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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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 coding space.
 Usually they are Deep Neural Networks e.g. a feed forward network or even more complex models such as Long ShortTer 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 L₂ 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:

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

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

s. t.
$$||X - L - S||_F^2 = 0$$
 (6)

where $ho(\cdot)$ 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:

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

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

- 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 I_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

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

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

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



The role of λ

- ullet 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:

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

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

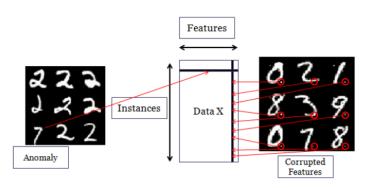
Notice two things:

- 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 $I_{2,1}$ regularization

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



The $I_{2,1}$ norm

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

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

- The I_{2,1} norm can be seen as introducting a I₂ norm regularization over each feature and then adding a I₁ 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.
- 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

$$\operatorname{prox}_{\lambda,g}(x) = \underset{y}{\operatorname{arg\,min}} g(y) + \frac{1}{2\lambda} \|x - y\|_{2}^{2}$$
 (18)

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

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

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

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

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

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

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

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

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

s.t.
$$X - L_D - S = 0$$
 (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 prox $_{\lambda,L}$ function of choice.
- If $c_1=\frac{\|X-L_D-S\|_2}{\|X\|_2}<\epsilon$ or $sc_2=\frac{\|LS-L_D-S\|_2}{\|X\|_2}<\epsilon$ 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.
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https://github.com/AlexThirty/SaMLMfTSA

Thank you!



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