



Master's thesis

Explainable Artificial Intelligence for Out-of-Distribution Detection

Using irregularities in machine learning explanations to detect when a model is faced with unusual data

Jonatan Hoffmann Hanssen

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Department of Informatics
Faculty of Mathematics and Natural Sciences

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Jonatan Hoffmann Hanssen

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Supervisors:
Hugo Lewi Hammer
Kyrre Harald Glette

Abstract

As Artificial Intelligence becomes a larger and larger part of society, the need for robust and understandable models becomes paramount. When neural networks are used in high-impact settings such as cancer detection or autonomous driving, we must require that they

Sammendrag

Here comes the abstract in a different language.

Preface

Generative Artificial Intelligence (AI) has not been used to generate or enhance any written text contained in this thesis. However, generative AI has been used for some programmatic tasks. Services such as GPT UiO have been used for code debugging, for generating TikZ code used for creating diagrams, and for generating some boilerplate Python code. All data and personal information have been processed in accordance with the University of Oslo's regulations, and I, as the author of the document, take full responsibility for the validity of any generated code used as part of this work.

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OOD	Out-of-Distribution
DL	Deep Learning
ID	In-Distribution
CAM	Class Activation Mapping
GradCAM	Gradient Class Activation Mapping
GAP	Global Average Pooling
MSP	Maximum Softmax Probability
LIME	Local Interpretable Model-Agnostic Explanations
MLS	Maximum Logit Score
MSP	Maximum Softmax Probability
RMD	Relative Mean Absolute Difference
QCD	Quartile Coefficient of Determination
CNN	Convolutional Neural Network
SLIC	Simple Linear Iterative Clustering
FFNN	Feed Forward Neural Network
CV	Coefficient of Variance
GBP	Guided Backpropagation
ML	Machine Learning
LRP	Layer Relevance Propagation
XAI	Explainable Artificial Intelligence
AI	Artificial Intelligence
AUROC	Area Under Receiver Operating Characteristic
AUPR	Area Under Precision Recall Curve
ROC	Receiver Operating Characteristic
FPR	False Positive Rate
TPR	True Positive Rate
FPR95	False Positive Rate at 95% Recall

Preface

I would like to thank my dog and Ed Bickley, who is still at large.

Preface

Chapter 1

Introduction

1.1 Motivation

Machine Learning (ML) generally, and Deep Learning (DL) specifically, have seen a tremendous increase in performance in recent years, performing comparable to humans in tasks such as image classification, speech and handwriting recognition, as well as many others [1]. Consequently, DL methods have been deployed in a multitude of fields and have become a part of our daily lives through their role in web search, text translation, computer vision, and in many other technologies which are taken for granted. In medicine, deep learning has the potential to provide faster and more accurate detection of diseases by being trained on cases from thousands of previous patients [2]. Despite this, "surprisingly little in health care is driven by machine learning" [3].

To explain this discrepancy, we should consider that despite their impressive performance, the application of deep learning methods is not without drawbacks. Firstly, deep neural networks are inherently unexplainable due to the large number of parameters that any non-trivial network has. State of the art models will perform millions of operations to evaluate a single data point, and it is therefore impossible for humans to comprehend and explain the entire process which lead the model to make a particular decision. In medicine, this is a major limitation of deep learning methods, as both doctors and patients expect to be able to understand why a decision was made [4].

Secondly, although neural networks may attain high accuracy on test data and appear to have learned great insights about the tasks they are employed in, they often lack robustness and can suffer large drops in performance on data points which are slightly different from the training data. As [5] has shown, it is possible to create data points which are imperceptibly different from normal data points, yet still fool otherwise high performing models. More problematically, unlike humans, who recognize when they are faced with a novel situation where their expertise might be lacking, DL methods will predict equally confidently on data points which are far outside the data they have been trained on [4].

These two problems lead to the fields of XAI, and OOD detection. XAI attempts to explain the reasons why a model came to a decision, which helps to remedy the black-box nature of complicated DL models. In a healthcare setting, such explanations can be inspected by medical practitioners to confirm the diagnosis, and can be used to give patients information about why decisions regarding their health were made. OOD detection attempts to uncover when a data point is too different from the training data to be classified reliably. These methods could alert medical practitioners when such data points occur, thus avoiding potentially fatal misclassifications.

Both of these fields have seen increased interest in recent years, and are vital parts of any integration of DL in medical settings. This thesis will focus on OOD detection, but will attempt to use methods inspired by XAI to improve detection performance. The overarching intuition is that by inspecting the explanation of a model on a specific data point, we may be able to uncover flaws or irregularities in the explanation which could help us determine whether the data point is OOD.

1.2 Problem Statement

As explained in the previous segment, OOD detection is a developing field, which has become more important in recent years as machine learning is being used for higher impact tasks, such as disease detection. Finding novel methods which improve a model's ability to detect when input is OOD is important to increase the robustness of machine learning models as they are used in these real-world scenarios. The field of XAI is concerned with understanding the inner workings of a model, and could thus offer insights which could help us detect unusual behaviour in the model as a result of OOD data points. The problem statement is thus as follows:

Can methods from the field of Explainable Artificial Intelligence be used to improve Out-of-Distribution Detection?

To answer this question, I introduce 2 objectives:

1. Develop OOD detection methods which rely solely on XAI explanations, and compare these methods
2. Develop theoretically sound proof of concept OOD detection methods that are inspired by insights gained from the field of XAI, and compare these methods on a variety of different benchmarks against existing OOD detection methods

1.3 Scope

As we will see in chapter 2, both the fields of XAI and OOD detection are very large, which make it impossible to explore all the possible ways one might combine XAI and OOD detection. Thus, it is necessary to restrict the scope of both the XAI and OOD detection methods used. In this section, I will describe the choices I've made and give a short explanation. In later chapters, the choices will be justified more thoroughly.

The field of OOD detection is primarily concerned with image classification tasks. Thus, my project will also deal exclusively with image classification datasets. Given this type of data, the choice of XAI algorithms naturally gravitates towards post-hoc, saliency based methods. The choice of OOD detection algorithms is not significantly restricted by the choice to deal exclusively with image data, but I will exclude methods which use outlier exposure to improve performance, or which require retraining of the model. These choices are informed by [6], which have found that post-hoc methods

1.4 Research Methods

Use ACM

1.5 Ethical Considerations

1.6 Main Contributions

Objective 1 is accomplished in chapter 2. Here, the fields of XAI and OOD detection are introduced, their respective taxonomies are explained and a selection of specific methods are explained in more detail. This chapter provides a good entry for machine learning researchers who wish a decent introduction to the two fields.

1.7 Thesis Outline

Chapter 2 gives a short introduction to machine learning, followed by a deeper look at the fields of XAI and OOD detection. Chapter 3 introduces my methodology; the methods I will use to compare and contrast XAI explanations on ID and OOD data, as well as a handful of OOD detection methods which integrate explanations into their functioning. Furthermore, I introduce the different datasets which will be used in chapter 4, among them the HyperKvasir gastrointestinal dataset [7]. Chapter 4 will first go into the results of the comparison between ID and OOD explanations, detailing the differences between different methods. Then, I will report the performance of the different OOD detection algorithms I have developed, on a handful of datasets, including HyperKvasir, CIFAR10 and ImageNet. After the experiments follow a discussion (chapter 5), where I reflect on the benefits and drawbacks of using XAI methods for OOD detection, and summarize the results from 4. Finally, the conclusion (chapter 6) concludes.

Chapter 1. Introduction

Chapter 2

Background

In this chapter I give a short introduction to important concepts in the field of machine learning generally, followed by a more in-depth look at the fields of OOD detection and XAI. Then, I give an overview of related works; papers which have attempted to use XAI for OOD detection. Finally, the datasets used in chapter 4 are covered.

2.1 Machine Learning

Machine Learning is the field of algorithms that are able to learn from data, as opposed to being explicitly programmed. Such algorithms use statistical methods to learn relationships in data, and use these relationships to generalize to unseen data. More formally, [8] gives the following definition of machine learning algorithms:

Definition. A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T , as measured by P , improves with experience E .

Thus, machine learning is a different paradigm from traditional problem solving, where programs are made to solve problems by following explicit rules. For example, a traditional image classification system attempting to differentiate between malignant and benign tumors might use hand-crafted rules which consider the texture, color and size of a tumor. As one might imagine, such rules will quickly become very complicated when we consider all the possible factors which might influence the appearance of a tumor. Using a machine learning approach, we would instead feed an algorithm with thousands of images of both benign and malignant tumors, and the rules could then be automatically updated until the algorithm predicted the correct category with a high enough accuracy.

Machine Learning is commonly divided into the three subcategories of supervised, unsupervised and reinforcement learning

2.1.1 Supervised Learning

Supervised Learning is a subcategory of machine learning where we have a dataset containing both inputs and desired outputs. In the example above, we could use supervised learning by creating a dataset of images of tumors (the input) and corresponding labels which indicate whether each tumor is malignant or benign (the desired output). The learning goal of the algorithm is then to associate images with the correct label. Because we know the correct answer, we are able to fine-tune the

algorithm automatically whenever it makes a mistake. However, supervised learning requires labeled data, which can be very costly, especially in the medical domain, where deciding whether a tumor is malignant or benign requires expert knowledge.

2.1.2 Unsupervised Learning

In unsupervised learning, we do not have any labels. In these cases, we might not know whether data points belong to different classes or not. Instead, we can use machine learning to uncover patterns in the data, for example by attempting to cluster the data into different groups and seeing if these groups are sufficiently separated. An example use case could be for fraud detection in a bank. By feeding financial transaction from many different users into an unsupervised learning model and asking it to perform clustering of the data, it might be possible to find a group of users whose transactions differ substantially from the rest, which might indicate that their transactions are fraudulent.

2.1.3 Reinforcement Learning

Reinforcement Learning deals with problems where we do not know exactly what the correct solution is, but we are able to assess whether a given solution is good or not. For example, when controlling a robot arm, it is difficult to say exactly what angles each joint should be for every millisecond when picking up an object, but if the arm does not pick up the object, we know the algorithm has failed. In these problems, the algorithm is trained through reinforcement, where good attempts are rewarded and bad attempts punished.

2.2 Neural Networks

Neural Networks are a class of machine learning algorithms, which have become the clear state of the art in almost all fields where machine learning is applied. Notable examples are computer vision, image classification, speech recognition, text and image generation and machine translation. Neural networks are loosely inspired by our own brains, where neurons are connected together and send information between each other. By connecting thousands of neurons together, neural networks are able to learn complicated relationships between the input and output.

2.2.1 Feed Forward Neural Networks

The Feed Forward Neural Network (FFNN), also known as a Multilayer Perceptron, traces its roots to the very beginning of machine learning, through the work of Frank Rosenblatt [9]. It forms the basic structure for neural networks which has been adapted and modified over the years to form more complex architectures such as convolutional, recurrent or residual neural networks. The basic structure of an FFNN is that the input values are passed through an affine transformation (a matrix multiplication followed by the addition of a bias), and then passed through an activation function, which produces outputs. These outputs can then go through the same process again, which constitutes a single "layer". By stacking several of these layers, with non-linear activation functions, an FFNN is able to learn arbitrarily complex mappings between inputs and outputs¹.

¹In fact, by the Universal Approximation Theorem [10], only a single hidden layer between the input and output is necessary, although this theorem does not give a way to construct such a network for any given function

Figure 2.1² shows a simple FFNN architecture with three hidden layers. In this case, the bias has been omitted for brevity. Here, we can see how all nodes of a layer are connected to the following layer. By using an activation function on the nodes of the hidden layer, before their values are sent to the next layer, we achieve the non-linearity required to learn complex patterns.

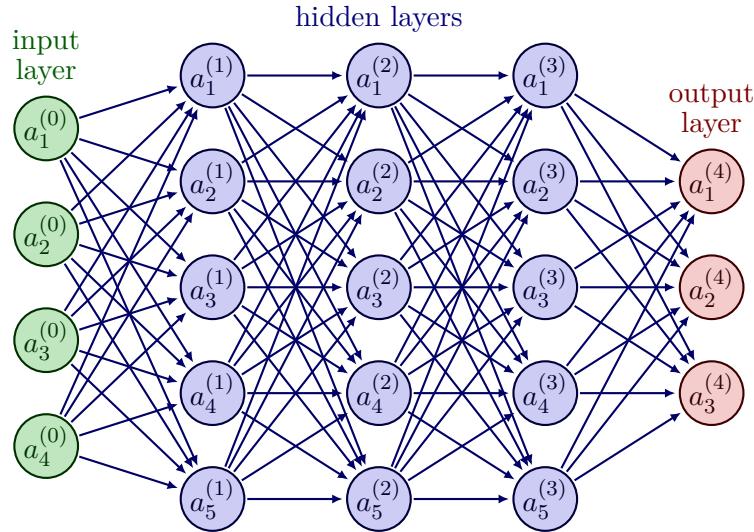


Figure 2.1: Figure showing a simple Feed Forward Neural Network, with nodes labeled. The number in parentheses indicates the layer number while the subscript indicates the node number within the layer.

Mathematically, a single layer can then be described as follows:

$$\mathbf{x}_{i+1} = \sigma_i(A_i \mathbf{x}_i + \mathbf{b}_i) \quad (2.1)$$

Here, the input \mathbf{x}_i is linearly transformed by the weights of the matrix A_i from the input space to the output space, then each value of the new vector in the output space is adjusted by an addition of a bias term, and finally an activation function (σ_i) is applied to each value. The size of the input and output layers is determined by the number of input and output features, respectively. Furthermore, the activation function of the output layer is also determined by the application, most commonly *sigmoid* for binary classification, *softmax* for multi-class classification and simply identity for regression.

2.2.2 Convolutional Neural Networks

FFNNs have some inherent flaws which make them unsuitable for working with high dimensional, spatially connected data, such as the pixels which make up an image. Firstly, each input of a FFNN is connected to every output of the following layer. If we want to connect the input pixels of a 224 by 224 image to a layer of 100 nodes, our first layer will have over 5 million weights, which is already quite a lot for a relatively small image. Furthermore, these weights will have to encode redundant information, because each pixel is considered separately. Consider a network attempting to detect the presence of a cat in an image. We would want the network to detect the cat regardless of whether

²Figure by Izaak Neutelings, "Neural Network with coefficients, arrows", TikZ.net, licensed under CC BY-SA 4.0, [https://tikz.net/neural_networks/].

it is in the middle, the right corner, or any other position in the image. In an FFNN, the weights connected to any of these positions in the image would then have to encode a cat detector separately from all the others.

Convolutional Neural Networks (CNNs) solve both these issues by using small kernels of weights which are "slid" across the entire input. By using the same weights across all positions of the image, we do not need to train separate detectors for different positions, giving us translation invariance. Figure 2.2 shows the functioning of a convolutional kernel on a 3-channel image. Each value in the output is a weighted sum of a neighbourhood of values in the input image, where the weights are defined by the kernel. As we can see, the same weights are used on all positions, drastically reducing the number of parameters that need to be tuned. In a 2d-convolution, the kernel has the same number of channels as the input, and is only slid across the height and width dimension. The kernel in this figure is a *Sobel Operator*, and detects vertical edges. In a CNN, the weights of each kernel are not specified manually, but rather learned through backpropagation.

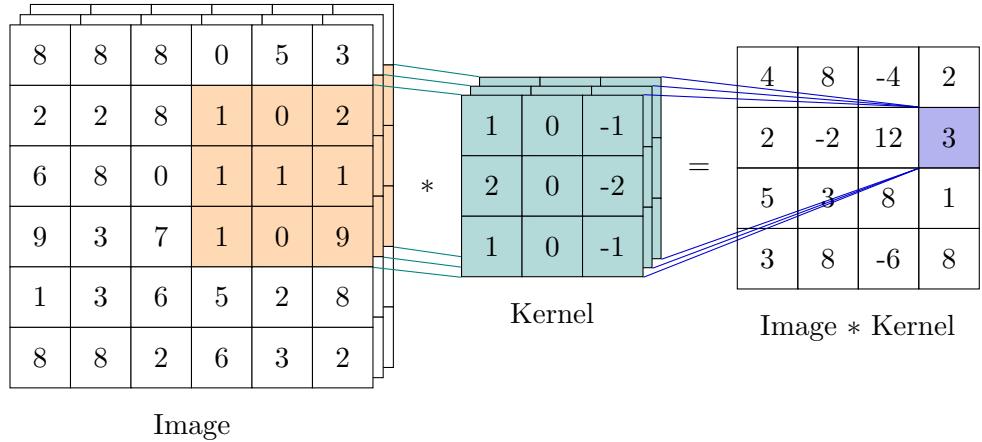


Figure 2.2: Figure showing a convolutional kernel applied to a 3-channel image.

By using several different kernels, we can detect many different patterns despite each kernel only detecting a single type. By using the outputs of all the kernels as inputs to a new set of kernels, we can use the same type layer structure as in an FFNN, allowing us to extract information in a hierarchical manner. It is common to see that trained CNNs have early layers that detect edges and texture, later layers that use these edge and pattern detections to detect larger shapes, while the final layers combine the shapes to detect entire objects [11].

By not evaluating every possible position in the input image, CNNs downsample the image, and are able to reduce the number of operations considerably. Simultaneously, this downsampling enables each subsequent layer to consider a larger area of the input image than the previous (a larger field-of-view), which allows larger patterns to be discovered. Simultaneously, it is common to use a larger and larger amounts of kernels on the new input, thus increasing the channel depth while the spatial dimensions are reduced. Between each layer, we use non-linear activation functions, similarly to how they are used in FFNNs.

After several such convolutions, we can flatten the output, either by aggregating each channel using Global Average Pooling (GAP) or a similar method, or we can simply

flatten all dimensions and consider the three dimensional feature map as a long vector of shape $C \times H \times W$. By doing this, we can pass the output to one or more linear layers, which can perform classification or regression on the extracted features and give us a final prediction. Figure 2.3 shows a high level overview of this process. Here, the input, which has only 3 channels, has its spatial dimensions reduced while its channel depth increases through consecutive convolutions. Finally, we have a certain number of channels in our final feature map, which are flattened (in this case with GAP) and processed through a linear layer to give a final prediction.

Input RGB Image:
3@224x224

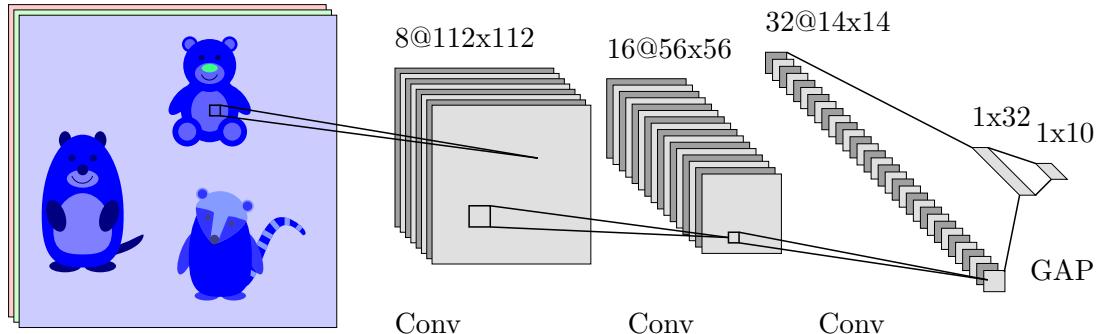


Figure 2.3: Figure showing a high level overview of how a CNN functions

2.3 Model evaluation

2.3.1 Metrics

OOD detection is essentially simply a binary classification problem. Thus, the metrics I will use in this thesis are those used for such problems. In the field of OOD detection, AUROC and False Positive Rate (FPR) are most commonly used. As such I shall focus on these metrics, as opposed to for example the Area Under Precision Recall Curve (AUPR).

Accuracy

Accuracy is the simplest metric used in binary classification. It is simply the ratio of correct predictions over all instances in the data set.

Accuracy has the advantage of being simple to understand and calculate, but it is very often insufficient. A simple (and quite common) scenario where accuracy fails to capture the performance of a model is any situation where there are large class imbalances. For example, imagine we have trained a CNN to predict whether a person has lung cancer or not, based on CT-scans of their lungs. As most people do not have lung cancer, we can imagine that such a dataset is highly imbalanced, for example that only 1 in 100 people actually have cancer. If a model simply predicts that no one ever has lung cancer, it will be correct in 99% of cases, and will thus have an accuracy of 99%, although it has missed every instance of cancer and is completely unusable in any real context.

For the purposes of OOD detection, accuracy is thus insufficient, as we have no guarantees that ID and OOD will be balanced. In fact, we expect OOD data to be relatively rare, given that the goal of developing an AI model is to ensure high

performance during deployment, which necessitates having training data which covers as much as possible of the data seen during inference.

Metrics utilizing the binary classification confusion matrix

Instead of simply considering whether a prediction was correct or not, we should take into account the different combinations of prediction and ground truth, considering positive and negative classes separately. Figure 2.4 shows the possible four possible combinations given a ground truth class and a predicted class.

	Predicted Positive	Predicted Negative
Actual Positive	True Positive	False Negative
Actual Negative	False Positive	True Negative

Figure 2.4: Figure showing the binary classification confusion matrix, denoting the four possible combinations created by the ground truth and predicted class. Green cells denote correct predictions, while red cells denote wrong predictions.

With these possibilities defined, we can begin to gain a clearer picture of the performance of a model.

Precision and Recall

Precision is the share of positive predictions that were actually positive. With a high false positive rate, we have a low precision, which means that the model is erroneously flagging many negative classes as positive. In an OOD detection setting, a model which flags many ID samples as OOD would have a low precision, if we treat OOD samples as the positive class.

Recall is the share of actual positive samples that were predicted positive. Recall tells us how many of positive samples we missed. In an OOD detection context, a model which lets many OOD samples slip by undetected will have a low recall score.

Precision and recall are often used together because evaluate the model in different ways that complement each other. If a model has both high precision and high recall, it does not erroneously flag many negative classes as positive, nor does it miss many positive classes.

Sensitivity and Specificity

Sensitivity and specificity is another pair of metrics that is commonly used for evaluating binary classification. Sensitivity is equivalent to recall; the share of positive samples that were correctly predicted as positive. Specificity is the share of the negative samples that were correctly predicted as negative. Sensitivity and specificity are also known as True Positive Rate (TPR) and *True Negative Rate*.

Threshold Independent Metrics

The previous metrics are a clear improvement over simply using accuracy. However, they still have the problem that they are all dependent on what threshold one sets when predicting something to be a negative or positive class. Thus, it becomes harder to compare different models by using these metrics. Indeed, by simply increasing the threshold of any classifier, we can increase the true negative rate. Similarly, by decreasing the threshold, we can increase the true positive rate.

Area under Receiver Operating Characteristic:

AUROC remedies this problem by looking at all possible thresholds, and calculating the TPR (equivalent to sensitivity, recall), and the FPR (equivalent to $1 - \text{specificity}$) for each possible threshold. With these values calculated, we can plot each point on a graph, giving us an Receiver Operating Characteristic (ROC) plot. Figure 2.5 shows this plot, for three different models.

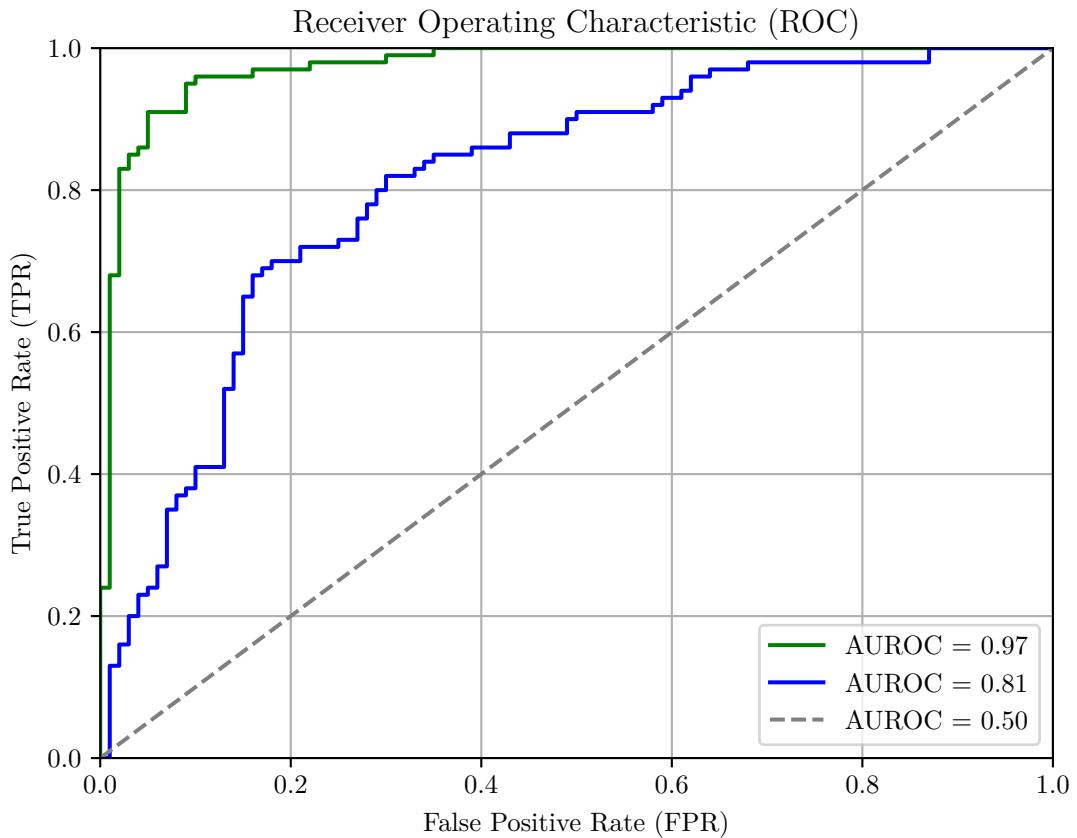


Figure 2.5: Graph showing the distribution of hypothetical ID, Near-OOD and Far-OOD data for an unspecified metric. The shaded region shows the overlap between the ID and OOD samples.

Once we have done this, we can calculate the integral under this curve, giving us the AUROC. If a binary classification model can perfectly separate the two classes, then all possible thresholds will either have 100% TPR or 0% FPR, giving an area under the curve of 1. If instead a model has no discriminative power, then the predicted values

of positive and negative classes are entirely random, and all changes to the threshold will increase one of the metrics at the expense of the other. Such a model would have TPRs and FPRs making a straight line of points, and an AUROC of 0.5. In between these extremes, we can evaluate different models, without having to consider different thresholds. 2.5 shows what the ROC-curve of a model with either 0.97 or 0.80 AUROC looks like, as well as that of a random classifier with AUROC = 0.50.

One important thing to note about the AUROC is that values lower than 0.50 do not mean that a model is worse than random guessing. This is because if a model is consistently wrong, we can simply choose the opposite category of what the model outputs, and gain a new model which is better than random guessing. For example, if a cat versus dog detector gave an actual image dog a higher chance of being a cat than an actual image of a cat in 95% of cases, it would have an AUROC of only 0.05. However, if we simply multiplied all outputs of the model by -1, we would suddenly have a model which correctly gives a cat a higher chance of being a cat in 95% of the cases, and an AUROC of 0.95. Thus, we really only care about getting AUROC scores far away from 0.50.

False Positive Rate at 95% Recall

False Positive Rate at 95% Recall (FPR95) is another way of comparing models without having to consider specific thresholds. Instead, we simply select the threshold which gives a recall (equivalent to TPR) of 0.95, and calculate the FPR at this threshold. The drawback to this metric as opposed to AUROC is that we do not get a general view of how the model performs. However, if we have a requirement that the model has a very high true positive rate, we may not care about how the model performs at any other threshold, and thus this metric is suitable. It is of course also possible to calculate this metric at any other recall value, depending on the application. However, in the field of OOD detection, FPR95 is the metric that is used in the vast majority of cases [6, 12–15].

2.3.2 Statistics: Bootstrapping and T-tests

Bootstrapping [16] is a way to get a better estimation of the true generalization error of a model, by performing the same experiments several times on resampled versions of the original dataset.

2.4 Explainable Artificial Intelligence

Below follows a thorough introduction to XAI, as well as detailed look at some important methods for explainability for neural networks applied to images. Specifically, saliency methods will be explained in detail, as they constitute a core part of my thesis.

2.4.1 The motivation for Explainable Artificial Intelligence

Given the impressive performance of DL methods, one might be convinced that these models do not need to be explainable or interpretable, and that we instead should just place our faith in the model without knowing exactly how it came to a decision. However, as [17] points out, "a single metric, such as classification accuracy, is an incomplete description of most real-world tasks". Small differences between the data distribution when the test data was collected and when the model is deployed may have a large impact on the model's performance, or the model may have learned artifacts or specificities in the training dataset which were also present in the test dataset, leading to a false

belief that the model has gained generalizable knowledge when it has not. By using explainable methods, we may reveal these shortcomings. In my case, this may also have the secondary effect of separating ID and OOD data points.

XAI is also especially important whenever the model is used in settings where its decisions have a high impact. If a model is used by a hospital for disease detection, both the patient and doctor will probably want to be able to understand why the model has found that a disease is present. For them, high performance on a test set of different cases may not be enough. As [2] states, "for the regulated healthcare domain, it is utmost important to comprehend, justify, and explain the AI model predictions for a wider adoption of automated diagnosis". In other high impact areas, such as autonomous driving, the impact of wrong decisions by the network can have fatal consequences, and customers and regulators will want to be absolutely sure that the models used are robust and base their decisions on relevant factors as opposed to quirks in the training data. Furthermore, the right to an explanation of an automated decision affecting a person is included in the EU's General Data Protection Regulation, which states that "In any case, such processing should be subject to suitable safeguards, which should include specific information to the data subject and the right [...] to obtain an explanation of the decision reached after such assessment and to challenge the decision." [18].

2.4.2 Taxonomy of Explainable Artificial Intelligence

This section goes through three axes which define an XAI method:

- Intrinsically explainable models versus post hoc methods
- Model dependent versus model agnostic methods
- Global versus local explanations

Intrinsically explainable models versus post hoc methods

Intrinsically explainable models are models which have sufficiently low complexity, such that it is feasible for a human to understand them without further modifications. Examples of such methods are linear regression, logistic regression and decision trees [19].

Post hoc methods are methods which are applied to the model after training. These methods do not aim to constrain the model to be interpretable, but inspect the model after training. For example, after using a convolutional neural network to classify a CT-scan of a tumour (which gave a prediction of malignant), we could run post hoc algorithms on the network which are able to extract which part of the image contributed the most to the prediction. Thus, post hoc methods remove the need for the model to be simple enough for a human to understand by extracting the relevant information for us.

Model dependent versus model agnostic methods

Model dependence/agnosticity denotes whether an XAI method uses specifics of a particular type of model to generate the explanation, or whether the method can generate an explanation without using specifics of the model at all. Explanations based intrinsically explainable models are clearly model dependent, while methods that only use the input and output of the model instead of looking at the internal operations

are model agnostic. An example of a model dependent method (which is not simply an intrinsically explainable model) is Class Activation Mapping, which requires a CNN with a specific architecture to function, while an example of a model agnostic method are Shapley values, which use the inputs and outputs to calculate the marginal effect of a single feature on the output value.

Global versus local explanations

Global explanations provide general relationships between the input features and outputs learned by the model over the entire dataset [20]. In this way, they can show how a specific feature affects the output in general, instead of just how it affects the output of a single point. These methods are ideal for finding trends in the data, but may not be suitable for a patient wanting an explanation for their specific case.

Local explanations do not describe general trends, but focus only on a single data point. These methods give insight into how the features influenced the prediction of a single data point, but these relationships may not hold for other data points, and as such these methods do not give the same insight into the general behaviour of the model.

2.4.3 XAI methods adapted to images: Saliency maps and segmentation

As explained in section 1.3, the field of OOD detection is primarily focused on image data, and as such this is the focus of this thesis as well. Thus, before delving into specific XAI methods, it is beneficial to elaborate on how XAI methods are adapted to images. When explaining tabular data made up of categorical and numerical values, it is often common to explain each feature by associating it with some change in the output prediction. For example, one might say that increasing the number of rooms in a house by one increases the predicted sale price by 30 000 NOK, or that the absence of a balcony decreases it by 25 000 NOK. But, given that images are made up of tens or hundreds of thousands of features (pixels), such an approach may not be suitable.

Firstly, given that we have so many features, it may no longer be interesting to know exactly how much each feature contributes to a prediction, given that we don't expect any single pixel to have a very large impact. Furthermore, inspecting the contribution of each individual pixel, like one might do for tabular data, is not even realistically feasible, due the overwhelming number of features. Given that our input is in the form of an image, which is best understood visually, as opposed to numerically, it is then natural to instead present the explanation in the same way.

These visual explanations take the form of saliency maps, as shown in figure 2.6. Here, we display the saliency values of all pixels in a heatmap, as opposed to numerically. Instead of considering the absolute values, we instead display the saliencies in relation to each other, such that the most important and least important pixel has colors on opposite sides of the colormap. In this way, it is easy and intuitive to see where the important regions of the image are, and we do not need to consider the absolute values of each pixel.

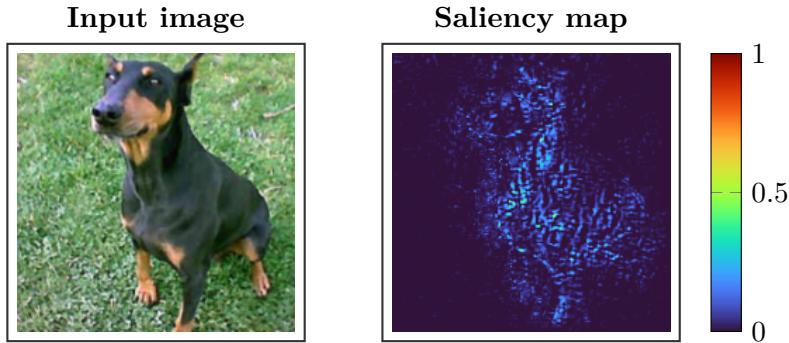


Figure 2.6: Figure showing an input image and the corresponding saliency map, generated by an XAI algorithm which shows the important pixels for the predicted class (Rhodesian Ridgeback). The colorbar and heatmap show the relative saliency for all pixels, with 0 being the least important pixel and 1 being the most important pixel

Secondly, many methods which are designed for data tabular data (which may have 10-20 features) are far too slow when the number of features may be over a hundred thousand. Methods such as LIME, Occlusion or Shapley fall into this category, as they permute the input at a rate which scales with the number of inputs.

A solution to this is to segment the image into larger regions, which are treated as one. As opposed to asking "how does the prediction change if we change this pixel", we instead ask "how does the prediction change if we change this *region*". All pixels in a region are then awarded the same amount of importance. This drastically reduces the dimensionality of the problem, and allows us to use a much larger range of methods.

Regions of pixels can be created in different ways. The simplest option is consider a window of a specific height and width, and slide this window over the image with a specific stride. By adjusting the stride and size, the number of dimensions can be adjusted. The benefit of such a simple approach is that the segmentation itself introduces no extra computation. However, a substantial downside is that each region can contain completely unrelated objects, because the regions are created without considering the underlying image. For example, if a 60 by 60 pixel region contains in its lower right corner a part of a dog, occluding this region could lead to a large change in confidence and thus high importance. However, it is not just the lower right corner that is awarded high importance, but the entire region, which may contain other objects or parts of the background which are not actually important.

By using more sophisticated segmentation methods, we can avoid this problem. Methods such as Simple Linear Iterative Clustering (SLIC) [21] create regions which can be considered more intuitive than simply using a rectangular sliding window. SLIC performs an iterative clustering of pixels, grouping similar pixels into larger regions called superpixels. The downside to this method is that the iterative, CPU-bound process introduces a considerable computational overhead. Figure 2.7 shows a comparison between the saliency map of the LIME algorithm applied to an image segmented using rectangular regions and to an image segmented using SLIC. As we can see, the rectangular segmentation means that the some of the grass in the background is given a high saliency, because it happens to be in the same region as the dog's head. Using SLIC, there are few regions which contain both grass and the dog, and thus the high saliency of the dog's face does not affect other parts of the image.

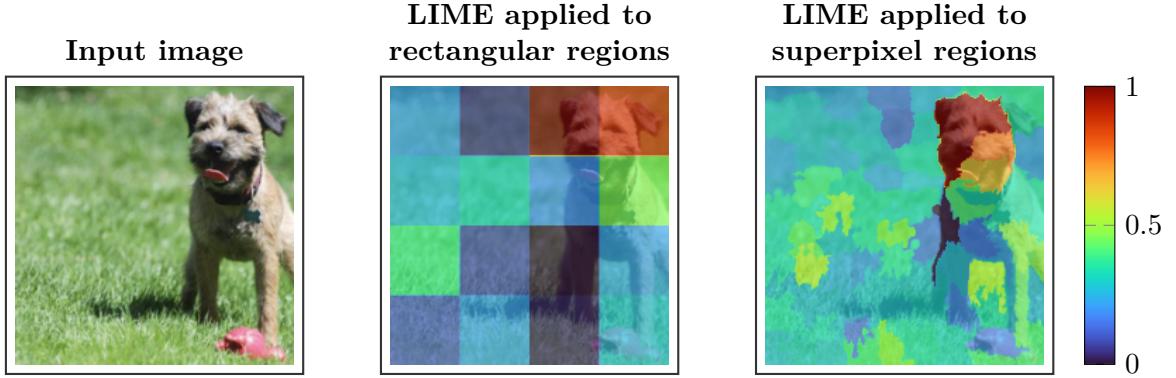


Figure 2.7: Figure showing a comparison between running the LIME algorithm on rectangular and superpixel regions

2.4.4 Specific methods

The following section goes through several specific XAI methods. This serves two purposes: Firstly, by explaining how commonly used XAI methods function in more detail, it is easier to understand how XAI methods work in practice. Secondly, this section also covers the specific methods that will be analyzed and evaluated as part of the rest of the thesis. By thoroughly detailing the functions of these methods in this chapter, it becomes easier to analyse and explain the proposed methods in chapter 3 and the results in chapter 4.

Local Interpretable Model-Agnostic Explanations (LIME)

LIME [22] is a post-hoc, model independent XAI method. The method is built on the idea that while the decision function of a large neural network (or any other large model) might be far too complex to easily interpret, it can most likely be approximated quite well by a simpler function, as long as we only look at the feature space around a single data point. For example, we could approximate a large feed forward neural network with a simple linear regression model, which can be intrinsically explained due to its low complexity.

To create a locally interpretable model, we need a neighbourhood of data points around our point of interest. To do this, we can sample a number of points from our dataset and weigh them by their distance to our original point. This sampling can be done in many ways, for example by calculating a mean and variance for each feature and sampling from a normal distribution. For image data, we can create new points similar to the image by masking out different regions of the image [19]. The distance measure depends on the type of data we are dealing with. Regardless, the distance values are passed through a smoothing kernel which can be tuned to adjust the size of the "neighbourhood".

With these new data points, we can generate new predictions using the original, complex model. Thus, we now have a series of points, each with a weighting based on their distance to our original point, and each with a predicted score from our original model. With such a dataset, we can train a simpler model, which will then approximate the complex model around the point of interest. By inspecting this simple model (for example the learned weights of a linear regression model, or the structure of a decision

tree), we can learn approximately how the complex model functions in a region around this single data point.

Occlusion methods

Occlusion methods are a family of post-hoc model independent XAI methods. They function by masking different parts of the image and inspecting the change in output score. If an area leads to a large drop in softmax score for the predicted class when masked, this area must have been important for the network when making the prediction. The mask can be as simple as replacing all masked pixels with a single color, such as gray [23], or they could use more advanced inpainting methods using generative models, for example by replacing a masked tumor with generated healthy tissue.

Regardless of the mask, one can easily calculate the importance of any pixel for a prediction by calculating the average change in the output score for all masks which contain the specific pixel [24]. Occlusion methods have the advantage of being completely model independent, since they do not consider the internals of the model. However, the computation can be expensive, because we need to run a forward pass for each position of the mask on the image. Figure ?? shows the process visually.

Class Activation Mapping (CAM)

Class Activation Mapping (CAM) [25] is a model dependent, post hoc XAI method, which is used on Convolutional Neural Nets (CNNs). For a specific output node of a model (for example, the one denoting the presence of a specific class, such as "cat"), CAM outputs a heat map showing which areas of the input image contributed to this node. In this way, CAM gives a visual explanation to which parts of an image the model focused on when making a decision to classify an image to a specific class. This method is model dependent, because it requires a specific architecture in the final layers of the network to work.

CAM is a relatively simple method to understand. It exploits the fact that various convolutional layers of CNNs actually behave as object detectors, even when the training objective is classification [25]. As [11] explains, the earlier layers "extract elementary visual features such as oriented edges, end-points [or] corners", which can be used by subsequent layers to detect higher-order features. In this manner, the final convolutional layer will detect very high level visual features, combining the extracted information from all the previous layers. This layer is composed of several feature maps, where each map can be thought of as denoting the presence of some specific feature across the original image. The authors perform global average pooling (GAP) on these feature maps, giving a single value for each map, which is followed by a single dense layer and the Softmax activation function. In this way, each output node in the final layer is a weighted sum of all the global average pooled feature maps from the final convolutional layer. This means that we can represent the areas of the image which were used to perform the classification by performing the same weighted sum on the actual feature maps instead, which gives us a heat map which we can overlay on the original image (after upsampling the feature maps).

Figure 2.8 shows the process visually. From this we can see that the resulting Class Activation Map (bottom right) gives an intuitive explanation for why the image in the top left gives a high score for the presence of the class "Australian Terrier".

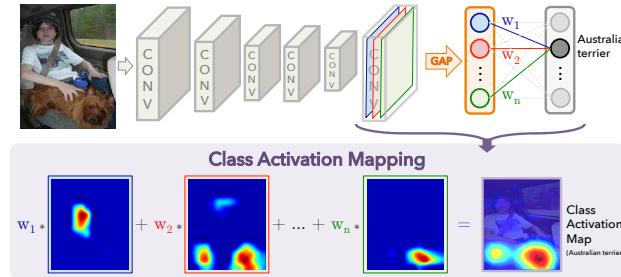


Figure 2.8: Figure taken from [25], showing the steps required to create a Class Activation Map

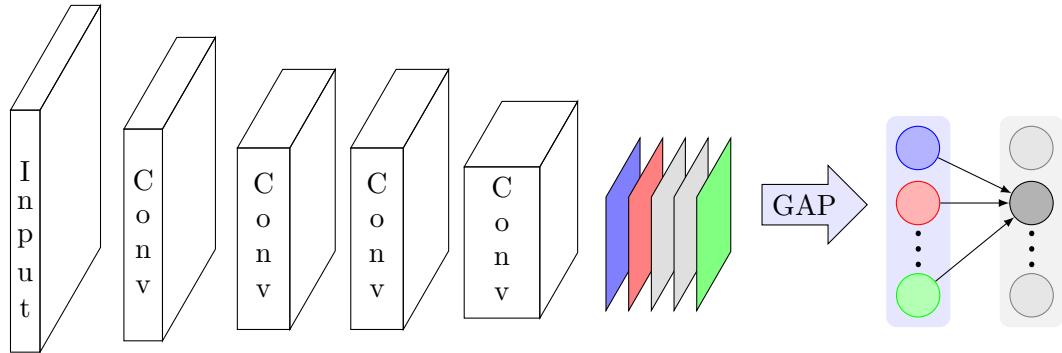


Figure 2.9: Figure showing a high level overview of how a CNN functions

Although CAM is an intuitive and effective method of visualizing the inner workings of a CNN, it has some downsides. Firstly, it is highly model dependent, requiring that the model only have a single dense layer after the convolutions. Although there are some state of the art models which only use a single dense layer, this still places a limit on what models can be used, or requires the simplification of models that use more than a single dense layer. [25, p. 4] notes a 1-2% drop in classification performance when performing this simplification. Secondly, the output of CAM is simply a weighted sum of all the feature maps after the final convolutional layer. As we move deeper in a CNN, we reduce the spatial resolution by downsampling, while increasing the number of channels (increasing the depth of the output while reducing the height and width). Because of this, the CAM will have a drastically lower resolution than the original image, often less than 10×10 , while the input image may be hundreds of pixels in both dimensions. Because of this, CAM can only show general areas, as opposed to pixel wise explanations.

Gradient Class Activation Mapping (GradCAM)

GradCAM [26] is an improvement on CAM, which generalizes the method to function with any CNN architecture, thus making the method much less model dependent and avoiding the performance drop incurred when simplifying the model with CAM. Instead of using the weights of a final layer to calculate a weighted sum of feature maps in the last convolutional layer, GradCAM uses gradients flowing from the relevant output node to the activation maps to calculate the weights for each feature map. Furthermore, the authors prove that this method is a strict generalization of CAM [26, p. 5], so that no information is lost by using gradients instead of weights.

Like the simplicity of the CAM method, the calculation of the weights using the gradients is also quite simple, as seen in Equation 2.2.

$$\alpha_k^c = \frac{1}{Z} \sum_i \sum_j \frac{\delta y^c}{\delta A_{ij}^k} \quad (2.2)$$

Here, c represents the index of the class we are interested in, k the index of the feature map, and i and j the width and height of the image. y^c is the element of the output vector y which corresponds to the class c , while A^k is the k 'th feature map. Z is equal to $i * j$, and simply normalizes the sum. Thus, we are actually just performing global average pooling of the gradients of A^k with respect to y^c , which gives us a single value we can use as the weight for this feature map. Doing this for all feature maps for a specific class gives us all the weights we need to calculate a weighted sum, which we can upsample and visualize to get an explanation for the decision of the CNN.

Thus, GradCAM improves upon CAM by making the method less model dependent. However, the explanations are still the same low resolution, which may not be ideal in all cases.

Guided Backpropagation

Guided backpropagation is another XAI method which utilizes the gradients of the network with regards to the input to generate an explanation.

Integrated Gradients

2.5 Out-of-Distribution Detection

This section discusses OOD detection, the field which attempts to tackle the second problem discussed in the introduction; that ML models have significantly worse performance on OOD data points and will often "fail silently", making completely wrong predictions with apparent high confidence [27]. OOD detection is a developing field, and still in an initial stage [28]. In 2017, [12] proposed a baseline OOD detection method. This section will discuss this method and the methods which follow it.

2.5.1 Motivation for Out-of-Distribution Detection

When training a model using supervised learning, we implicitly use the "closed-world assumption", which means that we assume that test data will be drawn from the same distribution as the training data [14]. However, when a model is deployed, the data we see may not obey this assumption. Without OOD detection, the model will behave in the exact same way when encountering OOD samples or in distribution (ID) samples, and may even claim to be highly confident in its prediction although the sample is far away from the distribution of the training data [29, p. 1]. In any system where models make high impact decisions, this is a huge problem. We do not want a model to claim high confidence when predicting if a woman has lung cancer if the model has only been trained on men, nor do we want a model to attempt to classify a rare disease that was not part of the training data. Thus, OOD detection methods are necessary, so that OOD samples can be caught before the model makes a prediction and dealt with correctly.

Intuitively, one might assume that distinguishing ID and OOD samples from each other can be solved by simple binary classification using a dataset of ID samples and

one of OOD samples. Indeed, if one has sufficient amount of high quality OOD samples, this can be done. However, this can be difficult to obtain in practice [14, p. 15], thus requiring more sophisticated methods of OOD detection.

2.5.2 Semantic versus covariate shift

The first distinction to make in OOD detection tasks is whether an OOD sample is OOD because of *semantic* or *covariate* shift. Semantic shift refers to samples with different classes than the ones the model is trained on. A picture of a giraffe would represent a semantic shift for a model trained to differentiate between different breeds of dogs, as a giraffe does not belong to any breed of dog. Covariate shift refers to samples which come from a different distribution while still belonging to one of the classes of the original data set. An image of a Beagle puppy could represent covariate shift for a dog breed classifier despite Beagle being one of the classes, if all ID images were of adult dogs. Likewise, an image of a dog in a dark room could represent covariate shift, if all the ID images were of dogs outside, in well lit conditions. Figure 2.10 shows this distinction visually. Here, we can easily see the difference between covariate and semantic shift; covariate shifted images come from the same classes as ID samples, while semantically shifted images come from completely unknown classes.

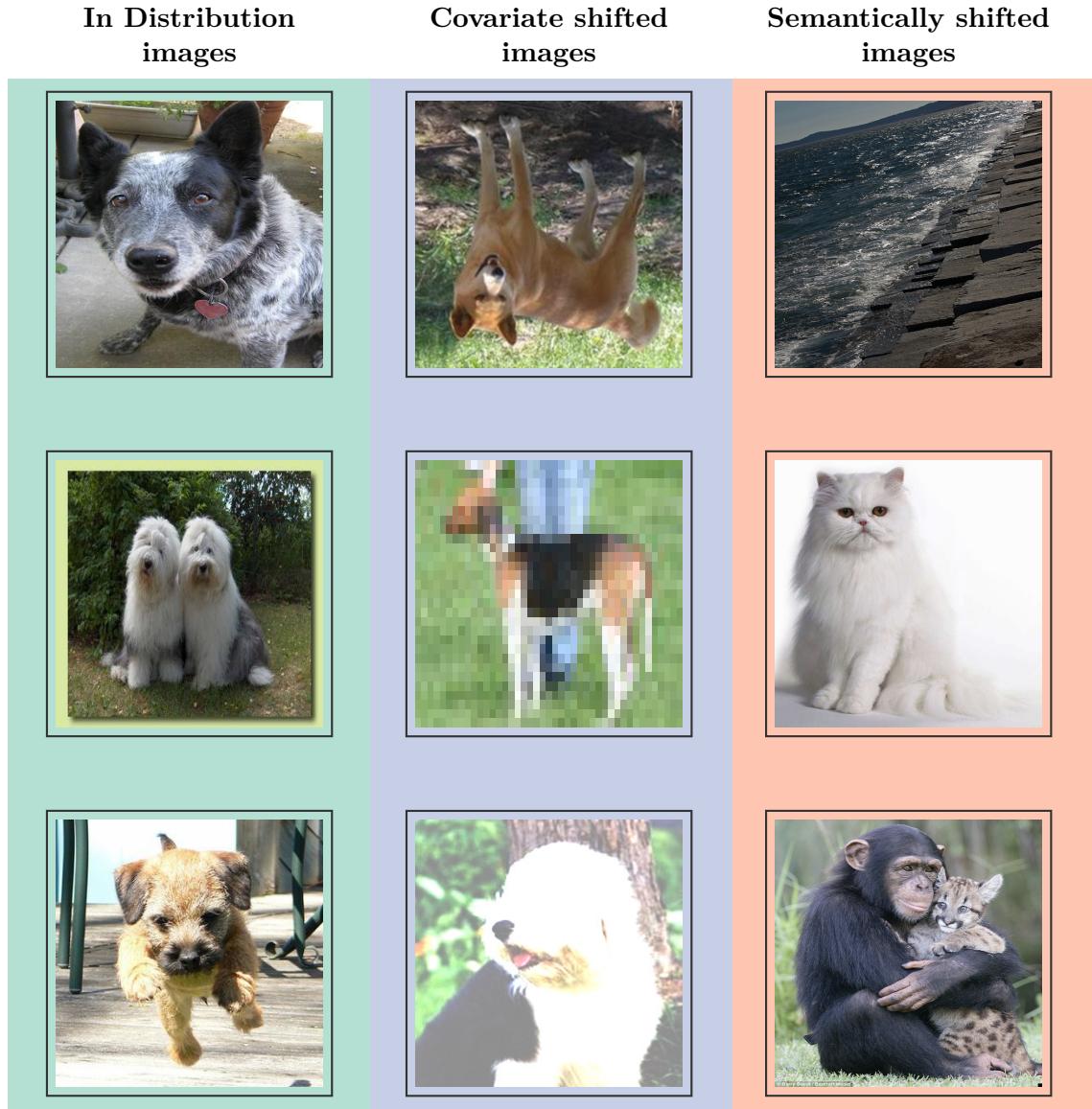


Figure 2.10: Figure showing in-distribution, covariate shifted and semantically shifted images for an imagined dog breed classifier. Images are taken from the ImageNet dataset

The detection of semantic shift, as opposed to covariate shift, is the main focus of most OOD detection tasks [14]. In many applications, it is expected that the model should be able to generalize its prediction to covariate-shifted data, and therefore the focus is on detecting semantic shift. However, the field of medical image classification is one where detecting covariate shift is also important, as the model should only make predictions on data points which are very similar to its training data [14].

Given that the detection of semantic shift has been the main focus of most OOD literature, my work will primarily deal with semantic shift as well. Thus, unless otherwise specified, when I refer to OOD data points, I mean data points which are semantically shifted, i.e that come from another class than those the model has been trained on.

2.5.3 Benchmarking

The performance of an XAI is hard to quantify, because the quality of an explanation is not easily reduced to a number. For OOD detection, performance is much easier to measure, as the problem can be described as a binary classification problem, with OOD and ID samples as the positive and negative class. Thus, we can calculate many different metrics and compare methods against each other. For OOD methods, the two most common metrics to report are FPR95 and the AUROC (see section 2.3.1). It is common to use ImageNet or CIFAR as the ID dataset, and calculate FPR95 and AUROC on other datasets which contain no overlapping class labels. When selecting OOD datasets, it is common to differentiate between **near-OOD** and **far-OOD**. Far-OOD samples are samples which are drastically different from the ID samples, while near-OOD samples only differ slightly. For our cat-versus-dog classifier, a tiger and a wolf would represent near-OOD semantic shift, while a plane and a car would represent far-OOD semantic shift. As one might expect, detecting near-OOD samples is much harder.

In 2021, [14] defined a generalized OOD detection framework, and in 2023 [6] introduced a comprehensive benchmark of all relevant OOD methods under this framework, which allows for accurate comparisons of methods within the field. This benchmark is discussed in detail in section 3.2.1.

2.5.4 Methods

This section will follow the same outline as section 2.4; firstly, the overarching categories of methods will be discussed, followed by a more detailed look at a selection of specific methods within the field.

The field of OOD is separated into four categories of methods [14]:

- Classification-based methods
- Density-based methods
- Distance-based methods
- Reconstruction-based methods

All methods can also be categorized by whether they are post-hoc or training based. Post-hoc methods take an already trained network and attempt to extract information which separates ID and OOD samples out of the network during inference. These methods have the obvious advantage that they can work out of the box with large pre-trained network without requiring expensive training from scratch. Training based methods train the network in ways which maximize the difference between ID and OOD samples. These methods do not necessarily require OOD samples, but can train using auxiliary loss functions which amplify the differences in network behaviour when faced with OOD data as opposed to ID. Regardless, these methods come with a much higher computational requirement than post-hoc methods, as they require training from scratch or at least retraining using the new loss criterion.

Given the fact that post-hoc methods can be applied to trained networks out of the box, it is quite common to combine both post-hoc and training strategies to achieve the best performance.

Below follows a short explanation of each the four categories mentioned above.

Classification-based methods

Classification-based methods usually use the softmax score or logits of a model to attempt to distinguish OOD and ID samples. [12] made the observation that while the softmax score may be a poor indication of the actual confidence of the model on a single data point, it is still higher on average for ID samples as opposed to OOD samples. By using this simple distinction, they created a baseline model which separated OOD and ID samples. Using input perturbations and temperature scaling, [13] further improved on this method, by amplifying the difference in softmax score of ID and OOD data.

More generally, classification-based methods do not need to use the softmax score, but may attempt to find any metric which separates the distribution of ID samples from OOD samples. Figure ?? shows the probability density for an unspecified metric for both OOD and ID samples. The goal of classification-based OOD detection is to find metrics or training methods which make these probability densities have as little overlap as possible, such that they are easily separated by a threshold.

There are several state of the art methods which utilize a classification-based approach, and these make up a large part of the representative methodologies for OOD detection today [14, p. 8]. As such, I shall devote the majority of section 2.5.5 to classification-based methods.

Density-based methods

Density-based methods explicitly try to model the in-distribution [14], which is then used to detect outliers in low likelihood regions. Although the idea is intuitive, learning the distribution of the data set can often be prohibitively expensive, and thus these methods often lag behind classification-based methods [14].

Distance-based methods

Distance-based methods attempt to detect OOD samples by calculating their distance to ID samples. Many different distance measures are used, such as Mahalanobis distance to estimated Gaussian distributions, cosine distance to the first singular vector of the data set or Euclidean distance in an embedding space.

Reconstruction-based methods

Reconstruction-based methods are based on encoder-decoder frameworks, where the core idea is that the model will be much worse at reconstructing OOD data than ID. By measuring the reconstruction loss, we can detect OOD samples.

2.5.5 Specific methods

Below follows a more detailed look a selection of specific OOD detection methods.

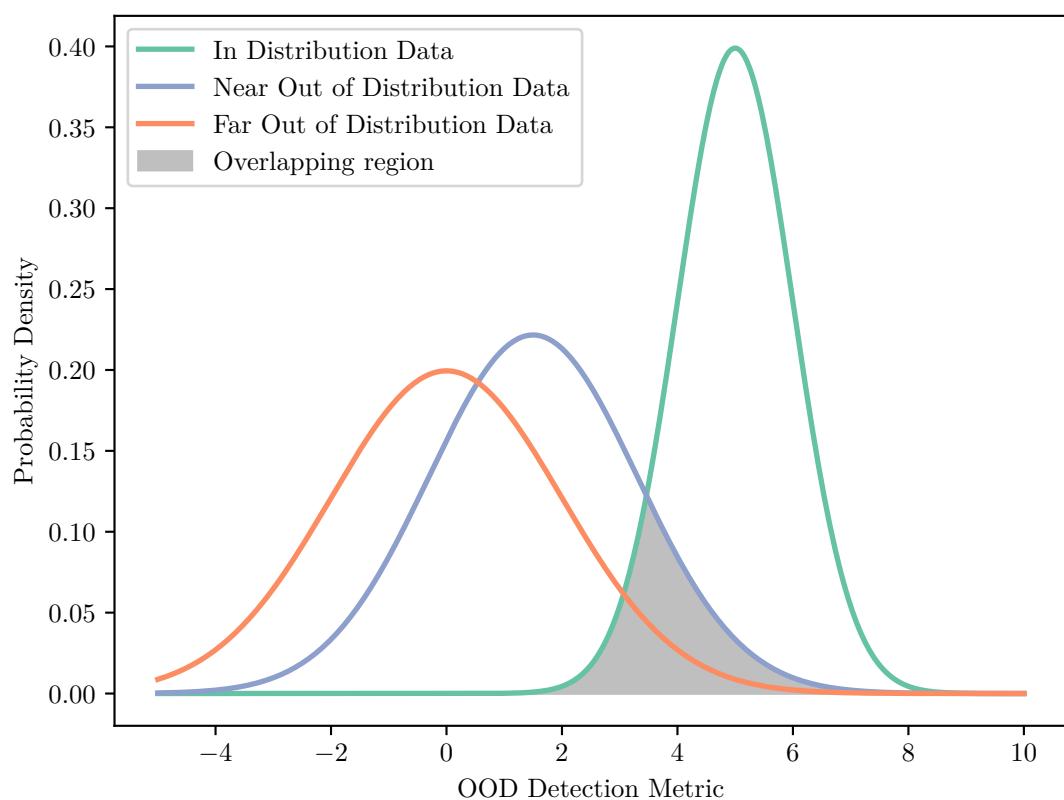


Figure 2.11: Graph showing the distribution of hypothetical ID, Near-OOD and Far-OOD data for an unspecified metric. The shaded region shows the overlap between the ID and OOD samples.

Baseline model

The baseline model created by [12] is extremely simple, yet effective. It simply compares the softmax score the predicted class to a threshold, and labels it as OOD if it falls below this threshold. Let us assume we have a model $f : \mathbf{x} \rightarrow \mathbb{R}^C$ that takes an input \mathbf{x} (which may be an image, a vector of values, or something else) and returns a vector of logits with length equal to the number of classes C . If we define a softmax score function

$$S_i(\mathbf{x}) = \frac{\exp(f_i(\mathbf{x}))}{\sum_{j=1}^N \exp(f_j(\mathbf{x}))}, \quad (2.3)$$

then the OOD detector has the following simple form, given a threshold δ :

$$g(\mathbf{x}; \delta) = \begin{cases} \text{in} & \max_i S(\mathbf{x}) \geq \delta \\ \text{out} & \max_i S(\mathbf{x}) < \delta \end{cases}, \quad (2.4)$$

This method reasonably well, because the softmax scores for ID data generally is higher than for OOD data. Two years later, [30] showed that this baseline could be improved in settings with larger datasets by forgoing the softmax normalization and instead only looking at the maximum logits, with the even simpler form

$$g(\mathbf{x}; \delta) = \begin{cases} \text{in} & \max_i f(\mathbf{x}) \geq \delta \\ \text{out} & \max_i f(\mathbf{x}) < \delta \end{cases}, \quad (2.5)$$

Perhaps surprisingly, both these methods are quite good at detecting OOD samples. However, there are still many ways to improve these methods, as will be shown in the following sections.

Virtual Logit Matching (ViM)

[15] attempts to improve OOD detection by calculating a score based on the feature, the logit and the softmax probability at once, as opposed to just one of them. By looking at all three elements in conjunction, they see an increase in performance over models which only rely on a single input source (such as the previously mentioned ODIN).

The reasoning behind not just looking at the logits or softmax probability is that there is a lot of information that is lost when going from features to logits [15]. Once we project the features down to logits, we have only class dependent information, and have lost the class agnostic information which is contained within the features. To show how this information is lost, the authors give an example based on null space analysis [31]:

Let us assume that we have a simplified network with only a single layer. Then, we have $\hat{\mathbf{y}} = W\mathbf{x}$, where $\hat{\mathbf{y}}$ is the vector containing the logits, \mathbf{x} is the feature vector of the input (with an additional 1 for the bias term) and W is the matrix containing the weights and biases transforming the feature vector into logits. A null space $\text{Null}(W)$ of a matrix W is the set of all vectors that map to the zero vector, such that $W\mathbf{a} = \mathbf{0} \iff \mathbf{a} \in \text{Null}(W)$. The null space of a matrix may be trivial (empty), but a matrix which projects vectors to a lower dimension have non-trivial null spaces. Given that the final layer of a neural network projects down to logits, which are the same dimension as the number of classes, this will almost always be the case. Because of the distributivity of matrix multiplication, we have the following:

$$W(\mathbf{x} + \mathbf{a}) = W\mathbf{x} + W\mathbf{a} = W\mathbf{x} + \mathbf{0} = W\mathbf{x} \quad (2.6)$$

The vector \mathbf{x} can be decomposed into $\mathbf{x}^W + \mathbf{x}^{\text{Null}(W)}$, where \mathbf{x}^W is the projection of \mathbf{x} onto the column space of W and $\mathbf{x}^{\text{Null}(W)}$ is the projection of \mathbf{x} onto the null space of W . It follows from this and equation 2.6 that when going from features to logits using the projection $W\mathbf{x}$, we lose all information contained in $\mathbf{x}^{\text{Null}(W)}$. [31] shows how this can be exploited by adversarial methods, by creating images with added noise derived from the null space of a matrix within the network, which are classified as if the noise was not present, despite having no resemblance to the original image. See figure 2.12.

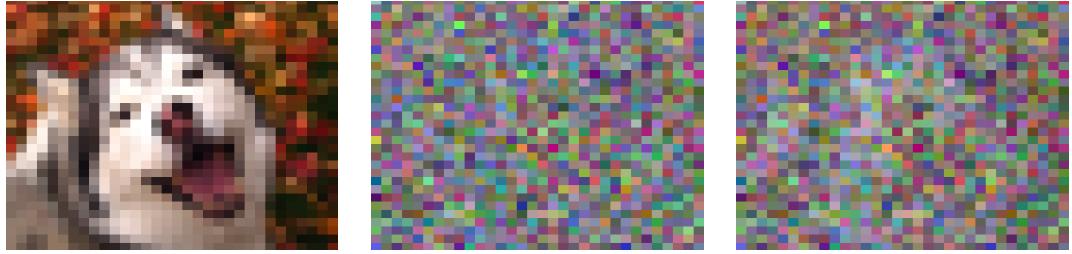


Figure 2.12: Image taken from [31]. Left: Original image. Center: Additive null space noise. Right: Final image, indistinguishable from original image according to the network the noise in the center column is sampled from.

From this, we can see that potentially large amounts of information can be lost when going from features to logits. Using this information, it is also possible to perform OOD detection, as shown by [31]. Another method which uses the features performs Principal Component Analysis (PCA) and looks at the residual information lost when using the first N principal components [32]. However, the information in the features is still class agnostic, and [15] aims to go beyond using just one input source and combine several elements of the network.

To do this, they propose using a *Virtual Logit*. The Virtual Logit is calculated as follows: First, they center the feature space, so that "it is bias free in the computation of logits" [15]. They then perform PCA as in [32], and calculate the residual of \mathbf{x} with regards to the principal components, which is the projection \mathbf{x} onto the null space of the principal subspace P . The residual represents the information lost when using the projection P .

$$\text{Residual}(x) = \|\mathbf{x}^{\text{Null}(P)}\| \quad (2.7)$$

This value is scaled based on the average values of the maximum logit across the dataset, and is appended to the rest of the logits as a Virtual Logit:

$$l_0 := \alpha \|\mathbf{x}^{\text{Null}(P)}\| \quad (2.8)$$

This now takes part in the computation of the softmax values, and thus is affected by the size of the rest of the logits. They call the softmax value of the Virtual Logit the *ViM score*. In this way, the ViM score represents the size of the residual in comparison with the predictions of the model. If the model is very confident, then the norm of the residual will be small in comparison, and the ViM score will be low. If the residual is very large, the ViM score will be higher, and more indicative of an OOD sample. In this way, [15] have combined information from the feature, the logit and the softmax probability level to perform OOD detection.

2.6 Related work

While the combination of XAI and OOD detection has been explored in many previous works, the majority of them focus on explaining why a data point was marked as OOD, as opposed to using XAI to aid the detection itself. Works like [33], [34] and [35] are papers which combine XAI and OOD for this purpose. Within network security, XAI has been as part of anomaly detection systems to detect malicious or faulty network traffic. Here, it has been used to explain detections ([36], [37]), but also to aid in detection itself by inspecting the explanations of the detection system ([38], [39]). These methods thus use XAI to aid OOD detection in a similar manner to my work, however they are strictly focused on sequential network traffic data as opposed to images, and are mostly concerned with detection "unnatural" data samples such as intentionally malicious traffic or that generated by faulty equipment, as opposed to natural OOD data caused by semantic or covariate shift occurring when a model is deployed.

[40] is the most relevant previous work. Here, the authors explicitly aim to use XAI to improve OOD detection on images. They do this by looking at saliency maps produced by a GradCAM-based XAI method (section 2.4.4) during inference, i.e the heatmaps that explain which parts of the image was most influential to classify the image as a specific class. Using these heatmaps, they perform distance-based OOD detection (section 2.5.4): By collecting all explanations for each image in the ID dataset, they are able to construct archetypical explanations, and can make clusters of explanations. To perform OOD detection, they simply compare the explanation of a new data point to the clusters of archetypical explanations, and mark it as OOD if it has a distance which is over a certain threshold.

This method performs decently on toy datasets, achieving scores similar to State-of-the-Art methods when using *Fashin MNIST* as ID and *MNIST* as OOD. However, this method fails catastrophically in more complicated scenarios, achieving an AUROC score of only 52% on *CIFAR10* vs *SVHN*, which is only marginally better than pure guessing and far below any other method. The paper thus ends with the authors concluding that "OoD detection approaches that are specifically designed for the purpose achieve in general better detection scores at the cost of an additional computational burden in the model's construction" [40].

For more potential related work, we can look to OpenOOD ([6]), which aims to provide a comprehensive benchmark of all relevant methods in the field of OOD detection. Out of all 41 OOD detection methods included in this benchmark, there are no methods which use XAI.

From the absence of any relevant method utilizing XAI in OpenOOD and from the poor results of [40], we can see that the potential for a truly effective OOD detection system using XAI has not been fully realized in any previous work.

2.7 Summary

In this chapter, I have given a thorough introduction.

Chapter 2. Background

Chapter 3

Methodology

The core of this work is the

As shown in the preceding chapter, there exists a plethora of XAI methods, which exploit gradient information, differences in output scores when altering model inputs, marginal contributions of input features, as well as many other intricacies of deep learning models. The core idea of this master thesis is that these methods, in their attempt to explain a model decision, may also inadvertently extract information which is valuable for OOD detection. Thus, there may be an unexplored potential in these methods to function not just as explanations, but also as classifiers which allow us to separate ID and OOD data. Intuitively, we might expect the explanations to be more spread out on OOD images, given that there are (by definition) no objects of interest in the image that the model can definitely be said to focus on. In contrast, we might expect an explanation on an ID image to be more focused on a specific area, which contains an object of interest. Furthermore, given that saliency methods give a numerical value to each region of the image, we might be able to extract information about the "OOD-ness" of an image by inspecting the magnitudes of these values. Intuitively, it makes sense that such values should be lower for OOD than ID, reflecting the higher uncertainty present in OOD data.

As an example, let us consider GradCAM. As explained in section 2.4.4, GradCAM uses the gradients of the weights within the final convolutional layer with regard to the output prediction, along with the final feature maps, to generate an explanation.

3.1 Proposed XAI methods for OOD detection

In this section, I introduce my proposed methods for OOD detection, which utilize XAI methods as part of their detection pipeline.

3.1.1 Stand-alone saliency methods

As we have seen from section 2.6, there has been little research into using explanations for OOD detection, aside from the work of [40]. Thus, I begin by presenting a simple baseline method which uses saliency values generated by XAI methods to calculate an OOD score.

Aggregate of Saliency

As mentioned previously, the field of OOD detection started with the simple baseline introduced by [12], which simply uses the Maximum Softmax Probability (MSP) (i.e the

confidence score of the predicted class) as a way to measure OOD. As such, I propose a similarly simple baseline when using explanations for OOD detection. The analogue of the maximum logit in an XAI context can reasonably be said to be the explanation generated of the predicted class (the class corresponding to the maximum logit). As explained previously, this explanation will take the form of an $n \times m$ saliency map. This saliency map is not a single scalar value, and does thus not make a suitable OOD score by itself. Instead, we may perform some form of aggregation on the saliency map (such as taking the mean, the max, the variance or some other form), and use this as the OOD score.

The intuition for this method is informed by the fact that there are many forms of aggregation over saliencies which one might reasonably expect to be different for ID and OOD data. As an example, let us consider the implications of aggregating in some way which captures the magnitude of the saliencies, such as the *mean*, the *norm*, or the *max value*. When we generate a saliency map using the predicted class, the XAI saliency method attempts to calculate a measure of importance for each region of the input image, with regard to this class. For ID data, as long as the model predicted correctly, we know that there really are regions of the input image which contain the predicted class. If we instead are looking at semantically shifted OOD data, we know that no input image contains any of the ID classes. Thus, when a neural network makes a prediction on such a data point, it will always be wrong, because it will always predict one of the ID classes. By generating a saliency map of this prediction, we are asking a method to decide how each region contributed to a false decision. Given that there are no objects of the predicted class, in any region, we should expect the saliency values to be lower than in an ID case, where such objects actually are present.

To further illustrate this theoretical justification, I present a simple example scenario (figure 3.1). Here, I imagine a model which has been trained to differentiate between different breeds of dogs. In the first case, it is given an image of a dog, and a prediction of "English Foxhound" is made, which happens to be correct. Generating an explanation for this prediction, each region of the image is given a measure of importance, calculated using gradient information, differences in prediction score on counterfactual examples or by other means. As there actually is an English Foxhound in the image, we expect that these methods generate saliencies which have a magnitude which is higher than if there was no dog present.

3.1. Proposed XAI methods for OOD detection

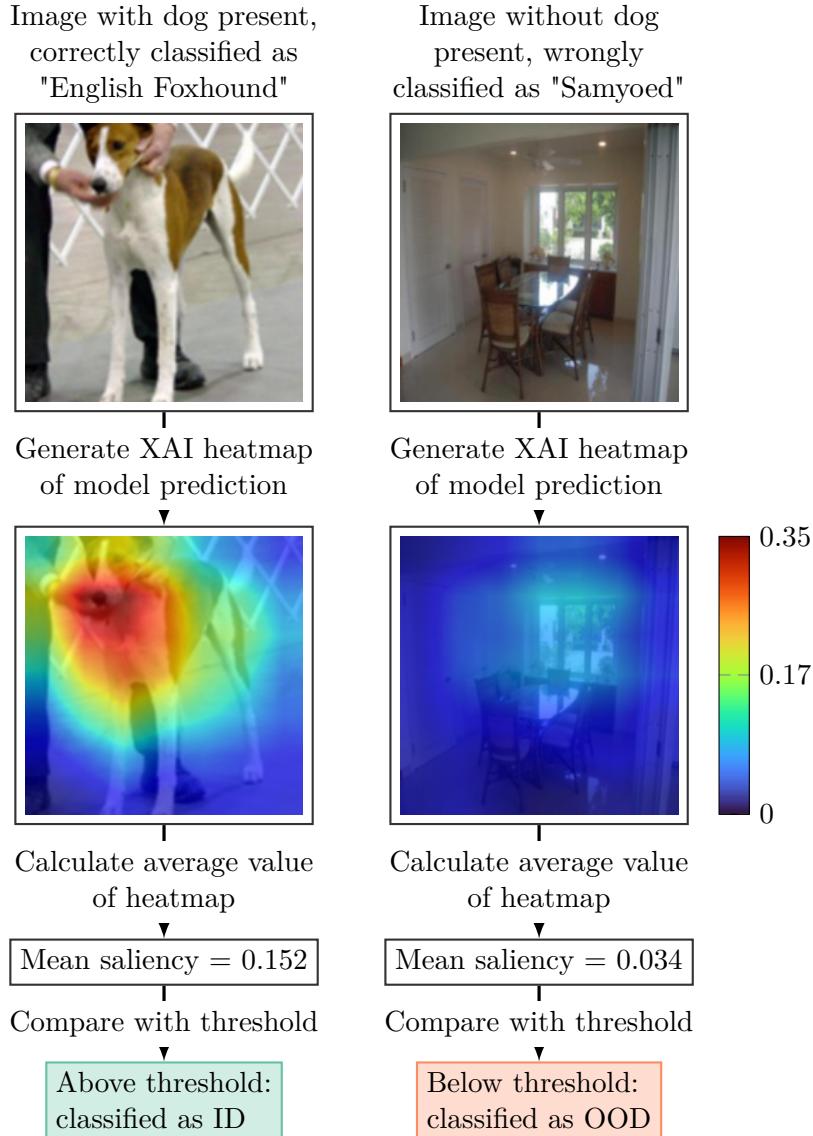


Figure 3.1: Figure showing the functioning of the Aggregate of Saliency OOD detector, using mean as the aggregation, in a hypothetical scenario where a model trained on images of dogs is shown an image with no dogs present. The heatmaps here show the maximum value of both saliency maps as dark red, reflecting the lack of normalization

In the second case, the model is given an image without any dogs present. Given that there is no class for images without dogs in them, the model will classify the image as one of the possible dog breeds. In this case, the model predicted the class of "Samoyed", a decision which can be considered essentially arbitrary. When a explanation is generated for this decision, the methods for calculating importance scores will most likely assign saliences to most regions, given that no region contains a dog. As such, if we calculate mean saliences for both the image with the dog and the one without, we expect the image with the dog to have a higher mean saliency. As long as we work with semantically shifted OOD data, it will always be the case that the prediction on OOD data is wrong, and thus we may also expect that the generated explanations in general output lower saliences.

Apart from aggregations which convey information about the magnitude of the

Chapter 3. Methodology

saliencies, we may also expect the variation or spread of the saliencies to be different between ID and OOD data. The intuition is that one might expect the heatmap on OOD data to be less concentrated and more spread out, given that there are no actual objects of interest present.

Figure 3.2 shows a hypothetical scenario in which calculating the spread could be beneficial in OOD detection. Like in the previous case, we imagine a model trained on dogs, which is fed two images, one which contains a dog and one which does not. In this case, we do not care about the magnitudes, but instead only the spread of the values in relation to each other, and thus the heatmap is normalized. As we can see, the heatmap is more spread out in the explanation where there is no dog present than for the image with a dog. By calculating a suitable metric, such as the Gini coefficient, entropy or another measure of spread, we can get a single number which represents how spread out the heatmap is, regardless of its magnitude. Using these values, we can define a threshold which is below most ID data and above most OOD data, allowing us to separate these distributions.

3.1. Proposed XAI methods for OOD detection

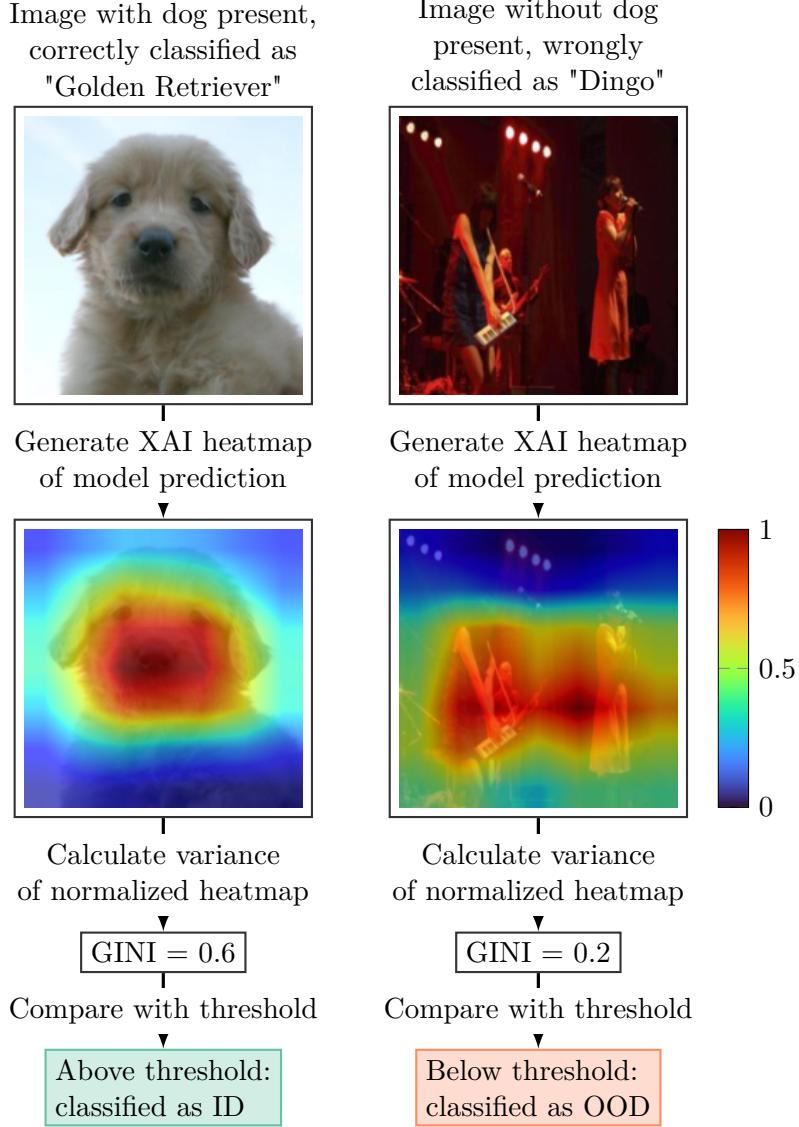


Figure 3.2: Figure showing the functioning of the Spread of Saliency OOD detector in a hypothetical scenario where a model trained on images of dogs is shown an image with no dogs present. The heatmaps are here based on the normalized values of each saliency map, meaning that magnitude information is ignored

With the intuition explained, we may now formalize the method. To define this detector mathematically, let us first define the necessary components. As in chapter 2, we assume we have a model $f : \mathbf{x} \rightarrow \mathbb{R}^C$. In this case, $\mathbf{x} \in \mathbb{R}^{D \times H \times W}$, i.e a D channel image of height H and width W . In addition, we define a XAI saliency mapping method $s : (f, \mathbf{x}) \rightarrow \mathbb{R}^{H_s \times W_s}$. This function takes the model f and an input \mathbf{x} and returns a H_s by W_s saliency map for the predicted class; the class corresponding to the highest logit. Finally, we define an aggregation function $A : \mathbf{x} \rightarrow \mathbb{R}$, where \mathbf{x} can be of any shape.

Thus, the OOD detector has the following form, given a threshold δ :

$$g(\mathbf{x}; s, A, \delta) = \begin{cases} \text{in} & A(s(\mathbf{x}, f)) \geq \delta \\ \text{out} & A(s(\mathbf{x}, f)) < \delta \end{cases} \quad (3.1)$$

An astute reader may note that aggregation functions are permutation invariant, meaning that all positional information from the two-dimensional saliency maps is lost when aggregating. This may seem strange, as it is primarily the positions of the different values that is important when using XAI methods for explaining model predictions on images. However, there is good reason to believe that for many image classification tasks, the positions of the points of interest in an XAI saliency map does not carry much discriminative potential. For datasets such as CIFAR10 and ImageNet200, there is a huge variety in the positions of the ground truth class (a dog may appear in the middle, the top right corner, or any other position and still be of the class 'dog'). As such, it is not a given that the removal of any positional information will be massively detrimental. Indeed, when [40] reflects upon the poor results of their saliency heatmap clustering for detecting OOD samples on CIFAR10, it is exactly this variability in position they highlight: "Indeed, the CIFAR10-C dataset does not afford the positional bias and low intra-class variability observed in the previous case studies: informative objects for the classes to be predicted appear in arbitrary parts of the image and have a high degree of compositional variability" [40].

Given the exploratory nature of this thesis, it is reasonable to try many different forms of aggregations. In the experiments, the following aggregations have been used.

Magnitude:

- Mean
- Median
- Vector norm
- Range
- Maximum
- Minimum

Statistical dispersion:

- Coefficient of Variance (CV)
- Quartile Coefficient of Determination (QCD)
- Relative Mean Absolute Difference (RMD)

The magnitude based aggregations are essentially self-explanatory. For the distribution based methods, some explanation is necessary. The Coefficient of Variance (CV) is an alternative to using standard deviation, which removes the effect of the magnitude of the values over which the standard deviation is calculated. The CV of a set of values is simply the standard deviation divided by the mean: $CV(\mathbf{x}) = \sigma_x / \mu_x$. For exploring whether the saliencies of OOD data is more dispersed or spread out than ID data, such a normalization is required, given that we do not expect the saliencies of ID and OOD data to have the same magnitude. Skewness is a measure of asymmetry of a distribution, and can tell us something about the outliers of the saliency maps and their location in relation to the rest of the values. The Gini coefficient is another measure of statistical dispersion, most commonly used to measure income and wealth inequality. The Gini-coefficient of a data set where all values are the same is zero, while it is 1 for a data set where all values are 0 except for one.

Explanation Clustering

3.1.2 Saliency integrated into existing OOD detection algorithms

Given the poor results of [40], one might expect that saliency maps on their own are insufficient to differentiate ID and OOD data.

Virtual Logit Matching with Saliencies

3.2 Datasets

With a thorough introduction to both XAI and OOD detection as well as methods which combine the two, I shall present the datasets that will be used to test the new method that I introduce in chapter ???. The two datasets used are OpenOOD ([6]) and HyperKvasir ([7]). OpenOOD is a comprehensive benchmark which can test the new method’s performance in a wide range of OOD scenarios, while HyperKvasir is a medicinal dataset which can be used to test the method in the specific use case of gastrointestinal OOD detection.

3.2.1 OpenOOD

As mentioned previously, OpenOOD was introduced in 2023 by [6] as an attempt to unify the performance metrics of the field, such that accurate comparisons of different methods could be made. Prior to this work, different methods were tested on different datasets, with different image preprocessing procedures, and with other externalities which inhibited effective comparison between methods [6].

OpenOOD includes 11 different benchmarks across Anomaly Detection, Open Set Recognition and OOD detection, three fields which are very closely related. Of these, 6 benchmarks are used to test methods for OOD detection. Each benchmark is defined by an ID dataset, with 6 or more corresponding OOD datasets, separated into Near-OOD and Far-OOD.

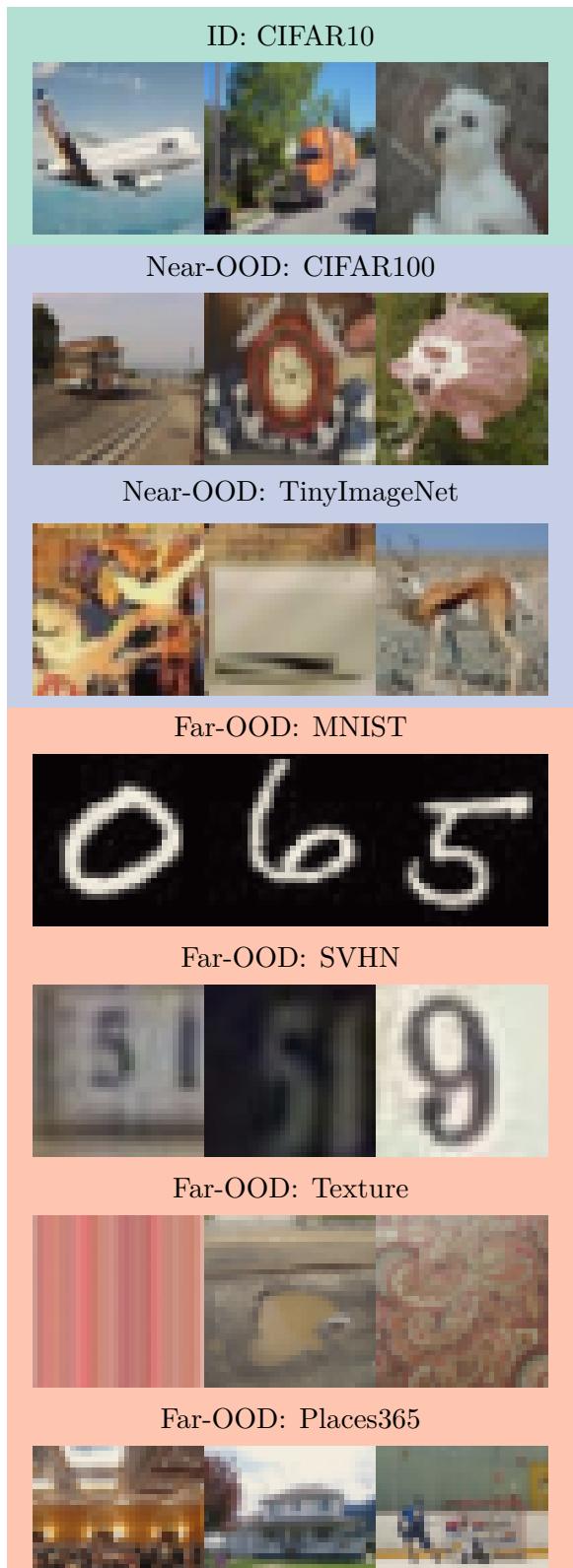
CIFAR10

CIFAR10 [41] is a 10-class dataset for general object recognition [6]. This dataset is commonly used in AI research [42]. Each image is 32×32 , and there are 50 000 training images and 10 000 test images. The ten classes are as follows: airplanes, cars, birds, cats, deer, dogs, frogs, horses, ships, and trucks. OpenOOD presents a series of Near-OOD and Far-OOD datasets which are used in conjunction with this dataset for evaluation. Table 3.1 presents a short description of each dataset and the number of samples.

In addition, a sample of images from CIFAR10 and the corresponding OOD datasets are shown in figure 3.3.

Dataset	Size	Description
CIFAR10	10 000	General objects
CIFAR100	10 000	General objects from same collection as CIFAR10
TinyImageNet	10 000	General objects
MNIST	10 000	Handwritten digits from 0 to 9
SVHN	10 000	Street view house numbers
Texture	10 000	Street view house numbers
Places365	10 000	Places, scenes, locations

Table 3.1: Hello



ImageNet200

Figure 3.4: Figure showing three example images from ImageNet200 and from the corresponding OOD datasets

3.2.2 HyperKvasir

HyperKvasir is the largest gastrointestinal (GI) machine learning datasets, containing 110 079 images and 374 videos collected during gastro- and colonoscopy examinations [7].

Dataset	Size	Description
ImageNet200	10 000	General objects
SSB-Hard	10 000	General objects
NINCO	10 000	General objects
iNaturalist	10 000	Handwritten digits from 0 to 9
Texture	10 000	Street view house numbers
OpenImage-O	10 000	General objects

Table 3.2: Hello

It is of utmost importance to detect and correctly classify disease found in the GI-tract, as the different diseases can range from minor annoyances to highly deadly diseases such as GI-cancer, which has a mortality rate of 63% [7]. Furthermore, the effectiveness of endoscopy in locating these diseases is highly dependent on the skill and knowledge of the human operator, with polyps in the colon having a 20% miss rate [43]. Thus, this is a field which could benefit greatly from computer aided diagnosis, but such an integration requires robust and trustworthy AI-systems which do not make erroneous decisions with high confidence. This makes HyperKvasir an ideal dataset to test a new OOD detection method in a more practical real-world scenario.

Of the 100 079 images, 10 662 have been labeled, with a total of 23 classes. HyperKvasir also contains segmentations and labeled video, however, I shall limit myself to the labeled images and to the task of classification, as per the scope of this thesis as outlined in section 1.3.

3.3 Networks

While it may be interesting to see how these new methods function on different network architectures, the combination of several different novel OOD detection algorithms and three different datasets already presents a considerable amount of evaluation. Thus, to focus the thesis on comparing different OOD detection methods against each other, I believe it is best to fix other parameters such as network architecture. With this in mind, I choose to limit myself to the ResNet [44] family of neural networks. In particular, I use ResNet18 for all tests, either one trained on 32×32 images (for Cifar10), or one trained on 224×224 images (for ImageNet200, HyperKvasir).

Aside from CNNs, Vision Transformers also perform exceptionally on computer vision tasks, and achieve state-of-the-art results in many settings [45]. On ImageNet, they are even dominant, and the top 10 models when considering (top-1) accuracy are all based on vision transformers, as opposed to CNNs.¹ As such one might question the choice of a CNN model, when newer and better models have been developed.

However, given that a large part of the XAI methods have been developed in the CNN paradigm, they are not easily adapted to vision transformers. Methods such as GradCAM and Layer Relevance Propagation (LRP) exploit specific parts of CNN architectures when generating explanations [46], and are thus difficult to use with different architectures. To be able to use a broad section of the representative XAI methods in use today, it is thus preferable to use CNNs as opposed to vision transformers.

¹<https://paperswithcode.com/sota/image-classification-on-imagenet>

3.4 XAI Saliency Methods

In the following section, I will describe the saliency methods I have chosen to use, and the specific ways I have used them.

3.4.1 LIME

As is common when applying LIME to images, I have used segmentations of the input image to reduce the dimensionality of the input that is fed into the LIME algorithm. During

3.4.2 Occlusion

3.4.3 GradCAM

GradCAM is a natural choice of XAI method, given that is a seminal work which has inspired a large number of other methods [47–49].

3.4.4 Guided Backpropagation

3.4.5 Integrated Gradients

3.5 Evaluation

3.5.1 Metrics

AUROC and FPR95 are the most common metrics used for OOD detection [6, 12–15]. In OpenOOD ([6]), AUROC is chosen as the primary metric used to rank methods against each other. As [6] by far presents the most comprehensive complete benchmark of all OOD detection methods to date, I have followed their methodology and used AUROC when evaluating my methods, while also calculating FPR95 as a secondary metric.

AUROC is agnostic to which class is the positive and which is the negative. Whether we consider OOD samples as 0 or 1, the result will be the same. However, the same is not true for FPR95, necessitating a choice of positive and negative classes. There is no correct answer, but [6] chooses to consider OOD samples as the positive class, to "align with ML convention". It is common to consider abnormalities, anomalies, or the unexpected as the positive class (for example, a cancer detection system would consider the presence of cancer to be part of the positive class). This aligns with the goal of OOD detection, which is to detect abnormal inputs with regard to the data the model is trained on. Thus, I have also followed this convention and considered OOD samples as positive, and ID samples as negative. In this case, FPR95 has the following interpretation: "If a specific threshold leads to 95% of OOD samples being correctly classified as OOD, what percentage of ID samples are then incorrectly classified as OOD"? In other words, FPR95 measures the rate of "false alarms" when 95% of actual anomalies are caught.

For both of these metrics, the calculations are done on each OOD dataset individually, as opposed to comparing all OOD samples to the ID dataset. Afterwards, the metrics of all Near-OOD and Far-OOD are averaged, giving us two general performance metrics which tell us how a method functions on either Near-OOD or Far-OOD.

3.5.2 Development and Test Sets

Given the scope of my thesis, which focuses on post-hoc OOD methods which do not use outlier exposure or require any form of training, there is no need for a training dataset. Despite this, there is still a chance of overfitting, due to the exploratory nature of developing an entirely new class of methods. By trying out different methods and by tuning different parameters to find out how one might best separate ID and OOD data using XAI, I am also biasing the results. Therefore, it may be possible that potential improvements in performance are not due to the increased quality of the method, but instead because of peculiarities in the specific datasets that the method is used on.

Thus, I have split all the datasets mentioned in 3.2 into development and test sets, and have performed all development of the methods exclusively on the development set. Only when calculating the final metrics have I used the test set, to remove any bias associated with performing multiple experiments on the same data. Due to the large amount of data available in the CIFAR10 and ImageNet200 datasets, and their associated OOD datasets, I have simply split all datasets into two equally large parts.

3.5.3 Bootstrapping

When evaluating a new method, it is not enough to simply report the results from a single experiment. Instead one should run the same experiment multiple times and perform statistical analysis to ensure that the results are robust. Therefore, I have bootstrapped the test set ten times during the calculation of the final test results. This makes it possible to report means and standard deviations of the results as opposed to a single point estimate. With these repeated experiments, it is also possible to perform t-tests comparing the new methods against baseline OOD detection methods.

3.6 Implementation

This section goes over the implementation details of my thesis.

3.6.1 Basic hardware and software

Python is the most popular programming language for data science and ML research [50], and as such it is my language of choice as well. Key libraries that I have used are *PyTorch*, *OpenOOD*, *Captum*, *Matplotlib*, and others. Below is a table of the key libraries and their version numbers.

Library	Version number	Short description
PyTorch	2.4.1	GPU-accelerated ML library
OpenOOD	1.5	Comprehensive OOD detection framework [6]
Captum	0.7.1	XAI methods integrated with PyTorch
Scikit-Learn	1.5.2	Various ML methods
NumPy	1.26.4	Efficient matrix multiplication and scientific computing
Matplotlib	3.9.2	Visualization library
Seaborn	0.13.2	Visualization library based on Matplotlib

All development and computation was done on a single computer with an Intel i7-8700K CPU and an Nvidia GeForce RTX 3090 GPU.

3.6.2 Method Evaluation: OpenOOD

As explained previously, OpenOOD [6] represents the most comprehensive benchmark for OOD detection methods. It is also a framework which easily allows for development and benchmarking of new methods, and is thus the ideal framework for the purposes of this thesis.

In particular, OpenOOD includes a "unified, easy to use evaluator" [51] that makes evaluating new methods very simple. All that is required is that new methods inherit from a base class (`BasePostprocessor`²), and override the calculation of OOD scores. Code listing 3.1 shows all the code required to create the Aggregate of Saliency OOD detector.

```
class SaliencyAggregatorPostprocessor(BasePostprocessor):
    def __init__(self, config, saliency_generator, aggregator):
        super().__init__(config)

        self.saliency_generator = saliency_generator
        self.aggregator = aggregator

    def postprocess(self, net: nn.Module, data: Any):
        predictions = torch.argmax(net(data), dim=-1)

        saliencies = self.saliency_generator(net, data)
        score_ood = self.aggregator(saliencies, dim=-1)

    return predictions, score_ood
```

Listing 3.1: Source code listing for the Aggregate of Saliency OOD detector

With this `postprocessor` defined, evaluating it on a specific dataset is similarly simple (listing 3.2):

```
resnet18_pretrained = get_network('cifar10')

ood_detector = SaliencyAggregatorPostprocessor(None, GradCAM, torch.mean)

evaluator = Evaluator(
    net=resnet18_pretrained,
    id_name='cifar10',
    postprocessor=ood_detector,
)

metrics = evaluator.eval_ood()

print(metrics)
```

Listing 3.2: Source code listing for evaluating methods within the OpenOOD framework

This code will calculate the OOD scores for all data samples in both the ID and OOD datasets, and subsequently calculate the AUROC and FPR95 for all the OOD datasets when comparing their OOD values to the values of the ID datasets. Code listing 3.3 shows this output when using the baseline MSP method.

	FPR@95	AUROC	AUPR_IN	AUPR_OUT	ACC
cifar100	61.36	86.51	84.20	85.05	95.56
tin	42.02	88.88	88.81	85.57	95.56
nearood	51.69	87.69	86.51	85.31	95.56 # average of two above

²In OpenOOD, `Postprocessors` are the OOD detection algorithms that generate an OOD score during inference

<code>mnist</code>	19.38	93.86	79.72	98.89	95.56
<code>svhn</code>	24.78	91.38	84.26	95.49	95.56
<code>texture</code>	43.31	88.68	91.01	80.97	95.56
<code>places365</code>	41.62	89.21	68.49	96.28	95.56
<code>farood</code>	32.27	90.78	80.87	92.91	95.56 # average of four above

Listing 3.3: Output of calling `evaluator.eval_ood` with CIFAR10 as the dataset and MSP as the detector

As we can see, OpenOOD allows for very easy evaluation of new methods. Furthermore, it allows for easy comparisons between methods, one of the stated goals of the framework [6]. This makes it an ideal framework for this thesis.

Modifications to OpenOOD

As explained previously, continually testing new methods on the same datasets will bias the final results. As of the writing of this thesis, there are no functionalities in OpenOOD which allow for creating development or test sets, all evaluations are done with entire datasets. For my purposes, which involve continuous exploration of different methods and careful inspection of the datasets, this is inadequate. Thus, I have made modifications to the `Evaluator` class such that it takes a `data_split` parameter during initialization, and have also modified the function `get_id_ood_dataloader` to accept this parameter and return the correct split accordingly.

Furthermore, there is no functionality for sampling from the datasets as opposed to using them as they are, which is necessary to perform bootstrapping and calculate the statistical significance of the results. This has been done by passing a seed to the `Evaluator` class, which, if defined, will be used to seed a random sampling operation on the datasets. By instantiating several `Evaluator` classes with different seeds, we can bootstrap the evaluation and perform statistical analysis on the results.

3.6.3 Implementation of Saliency Methods

There are many libraries which implement XAI methods [22, 52, 53]. When these implementations were suitable for my purposes, I used them. However, given I am not using these explanations for their original purpose (elucidating why a model came to a specific decision), there are many cases where the current implementations are inadequate. The two main problems are lack of access to the raw saliency values and slow speeds.

GradCAM

GradCAM has been implemented from scratch in PyTorch. There are several libraries which implement GradCAM [52, 53]. However, given that these libraries are concerned with simply producing heatmaps that users can inspect, they do not output the raw saliency values, but upscale the saliencies to match the input image dimensions. As explained in 2.4.4, GradCAM uses the final feature map to generate an explanation, which usually has a spatial dimension which is far smaller than the input image (e.g. 7×7 versus 224×224). When overlaying these values on the input image, it is common to use bilinear interpolation [53], which interpolates all 224×224 positions based on the original 7×7 saliency map. For visualizations, this is reasonable. When attempting to use this data to separate ID and OOD data however, this is undesirable. Bilinear interpolation introduces new values, which changes many statistical qualities of the saliency values.

This may reduce the separability of different samples. Furthermore, given that these new values do not add any new information, it is inefficient to involve these upscaled saliency maps in any computational operation.

Although it is relatively simple to modify the source code of these libraries to remove the interpolation, GradCAM is not very difficult to implement, and as such I have simply used my own implementation.

LIME

LIME has an implementation for Python, written by the original authors [22]. However, this implementation is not suitable for my purposes. The main issue is that it is far too slow, being implemented with NumPy which restricts the computation to the CPU. Furthermore, [22] also returns full size heatmaps, although the actual number of saliency values used to create this heatmap is far smaller than the number of pixels in the image.

Thus I have implemented LIME myself, using PyTorch whenever possible.

Occlusion

Captum [52] is a library of XAI methods implemented in PyTorch, and this library contains a suitable implementation of occlusion. As explained previously, occlusion occludes parts of the image and compares the prediction scores before and after the occlusion. By occluding all parts of the image, we can get a saliency value for all positions. Occlusion is usually done using a sliding window, similar to a convolutional kernel, which is slid over all parts of the image. Such a window is rarely a single pixel, because it is often not interesting to see how a single pixel contributes to a prediction, but rather a larger region. What this means is that the final heatmap, although it is the same size as the input image, actually contains far fewer unique values. To avoid performing computations on thousands of repeated values, I reduce the size of the heatmap by sampling one pixel from each of the positions the sliding window has been applied, which can be efficiently done using a 1×1 MaxPooling kernel with a stride equal to the stride used during the occlusion.

Guided Backpropagation and Integrated Gradients

Captum also contains a suitable implementation for guided backpropagation and integrated gradients, which I have utilized in essentially unmodified forms. By definition (see section ?? and ??), these methods return saliency maps over the entire input image dimensions. This separates them from the other methods, which return a far lower number of distinct saliencies, which are upscaled or transformed to the entire image (LIME and Occlusion output the same values for all pixels within a segment, GradCAM outputs an amount of saliencies corresponding to the final feature map, which is then upscaled). Because of this, the saliencies returned are exactly equivalent to the raw values I require, and no modifications are necessary.

However, this lack of dimensionality reduction also poses a technical challenge when we wish to store these saliency maps for later data analysis. For example, storing all the saliencies, without dimensionality reduction, for ImageNet200 and its associated OOD datasets would require 28 GB. Thus, instead of storing the saliencies themselves, I calculate the aggregate values during saliency generation and store them instead. This has the downside that if a new form of aggregation is to be tested, the whole dataset of saliencies has to be generated again. However, the decrease in storage requirements is

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immense, being between a 1000 and 10 000 times decrease depending on the number of aggregates stored.

Chapter 4

Experiments and Results

This chapter contains my findings. In the first section, I show how different forms of aggregation over saliency maps separate ID and OOD data points. This step is important, because it informs the choice of aggregation used in the Aggregation-of-Saliency OOD detection method. I report AUROC for different forms of aggregation over the three datasets. This is done on the validation sets, to avoid biasing the final results.

In the second section, OOD detection on the test sets is performed, and the AUROC and FPR95 for each method on each dataset is reported. In addition, I perform statistical analyses to investigate whether my XAI OOD detection methods outperform baseline methods.

4.1 Data Analysis of Explanations

This section will detail how various XAI methods generate explanations which differ between ID and OOD. The section considers each dataset individually. For each dataset, I first present the level of separation achieved by the two baseline methods MSP and Maximum Logit Score (MLS), to give a general intuition about how easily the ID and OOD datasets are to separate. Following this, I go through the different XAI methods and their different statistical qualities.

4.1.1 ImageNet200

ImageNet200 is a suitable dataset to begin with, given ImageNet’s ubiquity in AI research. Figure 4.1 shows the distribution of the maximum softmax score and the maximum logit. Here, we see that there is a decent amount of separation between ID and OOD data points, even with the simple baseline methods introduced by [12] and [30]. Separating the distributions using MSP, we get an AUROC score of 0.834 for Near-OOD and 0.915 for Far-OOD. Using MLS, we get an AUROC score of 0.833 for Near-OOD and 0.903 for Far-OOD.

LIME

With the baselines reported, we turn our attention to the first XAI saliency method, LIME. Figure 4.2 presents graphs representing the two main forms of aggregation that has been applied; those which consider the magnitude of the saliencies and those which consider the statistical spread. These two forms are here represented by the mean and the Gini-coefficient.

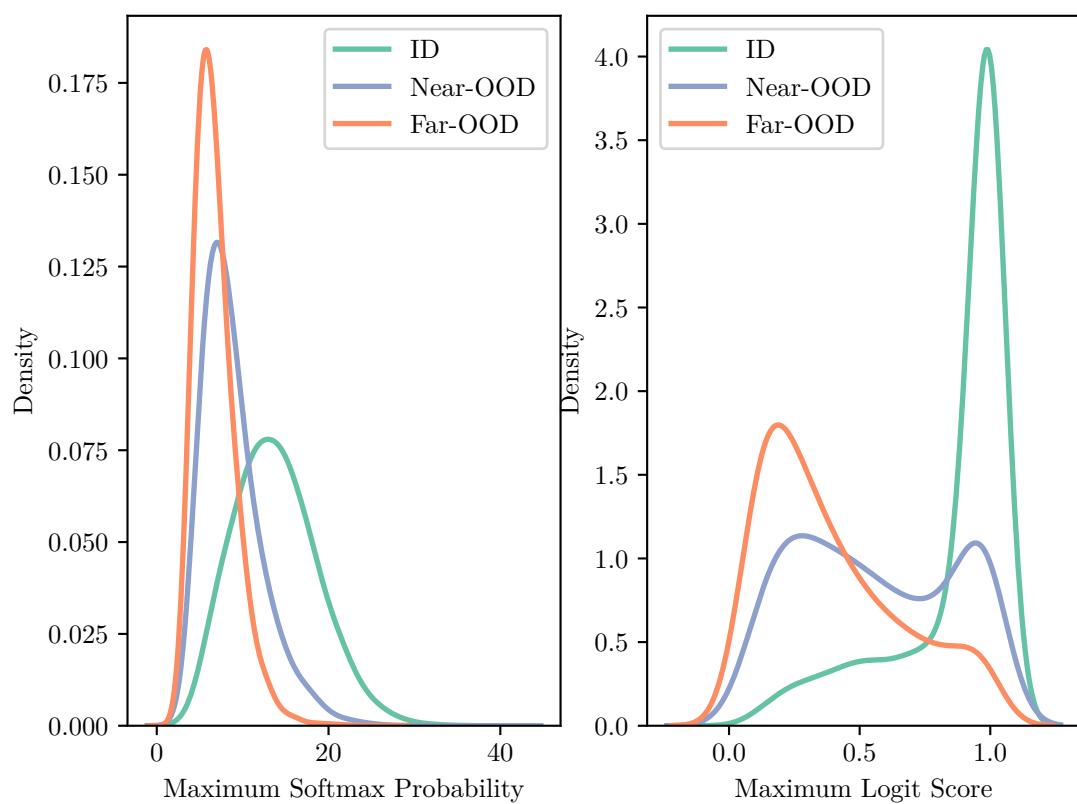


Figure 4.1: Graph showing the distribution of hypothetical ID, Near-OOD and Far-OOD data for an unspecified metric. The shaded region shows the overlap between the ID and OOD samples.

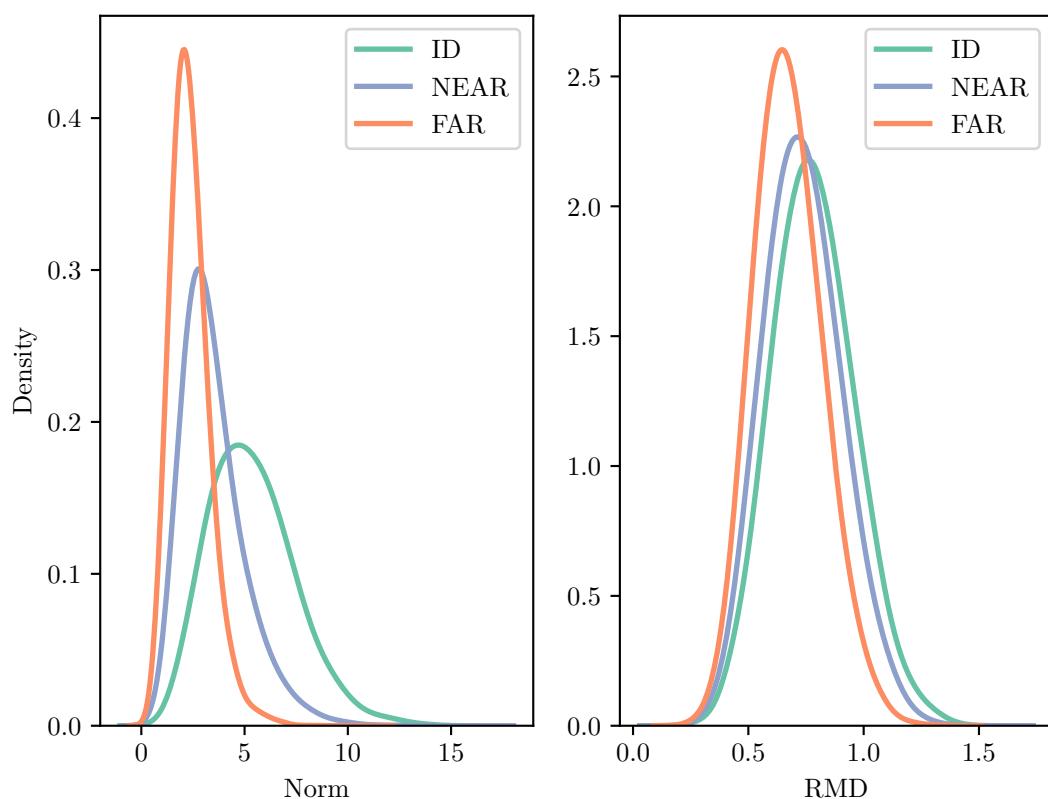


Figure 4.2: Graph showing the distribution of hypothetical ID, Near-OOD and Far-OOD data for an unspecified metric. The shaded region shows the overlap between the ID and OOD samples.

From the figure we can see that for LIME on ImageNet200, it is indeed the case that saliences are higher for ID data points than for OOD data points. Using the vector norm to distinguish ID and OOD, we get an AUROC of 0.814 on Near-OOD, which is slightly lower than the baseline methods, and 0.925 on Far-OOD, which is actually higher than the baselines. These results are far better than those attained by [40], the only other related work which has attempted to use saliency maps to separate ID and OOD data. This work achieved an AUROC score of only 0.52 when used on datasets which were not just small toy datasets, which is for all practical purposes equivalent to guessing. This large improvement suggests that the usage of raw saliency values, rather than normalized heatmaps (as was used by [40]) is highly consequential for the performance of XAI OOD detection algorithms.

Measuring the statistical spread using RMD, we find that there is indeed also a higher spread in ID data when compared to OOD data. However, in this case the overlap is substantial, which is reflected in the AUROC scores attained when discriminating using RMD: The Near-OOD AUROC score was 0.594, and the Far-OOD score was 0.695. In both cases, the scores attained are far lower than the both of the baselines.

Table 4.1 shows the AUROC scores for all forms of aggregation on LIME, as well as the previously mentioned AUROC of the baseline methods. In addition, the correlation between the aggregates and the maximum logit and maximum softmax score is reported, which gives insight into how XAI saliency maps are related to the prediction confidence of the model.

Aggregation type	Baselines		Magnitude of saliencies							Statistical dispersion		
			Mean	Median	Norm	Range	Max	Min↓	CV↓	RMD	QCD↓	
Aggregate	MLS	MSP										
Near-OOD AUROC	83.3	83.4	78.8	69.3	81.4	77.1	78.1	54.3	53.7	59.4	53.2	
Far-OOD AUROC	91.5	90.3	88.1	75.2	92.5	90.2	91.4	58.8	49.3	69.5	49.8	
Correlation with MLS	-	-	0.75	0.60	0.71	0.45	0.54	0.08	-0.01	0.08	-0.01	
Correlation with MSP	-	-	0.61	0.48	0.61	0.41	0.48	0.02	-0.01	0.09	-0.01	

Table 4.1: AUROC scores for lime on imagenet200. The highest value for Near- and Far-OOD is highlighted in bold. ↓ denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

From this table, we can note several interesting observations. Firstly, the aggregates which capture information about the magnitude of the saliences are highly correlated with both the maximum logit and the maximum softmax score of the predicted class. This is not unexpected, as LIME generates saliencies using differences in prediction values as different parts of the image is masked. If the predicted value is higher on average for ID data, then it is likely that the drop in predicted value when masking parts of the image is larger as well, leading to higher saliencies. Regardless, it seems clear that it is not only the correlation to the model output which explains the discriminative power of these aggregates, as we see that vector norm aggregation has lower correlation with MLS and equal correlation with MSP when compared to the mean, but has higher scores.

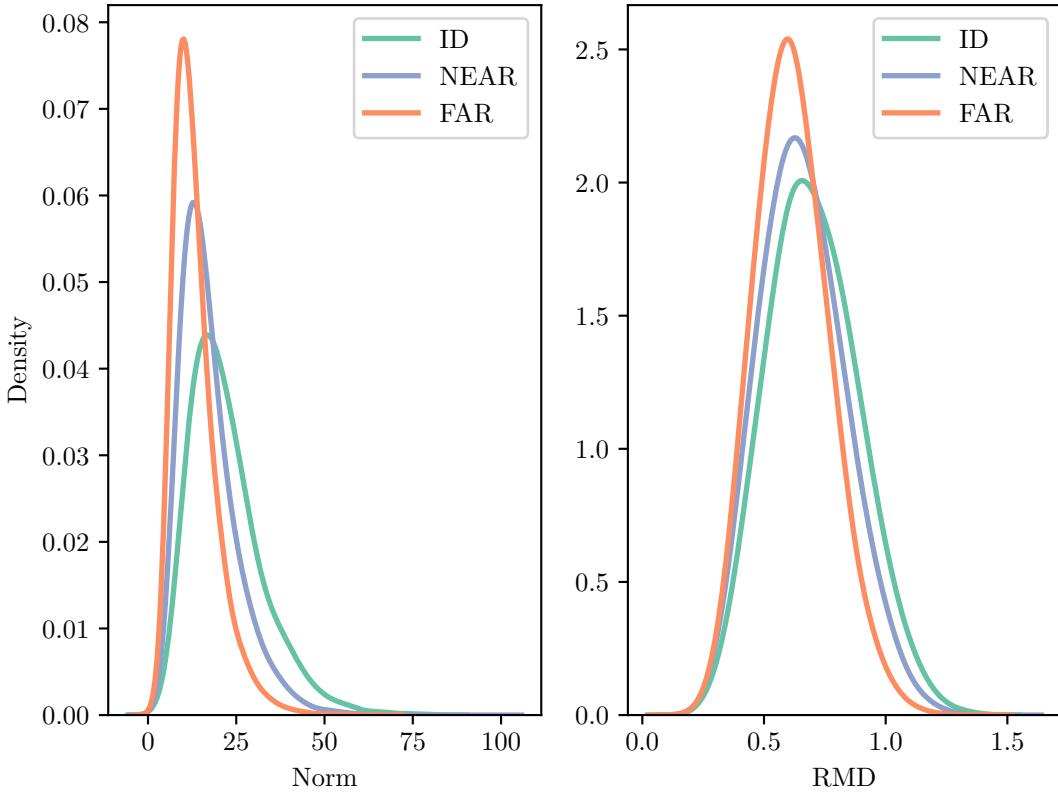


Figure 4.3: Graph showing the distribution of hypothetical ID, Near-OOD and Far-OOD data for an unspecified metric. The shaded region shows the overlap between the ID and OOD samples.

Secondly, we see that the magnitude based aggregations in general perform quite well, with vector norm in this case being the best. In contrast, the methods based on statistical dispersion perform poorly, putting into question the hypothesis that the saliency maps of ID data is more concentrated and less spread out than those on OOD data. Indeed, we see that while the RMD is higher on average for ID data, the QCD and CV is lower on average when generating saliencies using LIME. This further puts doubt on the idea that the spread of saliency maps is a reliable indicator of OOD-ness.

In general, the results from these aggregations are promising, and show that there is definite potential for OOD detection algorithms based on XAI outputs. However, the reader should note that these results are done on the validation set, and that no statistical tests have been done at this point. The statistical significance of using XAI saliency maps for OOD detection will be revealed in section ??, when the final testing is done on the test set and bootstrapping is performed.

Occlusion

Now, we turn our attention to occlusion saliency mapping. Looking at figure 4.3, we see that there is far more overlap between the ID and OOD densities than with LIME. From table 4.7 we see that this

Aggregation type	Baselines		Magnitude of saliencies							Statistical dispersion		
	MLS	MSP	Mean	Median	Norm	Range	Max	Min	CV	RMD	QCD	
Near-OOD AUROC	83.3	83.4	58.6	54.2	65.7	69.1	66.8	54.3	55.0	57.7	55.4	
Far-OOD AUROC	91.5	90.3	69.7	62.9	77.8	84.6	83.5	54.0	63.8	64.7	62.7	
Correlation with MLS	-	-	0.37	0.31	0.42	0.44	0.47	0.07	0.01	0.14	0.01	
Correlation with MSP	-	-	0.29	0.24	0.37	0.41	0.41	0.03	0.01	0.13	0.01	

Table 4.2: AUROC scores for occlusion on imagenet200. The highest value for Near- and Far-OOD is highlighted in bold. \downarrow denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

GradCAM

Aggregation type	Baselines		Magnitude of saliencies							Statistical dispersion		
	MLS	MSP	Mean	Median	Norm	Range	Max	Min	CV	RMD	QCD	
Near-OOD AUROC	83.3	83.4	83.3	80.3	83.8	80.5	81.9	59.2	50.8	51.8	51.7	
Far-OOD AUROC	91.5	90.3	91.5	87.6	92.9	92.2	92.8	56.1	63.6	64.9	64.8	
Correlation with MLS	-	-	1.00	0.94	0.97	0.69	0.81	0.49	-0.16	-0.12	-0.12	
Correlation with MSP	-	-	0.83	0.78	0.82	0.62	0.70	0.37	-0.11	-0.07	-0.07	

Table 4.3: AUROC scores for gradcam on imagenet200. The highest value for Near- and Far-OOD is highlighted in bold. \downarrow denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

Integrated Gradients

Aggregation type	Baselines		Magnitude of saliencies							Statistical dispersion		
			Mean	Median	Norm	Range	Max	Min↓	CV↓	RMD	QCD	
Aggregate	MLS	MSP										
Near-OOD AUROC	83.3	83.4	82.1	55.3	67.3	63.9	63.5	63.6	66.1	51.3	50.5	
Far-OOD AUROC	91.5	90.3	90.5	56.0	87.8	86.7	85.9	86.2	49.8	39.1	53.4	
Correlation with MLS	-	-	0.94	0.14	0.40	0.31	0.30	-0.30	-0.16	0.01	0.01	
Correlation with MSP	-	-	0.79	0.10	0.36	0.29	0.28	-0.27	-0.15	0.00	0.00	

Table 4.4: AUROC scores for integratedgradients on imagenet200. The highest value for Near- and Far-OOD is highlighted in bold. ↓ denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

GBP

Aggregation type	Baselines		Magnitude of saliencies							Spread of saliencies		
			Mean↓	Median↓	Norm	Range	Max	Min↓	CV	RMD↓	QCD↓	
Aggregate	MLS	MSP										
Near-OOD AUROC	83.3	83.4	73.7	55.7	77.4	71.3	71.8	69.9	50.2	52.8	51.5	
Far-OOD AUROC	91.5	90.3	81.7	51.1	92.3	90.7	90.6	89.7	43.5	72.3	50.7	
Correlation with MLS	-	-	-0.33	-0.08	0.45	0.25	0.25	-0.24	0.00	-0.01	-0.00	
Correlation with MSP	-	-	-0.30	-0.08	0.42	0.25	0.24	-0.24	0.01	-0.00	-0.00	

Table 4.5: AUROC scores for gbp on imagenet200. The highest value for Near- and Far-OOD is highlighted in bold. ↓ denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

4.1.2 CIFAR10

LIME

Aggregation type	Baselines		Magnitude of saliencies						Spread of saliencies		
	MLS	MSP	Mean	Median	Norm	Range	Max	Min	CV \downarrow	RMD	QCD \downarrow
Near-OOD AUROC	86.7	87.7	81.2	73.0	77.7	67.1	76.1	62.8	63.6	61.0	59.0
Far-OOD AUROC	91.4	90.8	86.1	77.9	84.0	74.5	81.9	59.6	59.0	61.2	53.2
Correlation with MLS	-	-	0.40	0.28	0.34	0.22	0.31	0.08	-0.00	0.11	-0.00
Correlation with MSP	-	-	0.29	0.20	0.23	0.15	0.22	0.06	0.01	0.08	-0.00

Table 4.6: AUROC scores for lime on cifar10. The highest value for Near- and Far-OOD is highlighted in bold. \downarrow denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

Occlusion

Aggregation type	Baselines		Magnitude of saliencies						Spread of saliencies		
	MLS	MSP	Mean \downarrow	Median \downarrow	Norm \downarrow	Range \downarrow	Max \downarrow	Min	CV	RMD	QCD
Near-OOD AUROC	86.7	87.7	79.2	69.3	84.5	79.5	75.6	83.7	68.3	66.3	51.5
Far-OOD AUROC	91.4	90.8	79.2	72.4	84.9	78.8	74.6	86.6	70.5	71.2	52.5
Correlation with MLS	-	-	-0.17	-0.28	-0.39	-0.39	0.00	0.68	0.01	0.71	0.00
Correlation with MSP	-	-	0.07	-0.16	-0.18	-0.24	0.26	0.87	0.02	0.68	0.01

Table 4.7: AUROC scores for occlusion on cifar10. The highest value for Near- and Far-OOD is highlighted in bold. \downarrow denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

GradCAM

Aggregation type	Baselines		Magnitude of saliencies						Spread of saliencies		
			Mean	Median	Norm	Range	Max	Min			
Aggregate	MLS	MSP							CV↓	RMD↓	QCD↓
Near-OOD AUROC	86.7	87.7	86.8	85.9	86.7	71.8	86.5	87.5	75.3	76.7	74.2
Far-OOD AUROC	91.4	90.8	91.4	91.2	91.4	80.7	91.2	90.7	78.8	80.1	74.5
Correlation with MLS	-	-	1.00	0.99	1.00	0.68	0.96	0.90	-0.47	-0.48	-0.45
Correlation with MSP	-	-	0.79	0.78	0.79	0.57	0.77	0.70	-0.42	-0.42	-0.41

Table 4.8: AUROC scores for gradcam on cifar10. The highest value for Near- and Far-OOD is highlighted in bold. ↓ denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

4.1.3 GBP

Aggregation type	Baselines		Magnitude of saliencies						Spread of saliencies		
			Mean	Median	Norm↓	Range↓	Max↓	Min			
Aggregate	MLS	MSP							CV	RMD	QCD↓
Near-OOD AUROC	86.7	87.7	52.4	51.9	86.0	84.8	84.8	84.4	51.4	54.1	50.3
Far-OOD AUROC	91.4	90.8	46.2	44.7	83.6	82.5	82.4	82.1	51.9	53.1	50.8
Correlation with MLS	-	-	0.01	0.03	-0.24	-0.21	-0.20	0.20	0.00	0.02	0.00
Correlation with MSP	-	-	0.02	0.03	-0.16	-0.15	-0.14	0.14	0.00	0.03	0.00

Table 4.9: AUROC scores for gbp on cifar10. The highest value for Near- and Far-OOD is highlighted in bold. ↓ denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

4.1.4 Integrated Gradients

Aggregation type	Baselines		Magnitude of saliencies							Spread of saliencies		
			Mean	Median	Norm↓	Range↓	Max↓	Min	CV	RMD	QCD↓	
Aggregate	MLS	MSP										
Near-OOD AUROC	86.7	87.7	52.4	51.9	86.0	84.8	84.8	84.4	51.4	54.1	50.3	
Far-OOD AUROC	91.4	90.8	46.2	44.7	83.6	82.5	82.4	82.1	51.9	53.1	50.8	
Correlation with MLS	-	-	0.01	0.03	-0.24	-0.21	-0.20	0.20	0.00	0.02	0.00	
Correlation with MSP	-	-	0.02	0.03	-0.16	-0.15	-0.14	0.14	0.00	0.03	0.00	

Table 4.10: AUROC scores for gbp on cifar10. The highest value for Near- and Far-OOD is highlighted in bold. ↓ denotes that ID data points more often have a lower score with this aggregation, and thus the output values have been negated (as described in section 2.3.1)

Chapter 5

Discussion

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Chapter 6

Conclusion

6.1 Future work

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