Report for Preliminary Study

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CMS DQM-ML4DC
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Outline

- Datasets
- Model
- Results
- Let find the cutoff (Application)
- Extended Investigation

Datasets

- JetHT
- 2016 Datasets
  - 259 Features
- Lumisection certification granularity
  - Good LS defined in Golden JSON
  - Rest of LS are bad

Datasets

- **Preprocessing**
  - **MinMaxScalar** Transformation
  - Consider Lumisection i and Feature j

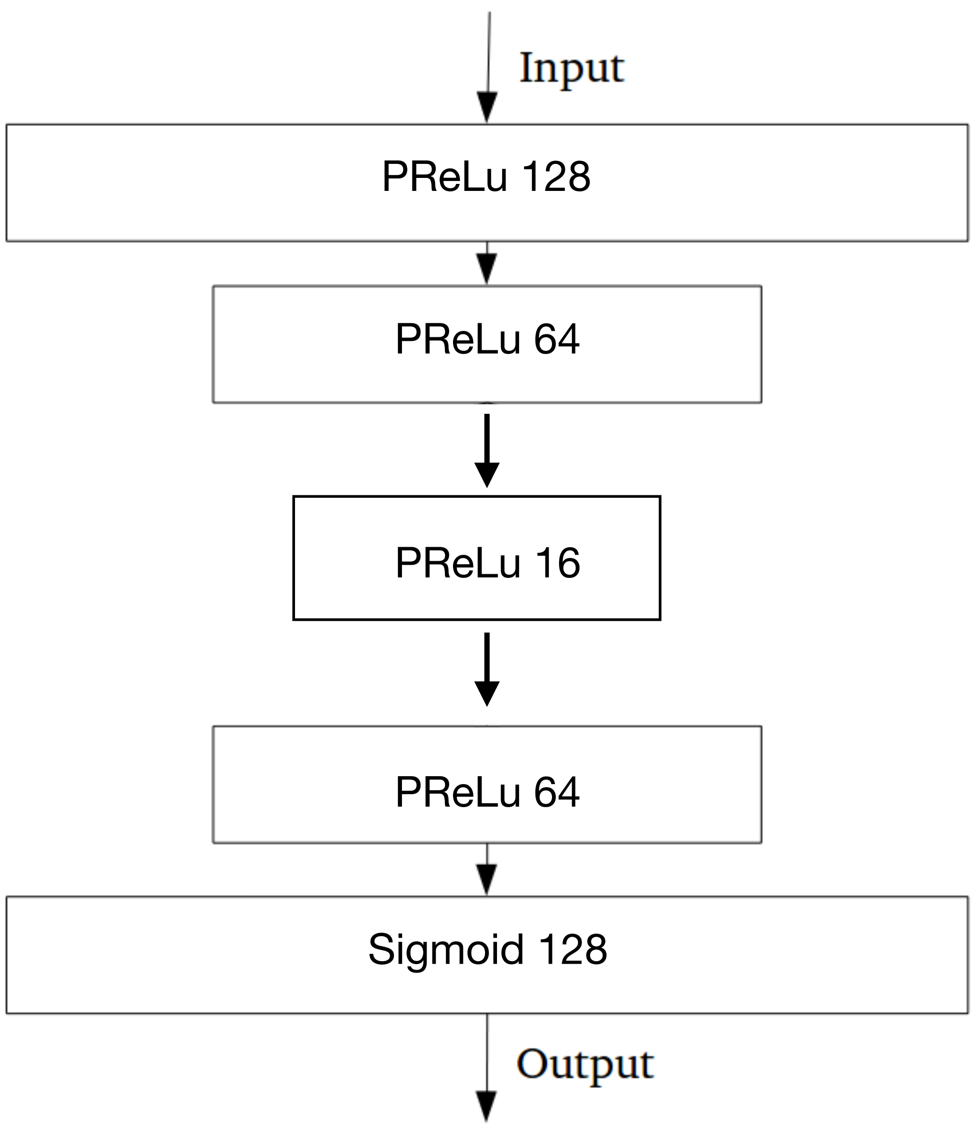
$$x'_{ij} \leftarrow \frac{x_{ij} - \min_{\forall i \in S_{\text{train}}}\{x_{ij}\}}{\max_{\forall i \in S_{\text{train}}}\{x_{ij}\} - \min_{\forall i \in S_{\text{train}}}\{x_{ij}\}}$$

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

Model

- 4 Flavours of Autoencoder
    - **Vanilla**
    - Sparse
    - Contractive
    - Variational
- No Neural-net
    - Isolation Forest
    - **Schölkopf’s One-Class SVM**

My Vanilla AE



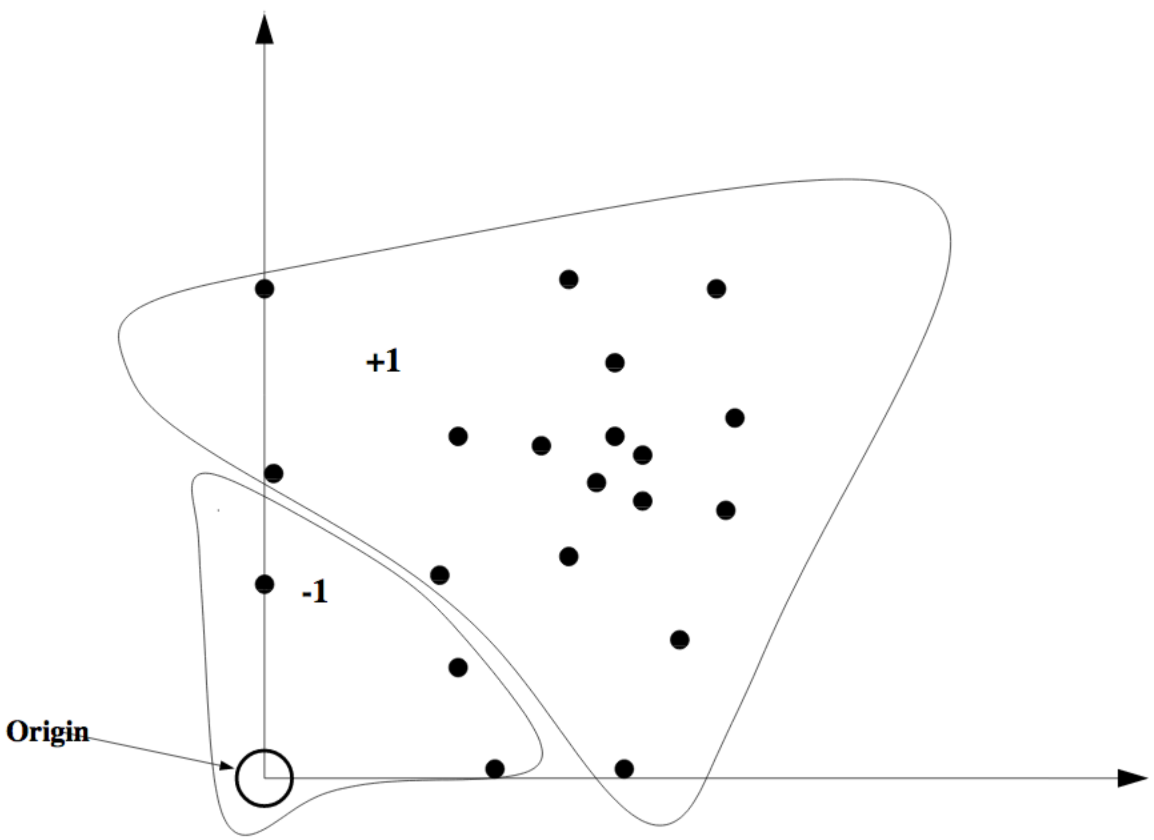
- Sigmoid fn. in output should bound between zero and one
- PReLu for the rest of activ. fn.

Training Dependency

- Truncated normal variable initializer
- Batch size 256
- EPOCHS 1200

Image modified from https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

Schölkopf's One-Class SVM



- Minimize (Soft margin)

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

- Under

$$w \cdot \Phi(x_i) \geqslant \rho - \xi_i; \xi_i \geqslant 0$$

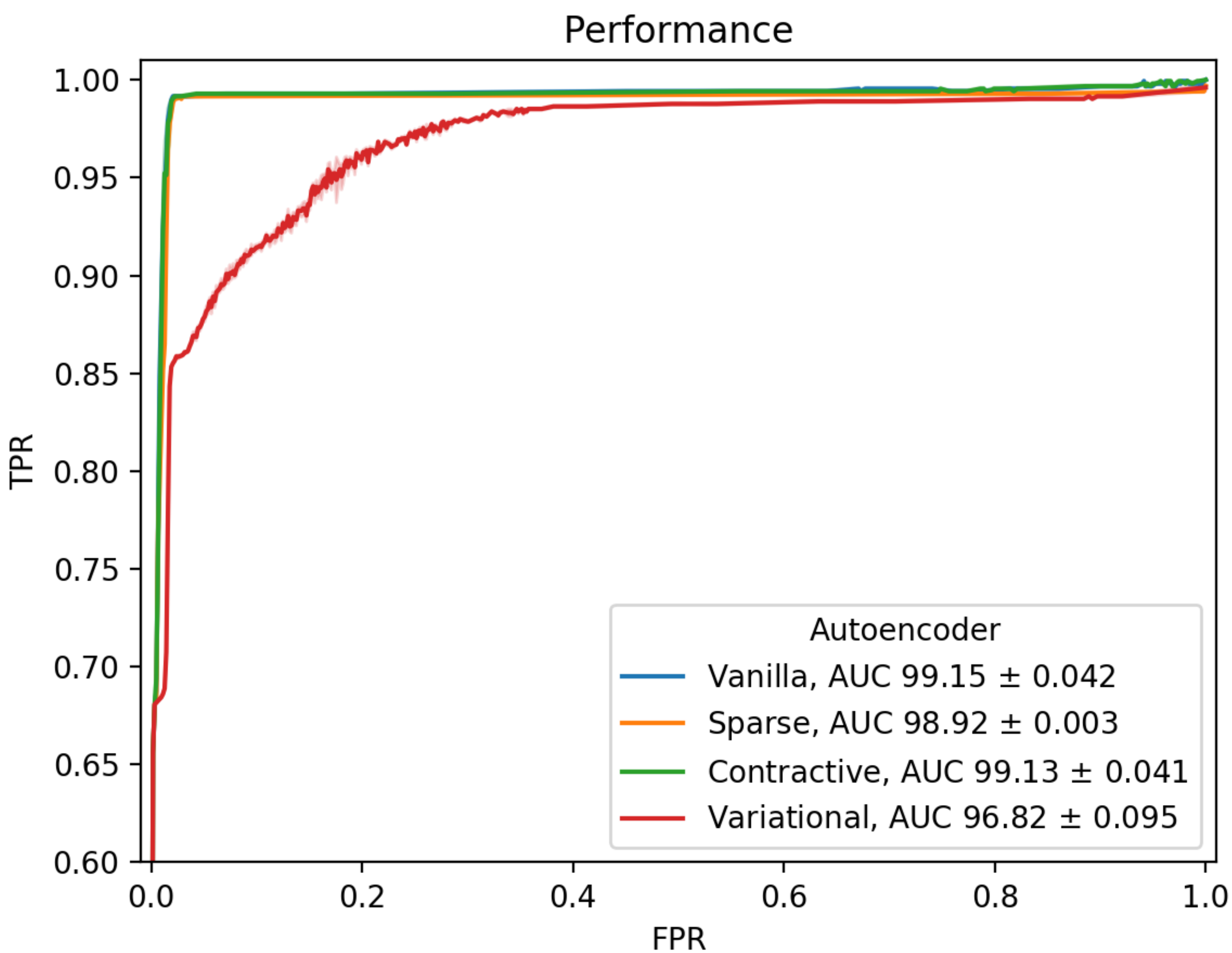
- **Kernel:** Gaussian Base Radial function (GBF)

- Determine by tangent distant from data point to hyperplane

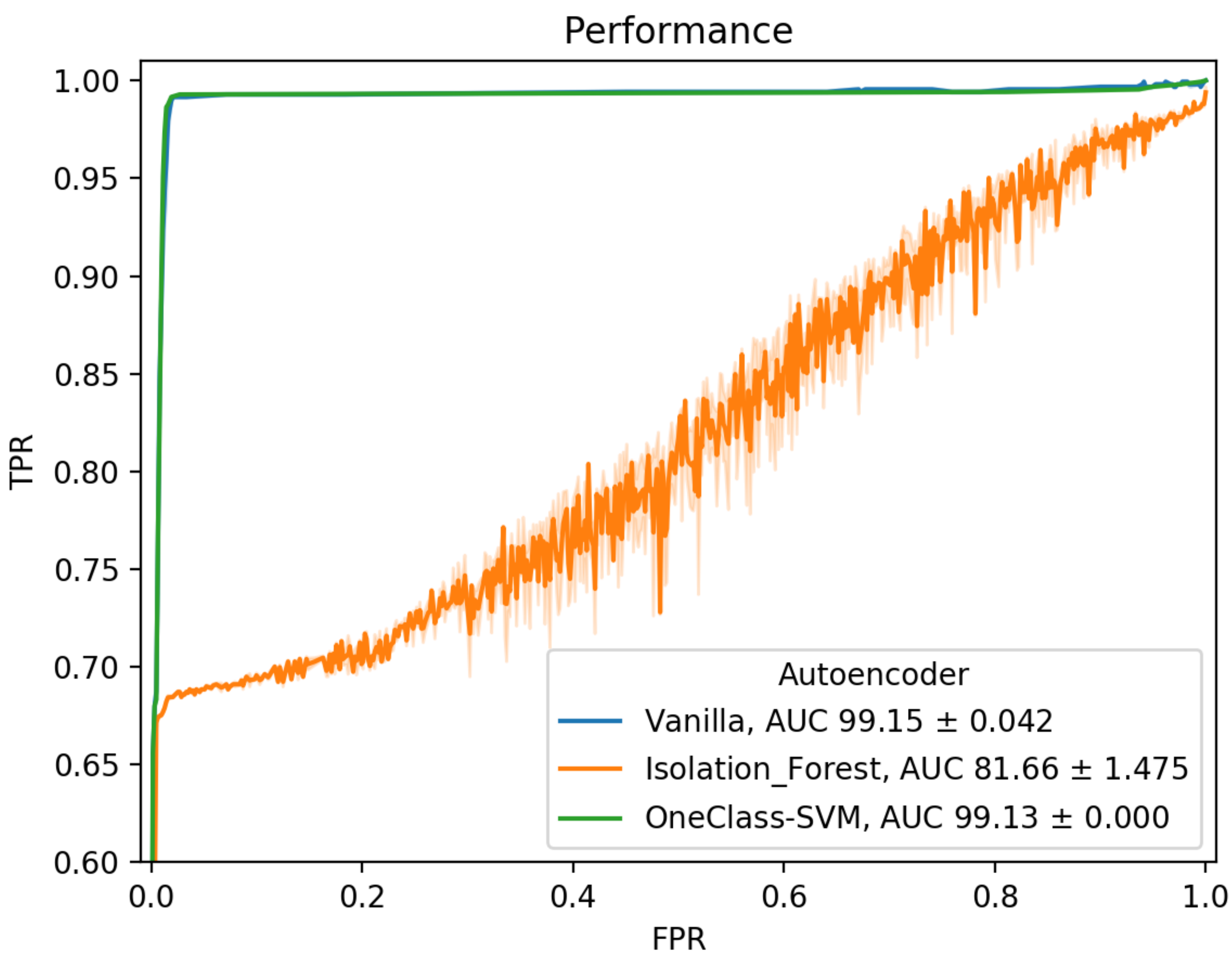
[1] http://www.jmlr.org/papers/volume2/manevitz01a/manevitz01a.pdf
[2] http://papers.nips.cc/paper/1723-support-vector-method-for-novelty-detection.pdf

Results

AE Performance



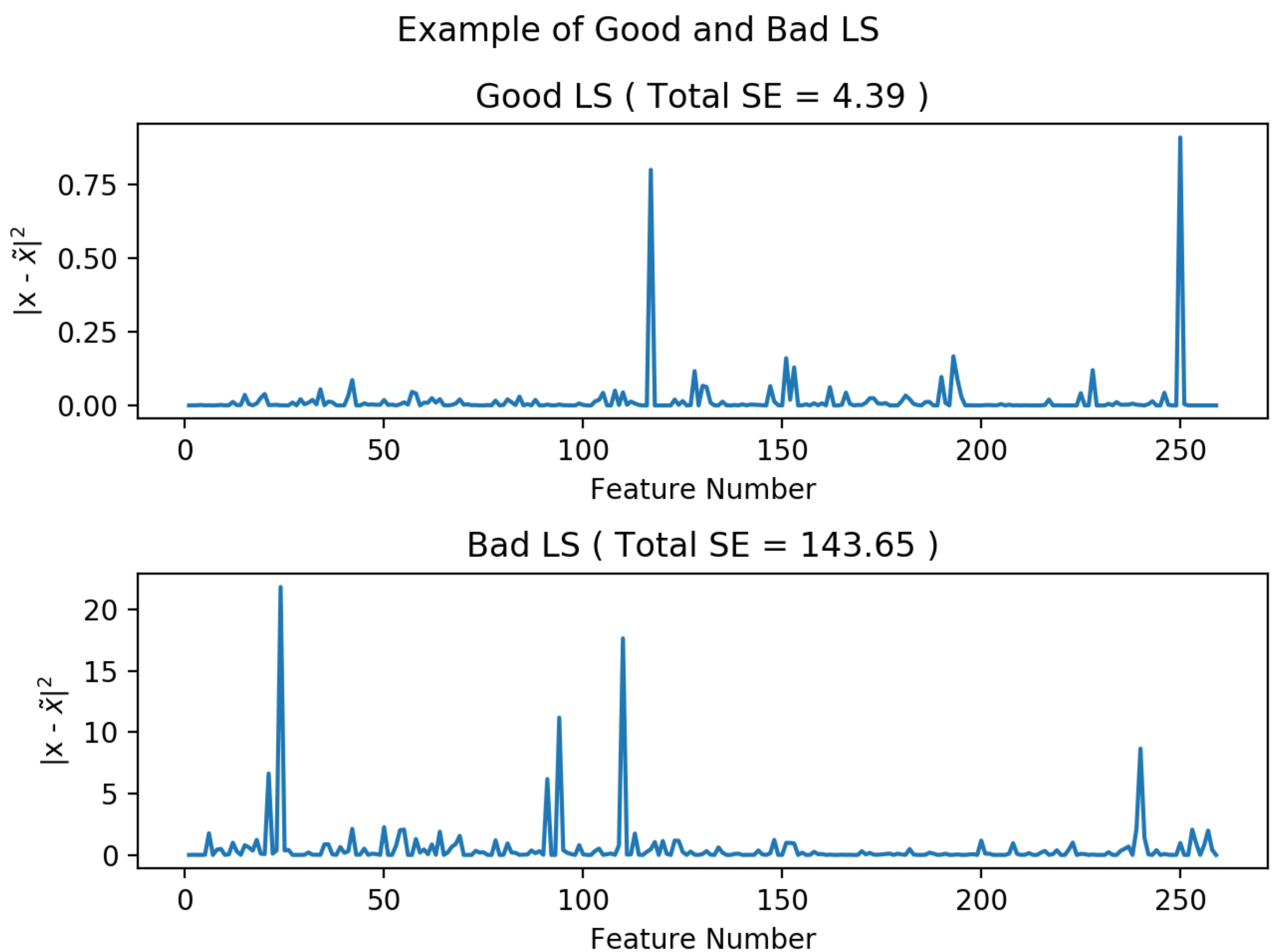
Vanilla vs no-NN Performance



Under configuration

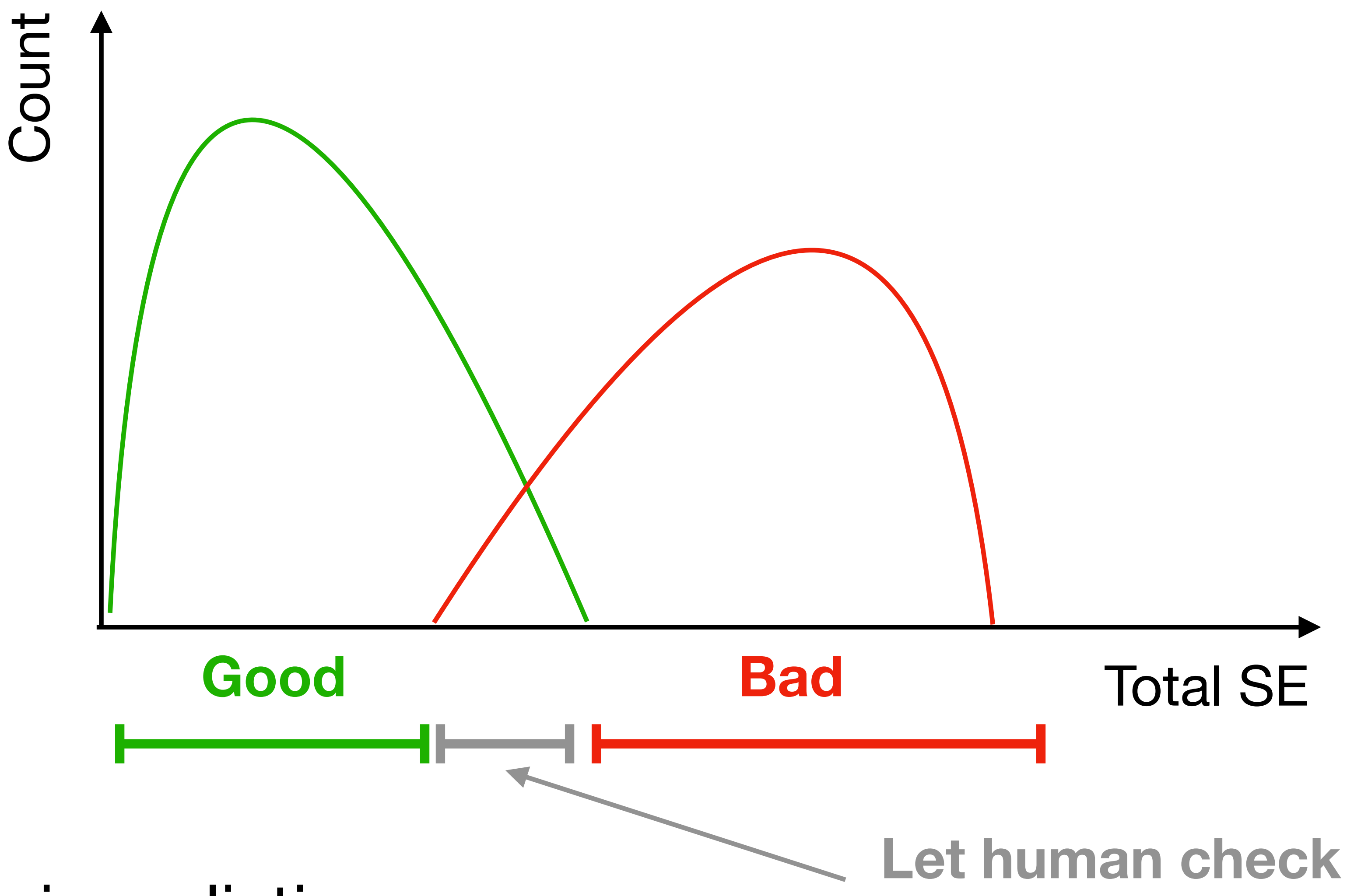
- Isolation Forest: tree = 200, sampling_size = 512
- OneClass-SVM: nu=0.1, gamma=0.1(inverse gaussian width)

Example from Vanilla



Find the cutoff

- **Expect** the total square error (SE) distribution to be like

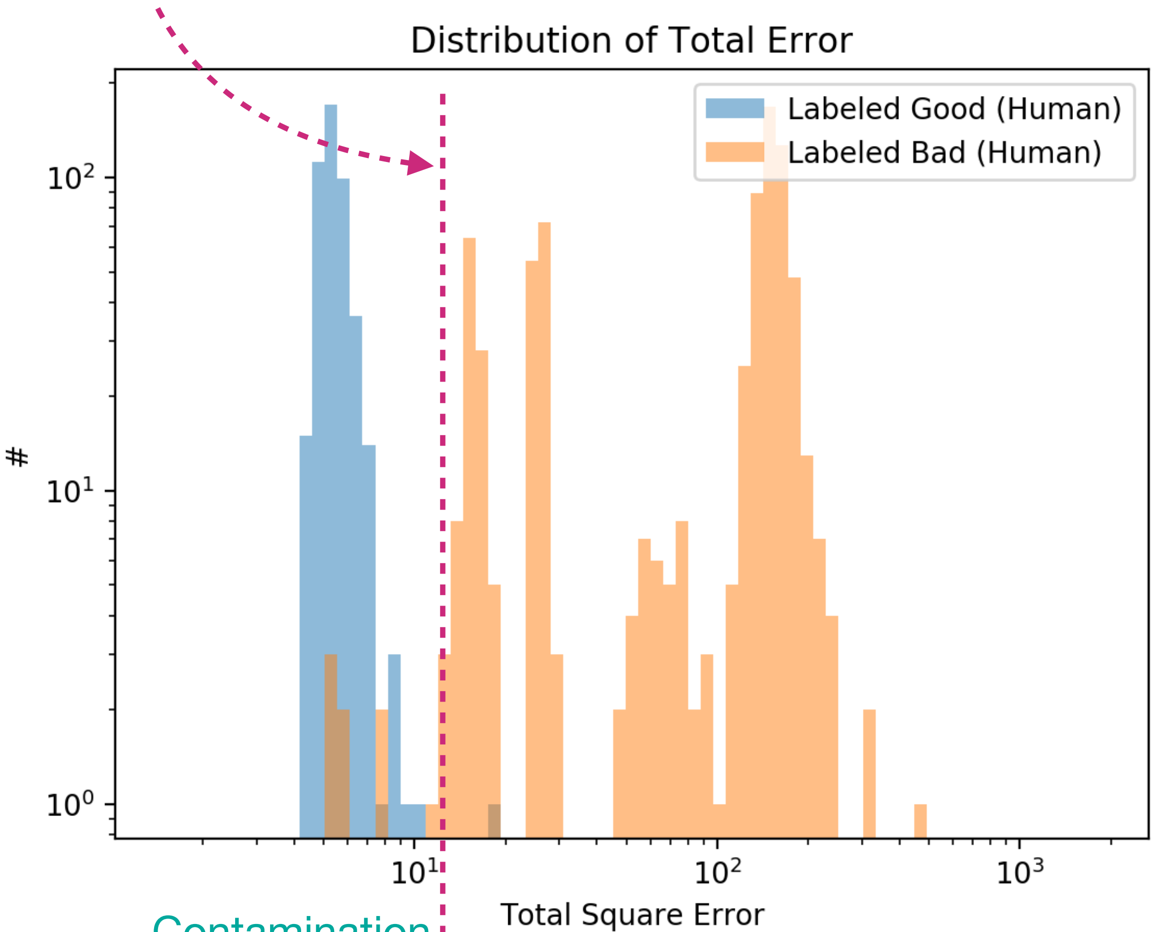


- Next slide is realistic..

Find the cutoff

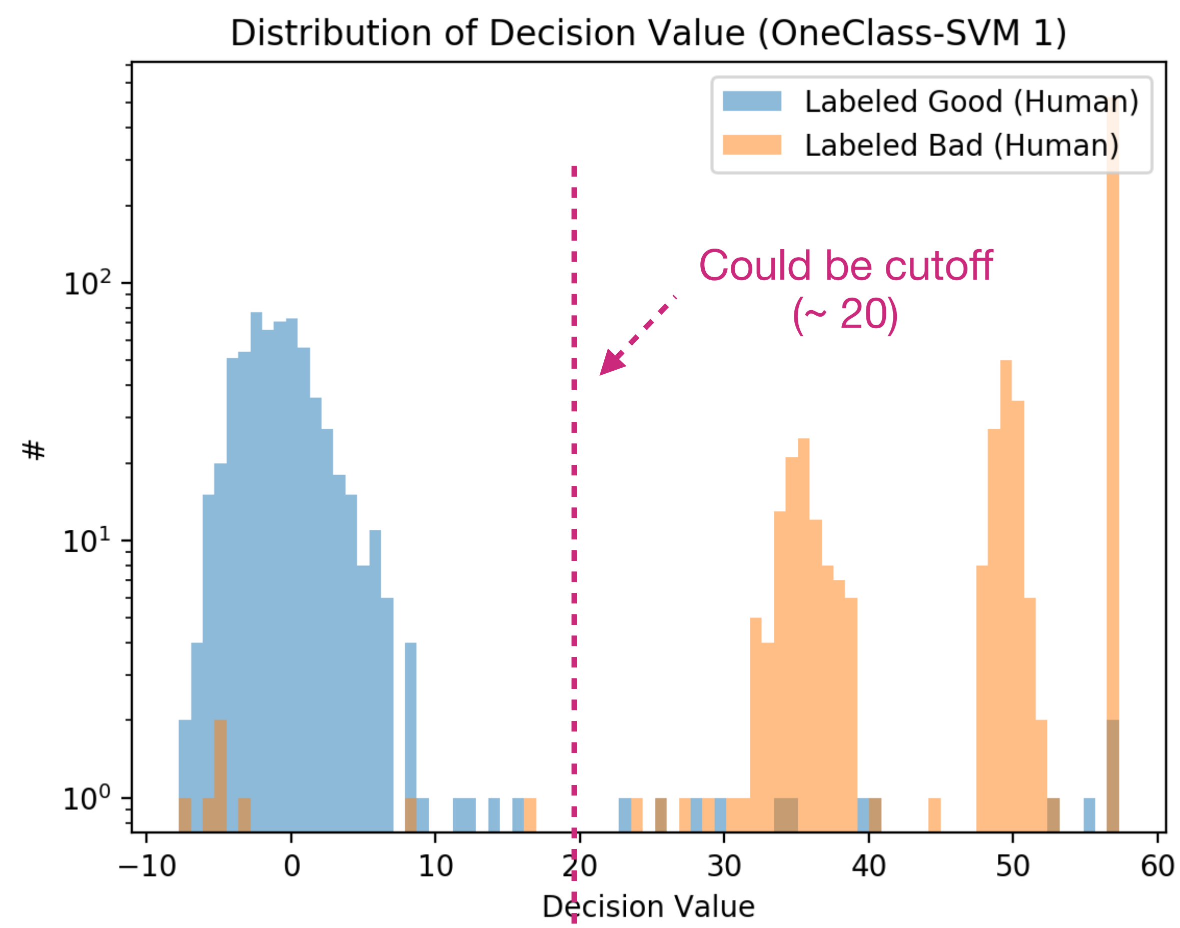
Vanilla AE

Could be cutoff
(~ 10)



Contamination
~ 1.5% in
Good LS

One-Class SVM



Contamination
~ 1.1% in
Good LS

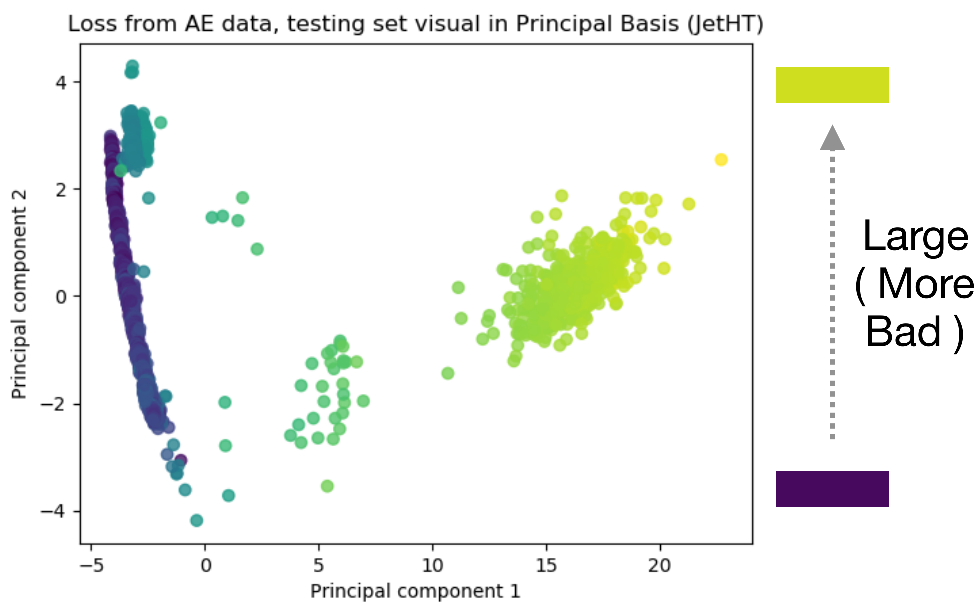
Contamination
~ 1.5% in
Bad LS

Spot the same Bad => Good LS

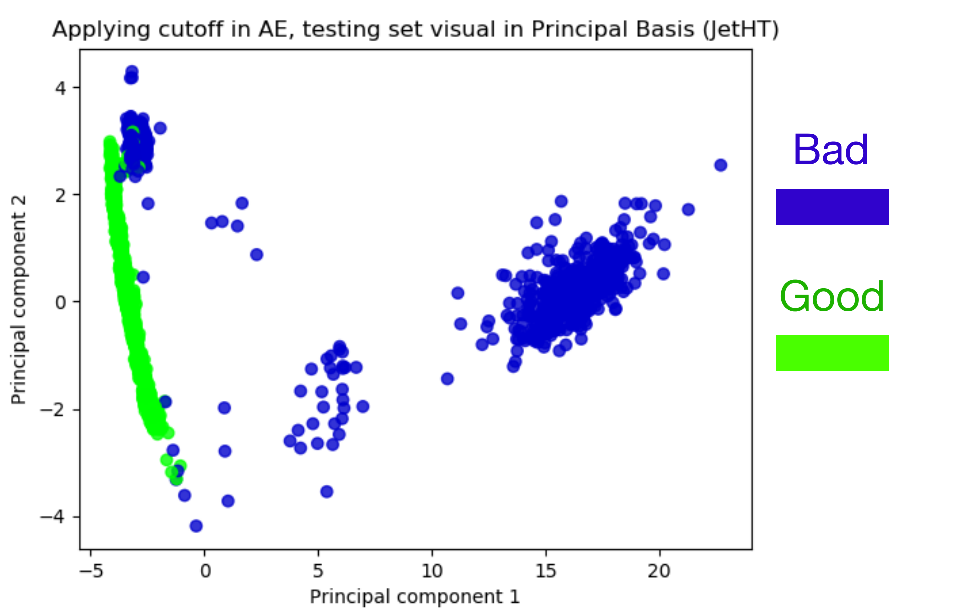
Extended Investigation

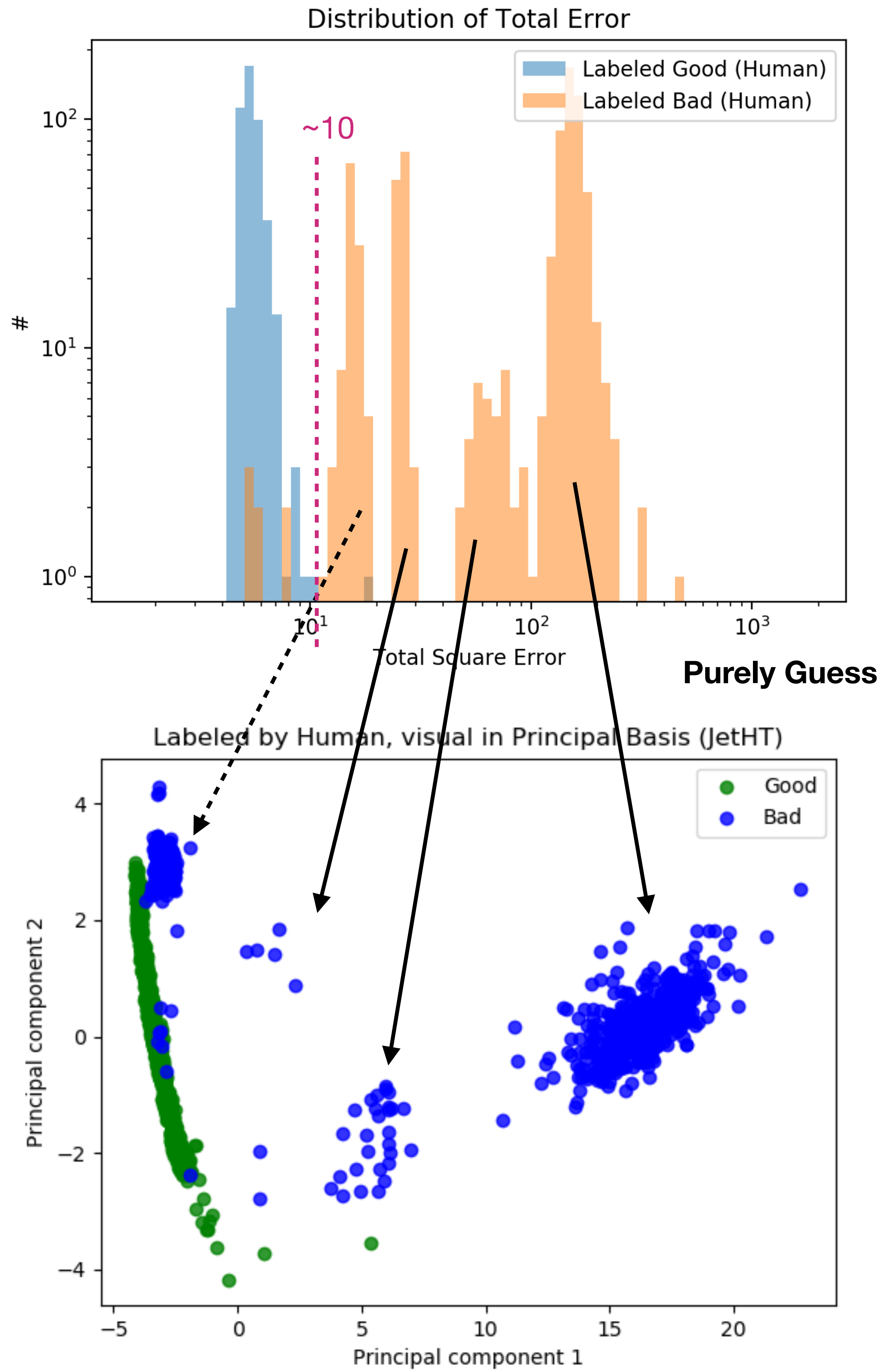
Loss value from Vanilla AE

Loss as color shading



Applying cutoff (MSE > 10.0 is bad)





Suspicious spot for 2018 datasets

- ~100k good LS and only ~1k in bad LS
- Found ~300 NaN value in some columns from new datasets
- Would be perfect if one who might use new datasets participate to help each other to inspect and discuss (not only for the model)

Backup Slide

Sparse Model

- Unsupervised
- Similar to Vanilla Autoencoder
- Tweak by **L1 Regularization (Prevent overfitting)**

$$\mathcal{L}_{\text{tot}} \equiv \frac{1}{N}\sum_{i}^{N}|x_i - \tilde{x}_i|^2 + \boxed{\lambda \sum_{j} ||w_j||}$$

Set $\lambda = 1e-4$

Contractive Model

- Unsupervised
- Similar to Vanilla Autoencoder
- Tweak by **Jacobi Matrix (Prevent variation in data)**

$$\mathcal{L} = \frac{1}{N}\sum_{i}^{N} |x_i - \tilde{x}_i|^2 + \boxed{\lambda ||J_h(x)||^2}$$

Set $\lambda = 1e-4$

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

Contractive Model

- Case PReLu activ. fn.

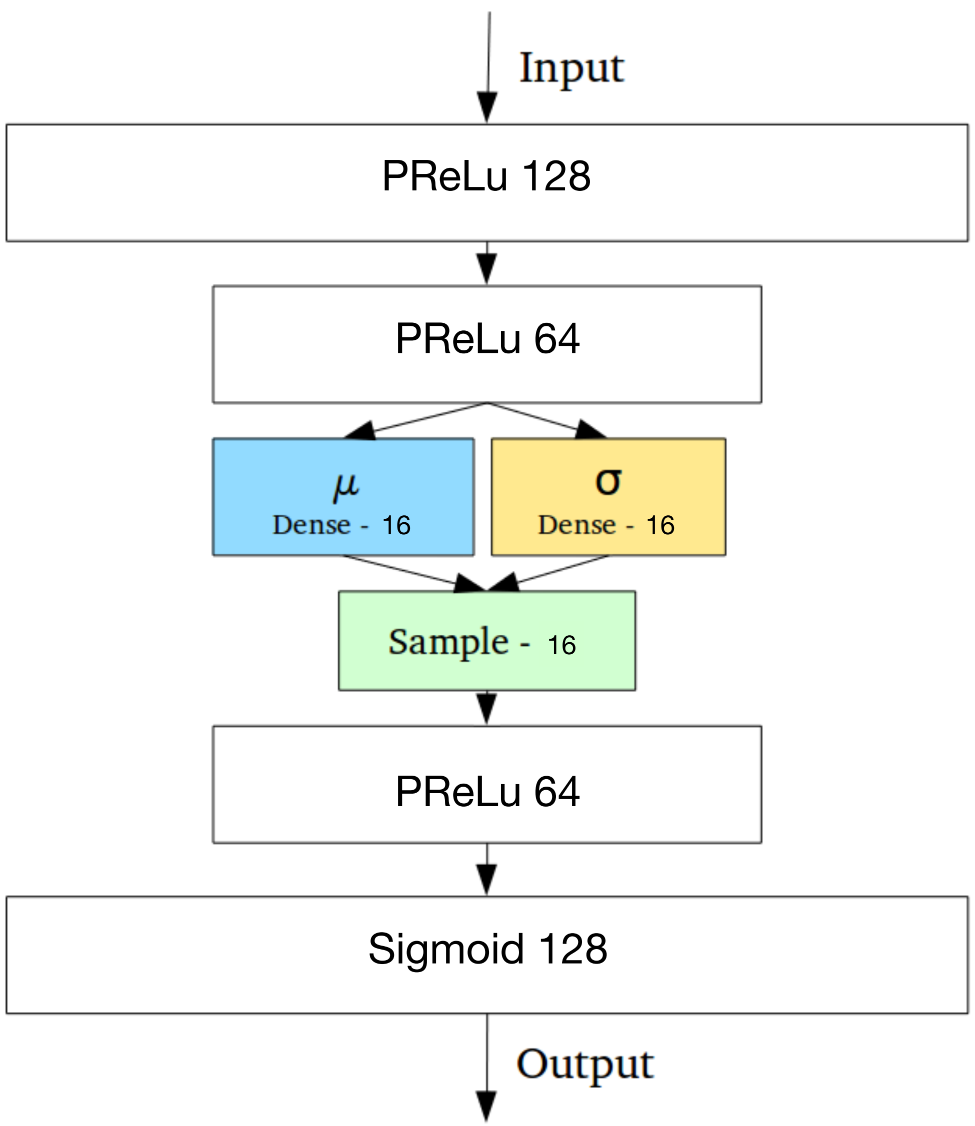
$$||J_h(x)||^2 \equiv \sum_j [\alpha_j H(-(w_{ji}x^i + b_j)) + H(w_{ji}x^i + b_j)] \sum_i (w_{ji})^2$$

- Case Sigmoid activ. fn.

$$||J_h(x)||^2 \equiv \sum_j [h_j * (I - h_j)] \sum_i (w_{ji})^2$$

Variational Model

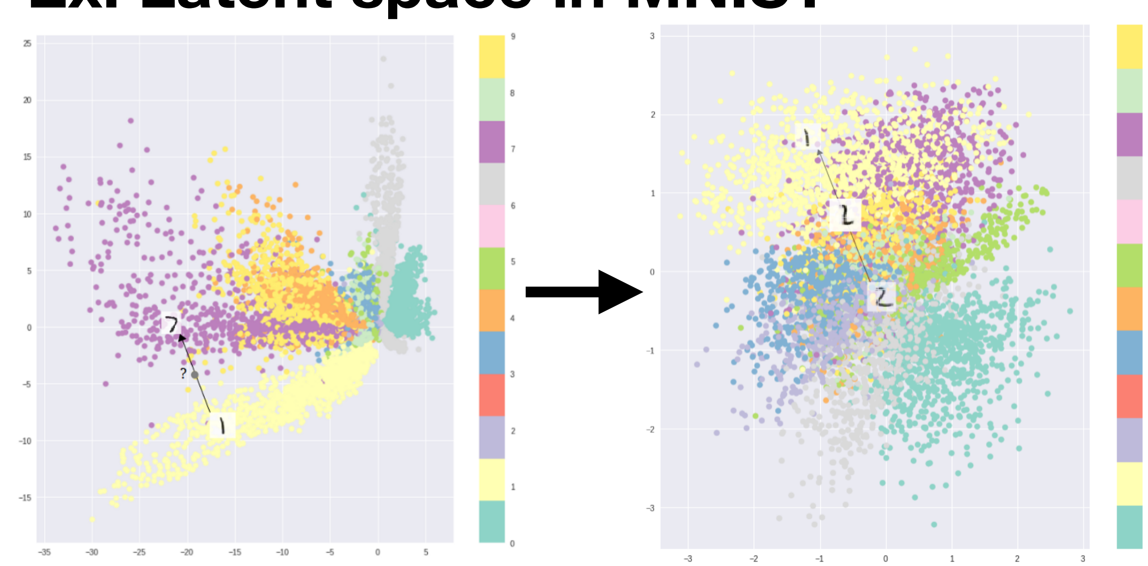
- Tweak by **Random Sampling in Encoding vector (Remove discontinuity in Latent Space)**



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

"Random new sampling by gaussian"

Ex: Latent space in MNIST



[1] https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

Variational Model

- Kullback–Leibler divergence

$$\mathcal{D}_{\mathrm{KL}}(p|q) \equiv < \log p - \log q >$$

- where p is observed value, and q is approx. fn.

- Since our q is gaussian, then

$$\mathcal{L}_{\mathrm{tot}} \equiv \mathcal{L}_{MSE} + \frac{1}{2}\sum_i(\mu_i^2 + \sigma_i^2 - \log(\sigma_i^2) - 1)$$

Isolation Forest

- Ensemble Forest from tree by subsampling (Ψ)
  - Iteratively picking up features and random value to contract the node (equivalent to step fn.)
- Anomaly score likely to be average depth of the instance over forest

$$s(x, \Psi) \equiv e^{-<h(x)>/c(\Psi)}$$

- Where
  - $h(x)$ is the depth in tree h
  - $c(\Psi)$ normalization factor growing as log2(Ψ) from branching