Outlier Detection for Data Certification

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Overview

1. Background
2. Objective
3. Datasets
4. Model
   - One-Class SVM
   - Isolation Forest
   - Autoencoder
5. Results and Interpretation
6. Summary

Data Quality Monitoring (DQM)

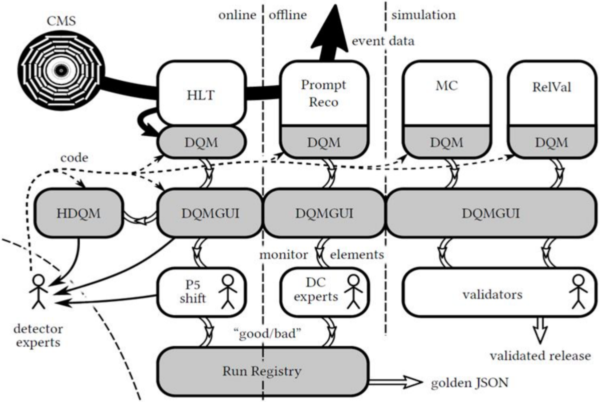


Figure: Tools and Processes of DQM, retrieved from M. Stankevicius

Data granularity in CMS (Offline)

- Reconstruct physics quantity 48 Hours after collision
- Offline shifters and detector experts check the dozens of distribution histograms to define goodness of data
- Certification is made on Run and Lumisection levels
- Lumisection is taken around 23 seconds for one interval

[1] M. Stankevicius, Data Quality Monitoring: Offline

Objective

- **Certify data quality in lumisection granularity**
- Reduce mannual work of the shifter
- Standardize data certification criteria

Expectation

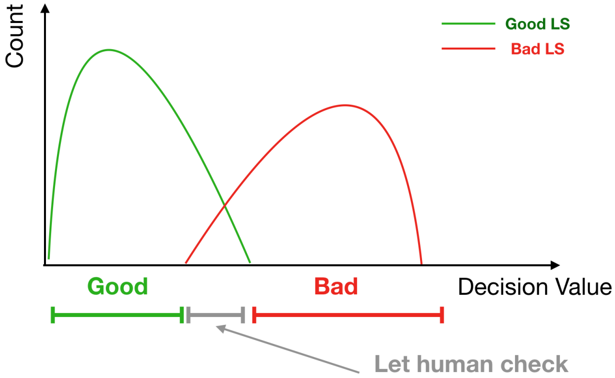


Figure: Three possible region of prediction

Datasets

- JetHT
- 2016 data from Run2
- 39 histogram of physics quantity e.g. JetPt, JetEta, JetPhi, etc.
- 259 Features (39×7)
- Good LS defined in Golden JSON else Bad LS

Histogram representation

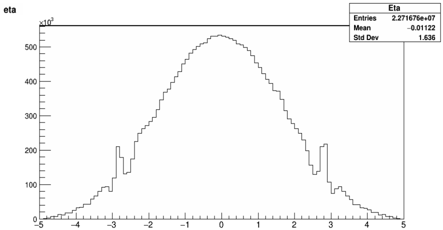


Figure: Example of Eta distribution

- Collection of physics objects e.g. photons, muons and so on
- Measurement quantity: Transverse momentum, eta, phi, etc.

1. Quantize [10%, 30%, 50%, 70%, 90%] of the histogram
2. Combine mean and rms
3. use these **7 values to represent one histogram**

Data Preprocessing

- MinMaxScalar Transformation
- Consider Lumisection i and Feature j

$$x'_{ij} \leftarrow \frac{x_{ij} - \min_{\forall i \in S_{\text{train}}}\{x_{ij}\}}{\max_{\forall i \in S_{\text{train}}}\{x_{ij}\} - \min_{\forall i \in S_{\text{train}}}\{x_{ij}\}} \tag{1}$$

- Then our datapoint should be in range [0, 1]

Semi-supervised Learning

- Unsupervised Models
  - Schölkopf's One-Class SVM
  - Isolation Forest
  - 4 Flavours of Autoencoder
- Only feed good LS for model training
- Consequently, it's falling into **Semi-supervised Learning** category

Schölkopf's One-Class SVM

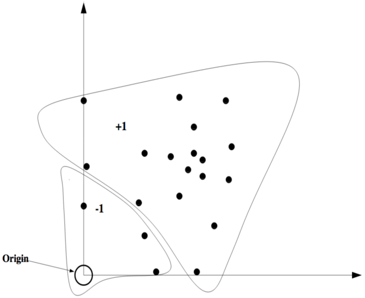


Figure: Scattering in latent space: retrieved from http://www.jmlr.org/papers/volume2/manevitz01a/manevitz01a.pdf

- Minimize (Soft Margin)

$$\frac{||w||^2}{2} + \frac{1}{\nu l}\sum_{i=1}^{l}\xi_i - \rho \qquad (2)$$

- Under

$$w \cdot \Phi(x_i) \geqslant \rho - \xi_i \ , \ \xi_i \geqslant 0 \quad (3)$$

- **Kernel**: Gaussian Base Radial function (GBF)
- Determine tangent distance from hyperplane

Isolation Forest

- Ensemble Forest from tree by subsampling (Ψ)
    - Iteratively picking up features and random value to construct the node (equivalent to step function)
    - Anomaly score evaluate from average depth of the instance over forest

$$s(x, \Psi) = \exp^{-<h(x)>/c(\Psi)} \tag{4}$$

- where
    - $h(x)$ is the depth in tree h
    - $c(\Psi)$ normalization factor growing as $\log_2(\Psi)$ from branching

[1] https://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/icdm08b.pdf?q=isolation-forest

Vanilla Autoencoder

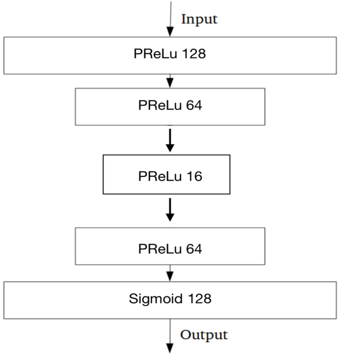


Figure: Body of Vanilla AE

- Concise the information into small latent space and reconstruct
- Loss function

$$\mathcal{L}_{\text{tot}} \equiv \frac{1}{N} \sum_{i}^{N} |x - \tilde{x}|^2 \qquad (5)$$

Sparse Autoencoder

- Similar to Vanilla AE
- Tweak by L1 Regularizaion (Prevent overfitting)
- Loss function

$$\mathcal{L}_{\text{tot}} \equiv \frac{1}{N}\sum_{i}^{N}|x-\tilde{x}|^{2}+\lambda_{s}\sum_{j}||w_{j}|| \tag{6}$$

Contractive Autoencoder

- Similar to Vanilla AE
- Tweak by Jacobi Matrix (Prevent variation in dataset)
- Loss function

$$\mathcal{L}_{\text{tot}} \equiv \frac{1}{N}\sum_{i}^{N}|x-\tilde{x}|^2 + \lambda_{\text{c}}||J_h(x)||^2 \tag{7}$$

- Jacobi matrix in our cases
  - PReLu activation function

$$||J_h(x)||^2 = \sum_j [\alpha_j H(-(w_{ji}x^i + b_j)) + H(w_{ji}x^i + b_j)] \sum_i (w_{ji})^2 \tag{8}$$

  - Sigmoid activation function

$$||J_h(x)||^2 = \sum_j [h_j * (1-h_j)] \sum_i (w_{ji})^2 \tag{9}$$

Variational Autoencoder

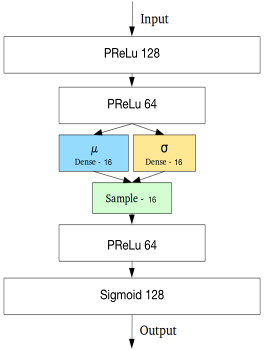


Figure: Body of Variaitonal AE retrieved from https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

- Random "new sampling" in latent space by gaussian random generator

$$\mathcal{Z} \equiv \mathcal{N}(\mu_i, \sigma_i) \qquad (10)$$

- Tweak by reduce discontinuity in latent space
- Loss function

$$\mathcal{L}_{\text{tot}} = \frac{1}{N}\sum_{i}^{N} |x - \tilde{x}|^2 + \mathcal{D}_{\text{KL}}(p|q) \qquad (11)$$

Variational Autoencoder

Theorem (Kullback-Leibler Divergence)

- *"How much information that loss after represent data with function"*

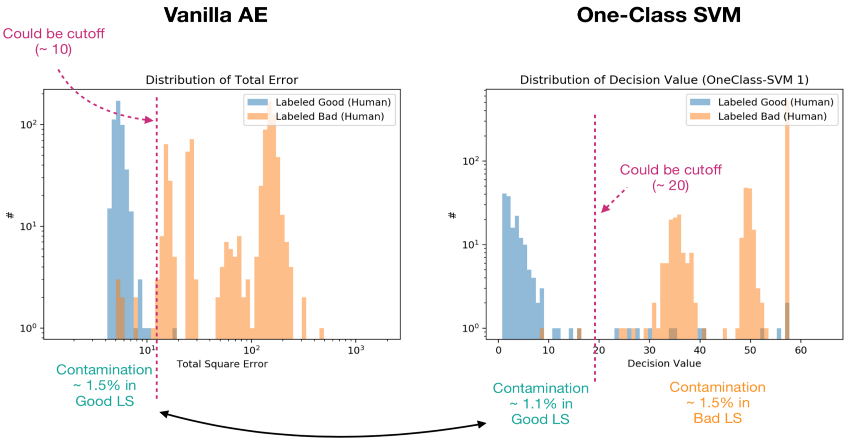
$$\mathcal{D}_{KL} \equiv < \log p - \log q > \tag{12}$$

- *Where p is observed value and q is approximaiton function*
- *Since our q is Gaussian function*

$$\mathcal{D}_{KL} = \frac{1}{2}(\mu_i^2 + \sigma_i^2 - 2\log(\sigma_i) - 1) \tag{13}$$

$$\mathcal{L}_{\text{tot}} = \frac{1}{N}\sum_i^N |x - \tilde{x}|^2 + \frac{1}{2}(\mu_i^2 + \sigma_i^2 - 2\log(\sigma_i) - 1) \tag{14}$$

Find the cutoff



Spot the same Bad => Good LS

Performance

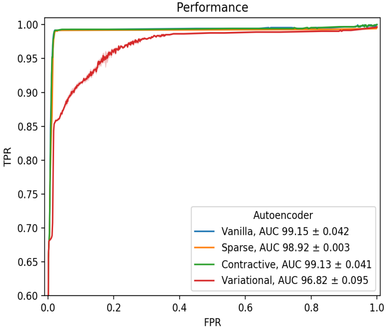


Figure: Various AE

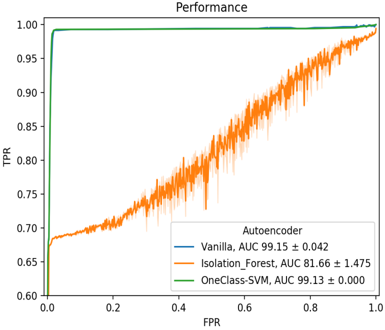


Figure: Vanilla vs SVM vs Forest

Example of Reconstruction

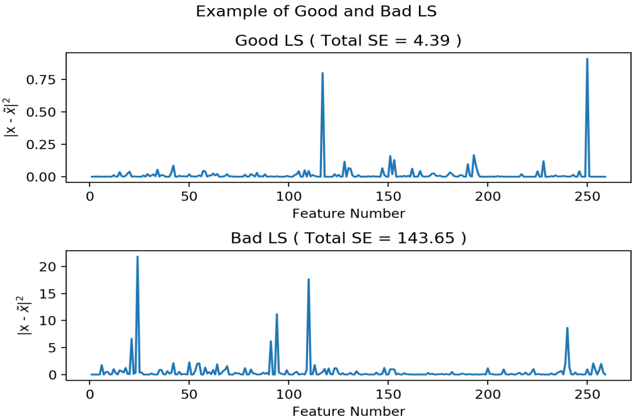
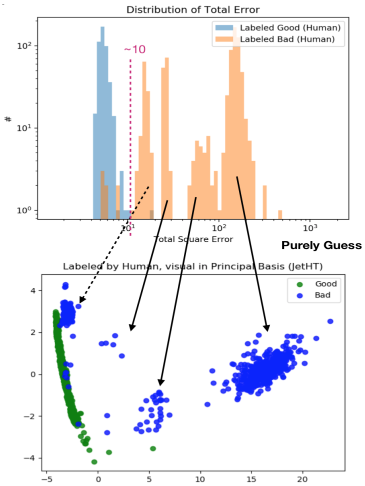
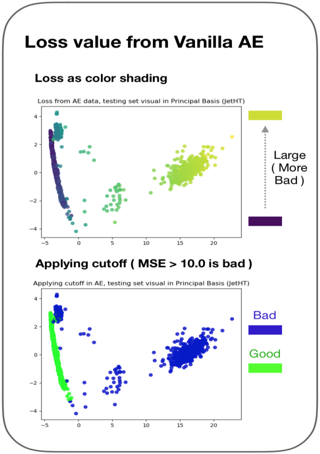


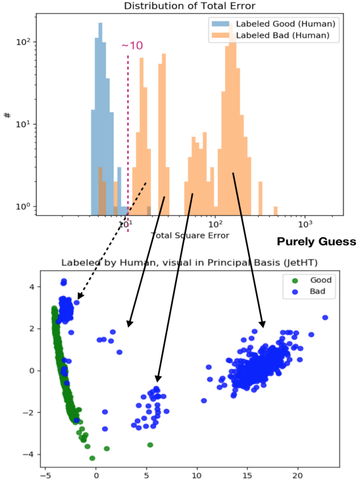
Figure: Reconstruction error from Vanilla AE

Extended Investigation



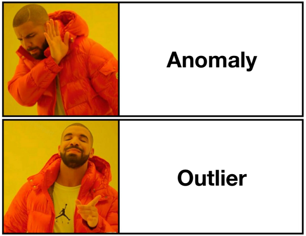
Extended Investigation





Summary

- Semi-supervised learning yield a remarkable result
- There is no grey zone from our model for this dataset
- There are 1-1.5% contamination from the prediction
- Bad LS could be divided into two parts
  - Bad with some pattern
  - Anomaly



Future work

- Good LS from Runregistry and DCs bits still suspicious not to be a ground truth
- Require simulation data
    - To be purely good LS for training
    - For testing the failure scenario

Thank you

Question?

Back up

ROC Curve

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