

Effectively using unsupervised machine learning in next generation astronomical surveys

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Abstract

In recent years many works have shown that unsupervised Machine Learning (ML) can help detect unusual objects and uncover trends in large astronomical datasets, but a few challenges remain. We show here, for example, that different methods, or even small variations of the same method, can produce significantly different outcomes. While intuitively somewhat surprising, this can naturally occur when applying unsupervised ML to highly dimensional data, where there can be many reasonable yet different answers to the same question. In such a case the outcome of any single unsupervised ML method should be considered a sample from a conceivably wide range of possibilities. We therefore suggest an approach that eschews finding an optimal outcome, instead facilitating the production and examination of many valid ones. This can be achieved by incorporating unsupervised ML into data visualisation portals. We present here such a portal that we are developing, applied to the sample of SDSS spectra of galaxies. The main feature of the portal is interactive 2D maps of the data. Different maps are constructed by applying dimensionality reduction to different subspaces of the data, so that each map contains different information that in turn gives a different perspective on the data. The interactive maps are intuitive to use, and we demonstrate how peculiar objects and trends can be detected by means of a few button clicks. We believe that including tools in this spirit in next generation astronomical surveys will be important for making unexpected discoveries, either by professional astronomers or by citizen scientists, and will generally enable the benefits of visual inspection even when dealing with very complex and extensive datasets. Our portal is available online at galaxyportal.space.

Keywords:

1. Introduction

Every so often in the history of astronomy, visual inspection of data has led to an unexpected scientific discovery. As the volume of data that astronomical surveys gather increases, the presence of increasingly rare phenomena within these datasets is essentially unavoidable. It is worth noting

that in astrophysics, what are observationally rare phenomena can actually be quite common and important but short lived (e.g., supernovae that only occur a handful of times per century in a given galaxy but play a crucial role in its chemical evolution). However, the likelihood of detecting such rare phenomena is decreasing, since much of the data we now gather cannot realistically be visually inspected.

The Sloan Digital Sky Survey Data Release 14 (SDSS DR14; Abolfathi et al. 2018) has obtained spectra of $\sim 3M$ galaxies and quasars. Since these were accumulated

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over nearly two decades, and intensively studied by the community, a non negligible fraction of the (high signal to noise ratio; S/N) data was in fact visually inspected by different people. This will surely not be the case for next generation surveys, that will generate ~ 10 times more data in $\sim 1/10$ of the time. For example, the Dark Energy Spectroscopic Instrument (DESI, Levi et al. 2013) which has completed commissioning, will observe $\sim 30M$ galaxies, and SDSS-V (Kollmeier et al. 2017) plan to obtain $\sim 6M$ stellar spectra and $\sim 25M$ spectra of the Milky Way interstellar medium (ISM). While the data rates increase a hundredfold, the number of experts available to inspect them remains more or less constant.

Since we will not be able to examine every spectrum these surveys will generate, we propose to enlist the help of unsupervised Machine Learning (ML) in order to prioritize. Unsupervised ML is the name of a broad family of tools that could be used to detect rare objects or trends. These tools include: (i) Clustering algorithms, which are used to detect groups of objects sharing similar features, (ii) anomaly detection algorithms, which are used to detect unusual objects, and (iii) dimensionality reduction algorithms. The latter family of tools facilitates clustering, trend finding, and anomaly-detection analyses, by representing a dataset in a low dimensional space that can be better visually (or otherwise) inspected. Since these algorithms are data rather than model driven, they have the potential to detect patterns in the data that we did not know existed, and therefore would not have searched for directly.

A wide variety of approaches to perform each of these tasks has been developed by the ML community. Python implementations of many of the most common approaches are publicly available in scikit-learn (Pedregosa et al. 2011). These are relatively easy to use, with conveniently homogenized user interfaces. These tools are flexible and could be tuned to produce useful results from most datasets. Many examples of application of these methods to astronomical data are available in AstroML (VanderPlas et al. 2012).

In this work we make use of both anomaly detection and dimensionality reduction, in the following subsections we briefly review both, focusing on recent usage in astronomy. For more comprehensive reviews of applications of ML in astronomy see Ball & Brunner (2010); Ivezić et al. (2014); Baron (2019).

1.1. Anomaly detection

Anomaly detection algorithms typically rank objects based on a definition of abnormality, where many such definitions exist. Three common general approaches are: (i) objects that are the least similar to other objects in the data, (ii) objects that reside in low density regions of the data, and (iii) objects that are not well reconstructed by a model of the data. However, there are many ways to measure similarity, a variety of methods to define and measure the density, and obviously, endless approaches to modeling data, lending to the richness of existing anomaly

detection algorithms. As could be seen in the examples below, all these approaches were successfully applied to astronomical datasets.

Applications of anomaly detection to spectroscopic data include Boroson & Lauer (2010) who detected anomalies in SDSS quasar spectra using the reconstruction error of a Principal Component Analysis (PCA) model of the data, i.e., the residual between the data and best fitting model. A more recent use of reconstruction-based anomaly detection is Ichinohe & Yamada (2019), where the model of the data (in this case X-ray spectra), was built using a variational auto encoder. Meusinger et al. (2012) used self organizing maps (SOM, Kohonen 1982) for anomaly detection in SDSS quasar spectra. Their unusual quasars were defined to be objects residing in low density regions of the 2D embedding of the data created via SOM. Distance based anomaly detection, was applied to SDSS galaxy and APOGEE stellar spectra by Baron & Poznanski (2017) and Reis et al. (2018) respectively, using an unsupervised Random Forest distance (Shi & Horvath 2006).

For light curve data, distance based anomaly detection was used by Protopapas et al. (2006) and Richards et al. (2012) with different definitions of similarity. Protopapas et al. (2006) worked with raw light-curve data and used the cross correlation distance. Richards et al. (2012) worked with extracted features and used Random Forest (in this case it was supervised, trained on labeled data). In an example that does not directly fit into any of the general approaches described above, Nun et al. (2014) used a supervised Random Forest to predict the class of unlabeled objects, and anomalies were detected as objects having unusual voting distributions. Nun et al. (2016) detected anomalies using an ensemble of anomaly detection methods.

An example of anomaly detection on imaging data is Shamir & Wallin (2014) who found peculiar SDSS galaxy pairs. As we discuss below, interpreting and understanding why an object was selected as anomalous by a given algorithm is often not trivial when dealing with spectroscopy or light curves. However, when inspecting the images of the objects detected in Shamir & Wallin (2014) their unusual features are manifest even to non experts in galaxy morphology.

1.2. Dimensionality reduction

Dimensionality reduction algorithms can be divided into types according to the quantity they try to preserve when representing the data in a lower dimensional space. Some algorithms, such as Multi Dimensional Scaling (MDS) try to preserve the similarity between all the objects. Other algorithms only try to only preserve the neighborhood, or nearest neighbors, but not the actual similarity values, e.g., t-SNE (van der Maaten & Hinton 2008). Auto-Encoders try to preserve information, in the sense that the data itself could be reproduced from the low dimensional representation, typically referred to as the latent space. In this work we use the Uniform Manifold Approximation and Projection (UMAP) algorithm (McInnes et al. 2018), which

tries to preserve the topology of the manifolds on which the objects lie between the low dimensional representation and the original data. See Gisbrecht & Hammer (2015) for a review of dimensionality reduction algorithms.

In recent years a number of works applied dimensionality reduction techniques to astronomical datasets and showed that the resulting embeddings contain useful information (in der Au et al. 2012; Meusinger et al. 2012; Jofré et al. 2015; Traven et al. 2017; Anders et al. 2018; Reis et al. 2018; Chattopadhyay et al. 2019; Cheng et al. 2020; Ralph et al. 2019). For example, Reis et al. (2018) created an embedding of the APOGEE (Majewski et al. 2016) infrared stellar spectra dataset using t-SNE. They showed that the location of a star on such a map contained information about its effective temperature, surface gravity and metallicity. In addition, groups of peculiar stars such as Be and carbon stars were clustered in specific locations on the map.

While it is clear that such maps can contain non-trivial information, it is not obvious how we can extract this information and potentially learn something new about the data. We suggest, as also done by in der Au et al. (2012), that one way to do this is by using the maps in an interactive way. Selecting and inspecting objects directly from the map enables studying the sample in detail. We will use such interactive maps of the data in the portal we present in Section 3.

1.3. Outline

In Section 2 we perform a comparison between various anomaly detection methods on a dataset of galaxy spectra from the SDSS. From the method comparison we draw conclusions that are general to any unsupervised ML application, and we discuss a number of challenges to the effective incorporation of these methods into our workflow with future surveys. In Section 3 we present the data portal that we are developing. We use unsupervised ML to construct as many useful but different human-inspectable summaries of the data as possible, and gather them in an intuitive and easy to use interactive portal. We showcase this approach with SDSS galaxy spectra. We summarize in Section 4.

2. The challenges with anomaly detection

2.1. Anomaly detection method comparison

The fact that many unrelated methods were successfully applied to astronomical data raises the question of how to choose which algorithm to use for a given project, or specifically, with next generation spectroscopic surveys. Is there, for a specific dataset, a single algorithm that is optimal? To try to answer this question we use a sample of 150,000 high S/N SDSS galaxy spectra, and apply four different anomaly detection algorithms; PCA reconstruction error, unsupervised Random Forest, Fisher Vector based anomaly detection, and Isolation Forest.

For PCA reconstruction error and Isolation Forest (Liu et al. 2008) we use the `scikit-learn` implementation. For unsupervised Random Forest we use the `scikit-learn` implementation of Random Forest, and our own code (available at github.com/ireis/unsupervised-random-forest) for calculating the anomaly score. We add to the comparison the results of the same algorithm from Baron & Poznanski (2017). For Fisher Vector based anomaly detection (Rotman. et al. 2019) we use our own implementation. The anomaly detection methods are described in more detail in Appendix B.

The galaxy spectra were obtained from the 14th data release of the SDSS SDSS DR14 (Abolfathi et al. 2018). We selected objects with `Class = GALAXY` from the `SpecObj` table and used only galaxies for which the rest frame spectrum contained flux values in the wavelength range of $3700\text{\AA} < \lambda < 8000\text{\AA}$ (for reference, the full wavelength coverage of the SDSS spectrograph is $3600\text{-}10,400\text{\AA}$). Out of these galaxies we selected the 150,000 with the highest S/N (according to the `SMedian` field in the `SpecObj` table). The preprocessing stage consisted of removing flux values marked as bad by the SDSS pipeline (i.e., flux values with inverse variance of 0), normalizing the spectra by the median, shifting the spectra to the rest frame according to the SDSS pipeline redshift, and interpolating the spectra to a fixed wavelength grid. We note that, as shown for example in Baron & Poznanski (2017), objects with incorrect redshifts can be found as outliers in this scheme. We use the normalized flux values as features for all the algorithms. Note that since we only consider high S/N spectra, we cannot compare the sensitivity of the different algorithms to noise.

Since a measure of success is not defined, unsupervised tasks are challenging to optimize. What constitutes a successful application of anomaly detection? In science we typically aim to detect a large variety of anomalies, and the sole detection of objects of a single kind is considered non-satisfactory. In all cases significant tuning of the hyper-parameters or implementations (the difference between implementation decisions and hyper-parameters is an implementation decision) was required to obtain satisfactory results. Tuning the hyper-parameters parameters was mostly based on trial and error (and the intuition that was built in the process).

As an example of hyper-parameter tuning, with Isolation Forest we used rank values instead of the normalized flux values (that is, we strip the marginal distribution of each feature), to get satisfactory results. Without this modification we obtained only objects with extreme emission line strengths. Due to a small difference between the `scikit-learn` implementations of Random Forest and Isolation Forest, Random Forest is not sensitive to the marginal distributions of the features while Isolation Forest is. This is because in `scikit-learn`, at each node of a Random Forest tree, the best split search grid is constructed from the feature values (of the objects in the node) themselves, while for an Isolation Forest tree the grid is a

linearly spaced set of values, between the minimum and maximum feature values. This example illustrates how implementation decisions can completely change the output of anomaly detection algorithms.

Additional examples for implementation decisions and hyper-parameters that we identified as having a major effect on the results include: (i) The properties of the synthetic data in Unsupervised Random Forest. This algorithm involves comparing the data to synthetic data that needs to be created by the user. There is infinite freedom in constructing synthetic data, and naturally, this affects the results. We were able to obtain useful results with a number of different synthetic data types. See also Shi & Horvath (2006) who compared two relatively similar methods of creating synthetic data and obtained very different results; (ii) The number of objects used to train a single tree in Isolation Forest and Random Forest. This hyper-parameter has a major effect on the behavior of these algorithms, and yet it is not built into `scikit-learn`, and requires wrapping around their implementation; (iii) The number of components in the Gaussian mixture model for the Fisher Vector method; (iv) The details of the reconstruction error calculation for PCA reconstruction error. We were only able to obtain satisfactory results when calculating the reconstruction error separately on relatively small regions of the spectra, and inspecting objects with the largest errors in different regions.

2.2. Consistency and significance of the discovered anomalies

After tuning the different methods we were able to obtain satisfactory results with all four of them. Examples of anomalies found by the different methods are given in Appendix B.1. Additional examples of anomalies found using Unsupervised Random Forest can be found in Baron et al. (2017), and additional examples of anomalies found using the Fisher Vector method can be found in Rotman, et al. (2019). These examples illustrate that each method is able to detect a diverse set of anomalies. All methods detected spectra showing type Ia supernova features, unusual emission and absorption line properties, chance alignments, and various calibration errors. On the other hand, the examples also show that all methods miss some interesting objects. Notably, it does not seem that different methods detect different *types* of anomalies, but rather different individual objects of the different types. For example, Table B.1 shows that all methods detect spectra with type Ia supernova features, but not the same ones.

Considering all the methods uncovered a satisfactory list of anomalous objects, it is not trivial to pick the best one. Worst, we found that there is little overlap between the anomalies detected by the different methods and the mean overlap between the top 500 objects from two different algorithms is ~ 20 . The overlap between the anomalies detected with variations of the same method is also small, and in fact not different from the overlap between anomalies from completely different methods. We further confirm

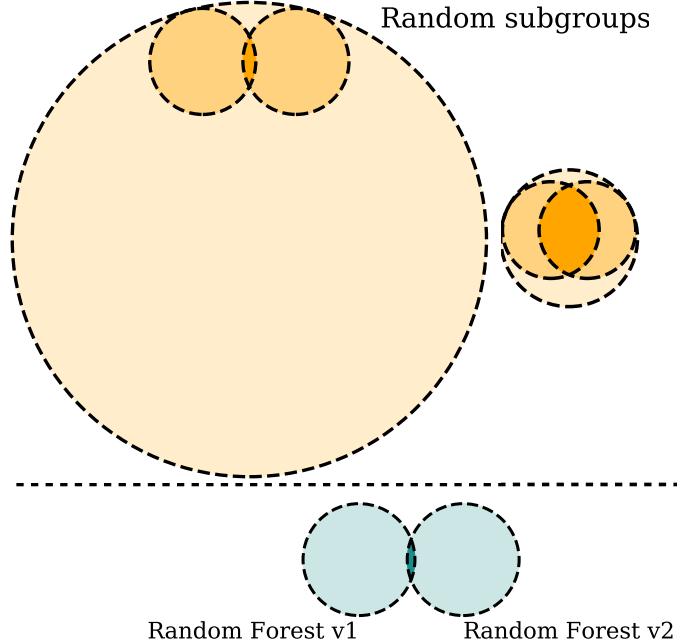


Figure 1: An illustration of how the total number of anomalies in the data could be estimated from the overlap between the anomalies detected by different methods. The top panels show Venn diagrams of a group of a given size ($n = 10,000$ on the left panel, and $n = 1,000$ on the right panel) and 2 randomly drawn subgroups of size $g = 500$. One can see the dependence of the overlap between the subgroups on the size of the original group. The bottom panel shows a Venn diagram of 2 sets of 500 anomalies, detected by the two implementations of Random Forest. The overlap suggests we are in a situation similar to the one in the top left panel, where there is a large number of anomalies in the data, $\sim 10,000$ in our case, of which we only detect small fractions. A quantitative estimation of the number of anomalies in the data is shown in Fig. 2.

that every method missed some interesting objects found by others. This suggests that a single anomaly detection algorithm does not produce in practice the most unusual objects in the data, rather the output should more appropriately be considered as a small subset of the unusual objects.

The overlap between the anomalies detected by different methods can teach us about the statistical significance of the anomalies. This is illustrated in Fig. 1. The top panels show Venn diagrams of two randomly drawn subgroups (each subgroup is analogous to the anomalies detected by a single algorithm) of size $g = 500$, which were drawn from a parent population (the parent population is analogous to the group of all anomalies in the data) of size $n = 1,000$ (right) or size $n = 10,000$ (left). The bottom panel shows Venn diagram of $g = 500$ anomalies detected by the two implementations of Random Forest, chosen here for example. The extent of the overlap between the two subgroups suggests that there are $n \sim 10,000$ anomalies in the data.

Estimating the number of anomalies in the data can be done quantitatively in the following way. Let us assume that there are n anomalies in the data. Let g be the

number of anomalies detected by each method, and $k_{i,j}$ the overlap between the anomalies detected by methods i and j . Further assuming that these sub-samples were uniformly drawn (see further discussion regarding this assumption below), we can estimate n given g and $k_{i,j}$, for each i, j . To calculate the expected k given n and g consider having a group of objects of size n , and a subgroup of size g . We are now randomly choosing, from the original group, another subgroup of size g . If $n \gg g$ the probability of a single randomly chosen object to be in the first subgroup is g/n . Choosing g such objects, the expected overlap is g^2/n . In this case we can easily estimate the number of anomalies with

$$n \sim \frac{g^2}{k}. \quad (1)$$

See Appendix A for the calculation without assuming $n \gg g$. Given the formula, an intersect of $k = 20$ between $g = 500$ anomalies detected by different methods suggests $n \sim 12,500$ anomalies in the data.

In Figure 2 we show the results of this calculation for each pair of anomaly detection methods we applied. $k_{i,j}$ is shown on the x-axis, and the resulting n is shown on the y-axis. The orange line represents $n(k)$ for random groups and the shaded orange region is its standard deviation, calculated numerically, by randomly drawing many groups and calculating the standard deviation of their intersects for different values of n . The largest overlap is between the PCA reconstruction and Fisher Vector methods (yellow-green line), for which $k_{i,j} = 29$ and $n = 8,525$. The lowest overlap is between one of the Random Forest implementations and PCA reconstruction (dark blue line), for this case $k_{i,j} = 8$ and $n = 31,716$. Note that the agreement between the two Random Forest implementations is lower than that of completely different methods. While not shown in the figure, this is also true for different implementations of any of the other methods we applied.

Taking this result at face value means that our dataset contains $\mathcal{O}(10^4)$ anomalies that would be picked up by either of these algorithms. As a consequence, by choosing only one algorithm, even if optimized, and visually inspecting a few hundred candidates, a common and manageable number, we will only assess $\mathcal{O}(5\%)$ of the true anomalies. This fraction is expected to further decrease as the number of objects worth noting will increase with the size of the data, but the number of objects inspected by a single person is not. Next generation spectroscopic surveys will contain one or two orders of magnitude more objects than what we have considered here, thus requiring a different approach.

For the sake of the discussion above we have made the assumption that each anomaly detection method detects a random group of anomalies. If this assumption were true, then the distribution of the anomalies detected by any single method would have been representative of the overall distribution of anomalies in the data. In such a case each single method would have the potential to detect all types of anomalies. This would be surprising, and indeed

does not hold in practice, as can be seen for example in Figure 3, where we show the S/N distribution of the top 100 anomalies from three methods. The fact that the three distributions are so different from each other makes it clear that the different methods are biased towards different types of objects. Note that if two methods are biased towards the same types of objects their intersect will be larger than that of randomly drawn groups and decrease our estimate of the number of anomalies in the data, and vice versa. The biased nature of the detected anomalies should thus increase the scatter in Figure 2 but not necessarily change the mean value. To get an unbiased sample, that has a better chance of detecting all types of anomalies, it is necessary to use an ensemble of different methods. This however does not obviate the need to examine many more objects than typically done.

Also, we used 500 objects per algorithm, but our results above are largely insensitive to that choice, in that as long as we use a few hundred objects per algorithm, we consistently get $n = \mathcal{O}(10^4)$. With more than a few hundreds, n starts to increase, likely due to false positives. Using less than ~ 200 objects per algorithm creates zero overlaps between the subsamples (and brings the difficulties of small number statistics).

2.3. Interpretability of the anomalies

Interpreting anomalies can be an even greater challenge than detecting them. All anomaly detection methods discussed above only produce a list of unusual objects and do not provide any indication as to what is unusual about a given object. This critical task is very time consuming, and prone to errors as there is no guarantee that our interpretation will be correct, i.e., that we indeed found the reason that an object was tagged as anomalous.

Interpretation becomes even more challenging when a single object is too complex to be easily inspected in a glance. This would be the case for spatially resolved spectroscopy, spectroscopic time series, or high resolution spectra, to give examples from the world of spectroscopy. As the complexity of the data increases, the question of what is unusual about a given object becomes more challenging but also more interesting. Furthermore, with the complexity, more objects will show some unusual features, or as often coined in the ML literature: when the complexity of the data is high enough every object is an anomaly. All the anomaly detection methods we have discussed are inherently designed for low dimensional data in which the anomalies are obvious and only need to be quickly and automatically detected. Progress will therefore come from a more streamlined interpretation, rather than more clever detection algorithms.

2.4. Unsupervised ML for high dimensional data

The challenges we discussed are both stemming from the complexity (or high dimensionality) of datasets and not their size. These challenges are not special to astronomy,

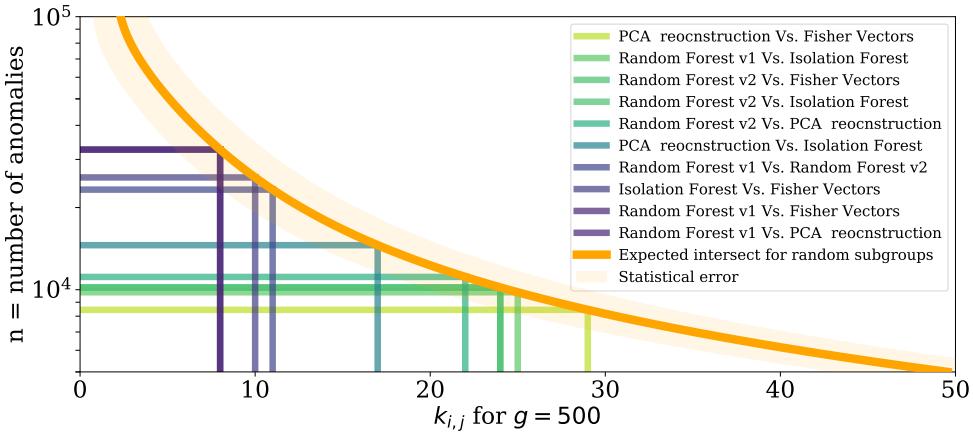


Figure 2: The overlap ($k_{i,j}$, x-axis) between the top $g = 500$ detected anomalies of different anomaly detection methods, and the resulting estimated total number of anomalies in the data (n , y-axis). The orange line is the expected size of a parent population given an overlap between two randomly drawn subgroups of size 500. If one assumes simplistically that there is a well defined group of anomalies from which different detection method pick random sub-samples, one can measure the size of the underlying group of anomalies. Using it only as a ballpark estimate, it seems that the underlying group is of order 10^4 , which is a few percent of the data. Random Forest v1 and v2 are two implementations of the same algorithm. The statistical uncertainty in the expected intersect is shown in light orange, while the Poisson uncertainty is omitted.

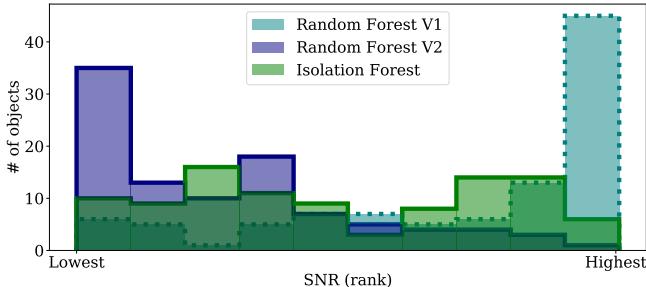


Figure 3: The Signal to Noise Ratio (S/N) distribution of the top 100 anomalies from 2 implementations of unsupervised Random Forest, and an implementation of Isolation Forest, on the SDSS galaxy spectra dataset. While one implementation of unsupervised Random Forest favors high S/N objects, the other favors low S/N object. This Isolation Forest implementation does not seem to show any S/N preference. This demonstrates how different detection methods or specific implementations are biased differently and produce inherently different outcomes. The x-axis is the S/N rank and not the S/N value, otherwise the S/N distribution dominates the graph. Note that our analysis is done with the highest S/N objects in the SDSS so that the lowest S/N objects in our sample still have high S/N.

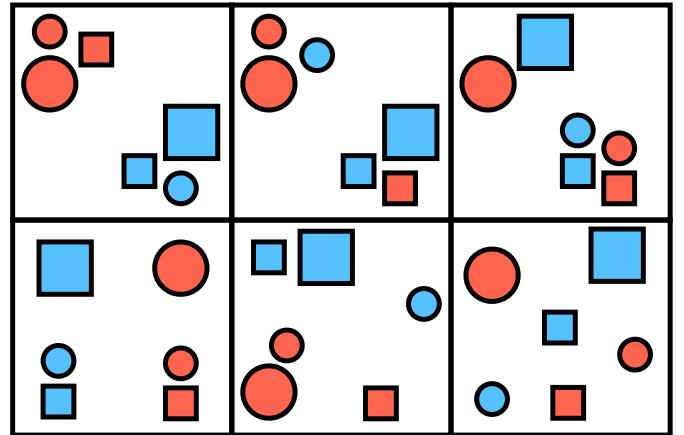


Figure 4: Six different ways of clustering the same data, none of which can be qualified as optimal. As the complexity of data increases, and each object is represented with more features, there could be many ways to divide the data into clusters (or similarly to define anomalies). While different from each other, all are conceivable. This is an illustration of the fact that in unsupervised ML there could be many possible answers to the questions we are asking. We should not look for the best answer, but instead find and inspect as many valid ones as possible.

and in fact **anomaly detection in high dimensional data is an active ML field of research** (Aggarwal & Yu 2001; Zhang & Zhao 2004; Müller et al. 2008; Kriegel et al. 2009; Müller et al. 2010; Keller et al. 2012, listing a few examples). See also Zimek et al. (2012) for a ML oriented review of this topic.

Before discussing possible approaches for handling high dimensional data we would like to emphasize that while we focus on anomaly detection, other unsupervised ML applications, such as dimensionality reduction and clustering,

suffer from the same issues. **For example, in high dimensional data there could be many different but informative ways to divide objects into clusters, and different clustering algorithms can produce different but valid outcomes.** This is illustrated in Figure 4 for the case of data with only three independent features. We see that these data can be divided into clusters in a number of different ways, without any single way being the best one.

The reason that anomaly detection, clustering, and

dimensionality reduction all suffer from the same issues, could be reduced to the definition of a pair-wise distance between objects in the data, which is the basis of many unsupervised ML methods. In complex data the relationship between two objects cannot be described by a single distance. If two objects are similar in one feature and different in another, there is no good way to include the information in a single number. As exemplified in Figure 4, is a red square more similar (i.e., closer) to a red circle or a blue square? Different definition of distance will give more weight to some features and less to others, and thus produce different outcomes for any unsupervised ML application based on this distance. Each different outcome has the potential of providing useful information. We note that not all unsupervised ML methods are based on a pair-wise distance (e.g., auto-encoders and Gaussian mixture models), but these methods suffer from the ‘curse of dimensionality’ as well.

A common approach for handling high dimensional data is working with subspaces, each subspace containing all the objects, but only a subset of the features. The advantage of this approach is that with small enough subspaces the issues arising due to the high dimensionality of the data disappear. In a small subspace the definition of distance becomes unique so there will be a single way to cluster the data, and define anomalies. The results we obtain are also easier to interpret, as we know why an object is an anomaly, or what is the common feature of cluster members, according to the subspace in which the anomaly or cluster were detected.

By working with subspaces one can resolve the two issues discussed above. One can scan many solutions, each from a given algorithm in a given subspace with its own merit, and with an easier path to interpretation, since an outlier in a limited subspace would be easier to understand, as we indeed show below. The subspaces can be defined using physical motivation, randomly, or even using ML. In most cases, using enough subspaces it should be possible to include any interesting property of the original data in at least one subspace. However, the unavoidable cost of having many algorithms, run within many interesting subspaces, is that there are many results to vet, more than can be realistically done by a single human.

3. Framework for the exploration of unsupervised ML results

One way to address the difficulty of having many different but useful outcomes, is collecting them in an easy to use tool so that they could be inspected by the community. In order to allow large numbers of people from the community to explore current and future datasets through the unsupervised ML lens, we are building an interactive graphical portal to large and complex datasets.

Data exploration portals are common in astronomy, a few examples are: SIMBAD (Wenger et al. 2000), Galaxy

Zoo (Lintott et al. 2008), The Open Supernova Catalog (Guillochon et al. 2017), ESASky (Baines et al. 2017), Marvin (Cherinka et al. 2018), and SkyPortal (van der Walt et al. 2019). An upcoming portal for anomaly detection in astronomical data is Astronomaly (Lochner et al. 2019). These portals are generally designed to inspect single objects in a convenient way, and thus cannot be used to explore large numbers of sources.

Compared to these portals, the key novel feature of our portal is machine-learned two-dimensional embeddings (or maps) of the data, that automatically group sources which are similar to each other, and from which objects can be interactively selected and inspected. The interactive maps should be used with the simple notion that similar objects are located close to each other. This makes detecting potentially interesting phenomena quite intuitive. Objects that are isolated on a map are interpreted as objects that are not similar to any other object in the dataset. Any structure in the ordering of objects suggests a continuous change in the properties of objects along the structure. A compact group of objects implies the objects share some common properties. While the maps are built using ML their usage is intuitive and does not require any prior knowledge in this field. Furthermore, by working in subspaces of the data, we can produce a number of such maps, each containing different information. As discussed above, when working with such subspaces, the interpretation of any unsupervised ML method, and specifically the 2D maps, is also made easier.

To illustrate the possible use cases of such a portal we apply it to the SDSS galaxy spectra dataset (same dataset as described in Section 2.1). In the next subsection we discuss the details of our portal as currently implemented for this dataset. A screenshot of the portal is presented in Figure 5. The portal itself is available online at galaxyportal.space, a user manual could be found at toast-docs.readthedocs.io. The source code is publicly available at github.com/ireis/portal.

3.1. Implementation details

Our implementation for the SDSS galaxies is intended to showcase the general approach described above, and the details can change in other implementations or in future versions of this portal. The main challenge in constructing the portal was creating interactive linked graphs containing large amounts of data. Since showing hundreds of thousands of points on a graph is both prohibitive and pointless, we implemented an adaptive graph that shows a random subset (with a fixed upper limit size) of the objects in the current frame, where more objects in a specific region could be seen by zooming in. Our code is based on the Bokeh library¹.

To create the maps of the data we first divide the spectra to a number of wavelength regions which are manually

¹<https://bokeh.pydata.org/en/latest/>

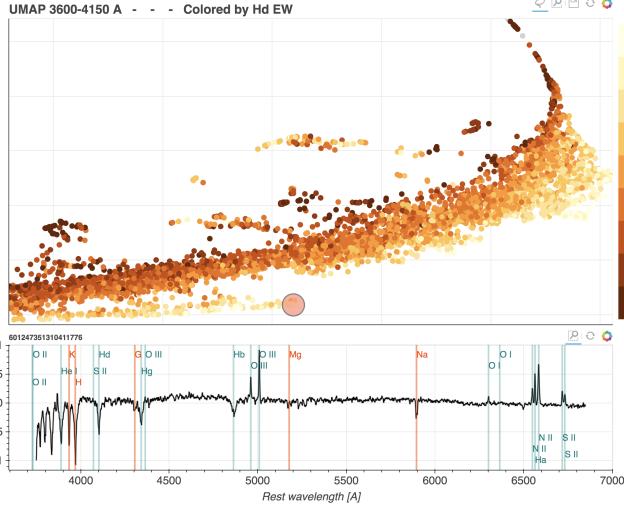


Figure 5: A screenshot from our data portal (galaxyportal.space), where one can study the SDSS galaxy spectra through an unsupervised ML lens. In the top panel, each point represents a galaxy, and galaxies with similar spectral properties are located close to each other in this abstract plane. In this specific embedding the similarities are based on the wavelength region $3600 - 4150\text{\AA}$. The map is further colored by the equivalent width of the $\text{H}\delta$ absorption line. This map and coloring are just examples of the many that we made available. The user of the portal can easily toggle between various embeddings and coloring schemes. In the bottom panel we see the spectrum of the galaxy that has been selected interactively in the top panel, where it is marked with a red circle.

defined according to the locations of common emission and absorption lines. These wavelength regions are examples of subspaces of the data. In each region the spectrum is normalized by the median flux value in the region. Next, Euclidean distances are calculated between the objects (i.e., a sum of the squared differences of normalized fluxes). Finally, we apply the UMAP algorithm to the distances to obtain the maps. In this work we use UMAP and not some other dimensionality reduction algorithm simply to provide a proof of concept for the portal. Generally, there is no need to select a single algorithm and it is possible to include results from a few different ones. While we do not follow this direction in the current work, we suggest that our interactive portal can be useful in comparing results of different dimensionality reduction algorithms. For example, it could be interesting to check if a cluster of objects in a map created using UMAP is also a cluster in a map created using t-SNE (or any other algorithm). This could be easily done with our portal, as it enables selecting objects on one map and viewing them on another (see below).

To illustrate the advantages of using maps created in subspaces of the data, let us consider a map constructed from the region of the spectrum containing the NaID doublet. An isolated group of galaxies on this map will most likely contain galaxies with unique NaID line profiles. On the other hand, on a map constructed from the entire spectrum, (i) there is no guarantee the same group of galaxies with unique NaID profile will appear as an isolated group,

since on such a map the galaxies could be grouped according to some other more prominent feature, and (ii) given an isolated group on the map it is hard to determine what is the unique feature shared by the objects in the group. Figure 6 shows an example of the first point, where objects clustered on a map created using the NaID region are no longer clustered on a map constructed from a different wavelength region.

In addition to the machine learned maps, we uploaded to the portal common galaxy diagnostics such as the BPT diagrams (Baldwin et al. 1981) from which objects can be interactively selected as well. All the embeddings in the portal are linked which allow the user to select objects on one map and display them on another. With this, it is easy to check, for example, where galaxies with unusual NaID profiles lie on the BPT diagram. This example is shown in the bottom left panel of Figure 6.

With the map displaying 2D information, it is easy to add a third one via color. The maps can be colored by various properties of the galaxies such as line ratios, the star formation rate, and the velocity dispersion. Most properties are taken from the SDSS value added catalogs, the rest were calculated by us. Coloring the maps is useful when learning the general location of different types of galaxies on the map. For example see Figure 5 where the UMAP is colored by the $\text{H}\delta$ equivalent width (EW). In this example the coloring can guide the user to the locations of post-starburst galaxies (strong balmer absorption is indicative of post-starburst galaxies, Poggianti et al. 1999). The bottom panel of Figure 5 shows one such post-starburst galaxy, located at the end of a one dimensional structure (the horizontal structure at the bottom of the UMAP) with increased $\text{H}\delta$ EW.

We included in the portal the results of all the anomaly detection algorithms that we used for the method comparison in section 2.1. The location of the anomalies on the different maps is useful for investigating the reason a given object was detected as an anomaly. It is also possible to order the anomalies according to either their location on the map, or any of the available galaxy properties, instead of viewing them ordered by their abnormality score, which is effectively quite random. This allows for a more efficient visual inspection process, as similar objects can be inspected and classified together.

Since anomaly detection is only one of the goals of our portal, we also include other features, that can be used when searching for trends. For example, the user can bin and stack spectra of objects on the fly, by selecting them on the maps, and binning them according to their coordinates or any of the available galaxy properties. A few example use cases for these features are presented below (Sections 3.2 and 3.3), more extensive instructions on how to use all the features are available in the online documentation at toast-docs.readthedocs.io.

It is important to discuss the applicability of our portal to larger datasets. The interactive maps can be used for data of any size, due to the zoom-in technique described

above. Creating the maps does not create a restriction on the size of the data, as the maps can be calculated in advance (so the time it takes to create them is not important). Another possibility regarding the creation of the maps is to learn the transformation from the high dimensional space to the low dimensional one using a subset of the data, and apply this transformation to the rest of the data. This approach also allows to account for new data. Another point is regarding the storage requirements. In our implementation all the data is loaded in random-access memory (RAM). This will not be possible with much larger datasets and a different approach should be taken. An important note in this context is that the infrastructure for viewing individual objects already exists for most astronomical surveys. For example, the SDSS created the **SDSS object explorer** that displays the spectrum of individual objects. In this web-page it is possible to select an object from a table or given its identifiers. This existing infrastructure could be easily connected to the 2D maps in our portal. Instead of accessing individual objects only from a table, they could be also accessed from the 2D maps.

3.2. Use case I: Anomaly detection

As a demonstration of the capabilities of the portal for anomaly detection, we focus here on a single map, constructed from the $\lambda = 5680 - 6120\text{\AA}$ region. As we show below, this restricted view alone uncovers multiple interesting phenomena. We detect galaxies as anomalies by manually inspecting the map. Namely we select and inspect all objects that are either isolated or located at extreme ends of the 2D distribution of objects. The map showing the detected groups is presented in Figure 6 and a number of example objects are shown in Figure C.8. A full description of the findings is given below. Using the portal, it is possible to check which of the anomaly detection methods discussed in Section 2.1 found which groups of anomalies. This is done by displaying the detected anomalies of each method on the $\lambda = 5680 - 6120\text{\AA}$ map. Below we include the findings of this test.

In this wavelength region, the strongest features are the NaID absorption doublet (to which both cool stars and the ISM contribute), and the HeII emission line at 5876\AA . We find the following groups of unusual objects (for the more interesting groups we list a few examples in a table, more examples can be obtained from the portal itself):

- As could be expected, galaxies with extremely strong NaID absorption are located at an extreme end of the 2D distribution and are easily detected. They are shown in yellow in Figure 6. Such objects were found by all anomaly detection methods except for the Fisher Vectors based one.
- Similarly expected, galaxies with extreme HeII emission are found at another edge. They are shown in dark green. Such objects were found by all anomaly detection methods except for one of the implementations of Unsupervised RF.

- Galaxies with strongly blueshifted NaID are grouped together at a few locations. We mark them in blue. The largest concentration contains a few hundred galaxies, where the objects with the largest blueshifts are also the farthest from the bulk of the galaxies. Another small group of galaxies with blueshifted NaID contains a few galaxies in which the absorption is also stronger. The last group of these is characterized by a bluer continuum. Table C.2 lists a number of examples. Blueshifted NaID is a signature of outflowing gas. A sizable fraction of the objects we find are star-forming face-on spirals such as the ones discussed in (Heckman et al. 2000; Bae & Woo 2018). Another dominant population is composed of post-starburst galaxies. These are found using the portal by inspecting the locations of the strongly blueshifted NaID galaxies on the UMAP constructed from a region of the spectrum containing the $H\delta$ absorption, where post-starburst galaxies cluster, or by coloring the NaID map with the $H\delta$ EW. PCA reconstruction error, Fisher vectors, and one of the implementations of Unsupervised RF did not detect any of the objects in the main concentration of blueshifted NaID galaxies on the map.

- Galaxies with multiple component NaID are located in a single cluster on the map. They are shown in light red. Most galaxies in this group seem to be well described by two velocity components, but some show evidence of three. The images of the objects in this group all show that these objects are blended, suggesting the multiple components are coming from different galaxies at similar redshifts. Some of these objects appear in catalogs of galaxy clusters. Table C.3 lists a number of examples. Such objects were detected only by the Fisher Vector based method, and by one of the implementations of Unsupervised RF.

- We find a number galaxies with apparent redshifted NaID absorption. Four such objects are located in a small cluster on the map. These are shown in dark red in Figure 6. Three additional objects are found in the region of the map containing galaxies with strong NaID absorption (shown in yellow on the map). All these objects are listed in Table C.4. Inspecting the individual objects, it seems that different reasons cause the apparent redshifted NaID line. In SDSS J211635.95-004613.1, the emission lines are redshifted by the same velocity as the NaID line, while the H and K lines are centered on the systemic redshift (we take the SDSS redshift as the systemic redshift). On the other hand, in SDSS J141518.01+230841.0, the H and K line are redshifted with the NaID line, while the emission lines are blueshifted from the systemic redshift. In the second case a natural interpretation is an offset AGN (e.g, Comerford &

NaI D region UMAP

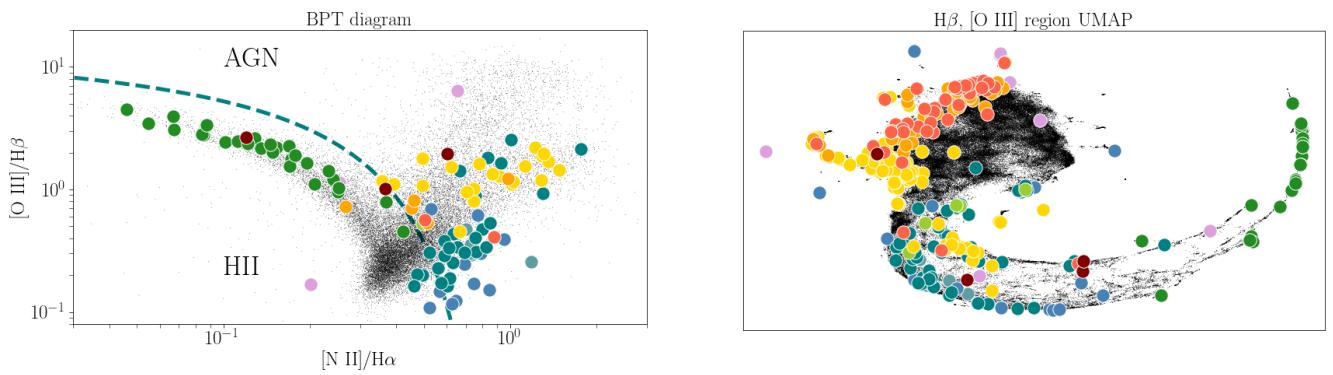
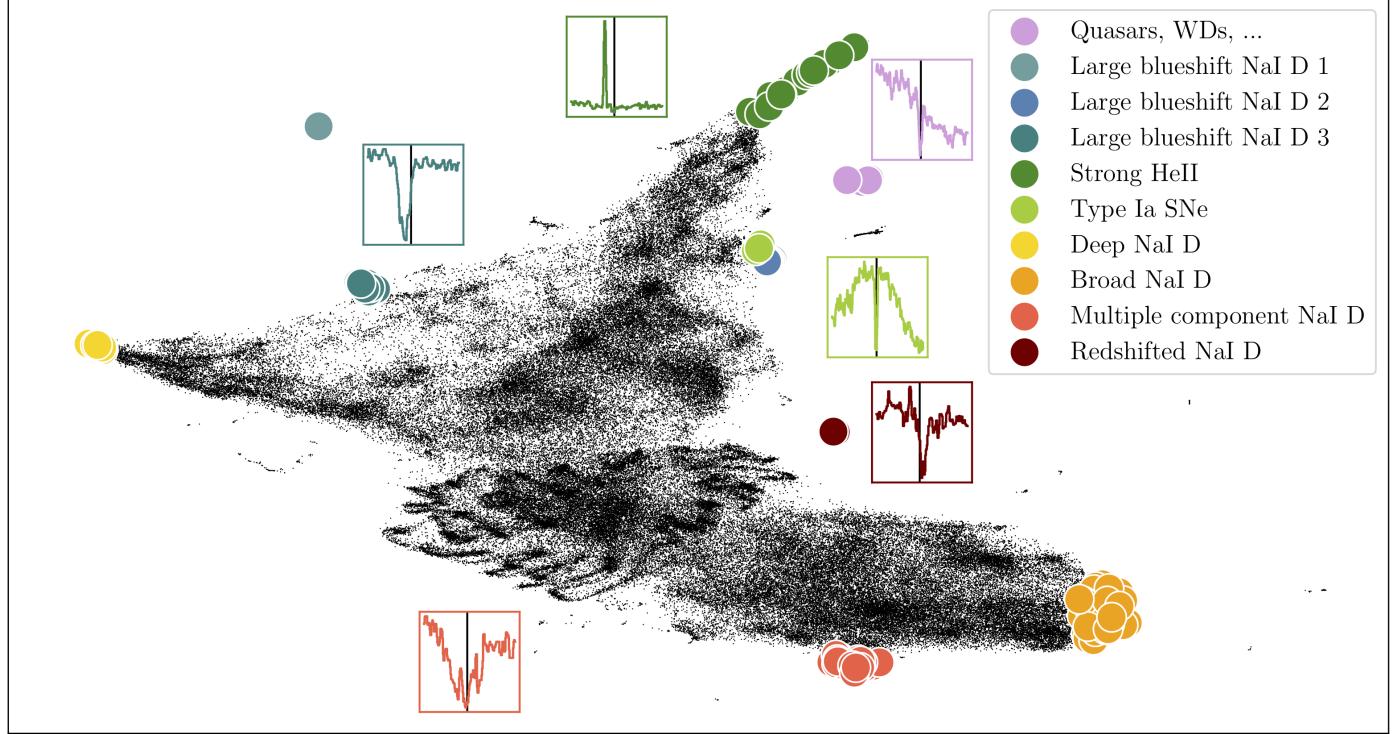


Figure 6: **Top panel:** A UMAP of SDSS galaxies constructed from the $\lambda = 5680 - 6120\text{\AA}$ region of the spectrum. Groups of unusual objects detected from the map are shown in color. Insets containing the NaID part of the spectrum for an example object are shown for select groups. **Bottoms panels:** The locations of the same galaxies with unusual NaID properties as in the top panel, on different embeddings. The bottom left panel shows the BPT diagram which separates AGNs from star-forming galaxies. The bottom right panel shows a UMAP constructed from the $\lambda = 4700 - 5100\text{\AA}$ region of the spectrum, containing the H β and [O III] lines. In the bottom left panel we can see that some of the unusual NaID groups lie in specific regions of the BPT diagram. The interesting finding is the galaxies with deep NaID absorption, who seem to be preferentially located in the AGN region of the BPT, while many galaxies with strong blueshifted NaID seem to be outliers on the BPT diagram. In the bottom right panel we see that the unusual NaID objects could not have been detected using this $\lambda = 4700 - 5100\text{\AA}$ map, illustrating that different maps contain different information. The locations of the unusual NaID objects here are also not random, suggesting correlations between various NaID and H β and [O III] properties. Interactive versions of all these maps, from which the unusual NaID objects and others were selected and inspected, are available at galaxyportal.space.

Greene 2014). Such objects were detected only by one of the implementations of Unsupervised RF.

- Another cluster on the map is composed of galaxies with an unusual slope of their SED in this wavelength region. They are shown in purple. Many of these objects were mistakenly classified as galaxies by the SDSS pipeline but are in fact white dwarfs and quasars. The objects that are indeed galaxies, such as SDSS J092034.87+511224.1 and SDSS J091959.69+513346.7 show broad emission features that we think are due to some error in the data acquisition or reduction. Such objects were detected by all the anomaly detection methods discussed in Section 2.1.
- Galaxies hosting type Ia supernova features in their spectra are also found in a small cluster. We mark them in light green. 8 of these galaxies, already found by Graur & Maoz (2013), are listed in C.5. Additional candidates could be found by inspecting the rest of the objects in the cluster. The clustering of these galaxies is due to the fact that the tell-tale feature of these supernovae, the deep Si absorption, falls partly within this wavelength region. Maps constructed with different wavelength regions, in which there are no prominent supernova spectral features, do not contain such a cluster. Galaxies hosting type Ia supernova features were detected by all the anomaly detection methods discussed in Section 2.1.
- Additional clusters (not shown in color) and objects that are isolated on the map show a variety of unusual behaviors. We find a small cluster of objects with chance alignment with brown dwarfs, objects with the wrong redshift determined by the SDSS pipeline, objects with bad sky lines subtraction, and some with unexplained absorption lines (likely due to a foreground or background source). Some of these galaxies are listed in Table C.6.

The bottom left panel of Figure 6 shows the locations of the detected anomalies on the BPT diagram. Note that some of the anomalous galaxies do not have detected emission lines and are thus not shown on the diagram. 3 groups of unusual NaID region galaxies also cluster on the BPT diagram: (i) Objects with strong NaID absorption are located in the AGN region of the diagram. (ii) Many of the objects with strongly blueshifted NaID are outliers in the BPT diagram, and have unusually low [O III]/H β line ratios given their (high) [N II]/H α ratios (line ratios refer to EW ratios). (iii) Objects with strong HeII emission are located in the star forming branch of the diagram.

To illustrate that different maps contain different information we show the locations of the same unusual groups of objects discussed above on a UMAP constructed from a different wavelength region in the bottom right panel of Figure 6. This map shows the $\lambda = 4700 - 5100\text{\AA}$ region,

containing the H β and [O III] lines. The unusual NaID groups are no longer clustered or isolated and would not be detected on this map.

3.3. Use case III: Trend detection

One method to detect trends is by inspecting how objects change along structures on the maps. In this example we use the $\lambda = 6400 - 6700\text{\AA}$ region map. This region contains the H α and [N II] lines. Objects that lie along geometrical structures on the map are expected to show continuous changes in these features. The user of our portal can select a specific region on the map and a specific direction, and stack the galaxies in bins along the chosen direction. This procedure takes a few button clicks on the portal. Figure 7 shows an example. What is found in this case is that the galaxies are ordered according to a combination of the emission line width and the H α to [N II] amplitude ratio. In general the emission features are more AGN-like towards the stack colored in yellow. In Figure 7, the AGN-like features are apparent as decreased H α to [N II] ratios towards the yellow stack. We have confirmed this point by inspecting the locations of objects at different parts of the sequence on the BPT diagram.

Trends can be discovered by looking for correlated changes in other regions of the spectrum. With well known samples or object types, one will mostly find trivial trends (e.g., emission line amplitudes that are correlated). In this example, however, we find that the equivalent width of the NaID absorption correlates with the width of the emission lines in the H α -[N II] complex, and with the H α to [N II] line ratio. We see that the stacks with wider emission lines and with lower H α -[N II] ratio have stronger NaID absorption. The bottom left panel of Figure 6 shows a similar trend as objects with deep NaID absorption lie in the AGN region of the BPT diagram.

While this example is only intended to illustrate how the portal could be used for detecting possible trends, it might be worthwhile to mention related work on the spectral features involved. Nagao et al. (2006) showed that in star-forming galaxies the H α -[N II] ratio is a metallicity indicator (but note that in our case at least in some of the objects there is an AGN contribution to the emission lines). In addition, the width of the narrow emission lines is known to correlate with the stellar mass of the galaxy. The NaID line, as mentioned above, gets a contribution from both the ISM and from cool stars.

4. Summary

We apply various anomaly detection methods to the same dataset of 150,000 SDSS galaxy spectra, and show that while they all succeed, they disagree on most of the top few hundred outliers. This naively surprising result is a natural manifestation of the fact that for high dimensional data there could be many different yet reasonable answers to the questions we ask of any unsupervised ML algorithm.

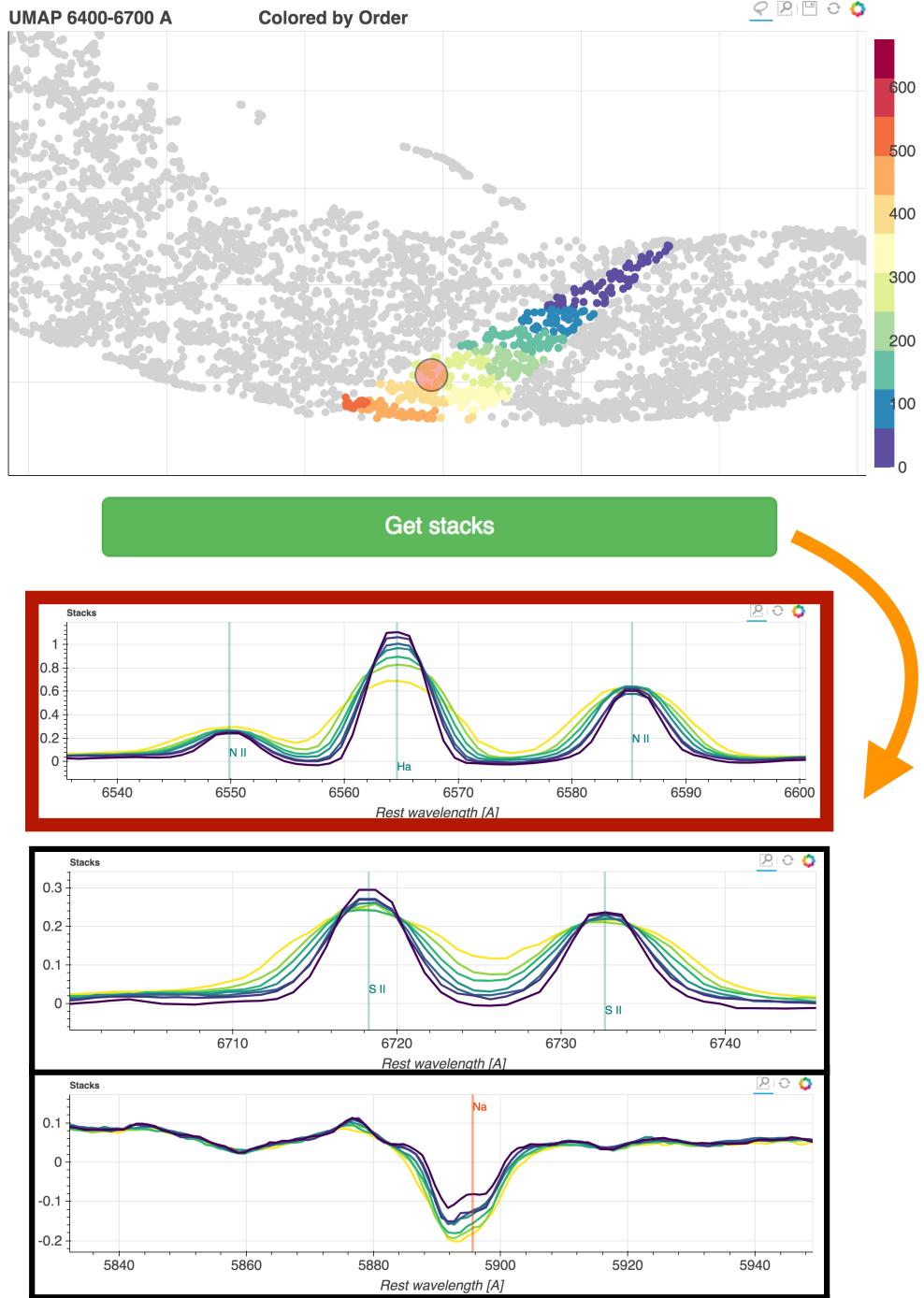


Figure 7: An example of trend exploration. The top panel shows a part of the $\lambda = 6400 - 6700\text{\AA}$ map, from which some of the galaxies are selected (the ones that are colored). The galaxies are ordered according to their location on the map, with color following the order. The bottom panels show different wavelength regions of the stacked spectra of the galaxies binned according to this order. In the example shown here the galaxies seem ordered by a combination of the line width and line ratio. The yellow lines have more AGN-like emission features; broader emission lines and higher [N II] to H α line ratio. In this example we also see a non-trivial correlation with the NaID absorption line that seems stronger in the AGN-like galaxies. Note that the coloring scheme of the map is different from that of the stacked spectra. Also, the orange dot in the top panel represent the currently selected object, and is not important in this plot.

As a consequence, any single method will only output a small subset of the answers we wish for.

In order to increase our chances of making discoveries, a practical approach is to accumulate many different results of unsupervised ML and make them available for inspection by the community in an easy and intuitive way. For this, we are developing an exploration tool for astronomical data, that brings together interactivity and unsupervised ML. The main feature of the portal is 2D embeddings, or maps, of the data, where objects that are similar in a given subspace are located near each other.

We demonstrate and develop our portal using the dataset of SDSS galaxy spectra. For this dataset we built several maps, each constructed using a different wavelength region. We also include several additional embedding (e.g., the BPT diagrams), various coloring schemes using metadata, and the results of a number of anomaly detection methods.

We show how such tools and approach can allow for a more effective discovery process when interested in anomaly detection or when searching for trends and correlations. Additional uses include the search for objects of interest via similarity ('find me more objects like this one'; Reis et al. 2018), or for studying an object in context of its peers ('how similar is this objects to others from other perspectives?'). We believe such methods will soon be indispensable.

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Mathematics of the Universe (IPMU) / University of Tokyo, Lawrence Berkeley National Laboratory, Leibniz Institut für Astrophysik Potsdam (AIP), Max-Planck-Institut für Astronomie (MPIA Heidelberg), Max-Planck-Institut für Astrophysik (MPA Garching), Max-Planck-Institut für Extraterrestrische Physik (MPE), National Astronomical Observatories of China, New Mexico State University, New York University, University of Notre Dame, Observatório Nacional / MCTI, The Ohio State University, Pennsylvania State University, Shanghai Astronomical Observatory, United Kingdom Participation Group, Universidad Nacional Autónoma de México, University of Arizona, University of Colorado Boulder, University of Oxford, University of Portsmouth, University of Utah, University of Virginia, University of Washington, University of Wisconsin, Vanderbilt University, and Yale University.

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Appendix A. Number of anomalies given the overlap

To calculate the probability of obtaining an overlap of k without assuming $n \gg g$, consider a specific order of randomly choosing the objects, where the first three objects are in the subgroup, and the next two are not. The probability for this scenario is

$$\frac{g}{n} \times \frac{g-1}{n-1} \times \frac{g-2}{n-2} \times \frac{n-g}{n-3} \times \frac{n-g-1}{n-4}. \quad (\text{A.1})$$

We see that for any order in which the objects are chosen, the probability for choosing k objects form the first subgroup and $g-k$ from the rest of the group is

$$\frac{g(g-1)\dots(g-k) \times (n-g)(n-g-1)\dots(n-g-(g-k))}{n(n-1)(n-2)\dots(n-g)}. \quad (\text{A.2})$$

Multiplying by the number of possible orders to choose the objects, the probability to obtain an overlap of k can be written as

$$\frac{g!}{(g-k)!} \frac{(n-g)!}{((n-g)-(g-k))!} \frac{(n-g)!}{n!} \binom{g}{k}. \quad (\text{A.3})$$

Appendix B. Anomaly detection methods

In this section we briefly describe the four anomaly detection methods that we used in the method comparison, applied to the galaxy spectra, and uploaded to our portal.

1. PCA reconstruction error. This is an example for model-based approach for anomaly detection. PCA is used to model the data, and the anomaly score is defined to be the χ^2 between the model and the data.

Additional examples of ways to model the data that could be used instead of PCA include independent component analysis (ICA), non-zero matrix factorization (NMF), Auto-Encoder, and physically motivated models.

2. Unsupervised Random Forest. This is an example for distance based approach for anomaly detection in which the definition of distance definition is based on an ensemble of classification trees. The similarity between two objects is defined to be the number of trees in which the objects end up on the same terminal node when propagated through the tree. The distance is the inverse of the similarity. An unsupervised Random Forest, which is a Random Forest (Breiman et al. 1984) trained to distinguish between real and synthetic data, is an example for an ensemble of classification trees. Other tree ensembles that could be used with the same distance definition include supervised Random Forest, Extremely Randomized Trees (ERTs), and boosted trees (e.g AdaBoost, Freund & Schapire 1997). Many other distance definitions exist, the simplest one being Euclidean distance.
3. Isolation Forest. This algorithm does not fall into any of the general three approaches given in Section 2. In Isolation Forest the inverse of the anomaly score is defined to be the number of nodes an object goes through before being isolated (i.e, found to be the only object on a node), summed over all the trees in the ensemble. Isolation Forest is commonly used with ERTs, but in principle could be used with other types of classification tree ensembles.
4. Fisher Vector based anomaly detection. This algorithm is related to the density based approach for anomaly detection. Instead of using the density itself, the anomaly score is defined to be the contribution of an object to the Fisher Information the data holds about the parameters of the density distribution model. We used a Gaussian Mixture Model (GMM) to model the density of the data, as in this case the gradients of the density with respect to its parameters, which are needed for the calculation of the anomaly score, have an analytical formula.

Appendix B.1. Example results

We list examples of anomalies detected by the four methods in Table B.1. Additional examples of anomalies detected by Unsupervised Random Forest can be found in Baron et al. (2017), and additional examples of anomalies found using the Fisher Vector method can be found in Rotman. et al. (2019).

Appendix C. NaID anomalies specific examples

In this section we provide examples from the various types of galaxies detected as anomalies from the NaID UMAP, as described in Section 3.2. Figure C.8 shows example

spectra of a number of different types of such anomalies. For each object the left panel shows the entire SDSS spectrum, and the right panel shows the zoom in on the NaID region which was used to detect the objects. A number of example objects for the different types of detected anomalies listed in the following tables: Table C.2: galaxies with large blueshift NaID. Table C.3: galaxies with multiple component NaID. Table C.4: galaxies with redshifted NaID. Table C.5: galaxies hosting a type Ia supernova. Table C.6: Various additional types of anomalies.

SDSS name	comments	detected by
SDSS J091337.33+295958.4	type Ia supernova	Isolation Forest, PCA reconstruction error
SDSS J095153.06+010605.8	type Ia supernova	RF V2, PCA, Fisher Vectors
SDSS J140622.31+162900.4	type Ia supernova	RF V1
SDSS J142608.24+152501.9	type Ia supernova	PCA
SDSS J150407.51-024816.5	narrow emission lines unusually broad	Isolation Forest, PCA, Fisher Vectors
SDSS J150908.75+090220.9	narrow emission lines with redshifted wings	Isolation Forest, Fisher Vectors
SDSS J144104.37+532008.7	triple peaked [O III] emission lines	Isolation Forest, PCA, Fisher Vectors
SDSS J152620.42+155226.8	chance alignment of two galaxies (shifted set of emission lines)	PCA
SDSS J080105.42+344941.0	chance alignment of two galaxies (shifted set of absorption lines)	RF V2
SDSS J031248.68-010020.6	chance alignment with foreground star	Isolation Forest, PCA, Fisher Vectors
SDSS J083909.65+072431.5	calibration fault	Isolation Forest
SDSS J111817.05+534459.6	calibration fault	RF V2, PCA, Isolation Forest, Fisher Vectors

Table B.1: Examples for anomalies detected by the four methods used in the method comparison: PCA reconstruction error, Unsupervised Random Forest, Isolation Forest, and Fisher Vector based anomaly detection.

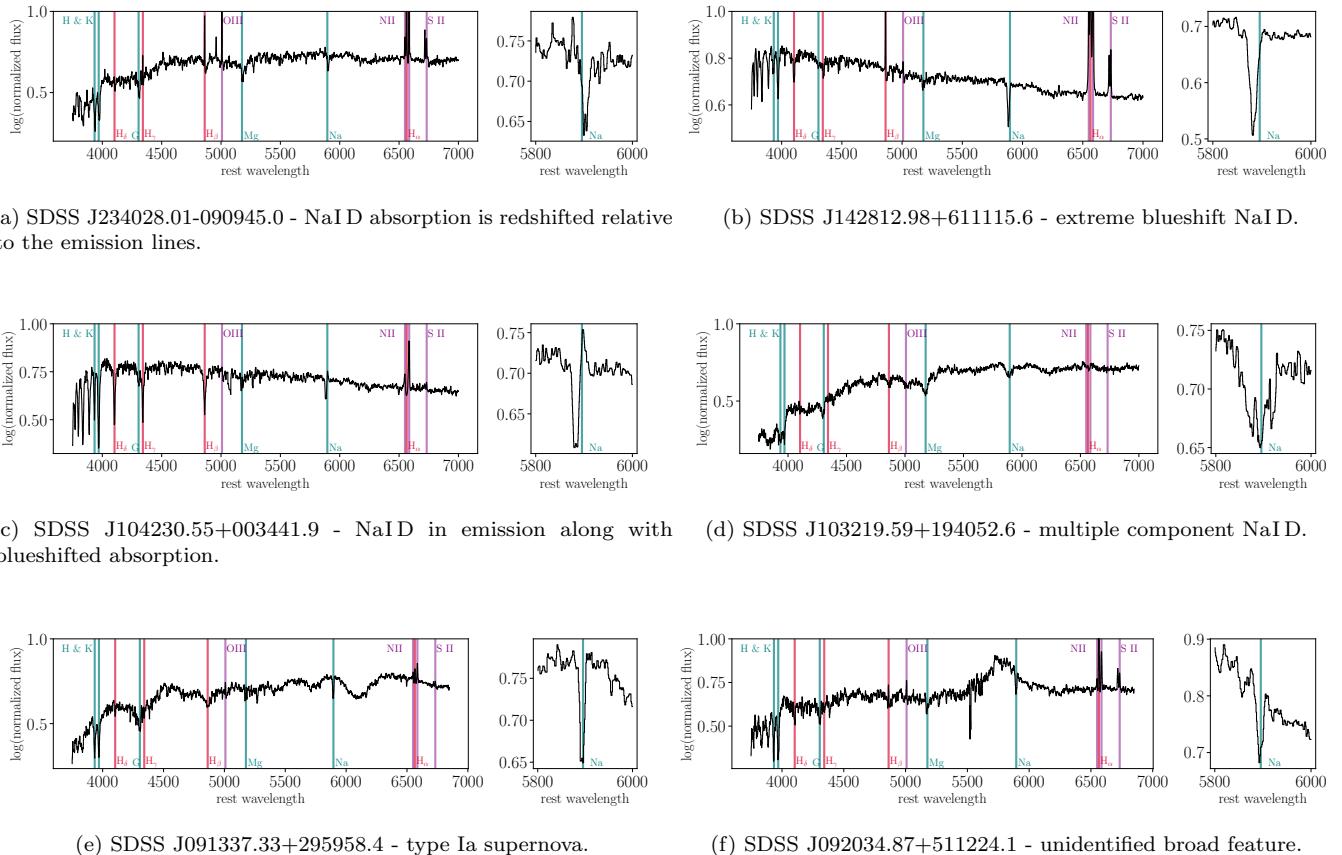


Figure C.8: Examples of galaxies with unusual NaID line profiles detected with our portal. The blue vertical lines mark the locations of common absorption lines, the purple vertical lines mark common emission lines, and the red vertical lines mark the Balmer series that can be seen in both absorption and emission.

index	SDSS name	comments
1	SDSS J142812.98+611115.6	SF
2	SDSS J094630.90+345500.6	Wolf-Rayet galaxy, SF, FOS
3	SDSS J104230.55+003441.9	PSB
4	SDSS J073856.16+320317.4	SF, PSB
5	SDSS J125427.34+022059.3	SF
6	SDSS J140621.04+252846.9	SB, ionized outflows
7	SDSS J125427.34+022059.3	PSB
8	SDSS J122715.39+062757.2	SF, PSB
9	SDSS J235047.12+143617.5	SF, ionized outflows
10	SDSS J141943.23+491411.9	SF, FOS
11	SDSS J083950.75+230836.1	SF, FOS
12	SDSS J025600.55+013829.5	SF, FOS
13	SDSS J031034.09+002938.7	SF, FOS

Table C.2: Examples for galaxies with extreme NaID blueshifts. Additional features are included in the comments column: SF = star forming emission lines, SB = star burst, FOS = face on spiral, PSB - post-starburst. Ionized outflows refer to the asymmetric profile with blueshifted wing of the [O III] line at 5007 Å. Wolf-Rayet classification was taken from SIMBAD and is based on Brinchmann et al. (2008).

index	SDSS name	number of components
1	SDSS J084344.28+385340.6	2
2	SDSS J211138.95+044126.8	2
3	SDSS J103219.59+194052.6	3
4	SDSS J110534.89+410524.2	2
5	SDSS J125856.36+385053.4	2

Table C.3: Galaxies with multi component NaID profile.

index	SDSS name	absorption	emission
1	SDSS J155157.88+203056.9	redshifted	blueshifted
2	SDSS J234028.01-090945.0	redshifted	blueshifted
3	SDSS J120525.71+510611.1	redshifted	multi-component
4	SDSS J125553.16+581948.6	redshifted	multi-component
5	SDSS J005555.93+003940.2	multi-component	redshifted
6	SDSS J141518.01+230841.0	redshifted	blueshifted
7	SDSS J211635.95-004613.1	multi-component	redshifted

Table C.4: Galaxies showing redshifted NaID absorption. The absorption and emission columns refer to the location of the features relative to the SDSS systematic redshift. The absorption column refers to the other absorption lines in the spectrum, e.g, the *H* and *K* lines. Note that blueshifted/redshifted are relative to the systemic SDSS redshift.

index	SDSS name
1	SDSS J080821.09+005035.3
2	SDSS J142608.24+152501.9
3	SDSS J095153.06+010605.8
4	SDSS J132301.39+243023.6
5	SDSS J140309.73+060754.3
6	SDSS J140237.96+034231.7
7	SDSS J091337.33+295958.4
8	SDSS J154024.75+325157.2

Table C.5: Galaxies showing type Ia supernova features in their spectra.

index	SDSS name	Comments
1	SDSS J073714.26+431414.9	chance alignment with foreground star
2	SDSS J152613.25+495322.5	chance alignment with foreground star
3	SDSS J083316.31+152314.6	chance alignment with foreground star
4	SDSS J143815.47+570445.1	chance alignment with foreground star
5	SDSS J142812.98+611115.6	extreme blueshift NaID
6	SDSS J052223.70+005916.4	calibration fault
7	SDSS J135124.77+054903.1	wrong redshift

Table C.6: Galaxies that are isolated on the NaID UMAP, suggesting unique properties, not similar to any other galaxy in the sample.