Anomaly Detection with Robust Deep Autoencoders

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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 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:

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

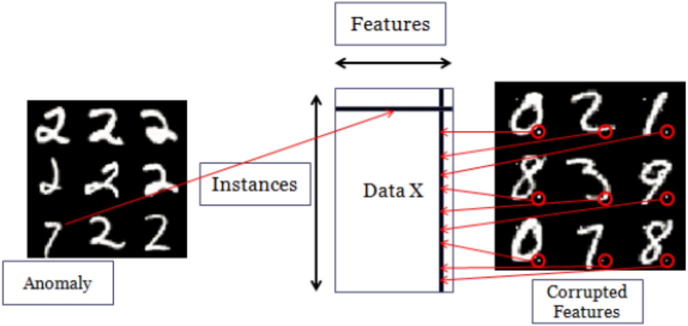
$$\text{s.t. } X - L_D - S = 0 \tag{12}$$

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

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

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

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

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

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

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

  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 $S_{ij}, j = 1, \ldots, N$)

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

  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 $sc_2 = \frac{\|LS - L_D - S\|_2}{\|X\|_2} < \epsilon$ we have early convergence.
- Set $L_S = L_D + S$.

Return L_D and S.

https://github.com/AlexThirty/SaMLMfTSA

Thank you!

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