The Federation

A novel machine learning technique applied on data from the Higgs Boson Machine Learning Challenge

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Data analysis in High Energy Physics

- Large datasets are typical in HEP
  - $\Rightarrow$ Because of resource constraints, often only a subset of data is used
- Background dominated data $\Rightarrow$ Imbalanced data
- Complex data
  - $\Rightarrow$ Undefined values
  - $\Rightarrow$ Categorical values

Problem: Training a model on a large dataset can take a lot of computing time and resources. How can this be mitigated?

What is the Federation?

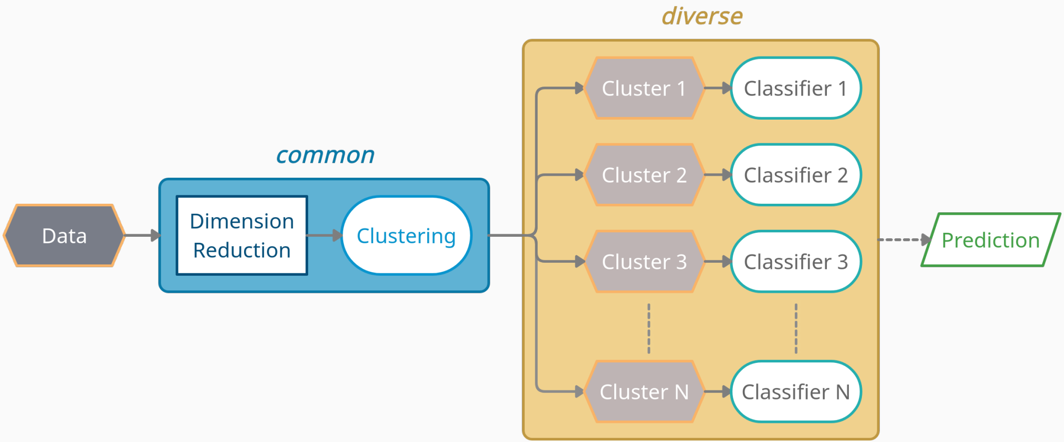
Idea:
1. Split data into smaller subsets and for each subset train a model.
2. Predict by using the ensemble of models

Issue: But how to split the data wisely and how to predict? $\Rightarrow$ Federation

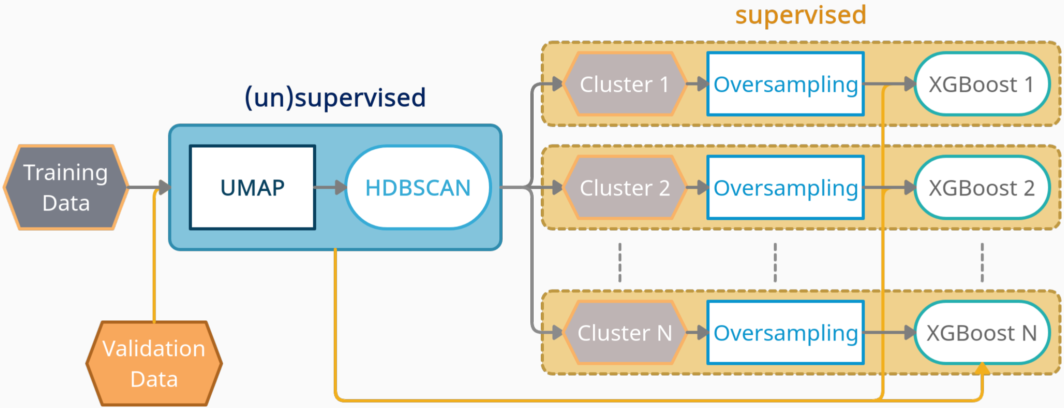
Definition

*"**federation**, the government of a federal community. In such a model there are two levels of government, one dealing with the* ***common*** *and the other with the territorially* ***diverse****."* `https://www.britannica.com/topic/federation`

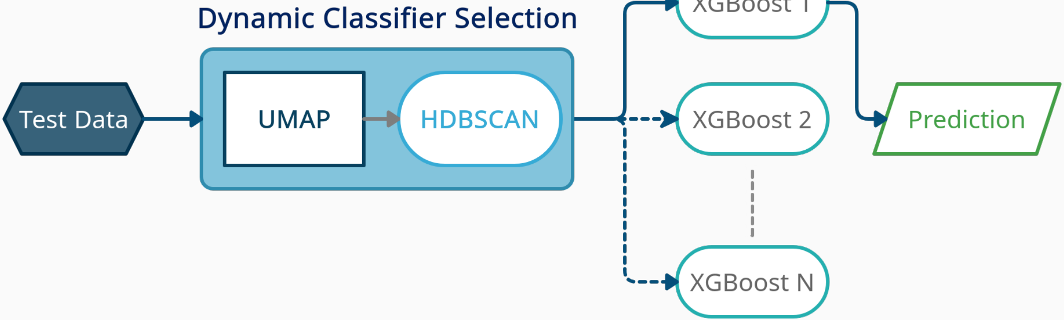
Federation – Concept



Federation – Training



Federation – Predicting



Data Sample

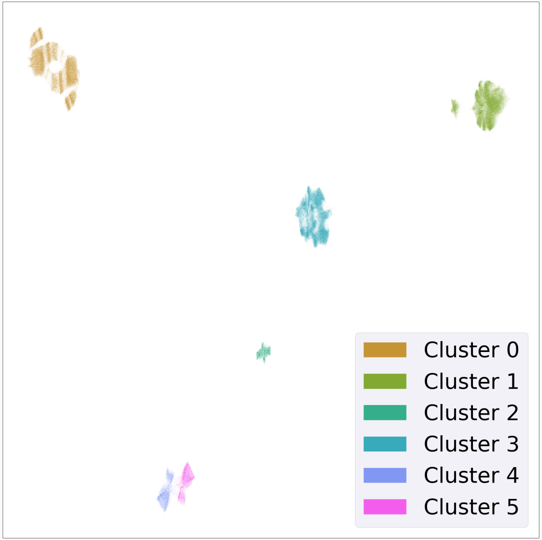
- Openly available dataset[1] from ATLAS
- Simulated $H \to \tau\tau$ signal and background events at $\sqrt{s} = 13\,\text{TeV}$
- Developed for the Kaggle Higgs Boson Challenge[2]
- Total of 30 features (some have *undefined* values)
  - → 17 kinematic features (including categorical: *PRI_jet_num*)
  - → 13 derived features
- Imbalance Ratio of IR ≈ 1.92 (IR $= \frac{N_{\text{sig}}}{N_{\text{bkg}}}$)
- 4 Subsets: training (250 000), validation (100 000), testing (450 000), unused (18 238)

[1] https://opendata.cern.ch/record/328

[2] https://www.kaggle.com/c/higgs-boson

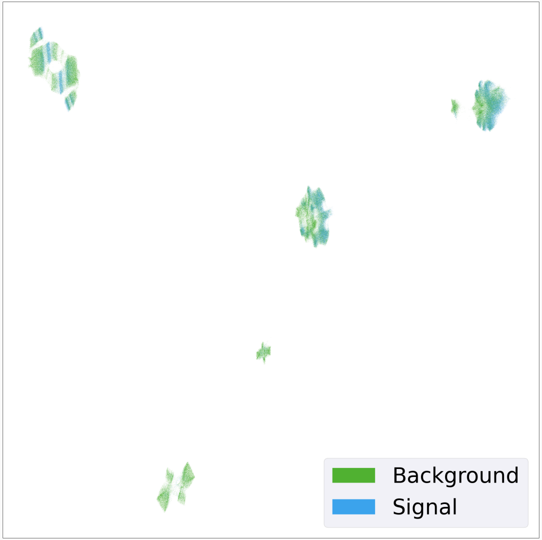
Federation – Visualization

- UMAP [1] reduces dimensions of training data from 30D to 2D
- HDBSCAN [2] finds 6 cluster in the 2D UMAP embedding
  - ⇒ 6 independent classifiers (federation members) are constructed



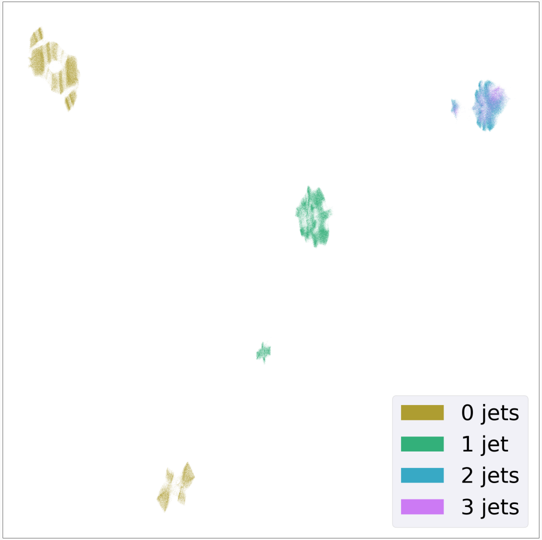
Federation – Visualization

- In some clusters, the majority of data points are background events
  - $\Rightarrow$ Oversampling is needed
- Cluster 0 has "signal bands" in local structure



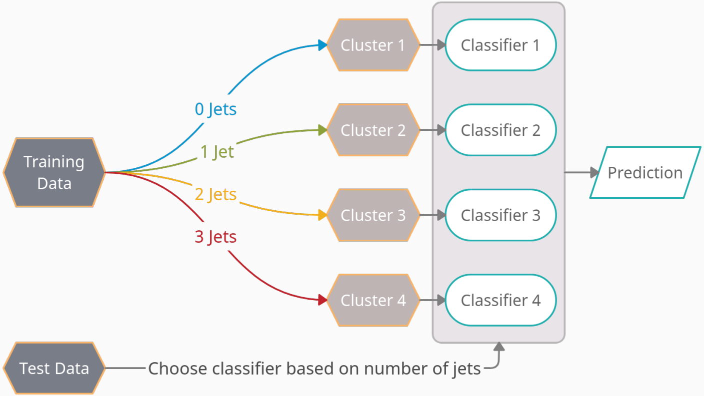
Federation – Visualization

- Global topology of the 2D-embedding is highly influenced by the number of jets feature



Baseline – Hand made clustering

- Clustering causes loss of statistics
  - ⇒ Performance of cluster based classifier degrades
- For a fair comparison, we chose as baseline a similar (feature driven) clustering
  - ⇒ Clusters based on number of jets



Performance evaluation

Figure of merit

- The evaluation metric from the Kaggle Higgs Bososn Challenge is used
  $\Rightarrow$ Approximate Median Significance (AMS)
- Predictions are sorted after the highest probability
- Only the N top predictions are marked as signal predictions

Finding the right threshold

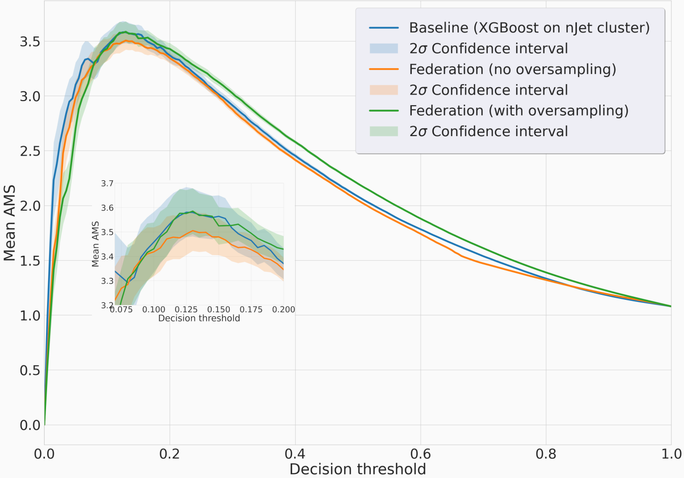
- Threshold scan on validation data
- Threshold with the highest AMS is used for the test data

Performance comparison

Method	Mean AMS $\pm$ Std	@Threshold
Single classifier	3.628 ± 0.036	0.160
Baseline (n-Jet clusters)	3.395 ± 0.067	0.090
Federation (no oversampling)	3.480 ± 0.037	0.145
Federation (with oversampling)	3.564 ± 0.041	0.145
Kaggle Challenge Submissions	**AMS**	
Winner (Gábor Melis)	3.80581	
Place 6 (Crowwork with XGBoost)	3.71885	

Bootstraped results ($N = 1000$) of test data

Federation – Performance plot



Mean bootstrapped ($N = 1000$) AMS of test data against decision threshold

Summary and Conclusion

- UMAP and HDBSCAN are the core of the Federation
  - ⇒ Creation of Federation members
  - ⇒ Used for Dynamic Classification Selection
- Oversampling the training data of the Federation members improves performance
- The training and predicting of the Federation members can be parallelized
- The Federation surpasses a comparable n-Jet based clustering approach

Thank you for listening!

References

[1] Tim Sainburg, Leland McInnes, and Timothy Q. Gentner. "Parametric UMAP: learning embeddings with deep neural networks for representation and semi-supervised learning". In: *ArXiv e-prints* (2020). arXiv: 2009.12981 [stat.ML].

[2] Leland McInnes, John Healy, and Steve Astels. "hdbscan: Hierarchical density based clustering". In: *The Journal of Open Source Software* 2.11 (2017), p. 205.

[3] Leland McInnes et al. "UMAP: Uniform Manifold Approximation and Projection". In: *The Journal of Open Source Software* 3.29 (2018), p. 861.

[4] Haibo He and Edwardo A. Garcia. "Learning from Imbalanced Data". In: *IEEE Transactions on Knowledge and Data Engineering* 21.9 (2009), pp. 1263–1284. DOI: 10.1109/TKDE.2008.239.

[5] György Kovács. "An empirical comparison and evaluation of minority oversampling techniques on a large number of imbalanced datasets". In: *Applied Soft Computing* 83 (2019). (IF-2019=4.873), p. 105662. DOI: 10.1016/j.asoc.2019.105662.

[6] György Kovács. "smote-variants: a Python Implementation of 85 Minority Oversampling Techniques". In: *Neurocomputing* 366 (2019). (IF-2019=4.07), pp. 352–354. DOI: 10.1016/j.neucom.2019.06.100.

Data Sample – Classifier

- Using XGBoost as baseline to compare with previous research
- Parameters based on XGBoost Paper[3]
    - max_depth $= 6$
    - learning rate $= 0.1$
    - loss $=$ AUC of Precision-Recall Curve
    - $\gamma = 0.1$, $\lambda_{reg} = 0$
    - 30 early stopping rounds
- Using validation set for validation

[3] PMLR 42:69-80, 2015

Data Sample – Figure of merit

Approximate median significance (AMS)

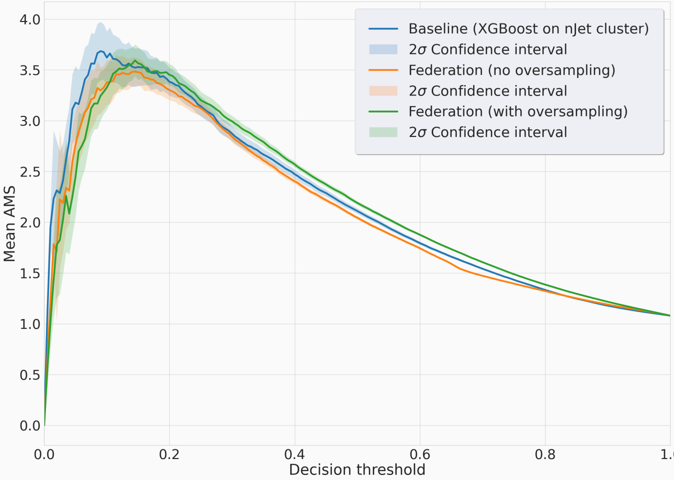
$$\text{AMS} = \sqrt{2\left((s + b + b_r)\log\left(1 + \frac{s}{b + b_r}\right) - s\right)}$$

$b_r = 10$ is a constant regularization term

$$s = \sum_{i=1}^{n} w_i \mathbb{1}\{y_i = s\}\mathbb{1}\{\hat{y}_i = s\}$$

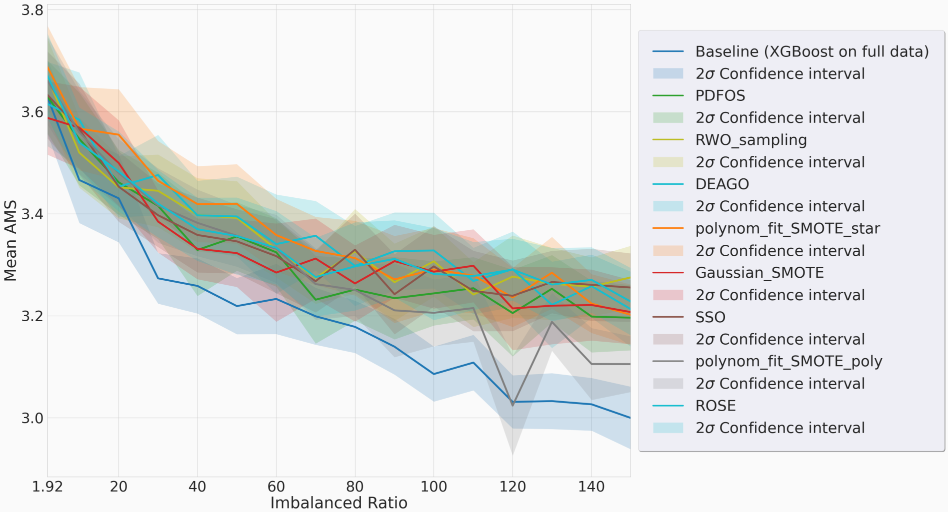
$$b = \sum_{i=1}^{n} w_i \mathbb{1}\{y_i = b\}\mathbb{1}\{\hat{y}_i = s\}$$

Federation – Performance plot



Mean bootstrapped ($N = 1000$) AMS of validation data against decision threshold

Oversampler performance comparison



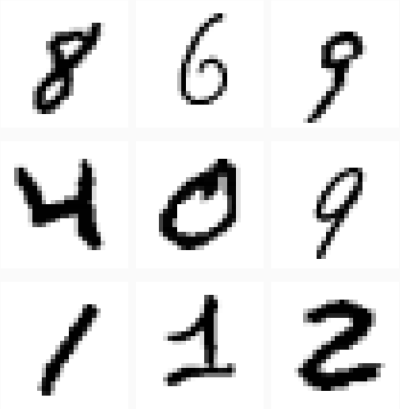
Mean bootstrapped ($N = 1000$) AMS against IR of training data for best performing oversamplers

Federation – Oversampler performance comparison

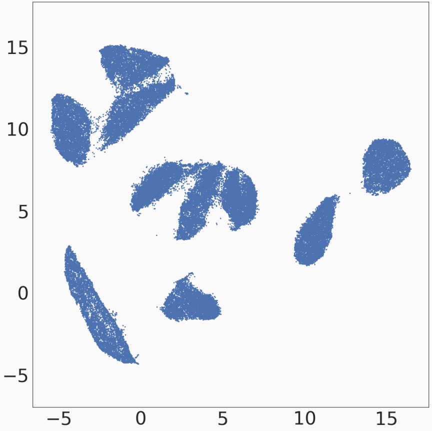
Method	Mean AMS $\pm$ Std	@Threshold
Federation (ROSE)	3.564 ± 0.041	0.145
Federation (PDFOS)	3.554 ± 0.040	0.145
Federation (polynom fit)	3.530 ± 0.034	0.160
Federation (RWO sampling)	3.529 ± 0.036	0.145
Federation (no oversampling)	3.480 ± 0.037	0.145
Federation (SMOTE)	3.451 ± 0.038	0.145

Bootstraped results ($N = 1000$) of test data

UMAP applied on MNIST



Lower dimensional UMAP embedding



Lower dimensional UMAP embedding

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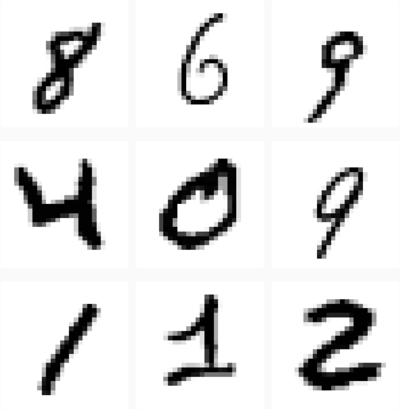
UMAP applied on MNIST



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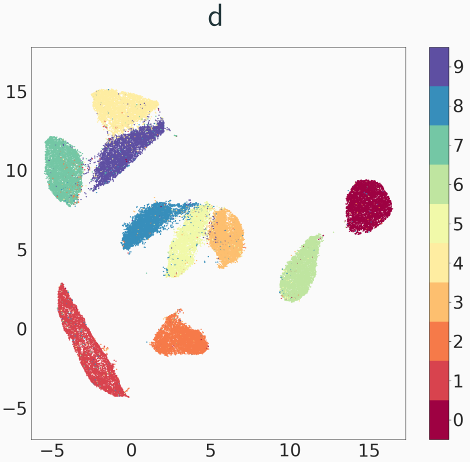

Lower dimensional UMAP embedding