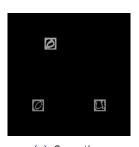
$$\lambda = 5.468$$



(a) \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

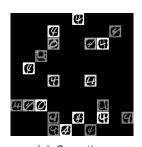
$$\lambda = 4.0$$



(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 was a SOTA method for outlier detection. It is based on the idea that outliers are few, different and separated 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

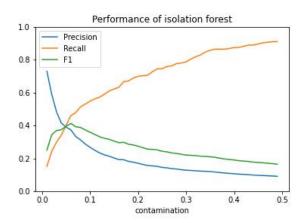


Figure: Isolation forest performance

- The best results 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.
- 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.
- 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 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.

Analysis

- Since data is unlabeled we don't have a clear benchmark for finding the correct value for λ .
- ullet I tried different values for λ to see how the number of outliers scales.
- 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	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 architectures w.r.t. λ

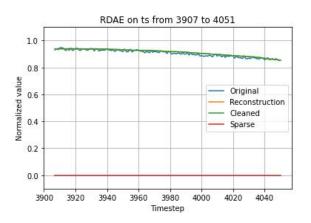


Figure: Example of a non anomaly subsequence for $\lambda=1.0$



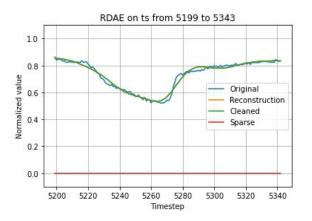


Figure: Example of a non anomaly subsequence for $\lambda=1.0$



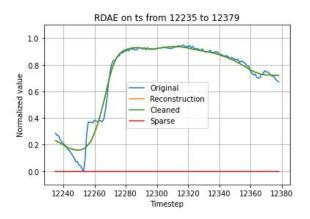


Figure: Example of a non anomaly subsequence for $\lambda=1.0$



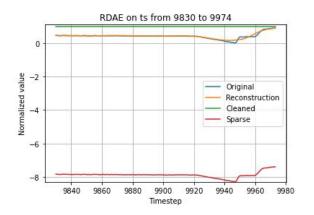


Figure: Example of a anomaly subsequence for $\lambda = 1.0$

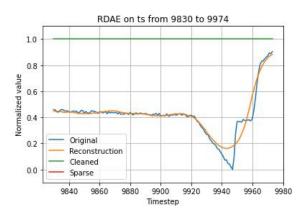


Figure: Example of a anomaly subsequence for $\lambda=1.0$

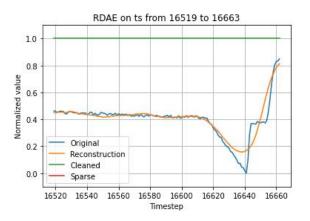


Figure: Example of a anomaly subsequence for $\lambda = 1.0$



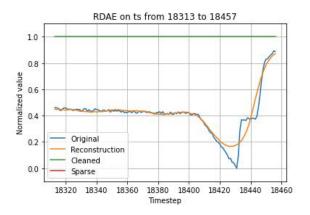


Figure: Example of a anomaly subsequence for $\lambda=1.0$

- 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.

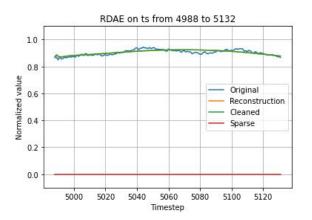


Figure: Example of a non anomaly subsequence for $\lambda = 3.3$



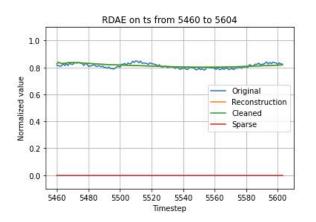


Figure: Example of a non anomaly subsequence for $\lambda = 3.3$



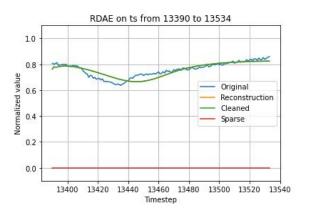


Figure: Example of a non anomaly subsequence for $\lambda = 3.3$

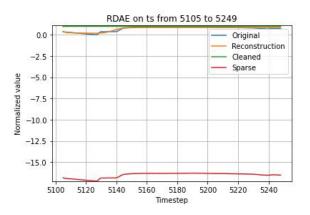


Figure: Example of a anomaly subsequence for $\lambda = 3.3$

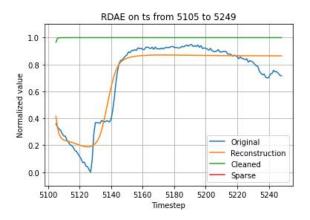


Figure: Example of a anomaly subsequence for $\lambda = 3.3$



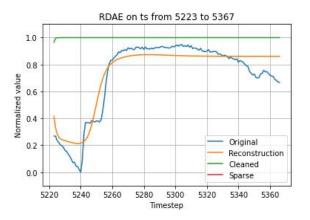


Figure: Example of a anomaly subsequence for $\lambda = 3.3$



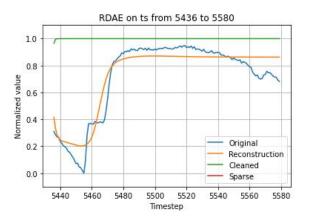


Figure: Example of a anomaly subsequence for $\lambda = 3.3$



- 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 (\sim 4 minutes for dense, \sim 20 minutes for LSTM, with the help of a RTX3070 laptop).

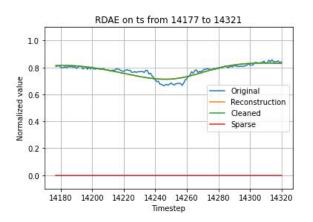


Figure: Example of a non anomaly subsequence for $\lambda = 3.3$



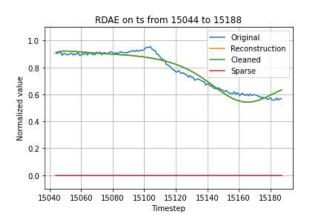


Figure: Example of a non anomaly subsequence for $\lambda = 3.3$

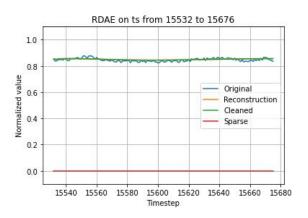


Figure: Example of a non anomaly subsequence for $\lambda = 3.3$

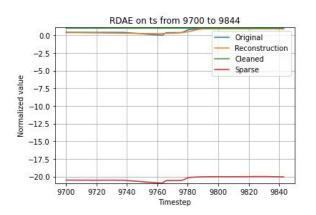


Figure: Example of a anomaly subsequence for $\lambda = 3.3$

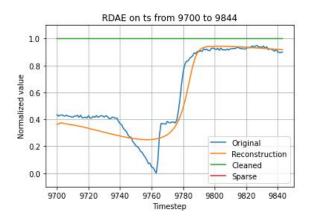


Figure: Example of a anomaly subsequence for $\lambda = 3.3$



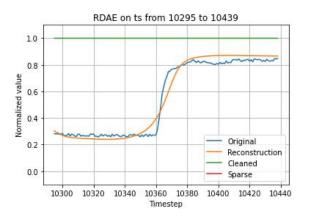


Figure: Example of a anomaly subsequence for $\lambda = 3.3$



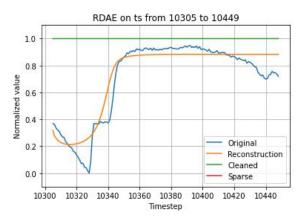


Figure: Example of a anomaly subsequence for $\lambda = 3.3$



- In this case, not all of the anomalies found reach the 0 value.
- Also in this case different anomalies found DO NOT overlap.
 So each of the failures is only recognized once. With GRU this happens in different parts of the subsequence.
- Also here the reconstruction is far worse than in the dense case.
- ullet Again we could increase parameters for better performance. Computation here required \sim 12 minutes with GPU.

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

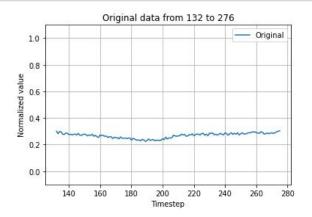


Figure: Example of an anomaly found by the isolation forest with outlier fraction of 0.001

Final comments

- The RDAE is a powerful tool for denoising and anomaly detection.
- 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.

Background Robust Deep Autoencoders RDAE training Results

https://github.com/AlexThirty/SaMLMfTSA

Thank you!



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