Signatures to help interpretability of anomalies

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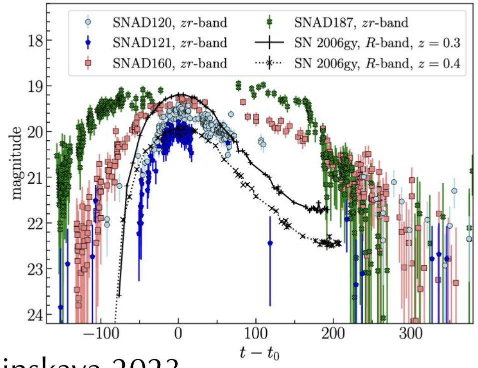
What is an anomaly ?

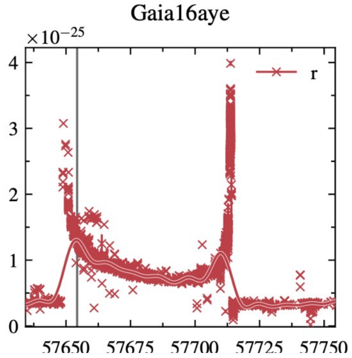
An anomaly is a pattern that does not conform to expected normal behavior, and is suspected to be generated by a different mechanism.

Some challenges :

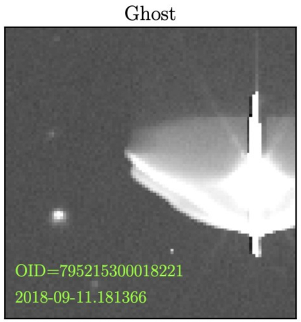
- Normal behavior may be not known
  - Usually in large data sets → Unsupervised learning, fast algorithms.
- Interpreting the underlying behavior/properties of anomalous data
  - Field expert knowledge needed



SLSN
Pruzhinskaya 2023



Binary microlens event
Pruzhinskaya 2019



Bogus finder
Malanchev 2021

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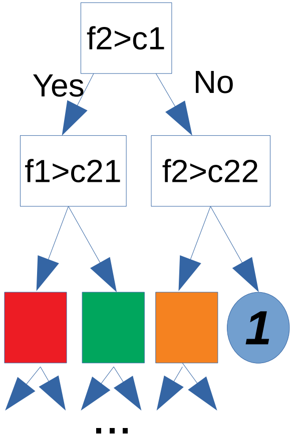
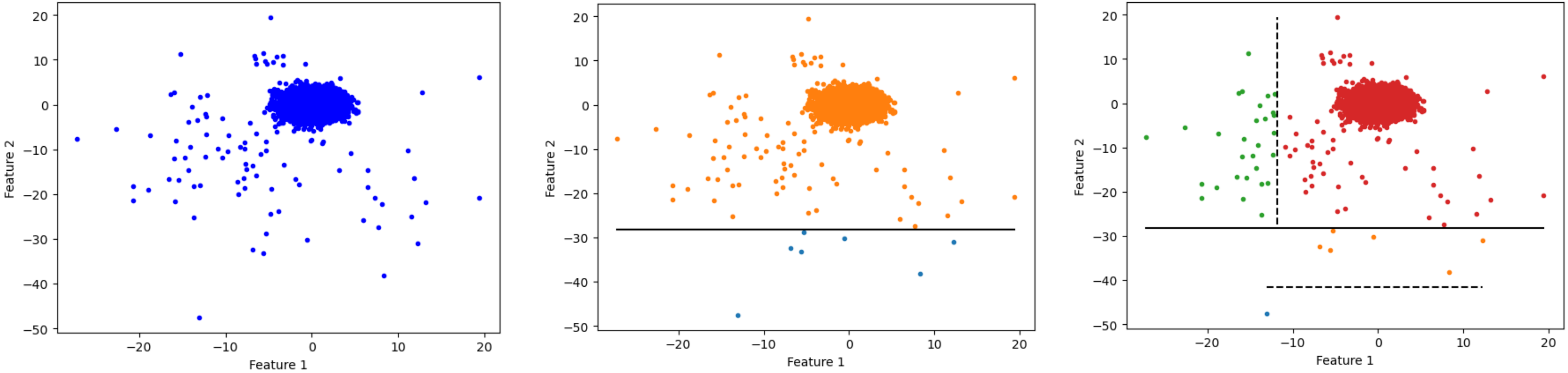
How to help the astronomer ?

- Find anomalies
- **Understand** Machine decision
- Find **more interesting** anomalies
- Discard uninteresting anomalies

Isolation Forest Density Estimation

- **Random Tree:**
  - Select a feature randomly
  - Select a random threshold within the range spanned by the feature for the (sub) sample
  - Repeat for each subsample
  - Stop when only 1 point in the sub-partition
- **Random Forest:**
  - Average depth on T trees (proxy for local density)

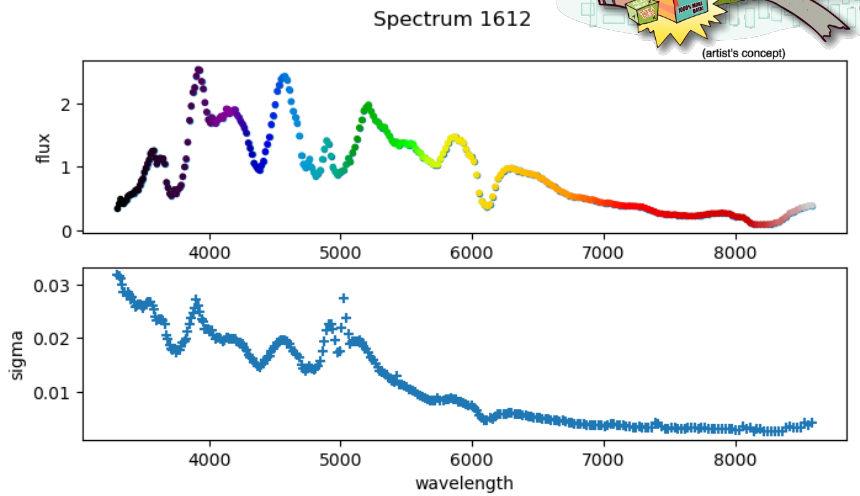




Depth 0 Depth 1 Depth 2

SNFactory dataset

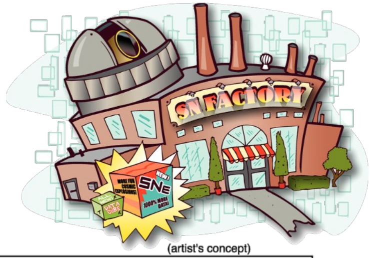
(artist's concept)



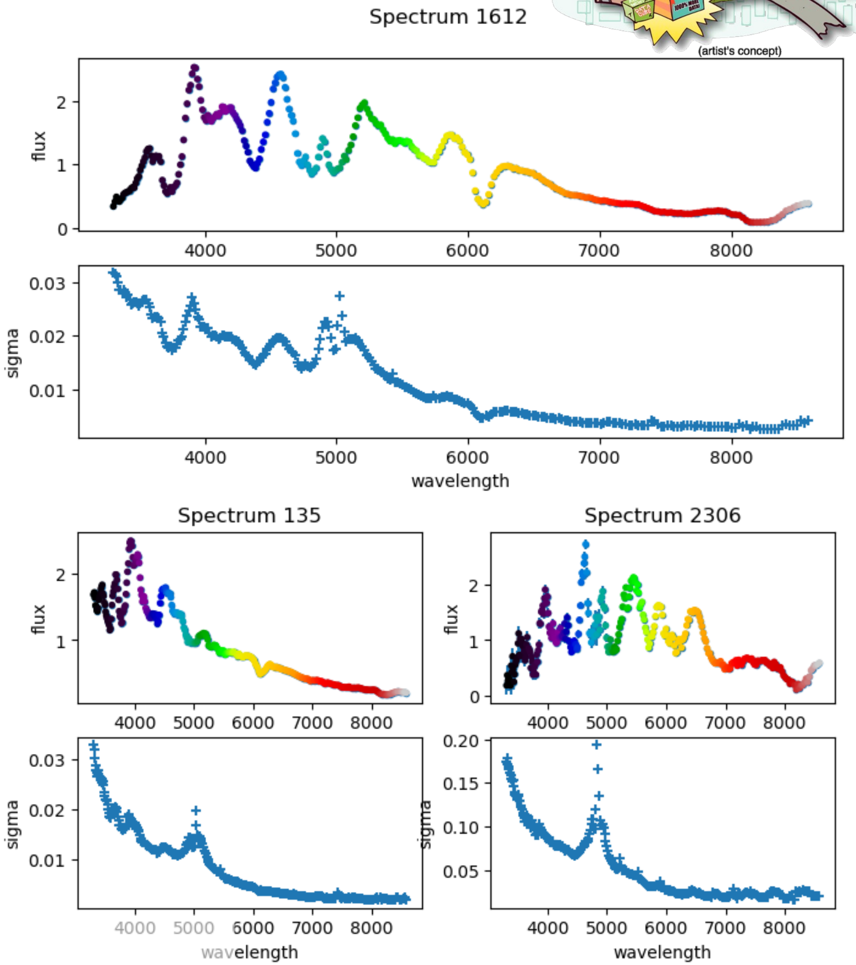
- Public astronomical dataset
  arXiv:2005.03462
  - **2323 spectra** of Type Ia supernovae
    - 288 spectral bins
    - With noise estimate

      → **576 features**

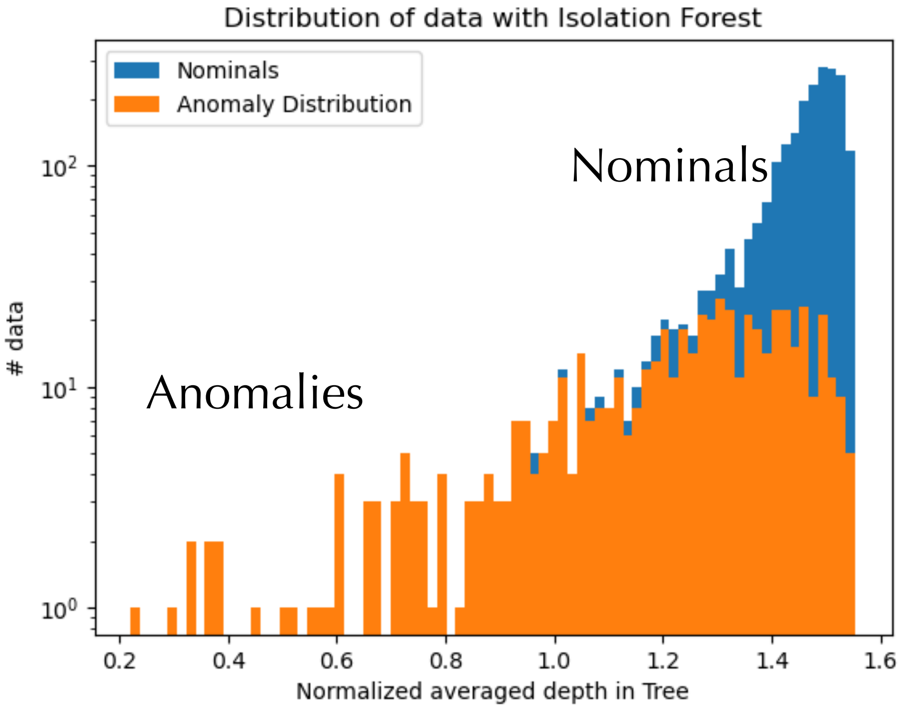
SNFactory dataset



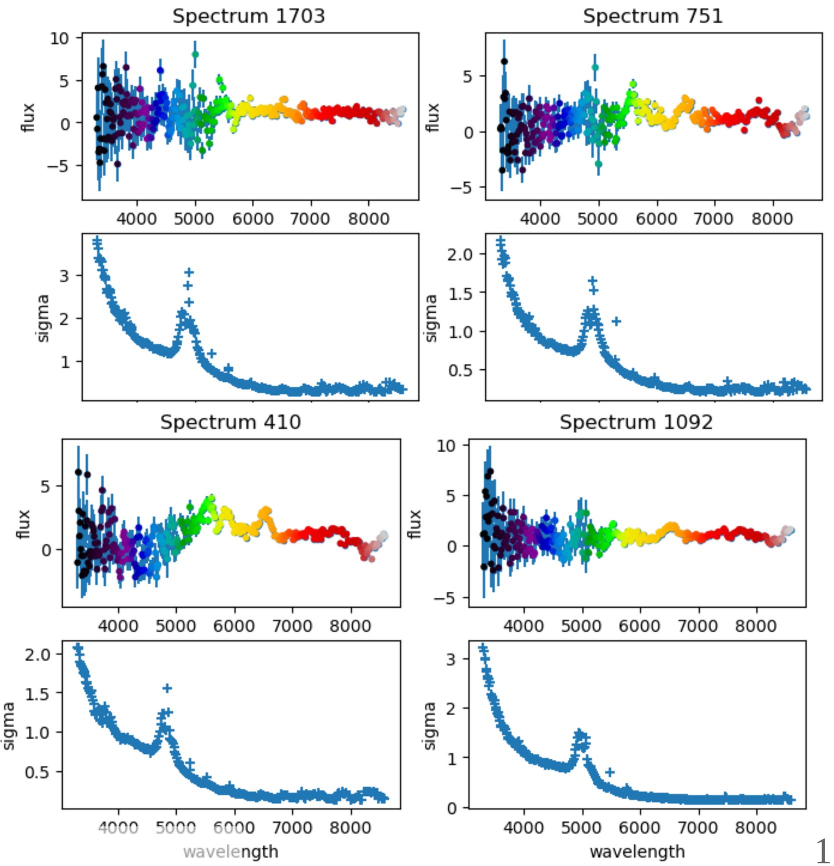
- Public astronomical dataset
- Interest of this dataset for anomalies
  - High **internal variability**
  - **Expert knowledge** for anomalies
  - Many **different class** of anomalies
  - **Noisy data** making the task difficult
  - Local **data artifacts**



Isolation Forest for SNFactory dataset



Top 4 outliers

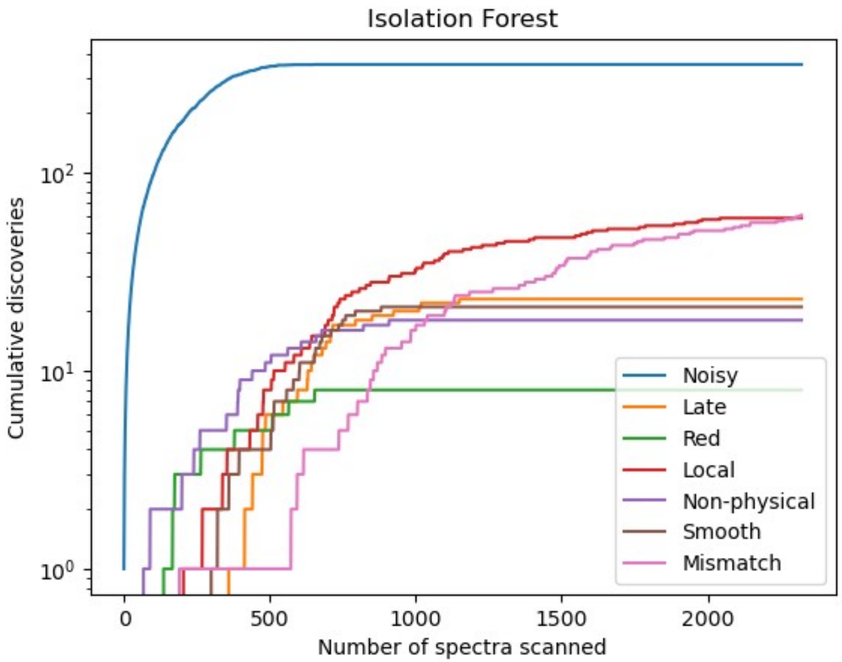


Outliers are anomalies of the **"noisy"** type

Discovery efficiency

- IF very efficient for **dominant anomaly**
  - → Noisy data dominate (AUC=0.985)

- Less efficient for **other classes**
  - **Rank** of last anomaly type dicovered: 360 (expected 326)
  - For non-noise anomalies : AUC=0.61

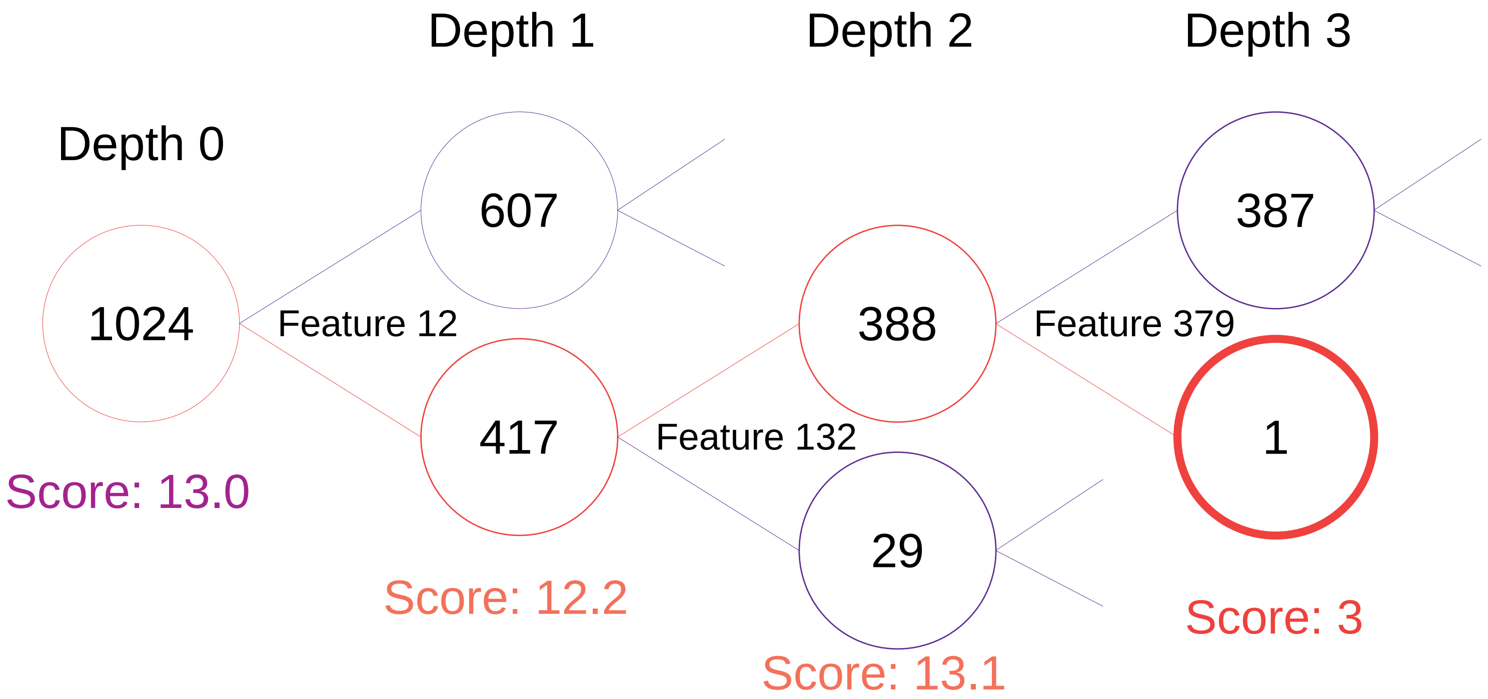


Some common Questions:

- **Why** are some data taged as anomalies ?
- Are there **different classes** of anomalies ?
- Can I improve discovery of **new anomalies** ?
- Can I find **more anomalies** of a given kind ?

Anomaly signature

- Anomaly score for 1 tree



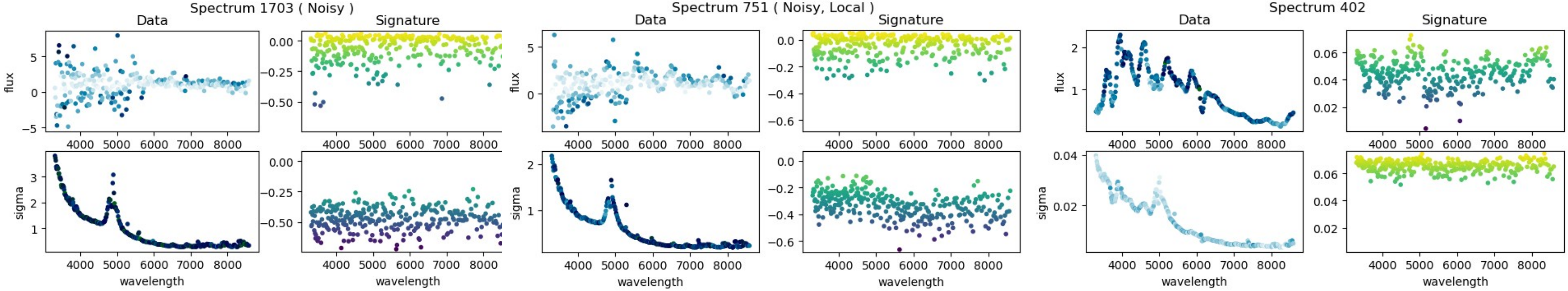
For this outlier :

Feature 12 = - 0.8 Feature 132 = + 0.9 **Feature 379 = - 10.1**

Signature & interpretability

Top 1 Anomaly | Top 2 Anomaly | Top 1 Nominal

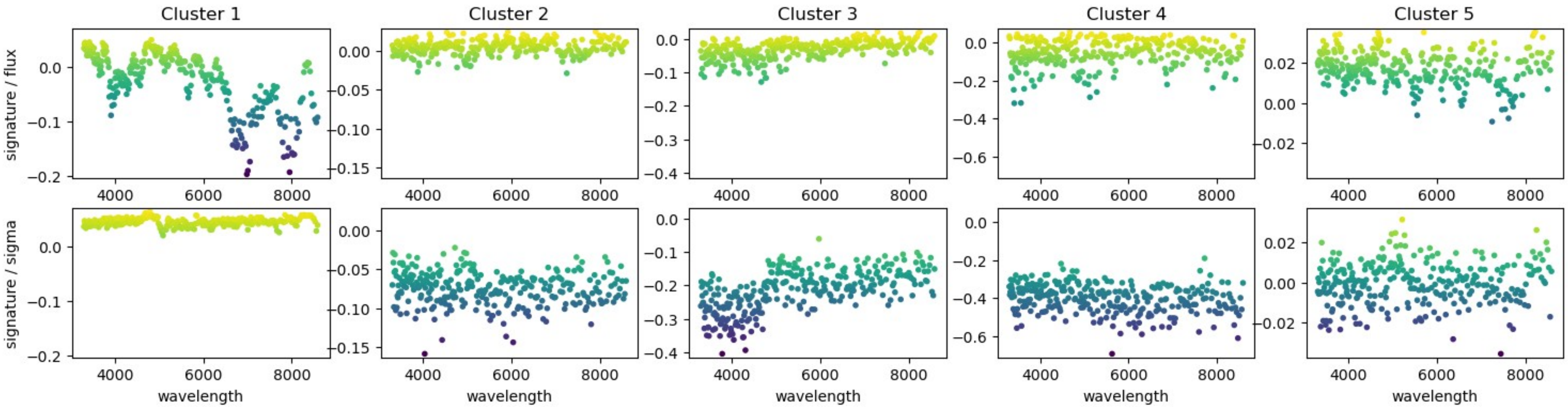
Data Signature | Data Signature | Data Signature



- Signature highlights where the data is anomalous
  - Negative score = anomalous
  - Interpretation : decision based on sigma
  - Positive score = nominal

Signatures & Clustering

- K-means on signatures for **top 10 % anomalous data** (232 spectra)
  - Very unbalanced : 90 % of those are tagged “Noisy”
  - Contains 7 % of nominals



- All anomalies belong to Cluster 1 !
- Only 39 elements : easier to analyse
- Still 2 classes of anomalies not found… + Choice of K is empirical

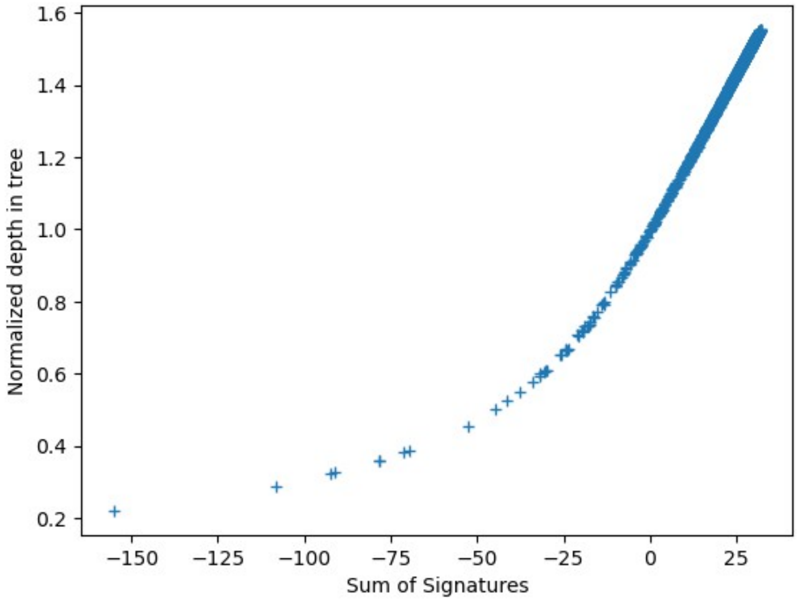
Recursive approach to novelty discovery with signatures

- Signature allow to derive a weighted anomaly score

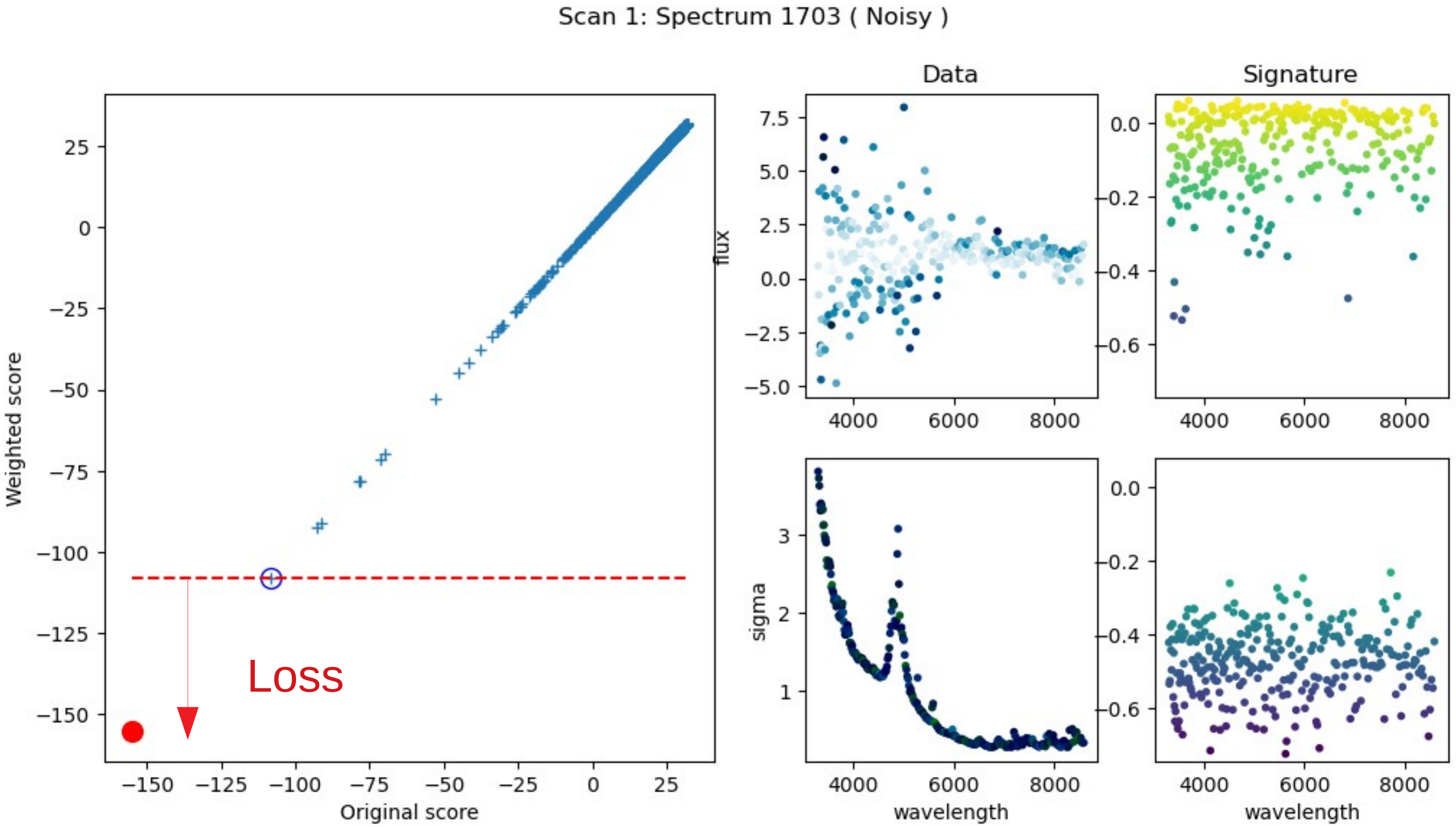
$$S^j = \sum_i \alpha_i S^j_{f_i}$$

  - Initialization of weights to 1

- For each data examined by the expert :
  - Tag as either wanted or unwanted
  - Update the weights / Hinge loss function
  - Propose to the expert the next mostly anomalous



Recursive approach to novelty discovery with signatures



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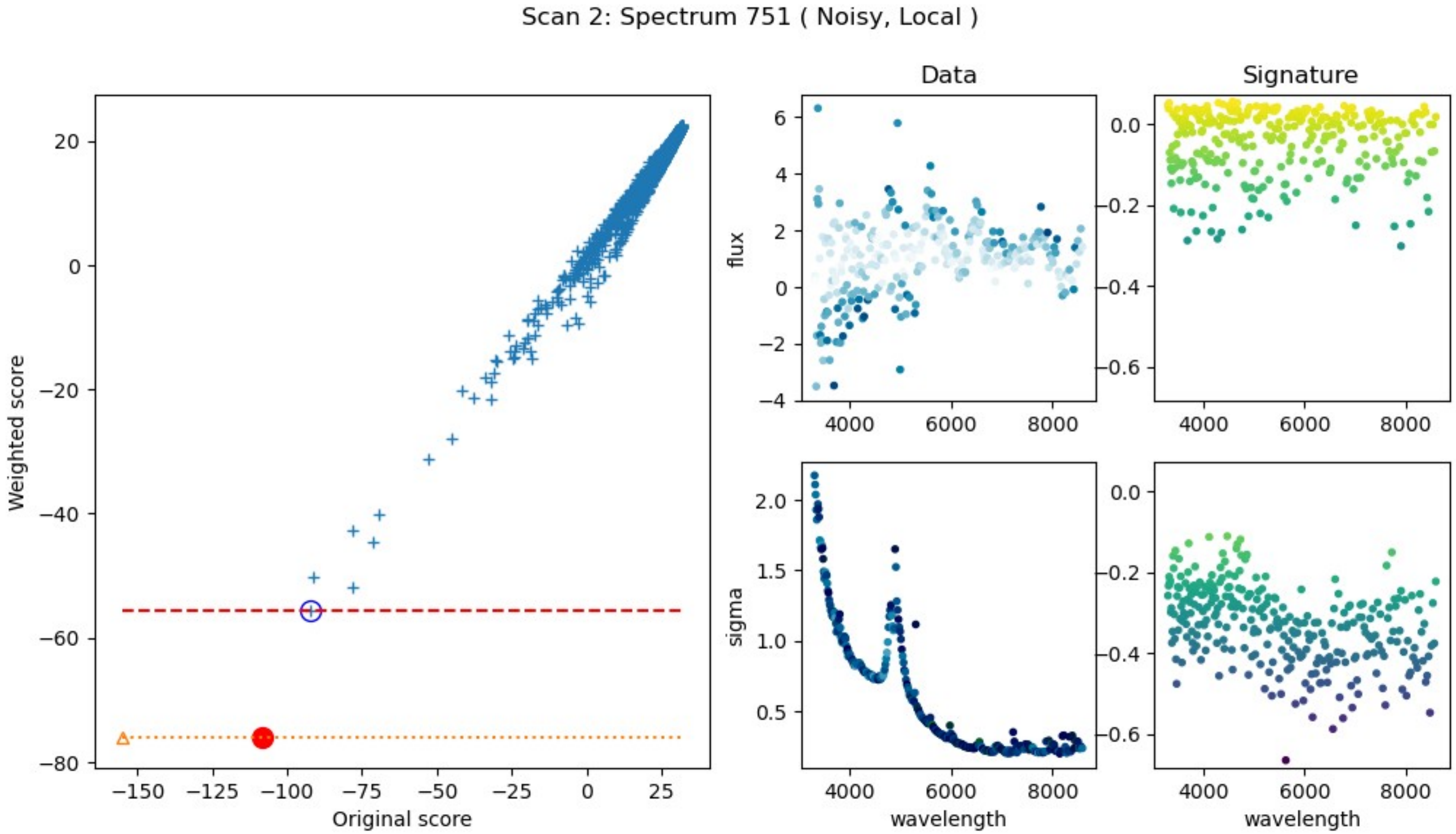

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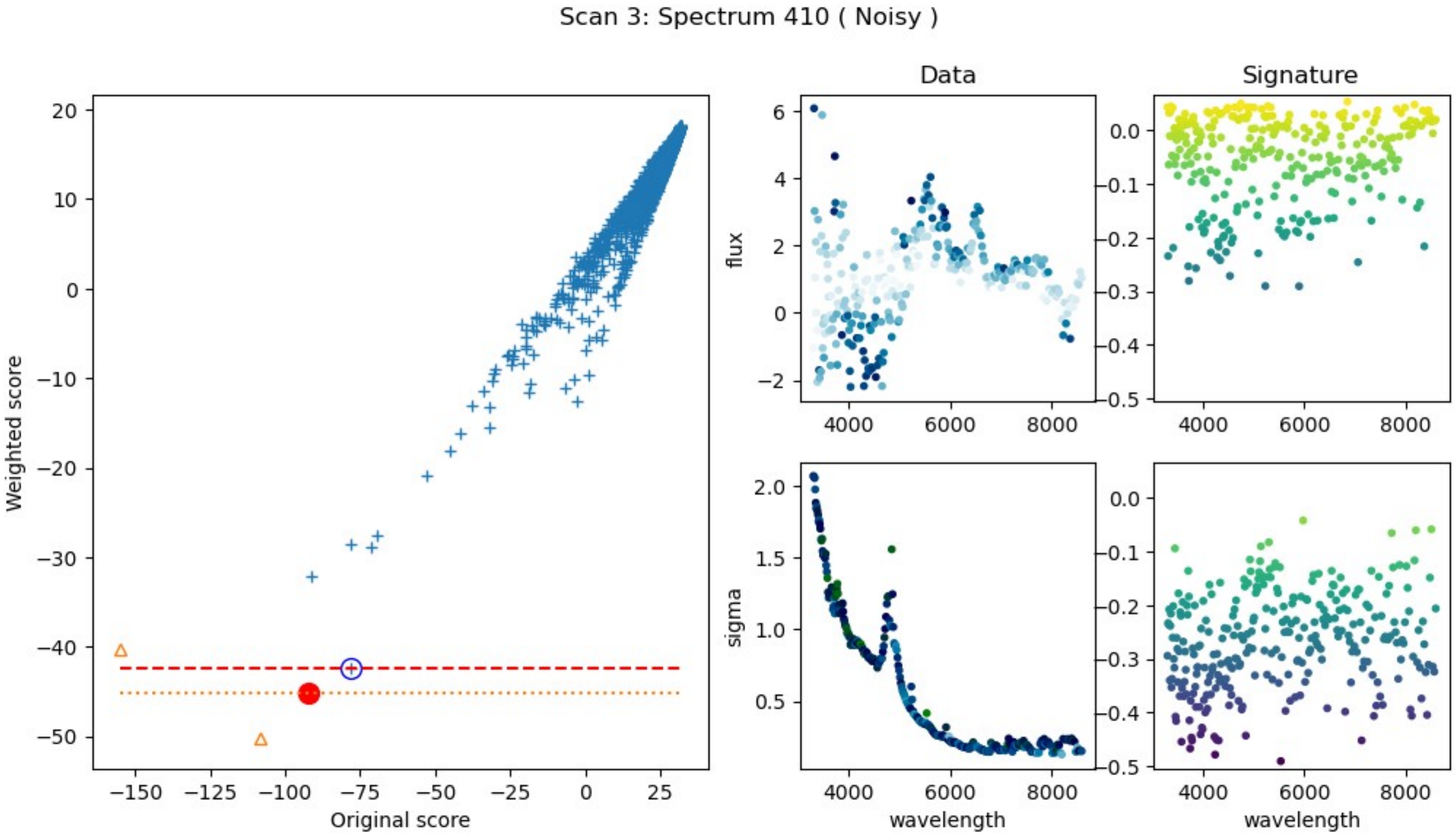

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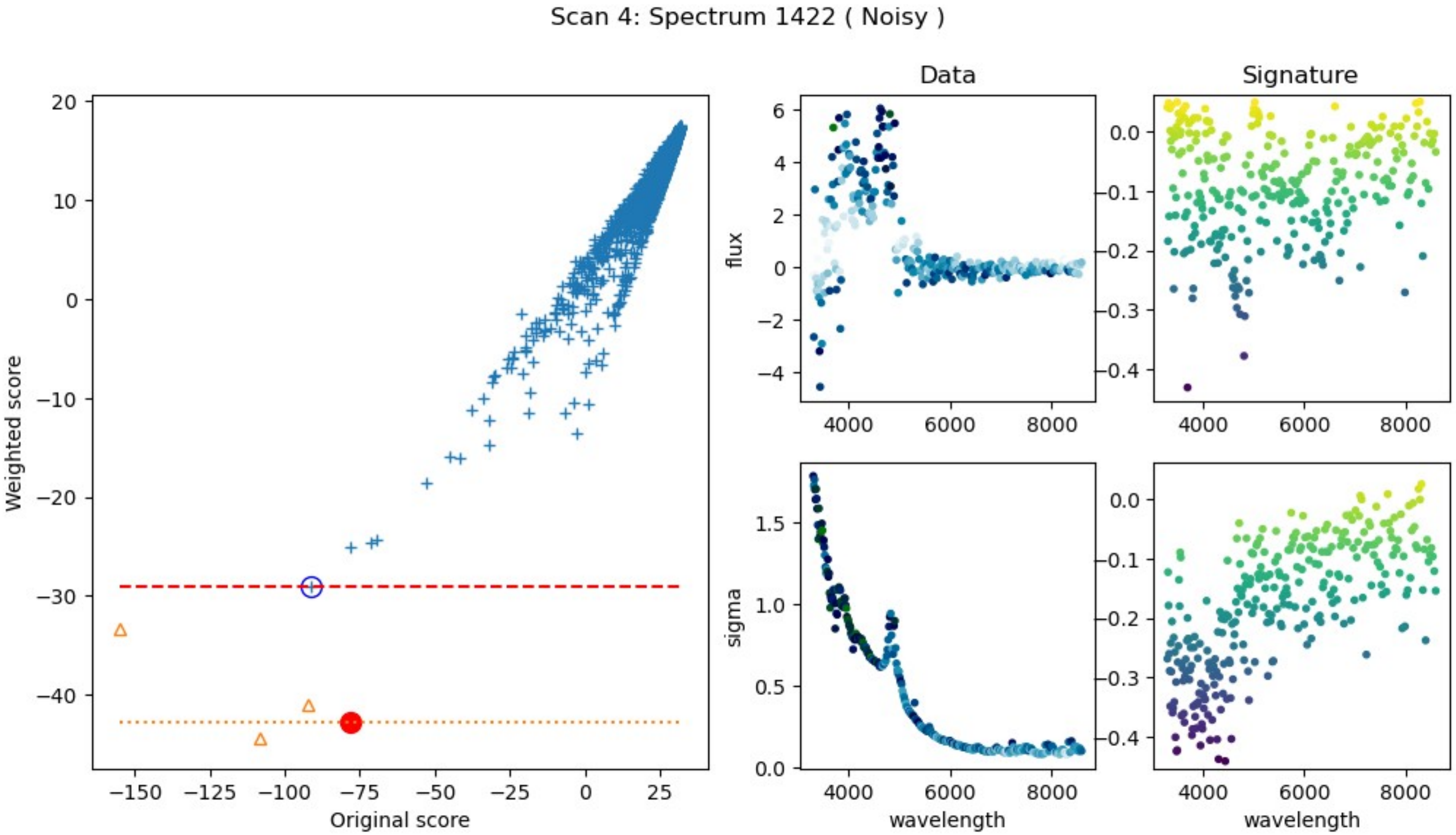

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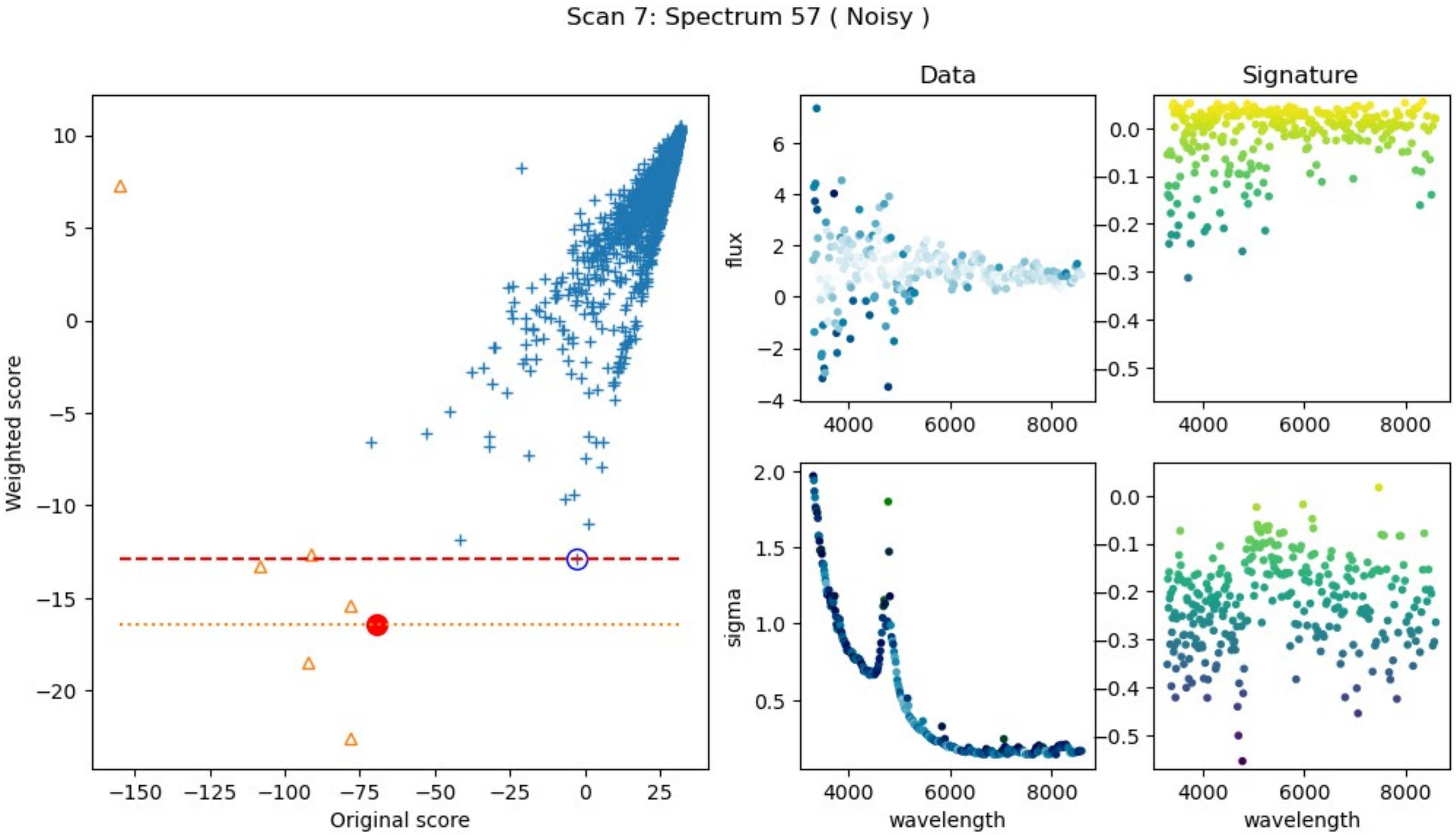

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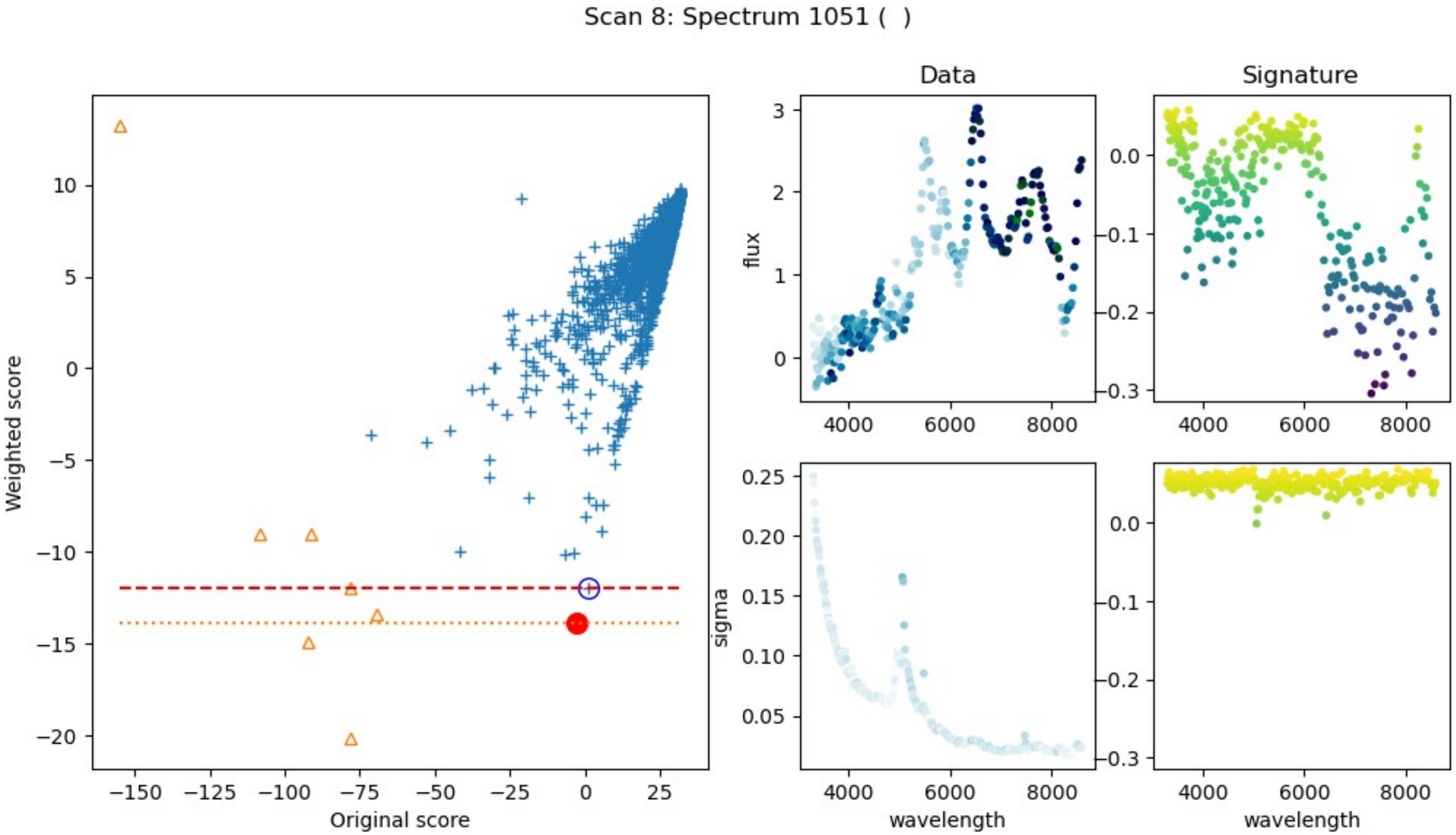

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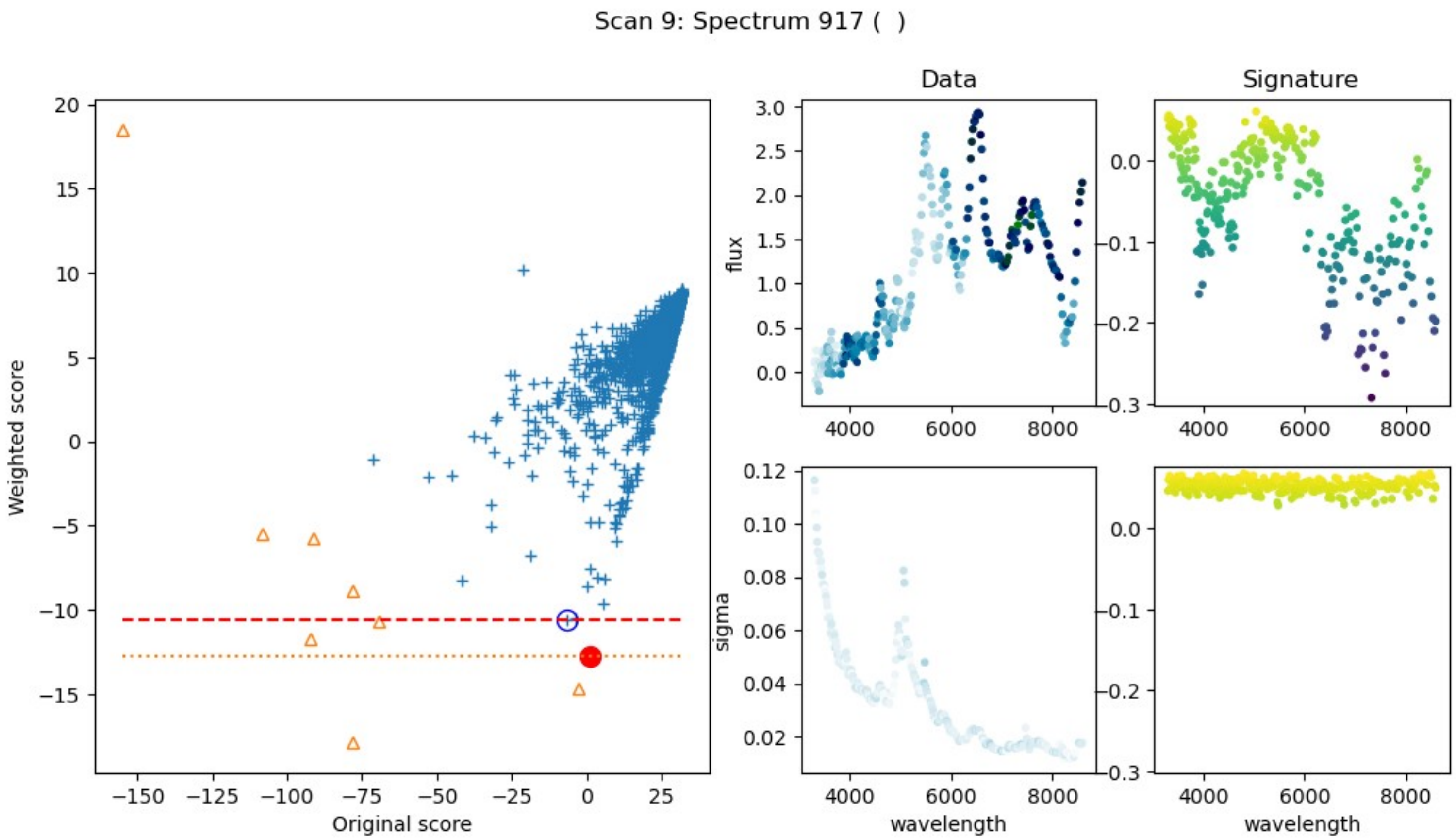

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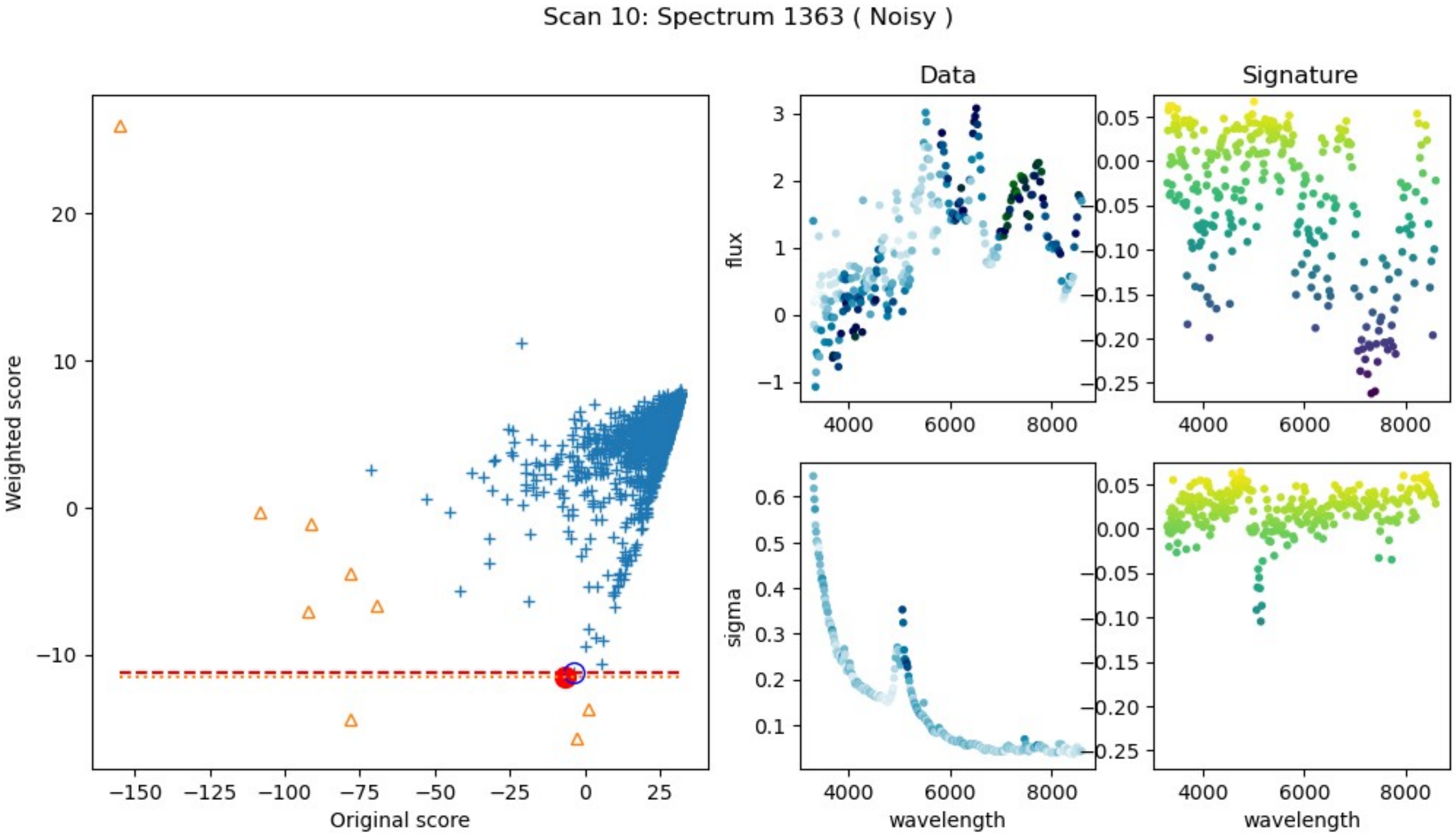

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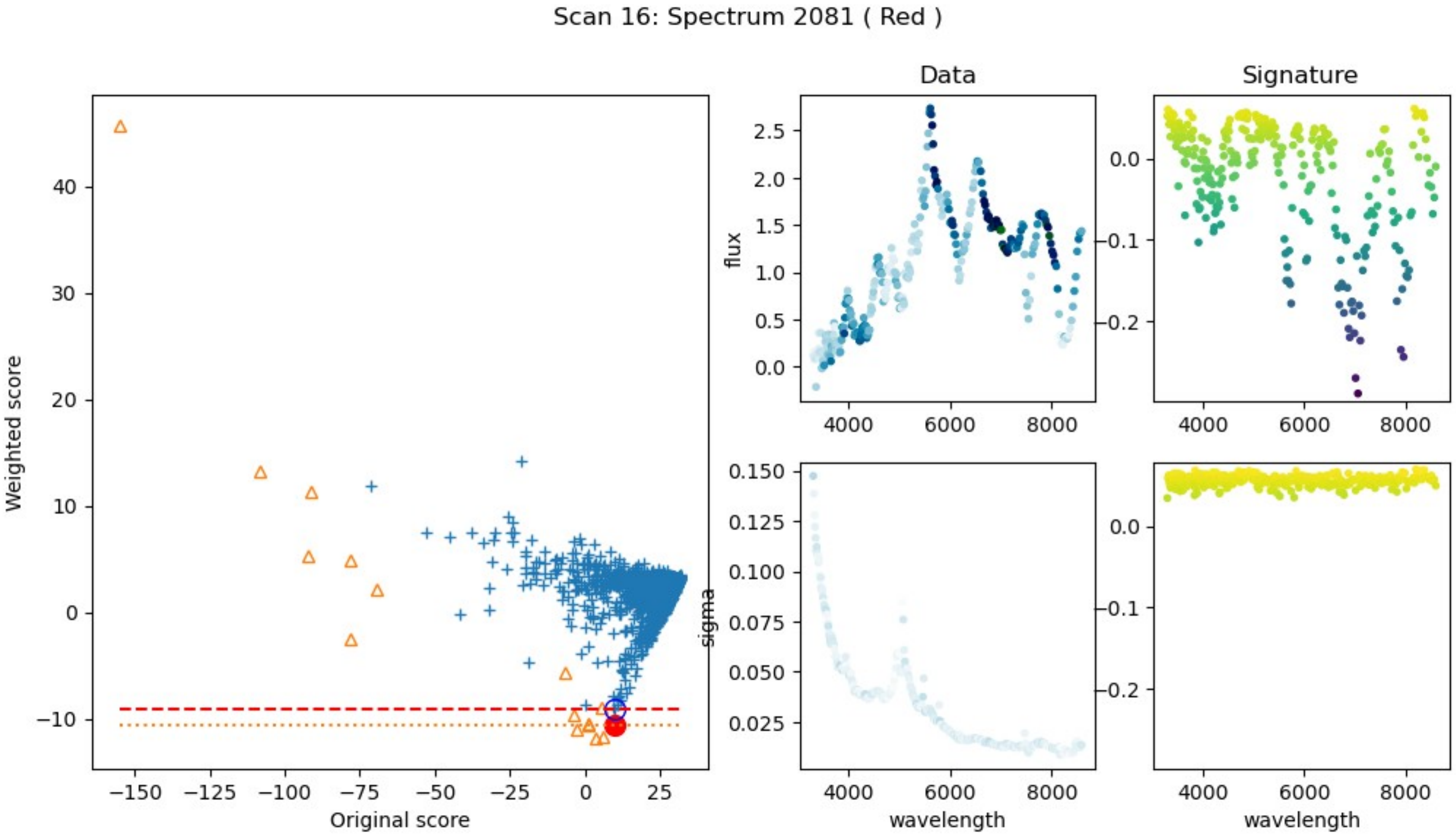

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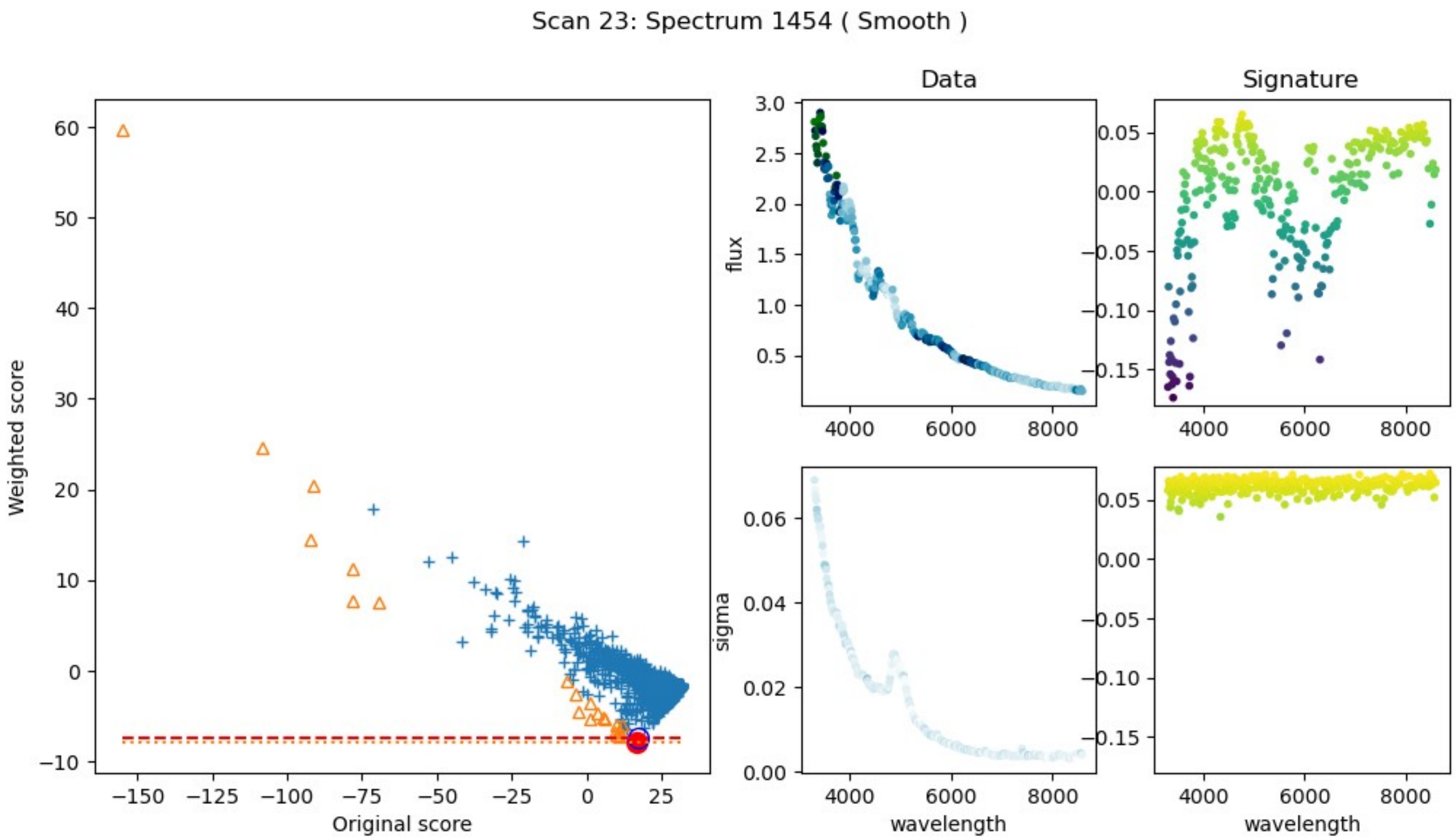
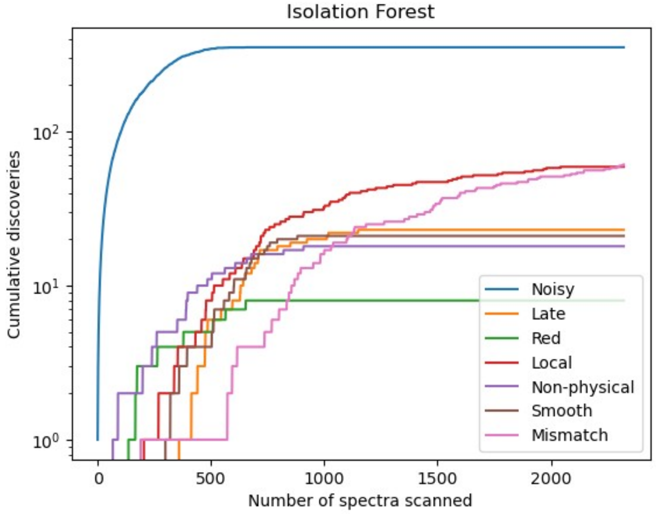


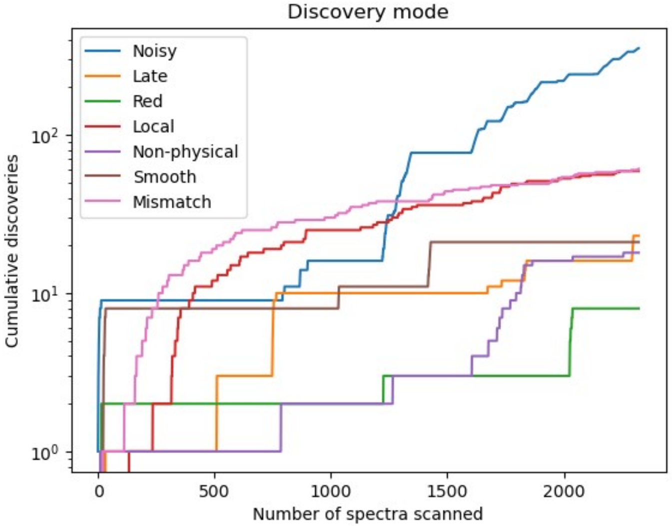
Different tasks :

Factor x3 speed-up in discoveries

- Isolation Forest
  - Default
  - *AUC(Noisy)*=0.98
  - AUC(Others)=0.60
  - Rank of last class=360



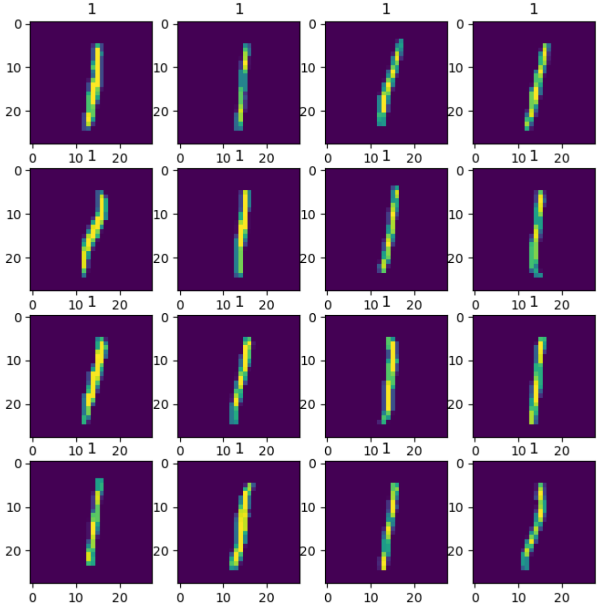
- Discovery mode
  - Optimize on novelty
  - AUC(Noisy)=0.25
  - AUC(Others)=0.51
  - ***Rank*** of last class=133



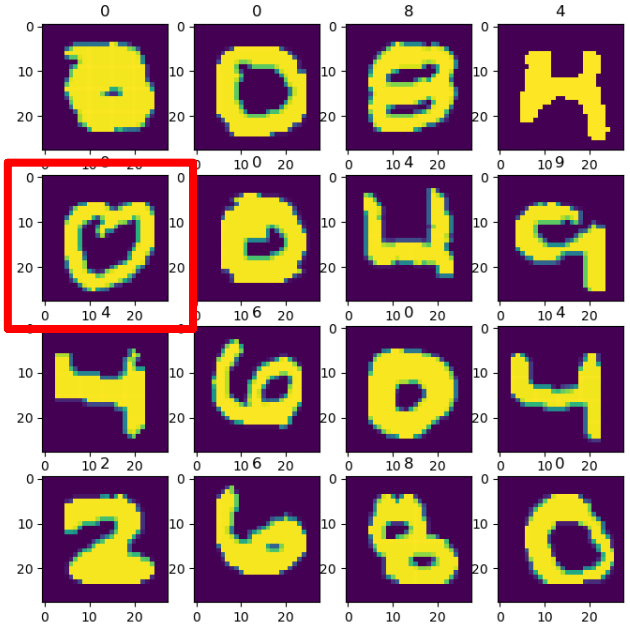
Using Signatures for Similar Anomalies

Anomaly search within MNIST:

- Handwritten digits
- Curated dataset

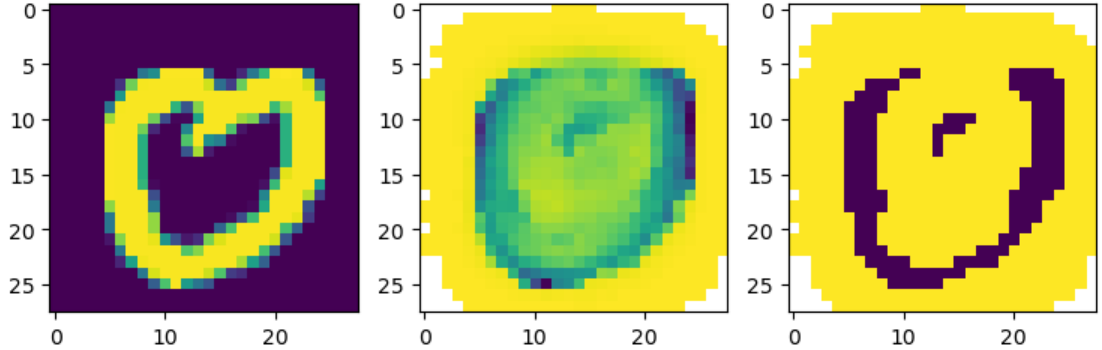


16 most Nominals



16 most Outliers

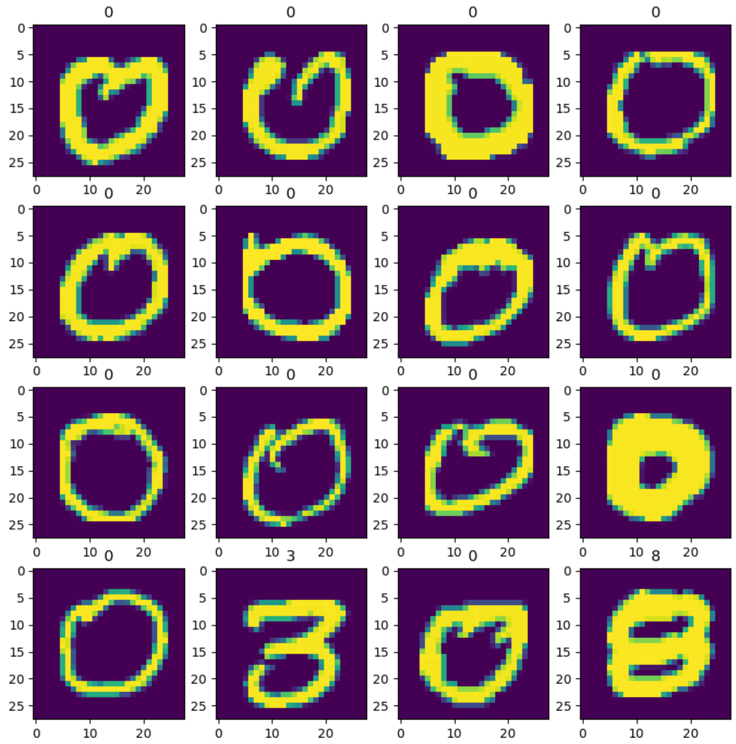
Using signature to select more of the same



Anomaly → Signature → Feature Mask

↓

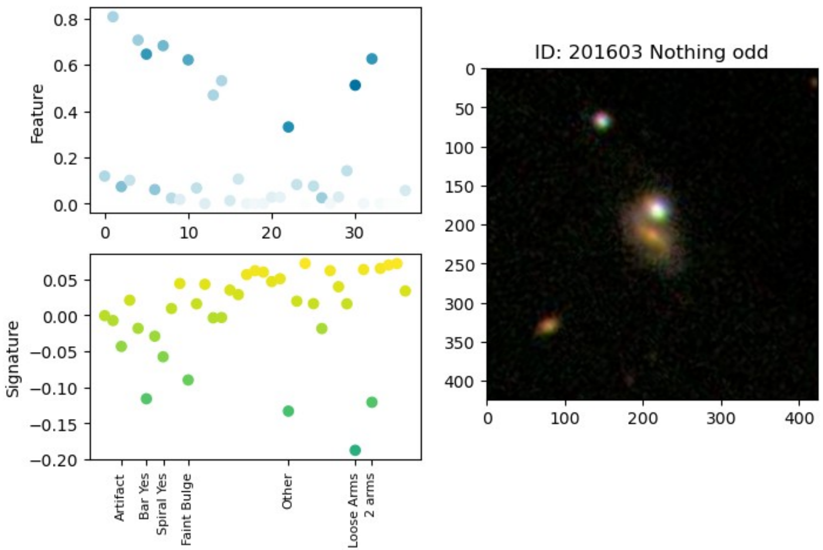
Retraining with selected features

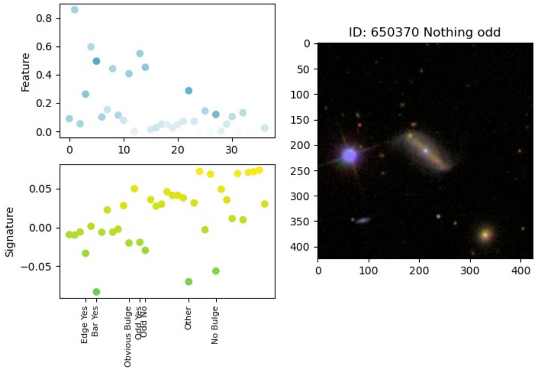


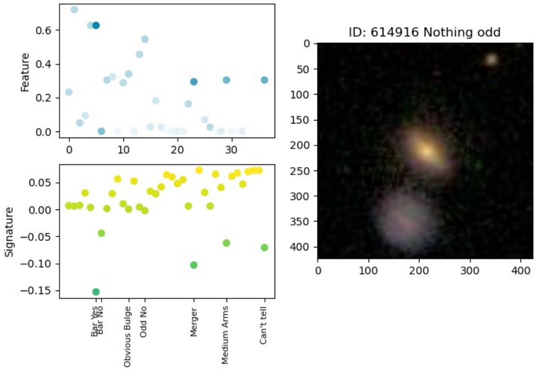
→ Similar Anomalies

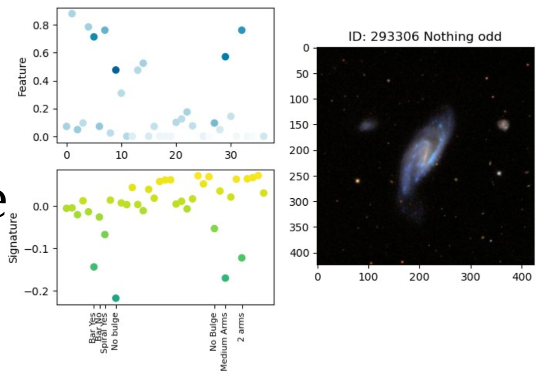
Galaxy Zoo 2 anomalies

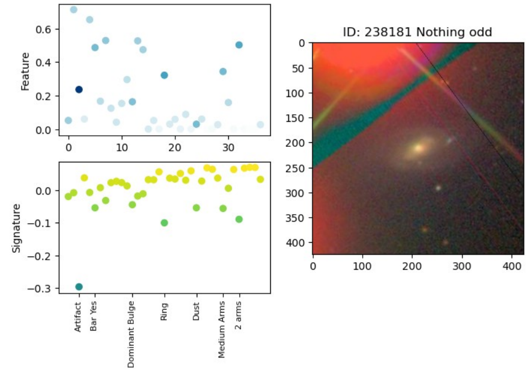
- Anomalies = Rare patterns in human decisions





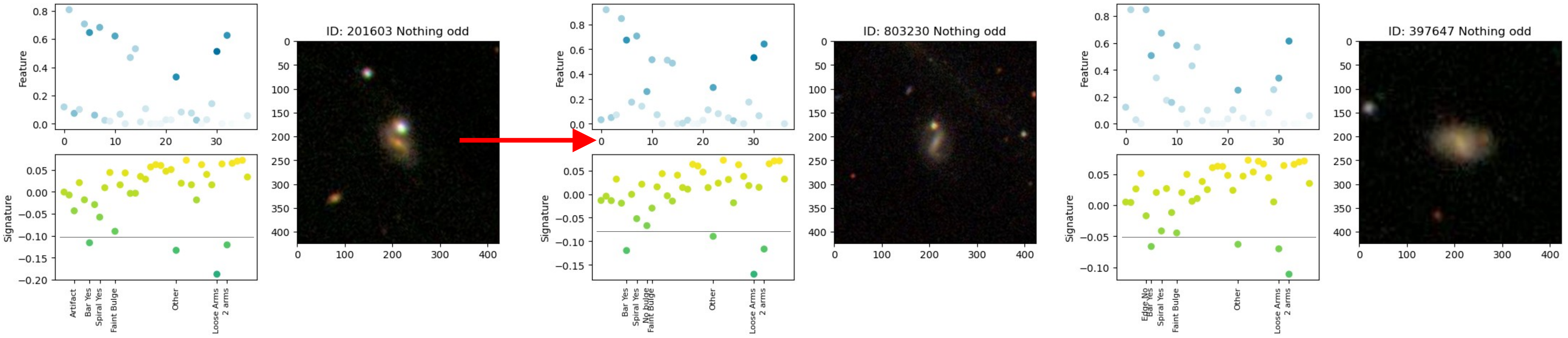


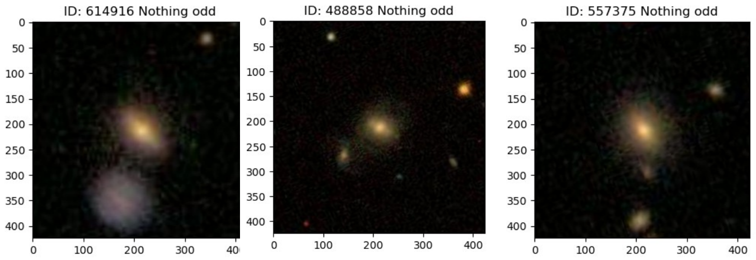




- No obvious pattern in signature
  - → **diversity**

Anomalies by similar signatures





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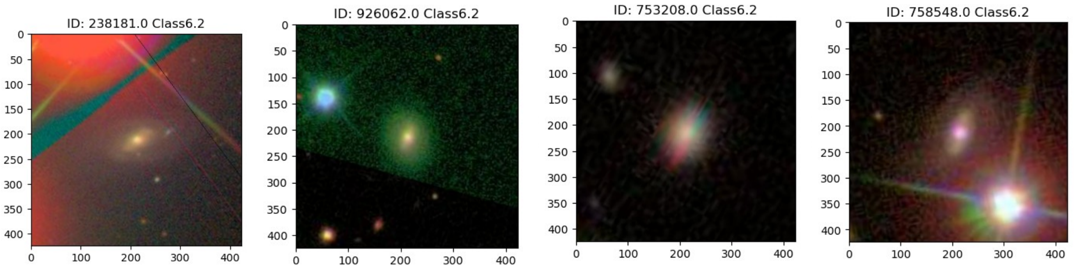

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Rare on "Merger + Bar"

Rare on "Artifact"

Conclusions

- **Anomaly Signature** is a metric for feature importance
- **Domain agnostic / method aware** (Isolation Forest)
  - Works with any tabluar data (features, vectorized images...)
- ***Many use cases:***
  - Interpretability of the decisions
  - Visualisation of outliers
  - Feature selection
  - Categorization of outliers
  - Active learning of anomalies

This is only the beginning !

Stay tuned on

SNAD

https://snad.space

https://github.com/snad-space/coniferest