Class Introspection: A Novel Technique for Detecting Unlabeled Subclasses by Leveraging Classifier Explainability Methods

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Abstract

Detecting latent structure within a dataset is a crucial step in performing analysis of a dataset. However, existing state-of-the-art techniques for subclass discovery are limited: either they are limited to detecting very small numbers of outliers or they lack the statistical power to deal with complex data such as image or audio. This paper proposes a solution to this subclass discovery problem: by leveraging instance explanation methods, an existing classifier can be extended to detect latent classes via differences in the classifier's internal decisions about each instance. This works not only with simple classification techniques but also with deep neural networks, allowing for a powerful and flexible approach to detecting latent structure within datasets. Effectively, this represents a projection of the dataset into the classifier's "explanation space," and preliminary results show that this technique outperforms the baseline for the detection of latent classes even with limited processing. This paper also contains a pipeline for analyzing classifiers automatically, and a web application for interactively exploring the results from this technique.

1 Introduction

1.1 Motivation

Training classifiers for machine learning tasks requires that the data is accurately and completely labeled for a specific application. However, in the real world there is often more structure to the data than is labeled—and this can have real-world consequences to how the model performs in production processes. Within each labeled class, there can be significant variations that the model picks up on but is invisible to the user—this is *latent structure* within the class. For an example of this latent structure, consider a hypothetical classifier to determine whether an image contains apples or oranges. Oranges tend to be uniformly orange, but apples can come in more than one color: red, green, yellow, etc. If the labels for the dataset are just `apple` and `orange`, then the information about the color of the apples is lost. The intuition here is simple: the classifier may know about the color difference between two types of apples, but still label both apples due to the training data available to it. Therefore, by using explainability techniques, a human can detect the different unlabeled subclasses by analyzing *how* the classifier determines the class of an instance.

As a less trivial but more impactful example, clinical trial results interpreting the efficacy of a drug's treatment via a classifier may not fully capture all the subgroups in the input. Are the reasons Person A and Person B respond to a specific round of treatment similar? How about why Person C did not respond? This may be down to some specific structure in the input data which may not be fully captured by training data labeling.

With current methods, it is difficult to determine this latent structure—especially with high-dimensional or complex data such as image, audio, or video inputs. Current state-of-the-art methods generally require either that an entirely new representation is trained (as in the case of mixture models (Bell 2021) which must relearn the data distribution), that instances be categorized manually (as in subgroup analysis (Lanza and Rhoades 2013)), or they are only suited to discovering individual anomalous instances (as in commonality metrics (Paterson and Calinescu 2019)). These methods are discussed more fully in Section 2.4, but in general they are not one-size-fits-all, and require a separate (new) model to detect latent structure. Instead, class introspection allows for the re-use of an existing classifier allowing for analysis to inherit the statistical power of the classifier.

1.2 Objectives

This project aims to provide a solution for the latent structure problem by leveraging explainability techniques to detect latent (unlabeled) subclasses in the input data, using a novel approach dubbed **class introspection**. This technique compares a classifiers decision making process for each point in a dataset, and within each predicted class performs clustering over the local model explanations. Crucially, this *reuses the existing classifier*, and does not require a separate model for detecting latent structure (in contrast to the current state-of-the-art). At a high level, the decision-making process of a classifier model will be different for different inputs—leading to clusters corresponding to fragmentation within input classes. This provides a level of auditability on the model training process, both by ensuring that models are producing results for the correct reasons and by allowing for the detection of deficiencies in the model setup priors; by detecting latent structure, possible errors in labeling can be detected in model training. Additionally, this technique is agnostic to both the architecture of the particular classifier model used and the particular local explanation method, al-

lowing for use in even black-box environments (where no knowledge of the classifier's internals is required).

2 Background

2.1 Overview

In this section, we will discuss the algorithms and methods that are fundamental to class introspection (namely, explainability and clustering methods). Additionally, this section discusses several existing algorithms for detecting structure in data and their limitations as compared to class introspection.

2.2 Explainability

A key issue facing machine learning is explainability (XAI). In current state-of-the-art machine learning models, the model outputs are generated opaquely—that is, the reasons that the model chooses to assign one label rather than another are inscrutable from the outside. While this may be fine in trivial applications such as face detection, in safety-critical applications the reasoning for why a model produces the outputs it does can be a literal case of life and death. Explainability allows for a model to be audited, and for faulty behaviors to be explained and calibrated away (Ghai et al. 2020). Even more crucially, explainability allows for a model's decisions to be trusted by other agents (like humans) (Došilović, Brčić, and Hlupić 2018).

What is an explanation? Explanations are, at their core, simply an indication of which input features are relevant for a specific output from a network, and for each how strongly (or not) these features contributed to the output. Typically this is represented numerically, where each input feature is weighted by its importance to the overall classification with respect to the other features (Došilović, Brčić, and Hlupić 2018).

In tabular data, numerically weighting input features trivially shows which inputs are important as the feature is clearly defined (i.e. each input feature is labeled). Image data is more complex, as the features do not carry the same amount of information per-feature as tabular data; explanations for this type of data show which regions of the image were important to a model's classification (see Figure 1).

Inherently Interpretable Models The easiest way to generate explanations for models is by using models that are inherently interpretable. There are two common model architectures with this feature: regression models and decision trees. Decision tree outputs can be simply explained by following the chain of decisions from the root node down to the eventual leaf representing the classification. Regression models are similarly simple, with linear regression and logistic regression:

$$\text{linreg}(\mathbf{x}; \mathbf{w}, b) = \mathbf{w}^\top \mathbf{x} + b \qquad \text{logreg}(\mathbf{x}; \mathbf{w}, b) = \sigma(\mathbf{w}^\top \mathbf{x} + b)$$

We can see that for each case, there is a one-to-one correspondence between the weight vector $\mathbf{w}$ and the input vector $\mathbf{x}$. Therefore, the relative importance of each input feature in
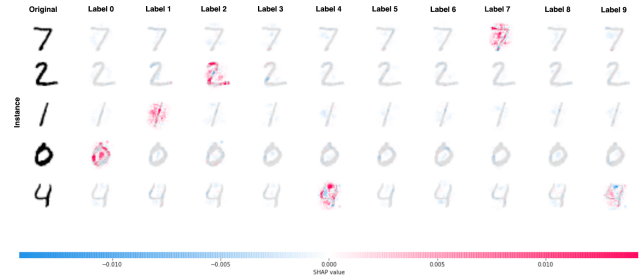

Figure 1: Example of a series of explanations of image data. Here, regions of the image that contribute positively towards the classification are red, and similarly blue regions denote negative contributions. Note that SHAP creates explanations for each instance for each label, regardless of true label. For more information, see Section 2.2.

$\mathbf{x}$ is directly encoded in the weights of the model—exactly an explanation.

Of course, using regression models or decision trees may not be an optimal strategy as these models are very limited in their capabilities. Another option is to converting an existing model as a whole into a more easily interpretable model architecture. For example, an interpretable model can be created with *Self-Explanatory Neural Networks* (SENNs) which are an extension of logistic regression (Teso 2019). This can use very few weights, and it is easy to determine the reasoning for any given classification as the weights correspond to a positive or negative linear combination of inputs. This approach, however, is limited in that some algorithms are not well-suited to interpretability. Algorithms such as deep neural networks are uninterpretable, and their performance cannot easily be matched by interpretable models.

Local Outcome Modeling If the model to be explained cannot be converted to an easily-interpretable model, it is still possible to create an explanation of its behavior using black-box explanation methods.

The simplest black-box approach is the Leave-One-Out (LOO) algorithm (Abdalla 2021). LOO simply segments the input features, and for each segment zeros out the segment and runs the model inference to determine how much the output changes. Despite LOO's apparent simplicity, this strategy is surprisingly effective at determining the salient regions of an input, and being a black-box algorithm means it can be broadly applicable to a diverse variety of algorithms (Abdalla 2021). Careful selection of segmentation algorithms can lead to very accurate saliency maps (see Figure 2). However, this flexibility comes at a cost. LOO is expensive to compute, as each segment requires a re-inference; additionally, this method does not take into account inter-dependencies between regions (Abdalla 2021). Additionally, this does not give per-feature saliency mapping, rather operating over superpixels—useful for individual explanations, but less so for comparing explanations between instances.

A more robust approach is to train a smaller model to explain individual predictions of a dataset (Teso and Kersting
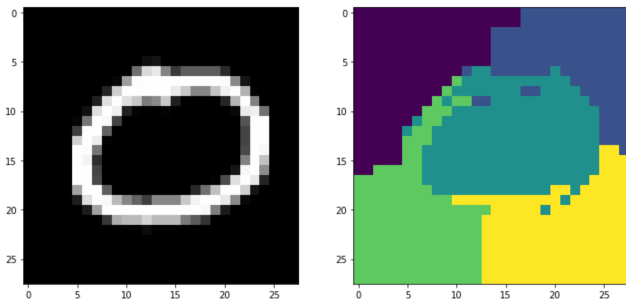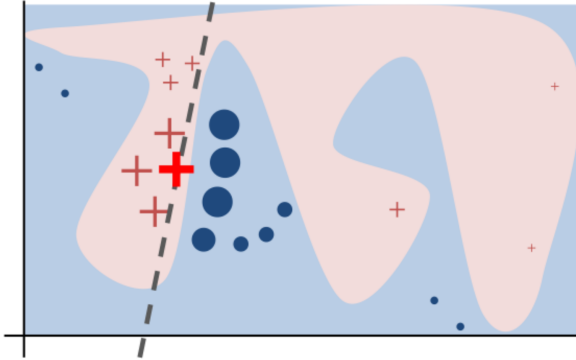
Figure 2: Example of LOO segmentation.

Figure 3: LIME local model. From Ribeiro et. al.(Ribeiro, Singh, and Guestrin 2016).

2018). This local approach has the benefit that the overarching model can be a black box while still providing explanations of the model behavior. This works because even if the decision surface may be defined by many uninterpretable features, a single point in that decision surface can be locally approximated. The most popular implementation of this approach is Local Interpretable Model-agnostic Explanations (LIME) (Ribeiro, Singh, and Guestrin 2016). LIME fits a flat plane against the decision surface, and infers the boundary by perturbing the input point to generate a cloud of points which are then all inferred by the model. While not being perfectly accurate, this is effective at broadly showing the explanation of the point inference and has the advantage of being model-agnostic. LIME still suffers from some the same limitations of LOO: each explanation requires multiple inferences (due to the input point perturbation), and to work over large dimensional data (such as images) superpixel segmentation must be used.

Neural Network Approaches A final approach is specific to neural networks: a series of techniques are available to compute the gradient of the class score with respect to the input pixels, yielding an effective explanation of which inputs are salient to the model's ultimate classification (Abdalla 2021). These methods are typically white-box, and operate over the specific structure of the neural network; this means that explanation method implementations need to be aware of the implementation details of the networks they are explaining.

Figure 4: Example saliency map generated with gradient ascent, depicting the saliency map from the top class prediction from a ConvNet (Simonyan, Vedaldi, and Zisserman 2014).

There are a several methods of achieving this, with the simplest being Gradient Ascent (Simonyan, Vedaldi, and Zisserman 2014). In gradient ascent, the gradient of the class label with respect to each input feature is computed via backpropagation all in one go, leading to a per-feature importance score across the image (Abdalla 2021). However, this can cause a very grainy saliency map (see Figure 4). A more nuanced approach is Deep Learning Important FeaTures (DeepLIFT), which compares the activations of network neurons to a "reference activation" (activations on a different instance) and can separate positive and negative contributions to give higher-quality results than Gradient Ascent (Abdalla 2021; Shrikumar, Greenside, and Kundaje 2019).

A popular library for generating these explanations is Shapley Additive Explanations (SHAP) (Lundberg and Lee 2017). SHAP represents explanations as a set of Shapley values (a measure of how important a contribution is to an overall whole borrowed from game theory) of the overall model, and computes these using a unification of several techniques (notably LIME and DeepLIFT) (Lundberg and Lee 2017). This approach generates high-quality explanations and is packaged into an easy-to-use Python library `shap` (Lundberg 2021).

SHAP is used heavily throughout this project, so it is

worth examining its underlying principles of operation. SHAP generates explanations for each label for each instance; for example for each numeral in MNIST SHAP generates ten sets of explanations: one for label `0`, one for label `1`, and so on. This is visible in Figure 1, where each instance (rows) has ten different Shapley value sets (columns). These Shapley values are not necessarily the same magnitude between data points (though in this project they usually are), and are typically similar within a dataset. SHAP operates over not only image data (with DeepSHAP) but works with other types of data, such as tabular data.

2.3 Hierarchical Clustering

Hierarchical clustering algorithms are a series of algorithms to form clusters over data where the number of target clusters is not necessarily known; contrasting against partitioning algorithms (such as K-means clustering) which require a knowledge of the cluster count to partition the dataset. Hierarchical clustering algorithms work by combining data points into clusters agglomeratively, and this property makes them incredibly powerful for analyzing unknown data as they are able to discover the data (Ester et al. 1996).

A commonly-used clustering technique is Density Based Spatial Clustering of Applications with Noise (DBSCAN). DBSCAN is able to efficiently handle clustering over a dataset with arbitrary-shaped clusters, and is able to achieve this with minimal required knowledge of the underlying dataset (as it is parameterized by a single hyperparameter) (Ester et al. 1996). This is achieved by picking an arbitrary point in the dataset and building a list of points reachable within a distance ϵ from that point (measured via a Euclidean distance metric). If that list is over a threshold number of points (typically 5), the list of points is given a cluster label—otherwise, it is marked as noise. This process is repeated until all points are either assigned a cluster or marked as noise.

However, due to DBSCAN's reliance on a Euclidean distance metrics, it is not suitable to very high-dimensional data. This is due to *curse of dimensionality*, which states that as the dimensionality goes up the more sparse the input space becomes for nearest-neighbor searching (Marimont and Shapiro 1979).

2.4 Latent Structure Detection

Class introspection is a novel technique, but the idea of identifying latent classes within a dataset is not new. A prominent application area of this concept is medical studies, where similarities between subgroups of patients need to be identified in order to determine the safety of a drug; for example, if certain members of the experimental group had different reactions to a research pharmaceutical, then it would be important to both identify fragmentation inside that group (i.e. had a reaction to a drug in different ways) and to identify common features between those individuals (e.g. similar ages, etc.) (Lanza and Rhoades 2013). Discovering these similarities is crucial, as treatment techniques can rely on a specific confounding variable in a population that is not readily captured by the available features.

Subgroup Analysis Subgroup analysis is a simple method of detecting latent structure. Subgroup analyses are performed by manually categorizing gathered data into subgroups based on some common characteristic of the data, and are typically examined by incorporating some moderating variable into a regression and interpreting the results (Higgins and Green 2011). However, because this grouping is inherently observational, this method is difficult to use effectively and is time-intensive. Additionally, the results of such analyses are subject to high Type I errors, as false positives are easy to make when manually grouping data (Lanza and Rhoades 2013).

Finite Mixture Models Finite mixture models are another way of determining latent structure (or structure in general) (Lanza and Rhoades 2013). Finite mixture models represent the data as a linear combination of component densities and maximize the likelihood of a specific configuration of models, and a common density function to use is the Gaussian normal distribution (Bell 2021). Gaussian mixture models optimize the probability:

$$p(x) = \sum_{m=1}^{M} P(m)\mathcal{N}(x; \mu_m, \Sigma_m)$$

where the probability $p(x)$ of a specific point is given by a sum of normal distributions moderated by mixing parameters $P(m)$ (Bell 2021). This probability is typically optimized by the expectation-maximization (EM) algorithm (Siedel 2011).

Finite mixture models can find latent structure, but they are limited in their effectiveness for this task. Finite mixture models are limited to discovering structure in the form of the basis functions chosen (e.g. Gaussians). Additionally, mixture models must re-learn the data distribution without any guidance from the original class labels which is computationally expensive(Bell 2021). FMMs also generalize poorly to high-dimensional data, as it is difficult to fit models in high-dimensional spaces. In general, these techniques are poorly suited to finding latent structure in complex data.

Commonality metrics A cutting edge technique in this area is the detection of rare subclasses via *commonality metrics* (Paterson and Calinescu 2019). This technique analyzes the input training classes for a given dataset and for each class determines the average activation in the penultimate neural layer for that class, and then scores each instance based on how similar it is to that average activation.

This is technique does not identify latent classes in and of themselves; rather, it identifies single instances that may be mislabeled or are significantly different than the average. Additionally, because the commonality metric approach operates over an average activation, large numbers of far-from-average instances will skew the whole commonality metric—potentially rendering the method less effective at identifying singular anomalous instances.

Clustering over neural networks Additionally, several recent techniques directly address the problem of unsupervised labeling of datasets. Broadly, these techniques intro-

duce a clustering step during the training of a neural network to improve the labeling performance of the network. Two such techniques are DeepCluster (Caron et al. 2019), and the self-labeling method proposed by Asano et. al. (Asano, Rupprecht, and Vedaldi 2020), where the loss function jointly learns the neural network parameters and the cluster assignments of the inferred features. DeepCluster itself simply uses k-means clustering to achieve this, and Asano et. al. use a more complex linear-programming-based method. Both, however, significantly outperform other feature-based learning approaches (Caron et al. 2019; Asano, Rupprecht, and Vedaldi 2020).

3 Methodology

3.1 Problem Formulation

The central problem to be solved is the discovery of latent subclasses in the input space. The aim is to find unlabeled (latent) subclasses within labeled classes in an existing dataset, with the hypothesis that these latent subclasses can carry additional information that is relevant to the authors of the classifier (see the examples in Section 1.1). The latent subclasses should be differentiated from one another without human intervention; that is to say, this should be an unsupervised technique.

This is, at its core, a clustering problem. In the ideal case (with no latent structure), each discovered cluster should correspond to a single true label in the dataset. However, in the case where latent subclasses exist within a class, we expect to see two or more cluster labels assigned to a single class label. In general, this method should take a dataset as input and the labels and output a list of cluster labels for each instance. As a baseline technique, simple heirarchical clustering could be performed; however, by using the explainability methods the resulting projection is hypothesized to be easier to cluster over.

3.2 Method Overview

Class introspection's central hypothesis is that even if a instances within a dataset is all labeled identically, the specifics of how a specific classifier *interprets* that instance can change significantly between those instances—and it is precisely that change that can be used to determine the existence of latent subclasses. In other words, this approach solves the subclass detection problem by leveraging an existing classifier, and through that the classifier's statistical power. Detecting these instance changes relies on the combination of several methods discussed in Chapter 2. The general process is described below:

1. Generate classifications for all instances in the dataset.

2. For each instance, create a local explanation of the classifier's decisions.

3. For each class:

   (a) Select all instances in the dataset classified as the selected class, and their explanations.

   (b) Run a clustering algorithm over the class's explanation.

   (c) **Multiple clusters indicate the existence of latent structure.**

Clustering over the instance explanations is possible as these explanations act as a *proxy* for the underlying instance. The explainability methods discussed in Section 2.2 produce saliency maps over the input features (Ribeiro, Singh, and Guestrin 2016; Lundberg and Lee 2017), and these saliencies are expressed as a tensor of saliency weights over the initial features. This is crucial: because these saliency maps are numeric, they can be interpreted just as easily as the original data—or even more easily, as discussed further on in this paper.

Because the explanations are simply numeric they can be clustered over, but the clustering itself is a challenge. Because the total class count is unknown, partitioning algorithms (e.g. K-means clustering) are not suitable to the task—if the total class count was known, the problem would be solved as we'd already know which subclasses exist. Instead, agglomerative clustering methods are appropriate for this use case, as they can operate over an unknown number of clusters. In this paper, DBSCAN is used to apportion the explanations into clusters—although others can be used (see Section 5.3).

Before clustering can be applied, the dimensionality of the data must be reduced. Clustering algorithms rely on (typically Euclidean) distance metrics, and as the number of dimensions increases the number of unit cells in that space increases exponentially, and so in these high dimensional spaces the nearest point can be extremely far away (Scarpa 2011). In this paper, principal component analysis is used to reduce the number of dimensions before clustering, yielding much better results.

At the end of the clustering process, the assigned cluster labels within each class are displayed as a histogram. The key insight here is that the cluster labels correspond to the similarity of the input images to each other, and if there are a large number of instances in two or more clusters those high-count are a candidate for a latent subclass.

Ultimately, this method requires human interpretation of the results as some of the detected latent structure may be intentional (e.g. in the apples-oranges example the classifier may not care about the different kinds of apple). Even so, the output from this algorithm is much more readily interpretable than attempting to audit the dataset and labels by hand.

3.3 Baseline

A simple baseline technique for detecting this latent structure is to ignore the explanatory methods altogether and perform clustering over the raw instance data itself. PCA is used to reduce the dimensionality of the data before being passed to the clustering algorithm, DBSCAN. This approach is similar to the commonality metrics methods described in Section 2.4, and is nearly identical to the methodology in Figure 5. To generate a dataset with latent structure, artificial latent structure is induced as in Section 4.1.

Running the baseline over the MNIST dataset yields a surprising result: the PCA and DBSCAN over the raw MNIST digits is not likely to determine when the artificial latent structure is present. Even with a hyperparameter sweep of the DBSCAN ϵ parameter, in some cases an optimal config-
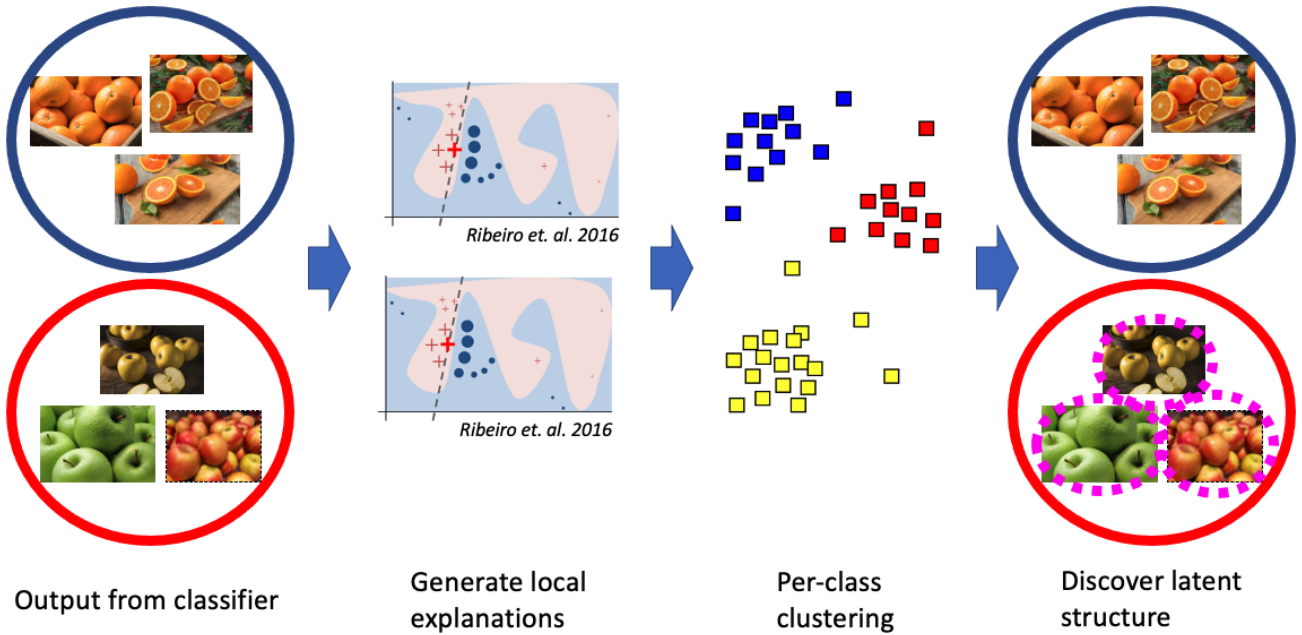
Figure 5: Class introspection methodology overview.

uration cannot be found where the bridged class has a significant split in cluster membership as opposed to the non-bridged classes. Figure 6 contains the output for the $(1 \rightarrow 8)$ bridging, and it is clear that the bridged class is not identified: no class contains any split in cluster membership, and some are entirely noise. However, some splits do work: in the case of the $0 \rightarrow 1$ split in Figure 7, the latent structure is successfully identified.

4 Experimentation

4.1 Artificial Latent Structure

To develop a pipeline to detect latent structure, we first need a dataset which contains latent structure. Unfortunately, it is difficult to find a dataset with such structure already in it. The challenge is twofold—either the dataset is simple enough that latent structure is virtually nonexistent, or the dataset is complex enough that detecting latent structure requires domain knowledge to detect. For a useful comparison of class introspection techniques, the dataset needs both the original class labels and labels for the latent structure to be detected. Creating these labels requires manually labeling every instance, which is both incredibly time-consuming and out of the scope of this project.

Clearly, another solution is needed. Instead of relying on existing datasets to have exploitable latent structure, we can *create* latent structure ourselves by "bridging" class labels together. This trivially creates latent structure, as both the instances for label A and label B are bound to the same class—and thus the new bridged class label has two distinct types of instance in it. This also has the benefit of giving labels corresponding to the original classes, as the original labels can be compared to the bridged labels to show which
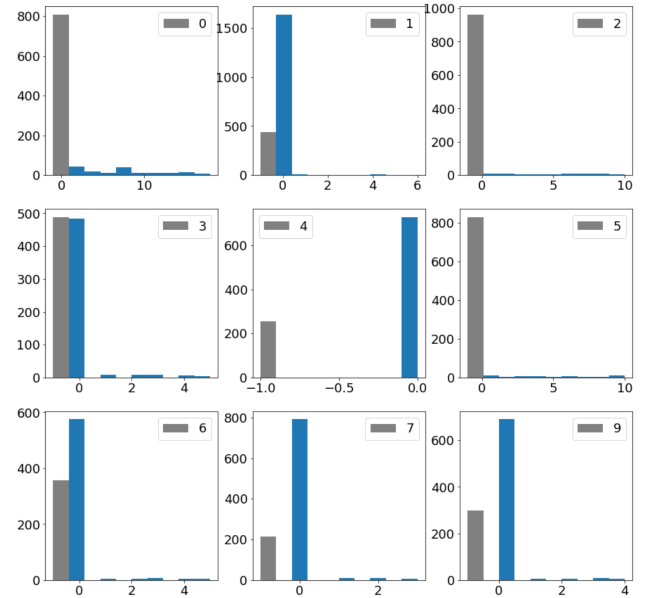

Figure 6: Detected class fragmentation from the baseline run against MNIST $1 \rightarrow 8$ with $\epsilon = 250$. Each blue bar represents a detected class from DBSCAN. Note how none of the classes show a major split in the assigned cluster labels (ignoring gray noise bars).

instances have been bridged. See Figure 8 for an example with MNIST with labels 1 and 8 bridged together.

This approach has limitations, however. The primary complication is the nature of the latent structure itself: bridging two classes can create a superclass with extremely obvi-
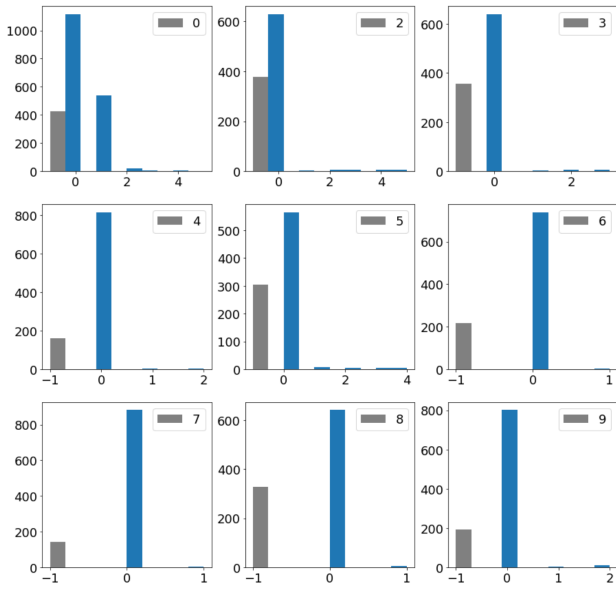
Figure 7: Detected class fragmentation from the baseline run against MNIST $0 \rightarrow 1$ with $\epsilon = 275$. Note how here, the latent structure is successfully identified (top left).

Figure 8: A demonstration of artificial latent structure with MNIST, here bridging the `1` and `8` classes. Note that the bridged classes have been highlighted.

ous latent structure, which may not align well with real-life latent structure. However, for the purposes of this project these effects have been ignored, as it is useful to have obvious latent structure to detect rather than very subtle structure in order to test the pipeline. Additionally, bridging class labels can lead to unexpected behavior whilst training models over a dataset with a small number of classes. This is a fundamental issue, as bridging two classes effectively removes one of the classes. For simple datasets, this can cause certain models to not learn the structure of the superclass but instead simply learn one of the other classes and segment the input space into "class and not class".

4.2 MNIST dataset

An appropriate multiclass dataset for the development of the class introspection algorithm is the MNIST dataset (LeCun and Cortes 2010) which contains $70,000$ handwritten digits (0 through 9) as 28 pixel by 28 pixel monochrome images. The MNIST dataset is a common dataset in machine learning as it is easily understood by beginners while still being complex enough to allow for meaningful analysis.

For the purposes of class introspection, it is an ideal dataset due to its relative simplicity and high class count. This high class count is crucial to avoid the issues with too few meaningful classes discussed above, as with a single bridged class there are still eight remaining classes.

SHAP and Keras Due to the fine-grained explanations required for class introspection, LIME's explanations were insufficient. A different explanation engine was required, and SHAP (with the DeepLIFT backend) is able to provide those explanations. Instead of operating over superpixels, SHAP uses DeepLIFT to backpropagate the contributions of ev-
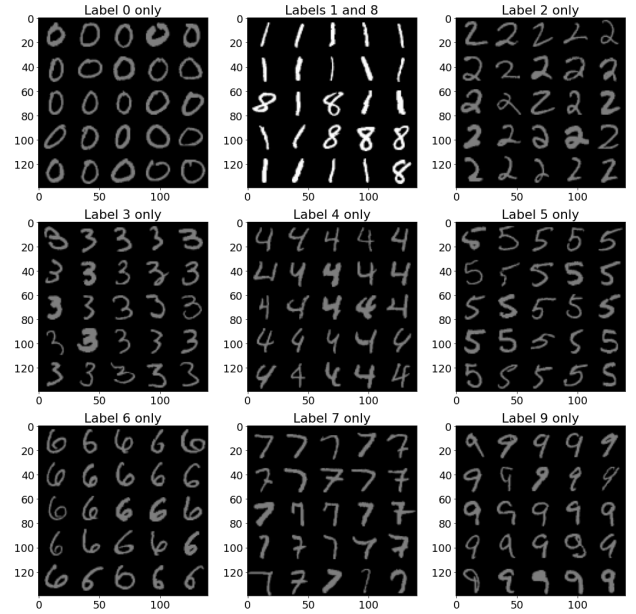
ery neuron to every feature in the input space (Shrikumar, Greenside, and Kundaje 2019; Lundberg and Lee 2017).

To keep the experiment simple, a relatively simple network architecture was chosen: fully-connected $784 \rightarrow 128 \rightarrow 128 \rightarrow 64 \rightarrow 10$ layers with ReLUs and a softmax activation. Training this network resulted in a 97.91% accuracy over the test dataset, which is expected over such a relatively simple dataset. Running SHAP explanations over the test dataset yielded a per-pixel saliency map, and this map is intuitively interpretably; as an example for an instance with a true label 7 the explanation for label 0 shows that the network expects a round shape, and because the instance does not match that shape the input features negatively contribute towards classification as a 0. For the same instance, the explanation of the true label 7 shows the shape of the 7 positively influencing the classification of a 7, yielding a classification of 7 for the instance (see Figure 9).

Again, the `1` and `8` digits were bridged together due to their dissimilarity, and the network was trained again (achieving an accuracy of 97.92%). Figure 10 shows another grid of SHAP explanations, note that there are no explanations in the `8` column as they have been bridged with the `1` column. Filtering just for instances in the bridged category shows a clear difference between the explanations for the `1` instances and the `8` instances.

The next step in the class introspection pipeline is to cluster the explanation to isolate the latent structure in the class. This poses several problems: the number of clusters is unknown, the data may not be linearly separable, and the data is high-dimensional. To solve the unknown cluster count, hierarchical clustering is used (DBSCAN). DBSCAN can handle clusters that are not linearly separable, making it suitable
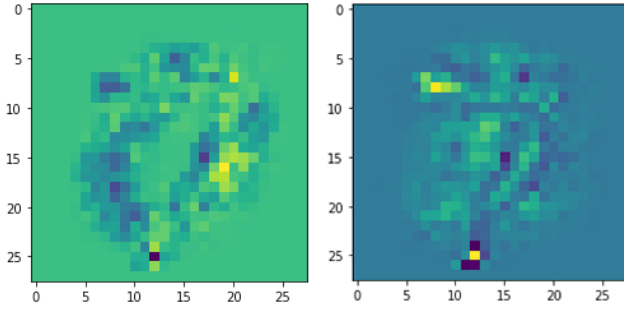
Figure 9: On the left: SHAP explanations over unbridged data, detail on explanation for label 0 and true label 7. Note the band of blue values in the shape of a zero, these are negative contributions (blue) from the features that would match label 0 and are missing on the 7. On the right: SHAP explanations over unbridged data, detail on explanation for label 7 and true label 7. Note the positive contributions (green) along the body of the glyph.
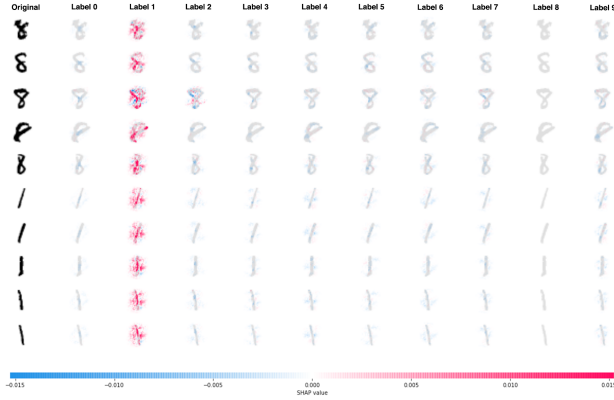

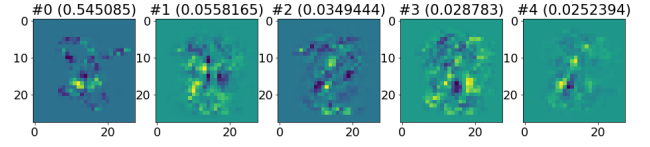Figure 10: SHAP explanations over bridged MNIST data.

Figure 11: PCA vectors for the 1 to 8 bridge, with the explained variance of each component.
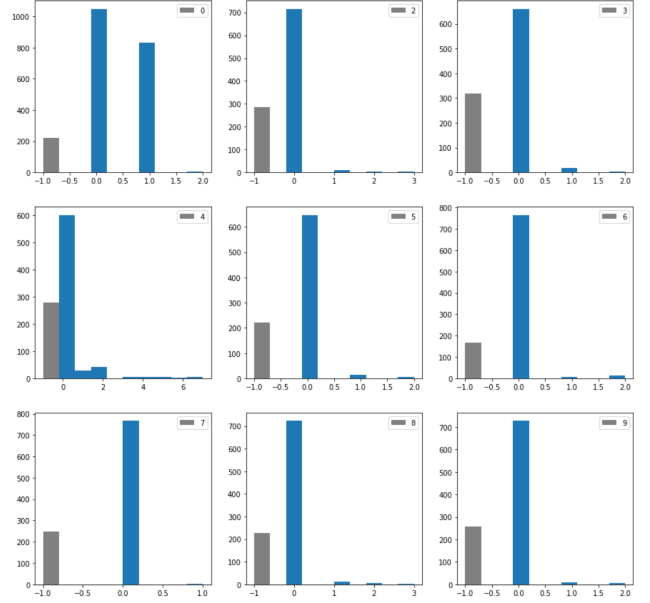

Figure 12: Intraclass fragmentation histogram viewed with DB-SCAN on bridged MNIST data (bridged labels 0 and 1). As before, the x axis is the class label and the y axis is the count of instances in that label. Note that in the bridged case $0 \rightarrow 1$ there are two main bars (+ a gray noise bar) and in the rest there is only one main bar.

Figure 13: Variance inside classes in bridged MNIST data (bridged labels 0 and 1). Note that the variance is highest in class 0 (the bridged class).

for this application (Ester et al. 1996). However, DBSCAN relies on a euclidean distance metric, requiring dimensionality reduction to avoid the curse of dimensionality.

In this case, PCA was used to reduce the dimensionality from 784 to 5 as a preprocessing step, yielding the principal components seen in Figure 11. PCA was calculated from the set of all explanations for instances the network predicted, giving a global set of basis vectors. Running DB-SCAN over this data with $\epsilon = 0.004$ yielded two distinct classes. As a control, all other classes were calculated using the same method, and this yielded the class membership visible in Figure 12. This shows that it is possible to find latent structure with this method. Additionally, even without DB-SCAN the latent class is visible in the variance explained by the PCA vectors, as seen in Figure 13.

To verify that this was not a fluke, this process was repeated for all possible pairings (45 in total). To facilitate this computation, a pipeline was created to automatically run all cases, and a web application was produced in order to view results. The code for both of these are available on Github[1].

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[1] https://github.com/pkage/class_introspection_krhcai

5 Discussion

5.1 Comparison to Baseline

Compared to the baseline method described in Section 3.3, the SHAP + PCA + DBSCAN method described above is very effective at determining the latent structure. This variation in performance is indicative of the difference in the type of data being processed. The baseline operates directly over the glyphs themselves, while the class introspection pipeline operates over the classifier's *explanations* of the glyphs. While similar, the distinction is important: in the baseline, the precise positions of the pixels are salient to the class representation, whilst in the explanations it is the specific neuron firings (and their intensities) that are salient. This allows the class introspection pipeline to group positive classifications by the specific neurons that are firing; the intuition being that the exact structure of the glyph does not matter so long as the specific neurons with that class are active which is fine tuned already by the classifier. Compare this to the baseline, which is relegated to determining the specific pixels that make up a class without the benefit of a trained neural network behind it.

5.2 Limitations

This experiment has shown that class introspection is a viable technique, but there are still several limitations in its current iteration. One main issue is that the explainability methods are imperfect. In most cases, SHAP or LIME produce saliencies that are reasonable, but in others they pick up on specific pixels that are assigned a saliency much higher than it's neighbors—or in fact, any other pixel in any other instance—by several orders of magnitude. This is infrequent, but care must be taken to avoid these outliers skewing the PCA vectors.

Another issue is the dependence on the DBSCAN hyperparameter ε. Without careful tuning, this can very easily yield a "collapsed solution", where the entire class is lumped into a single class, or a largely noise-filled clustering solution where most points are in the noise class or in minimum-cluster-size clusters. Future work here should be in adding checks to ensure that the class distribution is meaningful.

In a similar vein, PCA is ill-suited to image data. PCA does not preserve the structure of the image, rather flattening it out into a single-dimensional vector. This flattening ruins any sort of spatial correlation between features, and is extremely fragile to image scaling, rotation, transposition, etc. A better choice for future work is a proper computer-vision-based feature extraction method, such as Scale-Invariant Feature Transform (SIFT) or Histogram of Oriented Gradients (HOG). These techniques would preserve the feature positions in the saliency map, and allow for a higher-quality dimensionality reduction. In its current iteration, class introspection is ill-suited to complex image data (such as CIFAR or ImageNet) due to this limitation with PCA.

Fundamentally, class introspection is limited by the characteristics (and statistical power) of the classifier being explained. If the classifier does not learn the differentiating features of a class with latent subclasses and instead just treats that class as a catch-all, then class introspection is less effective at discovering that subclass. This is why the neural-network-based approaches were effective: the MNIST data was complex enough that the neural network had to actually understand the input features, and this allowed the bridged class to be easily discovered.

More fundamentally still, class introspection is an "unknown-unknown problem": namely, the number of latent classes is unknown—and even worse, the very existence of those latent classes is unknown. It is not unlike searching for a needle in a haystack without even knowing if the needle is there. Additionally, there is another problem: of these discovered subclasses, there is no way of knowing which ones of those subclasses are intentional or which are novel. This means that there will always have to be a human in the loop to determine which subclasses are relevant.

5.3 Future Work

The class introspection pipeline as it stands performs well in this paper, but there are areas that can be improved for more robust performance on a wider variety of data. A potential area of exploration is replacing the clustering algorithm with a Gaussian mixture-based approach, where each point could be maximized for the probability of being assigned a latent class instead of a definite class label being assigned to each point. This could help identify classes where the presence of latent structure is uncertain, but not definite.

Another direction of exploration is the even more involved technique of comparing not only the input saliency but the neuron activations chain through the last layers of the network for any particular instance. This would limit the technique to only neural networks, but may be a powerful tool for identifying subclasses as the last layers of the network can be effectively used for determining similarity of instances (Paterson and Calinescu 2019; Caron et al. 2019).

This technique has far reaching possibilities, as the ability to reliably discover latent classes has implications across diverse fields of data science and artificial intelligence research. For example, the ability to reliably detect latent structure in classifiers greatly benefits medical studies who may be looking for a robust alternative to subgroup analysis. More fundamentally, this technique may allow for the auditing of classifiers to ensure that the data they are trained on and the data that they work over is free of unknown and potentially unwanted subclasses that could reduce the overall effectiveness of the classifier.

5.4 Conclusion

Over the course of this project a technique for reliably extracting unlabeled (latent) subclasses from existing datasets has been developed, leveraging explainability techniques to take advantage of the statistical power of complex models. This provided an advantage over other approaches for capturing latent structure, and was demonstrated over an example dataset with artificially-induced latent structure.

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