Machine Learning Based Outlier Detection for Data Certification

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Overview

Data Quality Monitoring (DQM)

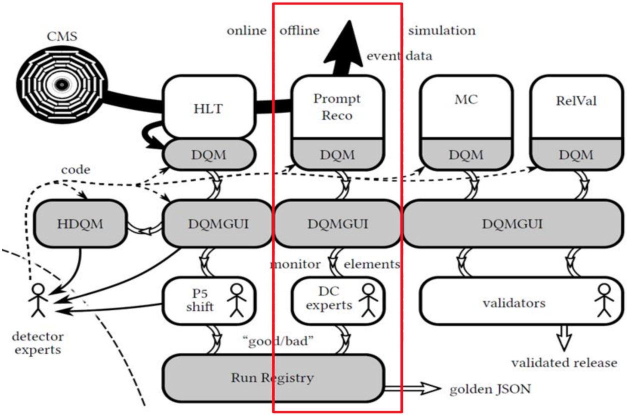


Figure: Tools and Processes of DQM, retrieved from M. Schneider, CHEP 2018

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(LS) is taken around 23 seconds
- Criteria for bad LS
  1. Runs tagged as bad by human (whole run)
  2. Automatically filter by DCS bits, beam status and etc. (LS levels)
  3. In rare cases are marked by DC experts (LS levels)
- The Golden JSON contains the list of all good LS

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

Objective

- **Certify data quality in lumisection granularity**
    - Classification on the basis of actual data distributions per LS
- Reduce manual work of DC Experts

Expectation

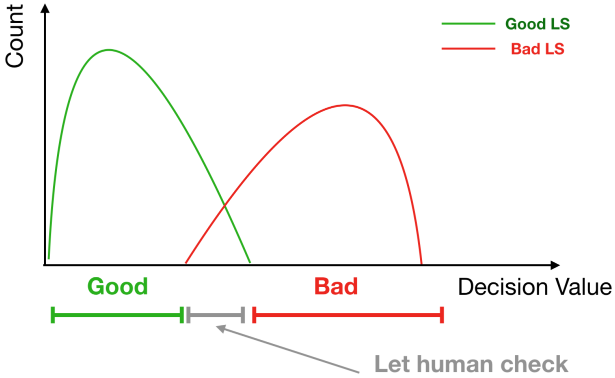


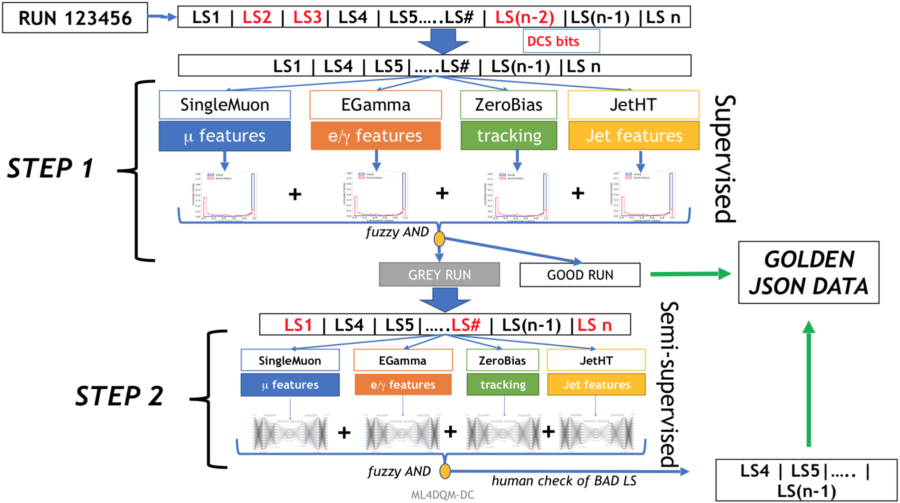
Figure: Three possible regions of prediction

Proposal For An Alternative approach: two steps

- The automatic DCS bit flagging will stay, ML applied on top of it
- Automatize the Data Certification procedure in two steps
  1. Provide a reliable quality **flag per Run using** grey-zone approach and **Supervised** models (artificial BAD data can be used for training)
  2. **Use Autoencoders** only on the grey-zone with the goal **to search for anomalous LS** and flag them automatically, human double check at this stage
- Using physical quantities as
  - **features** (pT, eta, etc) and
  - **objects** mapped to the relevant Primary Dataset (i.e tracks to ZeroBias, muons to SingleMuon ... etc)

  to better mimic the current DC procedure
- In this work, I will focus only on second step

[1] F. Fiori, ML Applied To Data CertificationStatus and Perspective



[1] F. Fiori, ML Applied To Data CertificationStatus and Perspective

Datasets

- pp collisions, 2016 data, PromptReco, JetHT
- Each lumisection (datapoint) contains
  - 39 histogram of physics quantity e.g. JetPt, JetEta, JetPhi, etc.
  - Represent one histogram with 7 numbers
  - 259 Features (39×7)
- Good LS defined in Golden JSON else Bad LS
- Data splitting
  - 60% good LSs for training
  - 20% good LSs for validation
  - 20% good LSs combine with bad LS for testing

Histogram representation

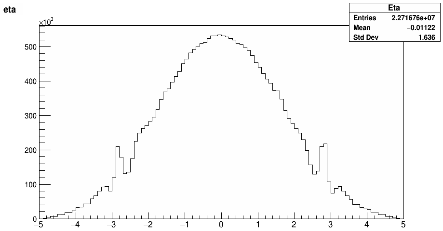


Figure: Example of Eta distribution

- Collection of physics objects e.g. photons, muons and so on
- Measurement quantity: Transverse momentum, eta, phi, etc. ▸ Click here to see all selected features

1. Quantize [0%, 25%, 50%, 75%, 100%] 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

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

- 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
- Feed only good LS for train and validate the model
- Testing with good LS and bad LS
- Consequently, it's falling into **Semi-supervised Learning** category

Schölkopf's One-Class SVM

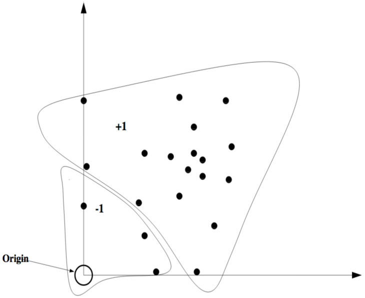


Figure: Scattering in latent space: retrieved from http://www.jmlr.org/papers/volume2/manevitz01a/manevitz01a.pdf

- 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

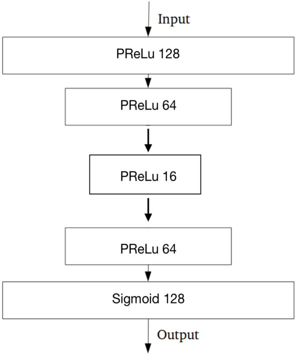


Figure: Body of Vanilla AE

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

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

- Truncated normal initializer
- Adam optimizer

Sparse Autoencoder

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

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

- where $\lambda_s = 10^{-5}$

Contractive Autoencoder

- Tweak by Jacobi Matrix (Prevent variation in dataset)
- Loss function

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

- where $\lambda_{\mathrm{c}} = 10^{-5}$

Contractive Autoencoder

- Definition

$$||J_h(x)||^2 \equiv \frac{1}{N}\sum_{ij}\left(\frac{\partial h_j}{\partial x_i}\right)^2 \quad (8)$$

- where h_j is activation function
- In our cases
  - PReLu activation function

$$||J_h(x)||^2 = \frac{1}{N}\sum_{j}[\alpha_j H(-(w_{ji}x^i + b_j)) + H(w_{ji}x^i + b_j)]\sum_{i}(w_{ji})^2 \quad (9)$$

  - Sigmoid activation function

$$||J_h(x)||^2 = \frac{1}{N}\sum_{j}[h_j * (1 - h_j)]\sum_{i}(w_{ji})^2 \quad (10)$$

Variational Autoencoder

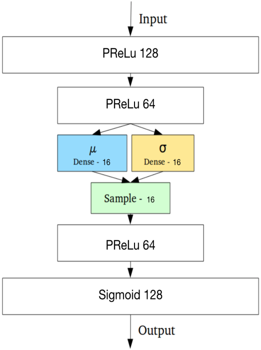


Figure: Body of Variational AE retrieved from https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

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

$$\mathcal{Z} \equiv \mathcal{N}(\mu_i, \sigma_i) \tag{11}$$

- Tweak by reduce discontinuity in latent space
- Loss function

$$\mathcal{L}_{\text{tot}} = \frac{1}{N}\sum_i^N |x - \tilde{x}|^2 + \mathcal{D}_{\text{KL}}(p|q) \tag{12}$$

Variational Autoencoder

Theorem (Kullback-Leibler Divergence)

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

$$\mathcal{D}_{KL} \equiv < \log p - \log q > \tag{13}$$

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

$$\mathcal{D}_{KL,i} = \frac{1}{2}\sum_{k}^{n_{latent}}(\mu_{ik}^2 + \sigma_{ik}^2 - 2\log\sigma_{ik} - 1) \tag{14}$$

$$\mathcal{L}_{\mathrm{tot}} = \frac{1}{N}\sum_{i}^{N}|x - \tilde{x}|^2 + \frac{1}{2N}\sum_{i}^{N}\sum_{k}^{n_{\mathrm{latent}}}(\mu_{ik}^2 + \sigma_{ik}^2 - 2\log\sigma_{ik} - 1) \tag{15}$$

Performance

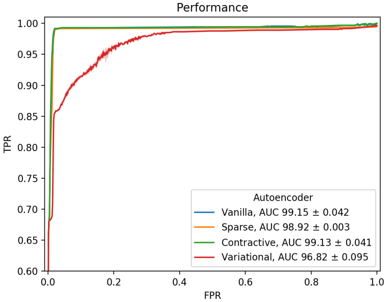


Figure: Various AE

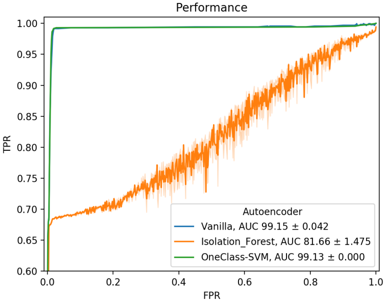
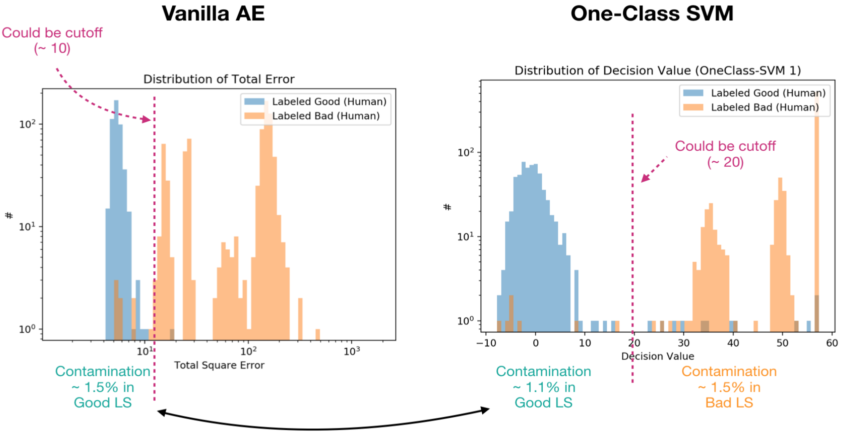


Figure: Vanilla vs SVM vs Forest

Under configuration

- **Isolation Forest** $N_{\text{tree}} = 200, \;\; \Psi = 512$
- **OneClass-SVM** $\nu = 0.1, \;\; \gamma = 0.1$(Inverse gaussian width)

Find the cutoff



Spot the same Bad => Good LS

Example of Reconstruction

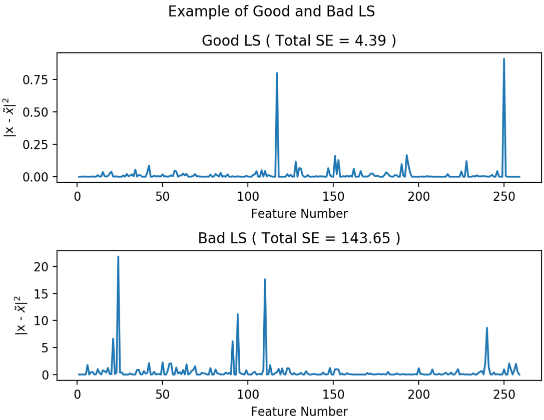
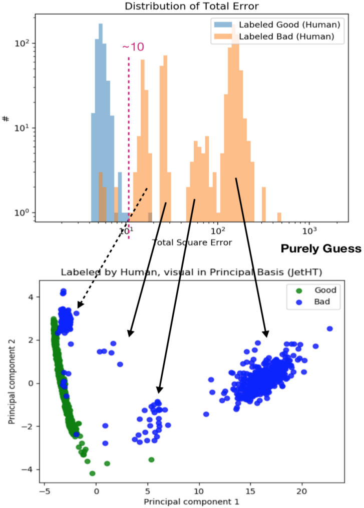
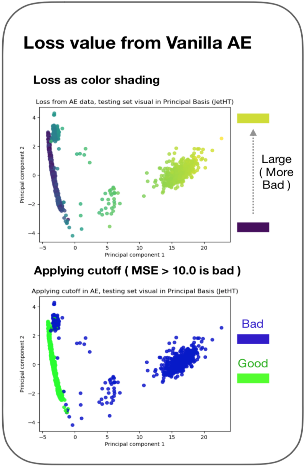


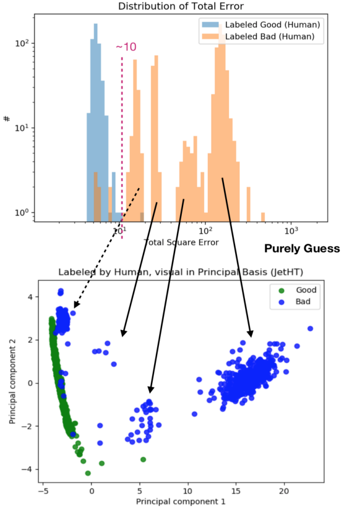
Figure: Reconstruction error from Vanilla AE

Extended Investigation



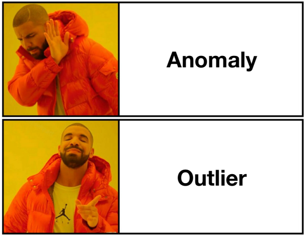
Extended Investigation





Summary

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



Future work

- Exploit the same technique in 2018 dataset
- 2018 data preparation still in progress
- Remove trivial bad LS (run tag and DCS bits) but take consider only bad LS that came from DC Experts

Future work

Let's have a look at principal component for JetHT PD

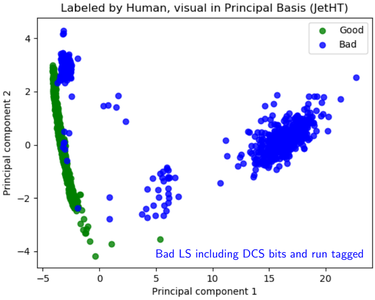


Figure: 2016 data

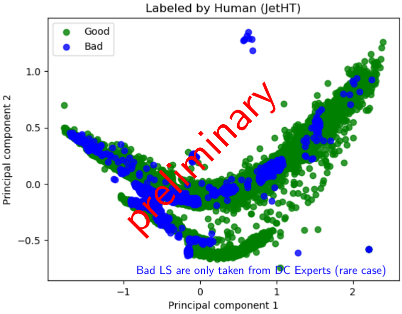


Figure: 2018 data

Acknowledgement

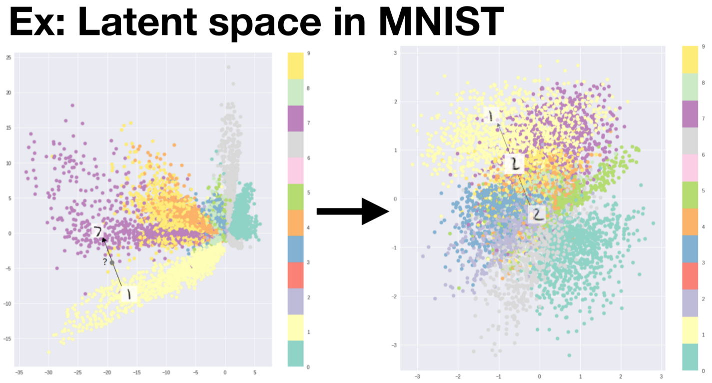
- CERN Summer Student program 2019
- Especially
  - **Marcel Andre Schneider**
  - Francesco Fiori
  - Kaori Maeshima
  - Adrian Alan Pol
  - Countless CMS DQM people :)
- GPU resources from IBM in collaboration with CERN Openlab

Thank you

Question?

Back up

Example of removing discontinuity in latent space



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