

# EVALUATING FEATURE ATTRIBUTION METHODS

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Dear Professor Abbosh,

In accordance with the requirements of the degree of Bachelor of Engineering (Honours) in the division of Software Engineering, I present the following thesis entitled “Evaluating Feature Attribution Methods”. This work was performed under the supervision of Dr Alina Bialkowski.

I declare that the work submitted in this thesis is my own, except as acknowledged in the text and footnotes, and has not been previously submitted for a degree at The University of Queensland or any other institution.

Yours sincerely,

Benedict Gattas.



# Acknowledgments

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# Abstract

This document is a skeleton thesis for 4th-year students. The printable versions show the structure of a typical thesis with some notes on the content and purpose of each part. The notes are meant to be informative but not necessarily illustrative; for example, this paragraph is not really an abstract, because it contains information not found elsewhere in the document. The L<sup>A</sup>T<sub>E</sub>X 2<sub>&</sub> source file (`skel.tex`) contains some non-printing comments giving additional information for students who wish to typeset their theses in L<sup>A</sup>T<sub>E</sub>X. You can download the source, edit out the unwanted material, insert your own frontmatter and bibliographic entries, and in-line or `\include{}` your own chapter files. Of course the content of a particular thesis will influence the form to a large extent. Hence this document should not be seen as an attempt to force every thesis into the same mold. If in doubt about the structure of your thesis, seek advice from your supervisor.

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# Chapter 1

## Introduction

### 1.1 Background

“State of the art” machine learning models now regularly achieve above expert-level performance in fields as diverse as medical imaging and language translation. However, lack of interpretability prevents their adoption in many of the fields that would benefit the most from them. These domains are often ones where the decisions made have a tangible impact on people’s lives. Decision-makers in those domains are unlikely to use the predictions made by a highly accurate but opaque model because of their requirement for trust and accountability.

The requirement for explainability is not in order to replace human experts, but to understand contradictions between expert and algorithm. For example, a radiologist might disagree with a diagnosis made by a model trained to predict pneumonia from chest X-rays, and attributing the error to a factor that one or the other relied upon would be helpful. Was the model relying on some unrelated part of the scan (a spurious feature) or was the radiologist failing to pick up on a subtle pneumonia differential? The former was observed in practice after applying an explanation technique to a convolutional neural network (CNN) trained on such data [1].

In the many domains that require trust, explanations for model predictions are as important as low rates of incorrect predictions. This is the counter-argument to the notion that a highly accurate model need not be interpretable to be effective: the premise of effectiveness requires a level of trust that a model relies on unbiased data and non-spurious features, two guarantees that are not at all provided by an objective function that seeks only to minimise prediction error. With poor visibility into the factors that a model relies upon, machine learning researchers tend to use model performance metrics as the basis for arguing a new model architecture is superior. This disconnect between performance in the sense of test set accuracy and

performance in the sense of accountability (lack of bias or spurious features) and reliability (sensical behaviour) is not ideal.

Interpretability in a Facebook algorithm recommending product categories, for example, might not be seen as important as interpretability in a cancer diagnosis model, though the possibility of unethical model behaviour from reliance on biased data is as tangible in both domains. One study of 200 sentiment analysis classifiers found several to have significant race and gender bias [2]. The consequences of errors can certainly be higher in some domains however - a poor Netflix recommendation is not as disastrous as a naive algorithm used in government decision-making, such as the “robo-debt” scheme recently employed by the Australian Government [3].

## Approaches to Interpretability

There is fortunately an active literature aimed at addressing this ‘black-box’ critique in machine learning. The top-level distinction among approaches is to either use inherently interpretable models to achieve explainability, or take complex, black-box models and find techniques to isolate and explain a piece of their complexity, such as an individual prediction.

The first approach includes model families with low complexity like linear/logistic regression, decision trees, k-nearest neighbours and Naive Bayes. Within these families are both parametric and non-parametric techniques, which demonstrates that lack of interpretability is more related to model complexity than a particular type of formulation - this empirically observed trade-off between accuracy and interpretability is discussed further in the next section<sup>1</sup>. Since many of these models are often too simplistic for obtaining competitive performance, the motivation to attack the ‘black-box’ critique from this angle is quite low. Instead, methods to introduce interpretability to modern, high-performance models are a more studied and popular approach to take in the literature, as in the second approach.

The second approach includes “feature attribution” or “feature importance” methods, which compute a weight score for each feature in the input space to measure its contribution to an output class. For example, a CNN classifier predicting “tree” would be expected to rely heavily on green pixels of leaves. This class includes model-specific techniques for neural network architectures, like those based on activations in a hidden layer, and model-agnostic techniques that are compatible with any model family. Within both sub-classes are a variety of techniques, with varying levels of model agnosticity and task compatibility. For example, some methods are

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<sup>1</sup>There is a view by some researchers ([4]) that in many domains the accuracy vs interpretability trade-off does not exist, and thus there is a responsibility to use equally effective, inherently interpretable models for high-stakes decisions where those are available.

designed solely for CNNs and are therefore mainly suited for image classification or related tasks.

Importantly there are both global feature attribution methods, which calculate each feature’s contribution to a model at large, as well as local methods, which attempt to explain a single prediction. This project has focused on the latter. Local methods are dominant in the literature for modern architectures - when the dimensionality of the data is high, such as in visual data, or when the number of parameters is too high to make conclusions about global model behaviour (as in most modern architectures) this tends to be the only effective approach to interpretability. An author of one local, model-agnostic method notes that understanding these models globally “would require understanding of the underlying prediction function at all locations of the input space” [5].

## Accuracy vs Interpretability

As deep learning and other state-of-the-art model families proliferate in their typical number of parameters, global behaviour has become even less explainable. Researchers maintain some intuitions about the impact of architectural design decisions, though not on predictive behaviour. For example, filters within a CNN model have been shown to act as ‘object detectors’ of patterns, shapes and other connected regions [6], though these per-layer intuitions don’t explain how a network of dozens of layers will determine a husky from a wolf (a recent approach in the literature, however, has looked at abstracting model behaviour into ‘concept’ vector encodings to capture model behaviour across filters and layers (Net2Vec [7], TCAV [8])).

Feature attribution methods can therefore re-introduce transparency into complex, non-linear models and highlight predictive biases in the context of individual predictions. They also can reveal unexpected features involved in a prediction, such as the spurious features mentioned in the previous X-ray data example, or bugs that could lead to exploitation of adversarial examples [9]. Note these methods do not seek to add causal interpretability to the models they are applied to, only to isolate and highlight a piece of complexity in a way that might make sense to an expert reviewing the explanation. This does not make them shallow - the benefit of the ‘post-training’ approach is that model designers have more flexibility in their choice of models, and fewer restrictive assumptions about model complexity are made<sup>2</sup>. More model-agnostic methods, with the least restrictive requirements, are not well understood in context with model-specific ones in terms of this accuracy

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<sup>2</sup>The counter-argument made by those who argue for the inherently interpretable model approach is that there is no guarantee these explanations are faithful to the model, and that they extend the authority of the black box instead of making it a “glass box” [4]. This is revisited in the **Discussion**.

and interpretability trade-off.

## Existing Literature

Some comparisons of feature attribution methods do exist, though typically either in a qualitative context, as a pairwise comparison, **cite** or within a single class of methods. They are not normally compared on speed/performance or adoptability in terms of task/model compatibility. They are however haphazardly compared on explanation quality, which is a difficult criteria to design. Lack of evaluation is partly due to differences in method formulation and therefore representation, but also this difficulty in finding objective proxy metrics for explanation quality.

## 1.2 Project Overview

This project has sought to evaluate a panel of feature attribution methods representative of different approaches to the interpretability problem. The aim was to highlight their relative strengths and weaknesses and thereby increase the understanding of the benefits of one method's approach over another.

Two other key contributions made over the course of the project have been a quantitative evaluation framework for explanation quality in the image classification context, and the development of a software package to collect image data explanations for multiple underlying methods at scale.

In summary the project aims have been to:

1. **Examine and evaluate** a panel of feature attribution methods using proxy metrics of explanation quality supported by analysis on performance, use cases and other qualitative criteria.
2. **Develop** an attribution software package for testing methods at scale with modular support for different metrics, methods and models, to make it easier for researchers to collect explanations and build more adoptable models.

## Project Scope

Section 1.1 introduced a broad motivation for interpretability, though this project has focused specifically on image classification for two main reasons.

Firstly, many interpretability techniques from before the deep learning era have been studied in this domain, and many deep learning specific methods continue to be developed and tested in this domain on modern CNN architectures. The natural ‘visual’ aspect of image data explanations has also made computer vision a dominant venue for interpretability research, with important applications such as medical imaging.

Secondly, well-annotated datasets and pre-trained, ‘off the shelf’ models are more easily acquired in this domain. This availability allowed for richer evaluation metrics and the removal of model training as a project requirement.

A more detailed scope is provided at the beginning of the Methodology section, including a description of the specific datasets, models, and feature attribution methods used.

## Report Overview

Chapter 2 examines the available feature attribution methods and existing approaches to method evaluation. Chapter 3 breaks down the project’s methodology in terms of particular milestones, including the software and evaluation metrics that were designed. Chapter 4 lists evaluation results from quantitative and qualitative standpoints. Chapter 5 provides a discussion on the project’s contribution and the limitations encountered, and finally Chapter 6 provides conclusions and recommendations for future work.

# Chapter 2

## Related Work

### 2.1 Scope of Research

In Chapter 1 (“Approaches to Interpretability”) a brief overview of feature attribution methods was provided with reference to a distinction between model-specific and model-agnostic methods. This is a common distinction in the literature and was also used to guide research in this project. The panel of methods chosen for evaluation ultimately consisted of a balanced selection from both approaches.

A major difficulty of this project was distilling the broad literature on these methods however. For the model-specific (neural network) family, different angles are commonly taken to calculate feature “relevance” or importance. These include generally:

- **Backpropagation-based** methods or ‘importance signal’ projections (such as activations in a hidden layer)
- **Gradient-based** methods, saliency maps and output sensitivity methods
- **Perturbation-based** methods and input occlusion techniques

This categorisation is based on two recent papers that make similar categorisations of explanation approaches [10] [11]. In this chapter a broad selection of methods based on traction over time, current popularity and representativeness of approach are described, though the reader should note there are more methods under each of those three than have been described here.

For model-agnostic methods, perturbation-based and other miscellaneous approaches are considered. Again the selection was based on traction and literature popularity.

First reviewed are traditional, visual approaches to interpretability to provide context to the task of feature attribution. After the exploration of feature attribution methods, a review of existing evaluation metrics and comparison studies is provided.

## Terminology

All methods are variously referred to as *attribution* methods in this project for any projection on the input space that highlights relevant features. Adebayo et al. (2018) instead refer to the broad category of “[...] visualisation and attribution methods aimed at interpreting trained models” as *saliency* methods, particularly in the context of image data [12]. Including by those authors, a *saliency map* is widely used as a catch-all term to refer to input space projections (individual explanations) in the context of interpreting deep neural networks for image data. However they also refer to a specific gradient-based method (Section 2.3.2).

Consensus on terminology is relatively lacking. Some researchers ([11]) describe attribution methods as a subclass of explanation techniques where contribution scores are specifically calculated for each input feature (i.e. excluding higher level ‘patterns’ which cause neuron activations, as in Zeiler & Fergus (2013) ([13]), (Section X) or the back-propagation class generally).

In summary, attribution methods is used in this report as a general term for explanation methods. Saliency maps, explanations and attributions are all interchangeably used for any attribution method’s output.

## 2.2 Traditional Approaches

### 2.2.1 Feature Projection

Visualisation tools for high-dimensional data are a popular way to gauge insight into expected model behaviour. These pre-learning, exploratory data analysis techniques include mathematical reductions like PCA and probabilistic techniques like t-SNE, projecting high-dimensional examples that are ‘similar’ into a visualisable 2D or 3D space [14] (Figure 2.1).

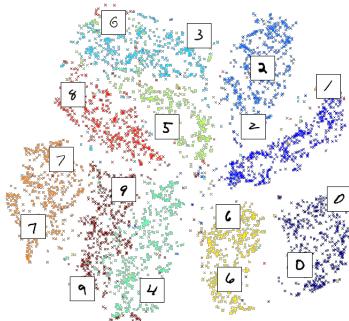


Figure 2.1: 2D embedding of 70,000 handwritten digits (0-9) from MNIST [15].

Other methods of clustering and dimensionality reduction are also widely used for interpreting data, and although useful for gaining an intuition on relationships

between features, they are not suited for explaining model behaviour as they examine only the input space itself.

### 2.2.2 Partial Dependence Plots

A partial dependence plot (PDP) is a tool to demonstrate the marginal effect of one or two features on a prediction outcome. It was proposed by Friedman in 2001 to interpret and visualise the features that the proposed gradient boosting machine relied upon (though it is limited to 1 or 2 input features such that it can be displayed) [16]. A partial dependence function  $\widehat{f}_{xs}$  can be calculated for some desired set of features S, by marginalising the model output over the set of ‘complement’ features C (all other features):

$$\widehat{f}_{xs} = \int \widehat{f}(x_s, x_c) dP(x_c) \quad (2.1)$$

It can be approximated with a Monte Carlo method. Friedman believed in 2001 that these might be used to help interpret “any black box prediction method” such as NN and SVM architectures, and that, “[...] when there are a large number of predictor variables, it is very useful to have a measure of relevance to reduce the potentially large number of variables to be considered” [16]. The mentioned relevance measure was defined only in the context of the decision trees which constituted the paper’s gradient boosting machine. Certainly, PDPs are suited for the low-dimensional feature spaces that were imagined in the pre-deep learning era, and are less suitable for high-dimensional input spaces such as in image classification. They are also restricted by an unrealistic assumption of independence among features.

## 2.3 Model-Specific Methods

Deep learning’s reputation for lack of transparency has led to many attempts to explain the predictions of complex NN architectures. This section examines representative attribution methods from the backpropagation-based, gradient-based and perturbation-based approaches overviewed in Section 2.1, with some emphasis on those developed in the context of CNNs (i.e. image data).

### 2.3.1 Backpropagation-Based

Methods in this class try to isolate an internal model signal, such as neuron activations in a target hidden layer, and map these signals back into the input pixel space. Zeiler & Fergus (2013) introduced the motivation for signal backpropagation as “[...] showing what input pattern originally caused a given activation in the feature maps” [13].

### Visualising Activations - DeconvNet, Guided Backpropagation

Visualisation of per-layer activations is one approach to explain inner model behaviour. It is different from other feature attribution approaches in that it seeks to visualise ‘learned features’ instead of the contributions of input space features. DeconvNet and Guided Backpropagation are two popular examples of the approach and are briefly described as two forerunners of the backpropagation (and gradient) approach.

Deconvolutional networks (DeconvNet) generate backwards projections of neuron activations, by reversing individual activations during a ‘deconvolution’ backwards-pass [13]. The procedure can be summarised as passing feature map output activations as input into ‘deconv’ layers, iteratively reversing activations and reconstructing input signals until the input pixel space is reached.

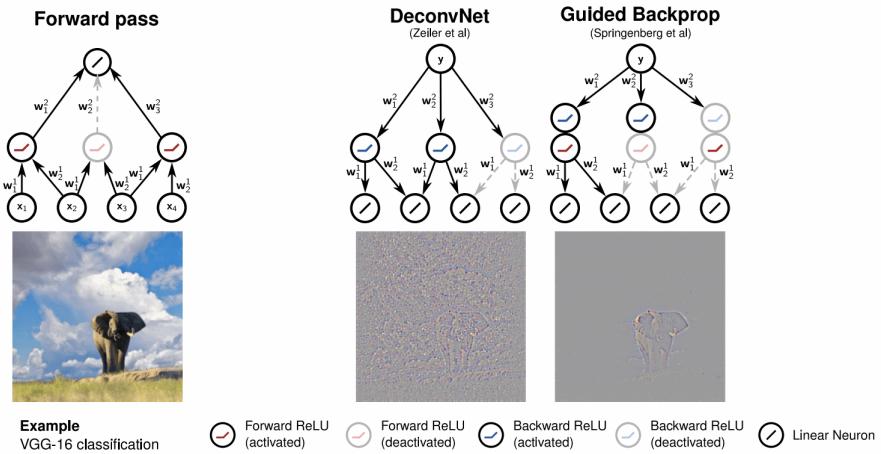


Figure 2.2: (Adapted from [11]) Illustration of DeconvNet and Guided Backprop.

Since it can target one layer’s activation at a time, the method is useful for understanding the hierarchical learned features that CNNs generate over multiple layers. Its limitation is that during the backwards pass, it ignores any negative inputs to ReLu activations that were zero’d out in the forward pass (deactivated activations in Figure 2.2).

Guided Backpropagation was an enhancement by Sprigenberg et al. (2014) that added an additional signal at each step by zero’ing the importance signal if it was a negative activation in the forward pass phase *or* negative in the backwards pass (the two intermediate signals in Figure 2.2 right) [17]. This stopped negative gradients in lower layers from decreasing the activation of the higher layer units which were the target, and this leads to sharper explanations than those created by DeconvNet [17].

## DeepLIFT

DeepLIFT (Deep Learning of Important FeaTures) [10] was created out of the motivation that the zero'ing of negative gradients by DeconvNet and Guided Backpropagation meant that neither are able to highlight inputs that contribute negatively to an output. In some sense they are therefore missing half the story of feature contribution / neuron activation. DeepLIFT's authors (Shrikumar et al. (2017)) also wanted to overcome the unaddressed saturation problem, which is that relevant neurons that contribute to a saturated output activation would not individually change the output if they were turned off (as might be tried in perturbation approaches).

DeepLIFT's innovation over previous backpropagation and gradient-based methods was to realise that where this problem existed, a single gradient value of an output with respect to an input value did not adequately or necessarily capture input contributions to an output. The authors' proposal was to find input contributions by instead calculating the absolute change in output with respect to a neuron's 'reference' activation.

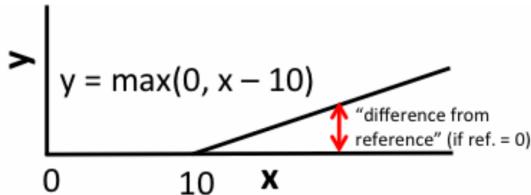


Figure 2.3: (From [10]) Difference-from-reference attributions can avoid bias terms.

Finding reference activations is an implementation difficulty. Generally, the authors propose all-zero input as a baseline (a black square for image data), and a better reference to be the average input over a background data sample [10].

Like other backpropagation methods, DeepLIFT is extremely fast to calculate as it requires only a single backwards pass to propagate an importance signal back into the input space. The authors also provide different formulations for practical implementation, and a relatively high-level public implementation [18]. The concept itself is also compatible with any NN architecture or application, unlike for example DeconvNets and Guided Backpropagation, designed for ReLu activation functions, and GradCAM (Section X) which was designed for CNNs.

## Other Backpropagation Methods

DeepLIFT is one of several modern methods to decompose a network's prediction onto input features using activation backpropagation. For brevity its main competitors, Layerwise Relevance Propagation [19] and DeepTaylorDecomposition [20], are omitted here but mentioned for the reader's reference.

### 2.3.2 Gradient-Based

These methods aim to explain a class output in terms of sensitivity in the input space by relying on a gradient function of the output<sup>1</sup>. The goal is to find the input features that make that prediction more or less confident: for example, for an output class of ‘tree’ they seek to answer “what makes a tree more/less a tree?”.

#### Saliency Maps

An early formulation of a local explanation method was provided by Baehrens et al. (2010) for any nonlinear classification algorithm (though developed in the context of Bayesian classification) [21]. The local explanation gradient vectors that this paper devised were based on class probability gradients, characterising how much a data point has to be moved for a predicted label to change.

Simonyan et al. (2014) later applied a similar idea to CNNs to create ‘class saliency maps’ specific to a given image and class [22].



Figure 2.4: (From [22]) Example of an image-specific class saliency map.

The formulation is based on finding the derivative of an output class with respect to an input image via back-propagation. The authors also formulate a method to generate an image that maximises the output class score for a particular class, to visualise the model’s ‘interpretation’ of a class.

This paper sparked great interest in CNN explanations and further interest in creating explanations from network gradients generally. Along with DeconvNet and Guided Backpropagation (developed relatively simultaneously with similar ideas) these three methods are the most historically popular and influential saliency techniques<sup>2</sup>. A drawback of saliency maps is that noisy images can be produced when a model does not distinguish between objects that are being predicted and nearby objects that are associated (i.e. a tree with leaves, in an image of a bird).

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<sup>1</sup>There is a strong overlap between gradient and backprop. methods: gradients as derivatives are approximated via backprop, and the weights updated by these gradients in training are the contributions to the neuron activations measured via backprop. techniques.

<sup>2</sup>Saliency maps are synonymous with gradient methods to the point where it is sometimes referred to as simply the ‘Gradients’ technique, as in Adebayo et al. (2018) [12], who may have done so to disambiguate the technique from saliency maps generally - see Section 1.1 (“Terminology”).

## Grad-CAM

Class activation maps (CAMs) are another approach aimed at understanding the behaviour of CNNs introduced by Zhou et al. (2015) [23], based on the motivation that deeper convolutional layers capture higher-level visual constructs while retaining spatial information [24]. While examining global average pooling (GAP) layers, a technique previously suggested for regularisation during training [25], the authors realised a final convolutional layer’s separate RGB channels (or ‘feature maps’) could be input into a GAP layer with outputs used as features in a fully-connected layer, just before the final softmax layer. The class-associated weights in that fully-connected layer can be combined with the original final convolutional layer feature maps to capture deep representations as object localisations/class ‘activation’ maps:

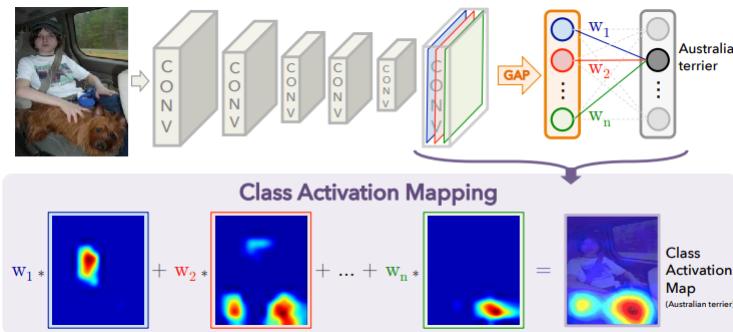


Figure 2.5: (From [23]) Summary of the CAM formulation. RGB channels are emphasised as inputs into the weighted sum that creates a CAM.

A major limitation of the CAM approach is that it requires specific CNN architectures without previous fully-connected layers, and a GAP layer to be added before the output softmax layer to generate the deep representations it visualises. As well as this being a hurdle to adoption, the representations are highly coarse and only roughly approximate class-associated regions (a reason for heatmap presentation).

Grad-CAM was proposed by Selvaraju et al. (2016) aimed at making CAMs applicable to a wider range of CNN models, and for visual tasks other than image classification [24]. It requires no alteration to model architecture. It still targets the final convolutional layer’s channels, as in CAM, but uses the *gradient* of an output class score with respect to these channels’ output activations to then globally-average-pool the gradients over the layer’s width and height dimensions. The importance weights produced can be visualised as a localised heatmap over the input space, though the authors also multiply a Guided Backpropagation output (Section 2.3.1) with the heatmaps to generate a class-discriminative, “high-resolution” version called Guided Grad-CAM (Figure 2.6).

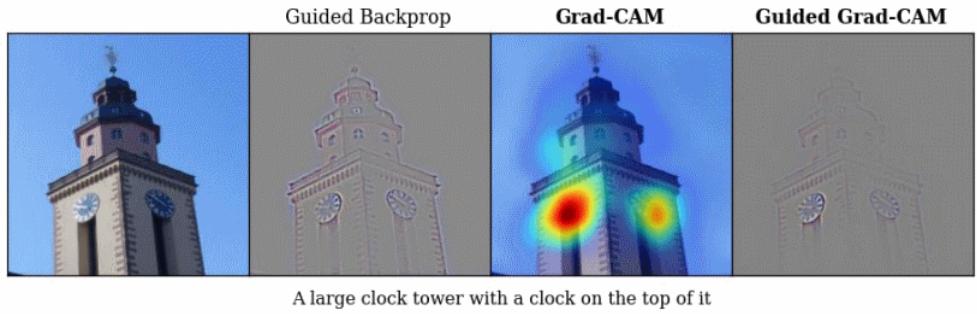


Figure 2.6: (Adapted from [24]) *Guided Backpropagation*, *Grad-CAM* and *Guided Grad-CAM* on an image captioning example from the Neuraltalk2 model.

One of Grad-CAM’s strengths is that its authors prove its effectiveness for a variety of use cases. These include highlighting causes of incorrect predictions (‘failure modes’), the effect of adversarial noise and causes of model confusion, and identifying training dataset bias<sup>3</sup>. Its application to a variety of models by other researchers ([26], [1]) is one testament to its authors’ claims on cross-model applicability and explanation quality, as well as its popularity in the literature (>2000 citations).

### Other Gradient Methods

Three other gradient-based methods are widely cited and relevant to discussion - Integrated Gradients [27], Gradient \* Input [28] and SmoothGrad [29].

Integrated Gradients is similar to DeepLIFT - instead of taking difference-from-reference activation as a signal of contribution, the approach is to integrate the possible gradients over all inputs (from 0 up to the activation caused by the input image) and then use this area under the activation function as an information measure of input relevance. It also addresses the saturation problem (Section 2.3.1) though is naturally expensive to compute. Approximating the integral requires a baseline example that can provide zero input score as a comparison, and the method is applicable to a variety of architectures (two other similarities with DeepLIFT).

Gradient \* Input was a simple proposal by DeepLIFT’s authors to sharpen the saliency maps of Simonyan et al. (2014) [22] by multiplying the gradient with the original input signal. SmoothGrad was another attempt to sharpen gradient-based saliency maps, that noted gradients as derivatives can fluctuate sharply at local scales. To compensate for the noise in the output explanation, they propose a local average of gradient values that can be computed based on random samples of the original input image with Gaussian noise added.

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<sup>3</sup>For example, they showed that a VGG model trained to classify nurses from doctors had learned to look at long hair to incorrectly label a female doctor a nurse, and the bias was because of gender-skewed training data.

### 2.3.3 Other Model-Specific Techniques

Backpropagation and gradient methods can be viewed as reflections of one approach based on a similar assumption: that propagating a relevant signal back through a neural network model is a means to explain how the signal was originally encoded. A third and more unrelated category of model-specific methods are perturbation techniques. These treat the underlying model as a true black-box by iteratively occluding patches of the input feature space in order to measure the change in output class score. Where the occlusion caused a noticeable change, the inference is that the region masked was important. Zeiler & Fergus (2013) ([13]) pioneered this approach in the same paper that proposed DeconvNets described in Section 2.3.1<sup>4</sup>.

An influential work by Fong & Vedaldi (2017) [30] formalised a meta-predictor framework that can *learn* masks via what they describe as a deletion minimisation problem. Summarised, the informative region is found by minimising the size of a small deletion mask that causes the output score to drop significantly. This mask generation framework leads to similar results as other methods mentioned so far (Figure 2.7). The authors rely similarly on gradients to extract information to solve their optimisation problem, but a key performance drawback is that *many* gradient calculations for successively increasing mask sizes are required.

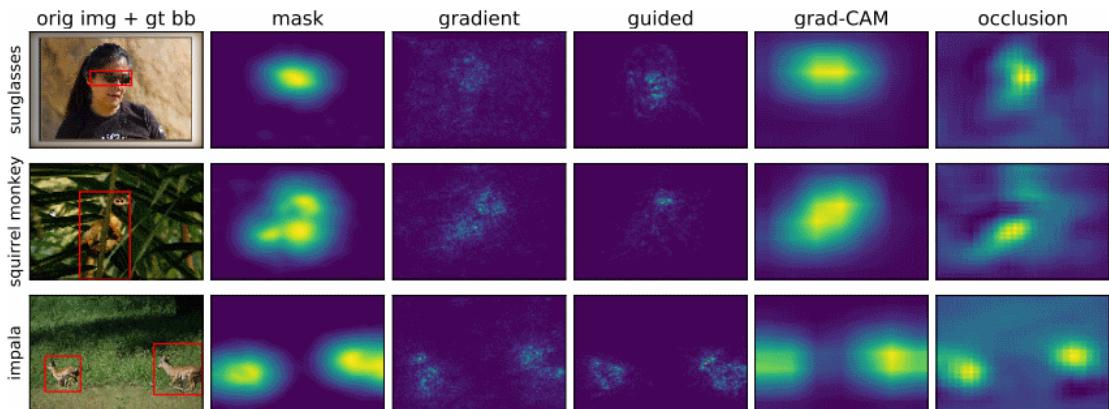


Figure 2.7: (Adapted from [30]) Comparison of methods discussed so far: Mask generation [30], Gradient (saliency maps) [22], Guided Backpropagation [17], Grad-CAM [24] and Occlusion [13]. Ground truth bounding boxes are labelled “gt bb”.

For completeness, some NN methods which do not attribute the contribution of input features specifically (or project internal model signals onto the input space) are not within project scope as a result, but are mentioned here. These are ‘concept vector’ methods that extract model behaviour across layers: Net2Vec [7] and Testing with Concept Activation Vectors (TCAV) [8].

<sup>4</sup>The grey-square masking method from the DeconvNet paper is usually referred to as ‘Occlusion’ in the literature.

## 2.4 Model-Agnostic Methods

In parallel to the literature aimed at explaining neural network model behaviour, a standalone approach in the interpretability literature is to find model-agnostic explanations. Similar to the motivation for perturbation-based methods (and with overlap), these are ‘black-box’ methods that make no restrictive assumptions about model architecture or classification task at all, and therefore can theoretically be applied to any model or task. Stark differences in approach and computational complexity still exist however. The most prominent methods in this sub-field are listed below.

### 2.4.1 Perturbation-Based

Described in Section 2.3.3, perturbing the input space (by toggling feature patches) is one way to isolate model behaviour. Changes in output score reveal importance in the occluded inputs. Several methods implement this intuition by training “surrogate”, interpretable models around the isolated features that are locally relevant to a single prediction. These include Local Interpretable Model-Agnostic Explanations (LIME) [31], Anchors [32] and similar variants [5].

#### LIME

LIME’s authors propose that non-linear, complex decision boundaries can be approximated locally around a single prediction via a simpler model that only relies only on the “neighbourhood” of the relevant input space [31].

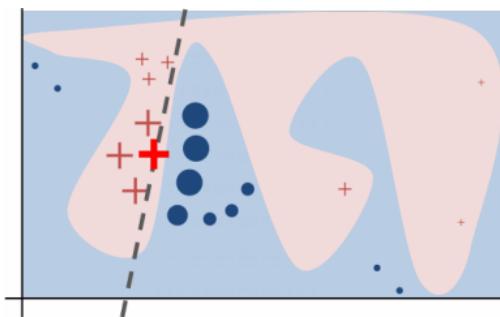


Figure 2.8: (From [31]) LIME’s intuition about complex decision boundaries.

To compute explanations, LIME trains an interpretable model (i.e. decision tree or Lasso regression) on permuted samples from a given instance, weighted by their proximity to the instance being explained. The training simply minimises mean-squared error based on the samples’ black-box predictions. Finally, the interpretable model’s weights on these proximal features (superpixels in the case of image data) represent the ‘explanation’ for the underlying instance.

The formulation in the paper is relatively vague however, particularly with regards to the size of the region of influence / neighbourhood that should be used for finding relevant features. The vagueness was potentially motivated by their intention to be agnostic about the choice of explanation model and the black-box model, though this leaves questions about the accuracy-interpretability compromise largely unaddressed. Generating samples and training models for each sample is also extremely performance costly. Even for a confident prediction and using many samples, instability from random sampling makes an explanation undesirably non-deterministic. This was noted by the authors [31]. The authors of the mask generation technique described in Section 1.3.3 note that LIME bears similarity to their perturbation approach, but takes significantly longer to converge and produces a coarser heatmap via super-pixels instead of their pixel-level attribution [30].

Despite these shortcomings, LIME’s simplicity and complete compatibility across all model families and classification tasks explains its high popularity among model-agnostic methods.

## Anchors

LIME’s problems motivated a more recent successor called “Anchors: High-Precision Model-Agnostic Explanations” by its original authors [32]. They replaced the use of simple local models with high fidelity if-then rules around a prediction, and give a framework for finding those rules efficiently. A rule (termed an ‘anchor’ explanation) is one that, “[...] sufficiently anchors an explanation locally, such that changes to the rest of the features of the instance do not matter” [32].

Formal ways to define the optimal region of influence (‘coverage’), build rule accuracy (‘precision’), and calculate rules efficiently were devised - three key improvements over their LIME proposal.

Though these anchor rules are highly interpretable, code available from the authors is limited and (possibly as a result) it has less popularity both in practice and in the literature. The GitHub repository provides for example a rough implementation for only text and tabular data and not image data [33].

### 2.4.2 Other Model-Agnostic Methods

#### SHAP Framework

Many methods have been listed so far and a reader may be fatigued of the variety. The SHAP framework (SHapley Additive exPlanations) by Lundberg & Lee (2017) was a push-back on this issue of method proliferation, showing links between many existing methods with a theoretical approach from game theory [34]. It has become extremely popular among researchers from all sub-fields in interpretability due to its

attractive formal properties and ‘outsider’ formulation, as well as its implementation approximations for many model families and a well-maintained GitHub repository to host those implementations<sup>5</sup>.

The game theoretic concept of Shapley values are a unique solution to the problem of calculating fair, marginal per-player rewards for the reward earned collectively in a cooperative game [36]. Since each player’s contribution may produce interaction effects with others, they are calculated by averaging contributions in all possible sub-coalitions of players. In the context of machine learning, if features are taken as players, the method can be applied to a prediction (the “payoff”) and it retains its per-player theoretical properties. These qualities include *efficiency*, which is that the sum of  $p$  constituent input feature contributions (Shapley value  $\phi_j$  for a feature  $j$ ) must equal the difference between a prediction of an input  $x$  ( $\hat{f}_x$ ) and an average for all inputs (an ‘expectation’ of model output  $E_X(\hat{f}(X))$ ):

$$\sum_{j=1}^p \phi_j = \hat{f}_x - E_X(\hat{f}(X)) \quad (2.2)$$

A key problem is that finding  $\phi_j$  requires iteratively computing outputs for all feature subsets including  $j$  and is therefore computationally infeasible for large input spaces<sup>6</sup>.

SHAP values are an implementable version of Shapley values. They connect Shapley value theory with local explanation techniques including LIME and DeepLIFT [34]. They are formulated as the difference between expected model output (approximated by an average background data sample’s prediction) and the instance at hand being predicted. The authors show that the game theoretical properties including efficiency apply to a whole class of ‘additive feature attribution methods’, both model-specific (e.g. DeepLIFT) and model-agnostic. They provide several model-specific approximations for implementing their attributions, one based on Integrated Gradients and another based on DeepLIFT.

## 2.5 Evaluation of Attribution Methods

Creators of feature attribution methods tend to provide visual comparisons with existing methods, as for example in Figure 2.7. An issue is that qualitative evaluation is implicitly left to the reader, who is encouraged to infer the author’s saliency maps are either equal in standing or more aesthetically pleasing than another method’s.

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<sup>5</sup>The SHAP paper has over 1000 citations and its GitHub has over 9000 ‘stars’ at the time of writing [35], despite only being published in late 2017.

<sup>6</sup>They are however commonly used in low-dimensional linear regression settings, like in economics for example, for calculating global feature importances when features are dependent [36].

Method creators *do* often suggest their own interpretability criteria, though this is done with little reference to criteria in the prior art. The interpretability field’s agreement on implementable standards for interpretability is therefore low. To some extent, the proliferation in attribution methods and variants can be attributed to these unfortunately subjective and still actively researched standards. In summary, two unresolved problems in interpretability research can be thought of as agreement on desiderata for interpretability, and lack of evaluation on any criteria *independent* of method creators. This thesis does not seek to tackle the first issue though makes a contribution in the form of saliency metrics. The main contribution is towards increasing independent understanding on common criteria.

Existing efforts to independently compare and unify methods are listed here. The SHAP framework can be thought of as one example as it shows how existing methods are related and that it demonstrates where one can be preferable. This research section therefore aims to:

1. Overview attempts like SHAP that have independently evaluated methods, performed ‘unification’ or comparison studies, or independently proposed desiderata for interpretability. This includes theoretical and practical standpoints.
2. Examine criteria that method authors have themselves proposed.
3. Describe existing software for generating explanations, that package several methods for visual comparison for use by researchers and practitioners.

### 2.5.1 Existing Studies

#### The Mythos of Model Interpretability [37]

An early, widely-cited contribution towards common interpretability criteria was made by Lipton (2016) to “define the discourse on interpretability” [37]. The proposed criteria were high level, coming from the view that different motivations for interpretability are what cause the many different interpretations of the word:

1. **Trust:** We should care about not just “how often a model is right, but also for which examples it is right”.
2. **Causality:** Does the model show cause-and-effect reasoning?
3. **Transferability:** Does the model generalise well?
4. **Informativeness:** What contribution does the model make towards increasing understanding of the application domain?

5. **Fair & Ethical Decision Making:** Can we show the model’s decisions conform to ethical standards?

Though it did help shape discourse by defining motivations for interpretability, the criteria are too high level to be useful for comparing one feature attribution method’s output to another’s.

### Towards a Rigorous Science of Interpretable Machine Learning [38]

Doshi-Velez & Kim (2017) provided an influential set of guidelines or “evaluation paradigms” for evaluating interpretability techniques, arranged in three levels of increasing abstraction [38]. This motivation was to provide a scientific basis for the different objectives in evaluation that method authors implicitly target (both qualitative and quantitative):

1. **Functionally-grounded:** How well the attribution method performs on quantitative criteria: ‘proxy’ metrics for explainability like weakly supervised object localisation (Section X).
2. **Human-grounded:** How much everyday people agree that an explanation is visually superior to another: user studies as an example.
3. **Application-grounded:** How well the explanation helps domain experts solve real tasks; such as a radiologist agreeing with fractures pointed out by a model trained on X-ray data.

Research on evaluation criteria below (Section 2.5.2) has focused on functionally-grounded criteria, since these are more common in the literature and since higher-level paradigms are difficult to compare objectively.

### Towards Better Understanding of Gradient-based Attribution Methods [39]

Similar to SHAP in motivation, an independent attempt at providing a unified framework for the gradient-based class<sup>7</sup> of attribution methods was provided by Ancona et al. (2017) [39]. In their work they prove conditions of equivalence between Layerwise Relevance Propagation and Gradient \* Input, and DeepLIFT and Integrated Gradients (Section 2.3). Another major contribution was to propose a generalisation for the ideal ‘additivity’ property that SHAP’s authors noted defined

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<sup>7</sup>The authors do not distinguish between backpropagation and gradient-based methods.

a class of methods (Section 4.3.4)<sup>8</sup>. This criteria was termed *Sensitivity-n*: “[...] when the sum of the attributions for any subset of features of cardinality  $n$  is equal to the variation of the output  $S_C$  caused by removing the features in the subset” [39].

Some of their key insights were that existing methods like DeepLIFT and Integrated Gradients show very high correlation, that the former therefore acts as an approximation of the latter in practice, and that on complex model architectures like InceptionV3, all gradient-based methods produce noisier saliency maps and less appealing explanations.

### Sanity Checks for Saliency Maps [12]

This paper by Adebayo et al. (2018), along with Lundberg & Lee (2017) (SHAP’s authors) and Ancona et al. (2017) above, have been the three main independent contributions towards understanding and unifying the model-specific set of feature attribution methods described in earlier sections of this chapter. This motivation was similar though more practical than theoretical: find an actionable methodology to help a practitioner / researcher decide between competing attribution methods.

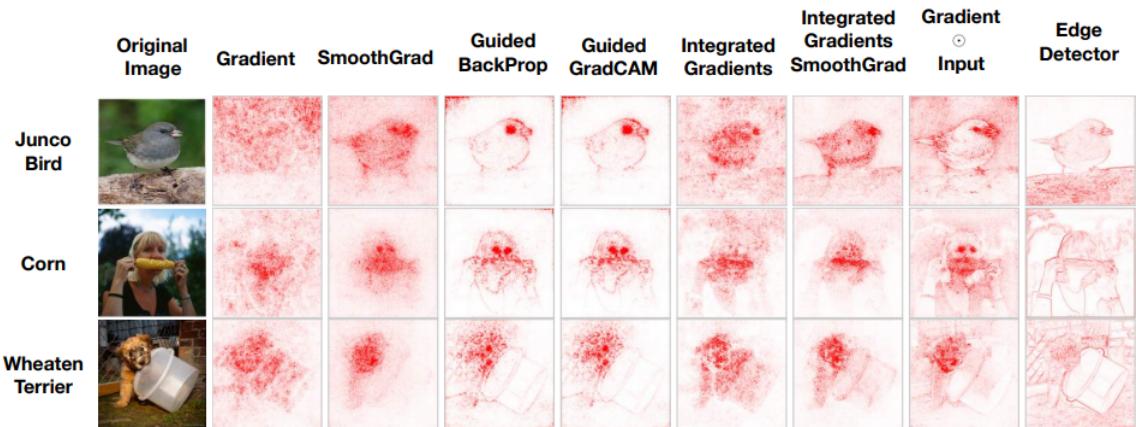


Figure 2.9: (From [12]) The panel of methods examined by Adebayo et al. (2018), all previously discussed in Section 2.3. They highlight that an edge detector alone can produce a mask similar to the output of some methods.

The methodology proposed was a set of two statistical randomisation tests (‘sanity checks’):

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<sup>8</sup>The authors actually reference the properties of *Completeness* (proposed by the authors of Integrated Gradients [27]) and *Summation to Delta* (proposed by the authors of DeepLIFT [10]), two variants of a similar idea to additivity.

1. **Model Parameter Randomisation Test:** A misleading attribution method could be insensitive to model parameters, so an untrained version of the same model with random weights should not produce a similar saliency map.
2. **Data Randomisation Test:** A misleading method could be dependent on training labels: a test with randomly permuted labels should therefore show significantly different saliency maps.

For comparisons between a normal attribution output and a modified one according to one of those two experiment conditions, the authors use similarity metrics including Spearman rank correlation and a structural similarity (SSIM) index. Note these metrics do not evaluate one method’s similarity with another: only the similarity with its modified version. Some insights are prepared from these metrics, like that Guided Backpropagation and Gradient \* Input show unexpected insensitivity (perform badly on the sanity checks).

One problematic point they emphasise though is that non-performing saliency methods may only be visually salient because they act like an edge detector (Figure 2.10). Although the work valuably points out that observers might have confirmation bias when viewing highlighted edges in a saliency map, this qualitative conclusion ignores the role of connected regions and pixel-wise attribution intensities, which some methods may have as a strength over others. These latter two criteria are arguably as important or more important for visual quality than edges alone, and the authors’ similarity metric results also do not relate to the standalone observation about edges.

### 2.5.2 Existing Criteria

#### Saliency Metrics (Quantitative Approach)

Some method authors however have made an effort to account for regions in method evaluation. In particular, ‘weakly supervised object localisation’ (WSOL) has been the technique used for evaluating saliency maps via bounding boxes derived from a segmentation algorithm (in natural image classification settings). It was first applied by Simonyan et al. (2014) while introducing the original saliency maps method (Section 2.3.2) [22]. Those authors used a colour segmentation algorithm on thresholded saliency maps, found bounding boxes on the segmented regions, and then submitted their annotations to an ILSVRC-2013 localisation challenge where they out-performed many fully supervised algorithms.

The paper that introduced CAM saliency maps (Section 2.3.2, [23]) used a similar technique and has been considered the seminal work for use of WSOL [40]. They chose a 20% quantile threshold for CAM values before finding the largest connected

component in each map. Unlike Simonyan et al. who only evaluated via the competition, CAM’s authors independently evaluate their derived bounding boxes using an intersection-over-union metric (thresholded at 0.5 to exclude instances where the method was significantly off). Their results on an ILSVRC validation set outperformed the benchmarks of localisation-trained models.



Figure 2.10: (Adapted from [23]) CAM’s predicted bounding box in green and the ground truth annotation in red (left in each sub-pane), and the original CAM (right in each sub-pane). Their IOU metric is calculated over the annotations.

Notably this IOU metric does not account for the weight of the attribution in any one pixel, which is relevant to most methods. The methodology also unfairly penalises more perforated-looking saliency maps due to relying on segmentation algorithms to find connected components and therefore ignoring pixel-level detail. On the one hand, connected components are more observer-friendly explanations of single objects (with an implicit assumption that the underlying model also cares about connected regions), though on the other hand some methods may be noisier and so may be punished harshly for having small, disconnected sub-regions yet still maintaining saliency in the ‘bigger picture’.

Dabkowski & Gal (2017) compensate for the latter problem by proposing an augmented localisation metric that takes a bounding box of the *entire* salient region, rather than just a thresholded and single-component subset of the saliency map [41]. A strong aspect of their work was to provide a “Max box” baseline in reporting localisation error: this reports the ground truth box’s overlap with the whole image. Where the localisation error is similar, this allows them to suggest the interpretability of their generated localisation boxes is similar to the ground truth boxes themselves.

Independently of the explainability literature, pixel-wise mask-based metrics have been developed for generic WSOL applications by Choe et al. (2020) [40], though it seems these have not been applied in the context of evaluating explainability techniques.

### Higher Level Criteria (Qualitative Approach)

Some authors sidestep the functionally-grounded approach to method evaluation to suggest “axioms” that fall more under the human-grounded paradigm. These criteria are summarised in Table 1.X, from lower to higher level qualities:

consistency between models input invariance

Across in the model-agnostic camp Ribeiro et al. (2016) have made the case for model flexibility as a strong criteria for explanation technique usability [42]. When comparing a tree-based model with a deep learning model, for example, neither a practitioner nor a researcher can get a fair idea of interpretability if two explanations are different in representation on account of different attribution methods. The observation by Ancona et al. (2017) that more complex architectures are not explained as well by current model-specific techniques also supports this argument (Section 2.5.1) [39].

#### 2.5.3 Existing Explanation Frameworks

Ancona et al. (2017) developed a software package called *DeepExplainer* to support their unified framework [43]. It implements a suite of the methods they showed relationships between: Saliency Maps, Gradient \* Input, Integrated Gradients, DeepLIFT and Occlusion (Section 2.3). It provides abstraction over these methods with some parameter specification allowed: .

Aimed at practitioners for auditing their models for bias, *FairML* was developed by Adebayo (2017) [44]. This package

There are no explanation frameworks for collecting both model-agnostic and model-specific techniques for saliency maps. Additionally, no automated method evaluation frameworks for WSOL-based evaluation are known to be available.

# Chapter 3

## Methodology

### 3.1 Overview

A panel of four local attribution methods were chosen for evaluation in this project, picked for representativeness of approach and their prominence in the literature. The panel was also a balanced selection from both ‘classes’ of method approach: model-specific (Section 2.3) and model-agnostic (Section 2.4):

1. **DeepLIFT:** Model-specific class, backpropagation-based approach (2.3.1)
2. **GradCAM:** Model-specific class, gradient-based approach (2.3.2)
3. **LIME:** Model-agnostic class, perturbation-based approach (2.4.1)
4. **SHAP:** Model-agnostic class<sup>1</sup>, generic approach (4.3.4)

Other methods could have been included in this panel though as related work has shown in 2.5.1 (particularly by Ancona et al. (2017)), similarities in formulation should allow conclusions on one method to apply to close relatives. Project constraints also meant that a decision on the panel breadth had to be made according to at least some criteria, and representativeness helps for comparing approaches (the main project goal).

This chapter is presented in order of project milestones achieved, from initial data collection through to fine-tuning of the evaluation metrics designed. The evaluation methodology itself can be summarised in terms of the dataset used, ‘off the shelf’ underlying models relied upon and the evaluation metric approach:

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<sup>1</sup>Due to its higher level formulation, SHAP has to be implemented for each model family. It’s therefore better described as *partially* model-agnostic.

1. **Dataset:** ImageNet validation set, with ground truth bounding box annotations usually used for object localisation training.
2. **Models:** VGG16 as the primary model, InceptionV3 and ResNet50 for supportive analysis.
3. **Metrics:** Pixel-wise and mask-based WSOL, extending related work in Section 2.5.2.

These are described in more detail in Sections 3.2, 3.3 and 3.8 below respectively. Finally, to support the metric analysis, qualitative analysis was also performed, though these results are left to the following chapter.

## 3.2 Data Collection & Annotation

The ImageNet Large Scale Visual Recognition Challenge (ILSVRC) uses a subset of the well-known, hierarchically-labelled ImageNet database [45]. The competition’s validation set consists of 50,000 images of 1000 categories, and includes annotations for ground truth class labels for image classification, and ground truth bounding boxes for object localisation.

This dataset was chosen because of the convenience of the bounding boxes for method evaluation, and the availability of models pre-trained on ImageNet. Images and bounding box XML files for all 50,000 instances in the 2012 validation set were acquired from an academically hosted torrent.

Each bounding box file contains one or several annotations (several if there are multiple instances of a single class, e.g. Figure 3.1), and each annotation contains the ImageNet class ID and  $\{x\text{-min}, x\text{-max}, y\text{-min}, y\text{-max}\}$  fields for the box<sup>2</sup>.

A script to draw rectangular annotations on the images was created to sanity check the acquired data. Example outputs are shown in Figure 3.1.



Figure 3.1: Collected ImageNet examples with annotations drawn.

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<sup>2</sup>These ImageNet ‘synsets’ IDs were converted to human-readable class labels using a script that connects to a standalone map of IDs to labels.

Much later into the project this script was upgraded to return the annotated image as a 2D array of 0's and 1's, with 1's inside the bounded regions to create a ground truth mask. The use of this mask for saliency calculation is described later (Section 3.8).

### 3.3 Models & Predictions

Deep CNN models are expensive to train, so the high-level Keras library was used to import image classification models pre-trained on ImageNet [46]. Three models were chosen representative of common modern architectures (summarised in Table 3.1). They acted as the underlying ‘black-box’ models being explained.

Model	Structure	Input Shape	Project Role
VGG16	16 stacked, 3x3 convolutional layers	224x224	Most testing / results
InceptionV3	Stacked modules of pooling + conv. layers	299x299	Supporting analysis
ResNet50	50-layer CNN with ‘residual layer’ connections.	224x224	Supporting analysis

Table 3.1: Pre-trained image classifiers used in the project.

To check each model was working, a script was written to automate prediction collection and interact with preprocessed examples from the collected data. All software in the project was developed to be agnostic about the underlying model, though some methods required specific hyperparameters like a layer target. These targets were set up in a high level struct-type object in a constants file.

### 3.4 Software Abstraction I

Each model requires input resizing and preprocessing in some form. An *ImageHandler* class was therefore designed to abstract from complexity related to different representations of a single image instance. All input/output file methods and getter methods for raw, expanded and preprocessed representations were stored in this class, which made enforcing model agnosticity and adapting methods (Section 3.7) much easier.

## 3.5 Initial Method Investigation

Public GitHub implementations for each of the four methods were sourced: Grad-CAM [47], DeepLIFT [48], SHAP [35] and LIME [49].

They were then run on some high-confidence instances fed into the VGG16 model (correct predictions with  $p > 0.75$ ) and their ‘out of the box’ saliency maps were then visually inspected. Examples are shown in Figure 3.3 over the page. Note different method formulations result in different explanatory features being highlighted, even for the same example and model prediction. Some other initial observations on each method were made:

- **GradCAM:** The heatmap represents the localisation characterised in the target layer (final convolutional layer). The Guided GradCAM variant (Section 2.3.2) was later used instead for a more discriminative version of the same saliency map.
- **DeepLIFT:** Attributions are relatively ‘noisy’, emphasise edges, and are higher resolution due to being captured in the original input shape.
- **SHAP:** Attributions are in the shape of the input to a target hidden layer, which accounts for its lower resolution.
- **LIME:** The method represents connected component ‘super pixels’ as the explanatory features, though in Figure 3.3 these appear patchy on the maze-like patterns on the coral, the texture of the hair on the monkey’s face, and the wheat in the field.

## 3.6 Software Abstraction II

Each method was wrapped in its own class with an *attribute()* function to return the array that represented its explanation output. Repeated logic in each method’s implementation was also extracted into an *Attributer* class fitted over these methods. This was a helpful prerequisite to adapting the methods for comparison. The functions in this class visualise figures, save returned NumPy arrays to results files, apply a colour map to highlight positive / negative attribution weights and the intensity of those weights, and normalise attributions between -1 and 1. This class is included in Appendix A and referred to in the class diagram in Figure 3.6.

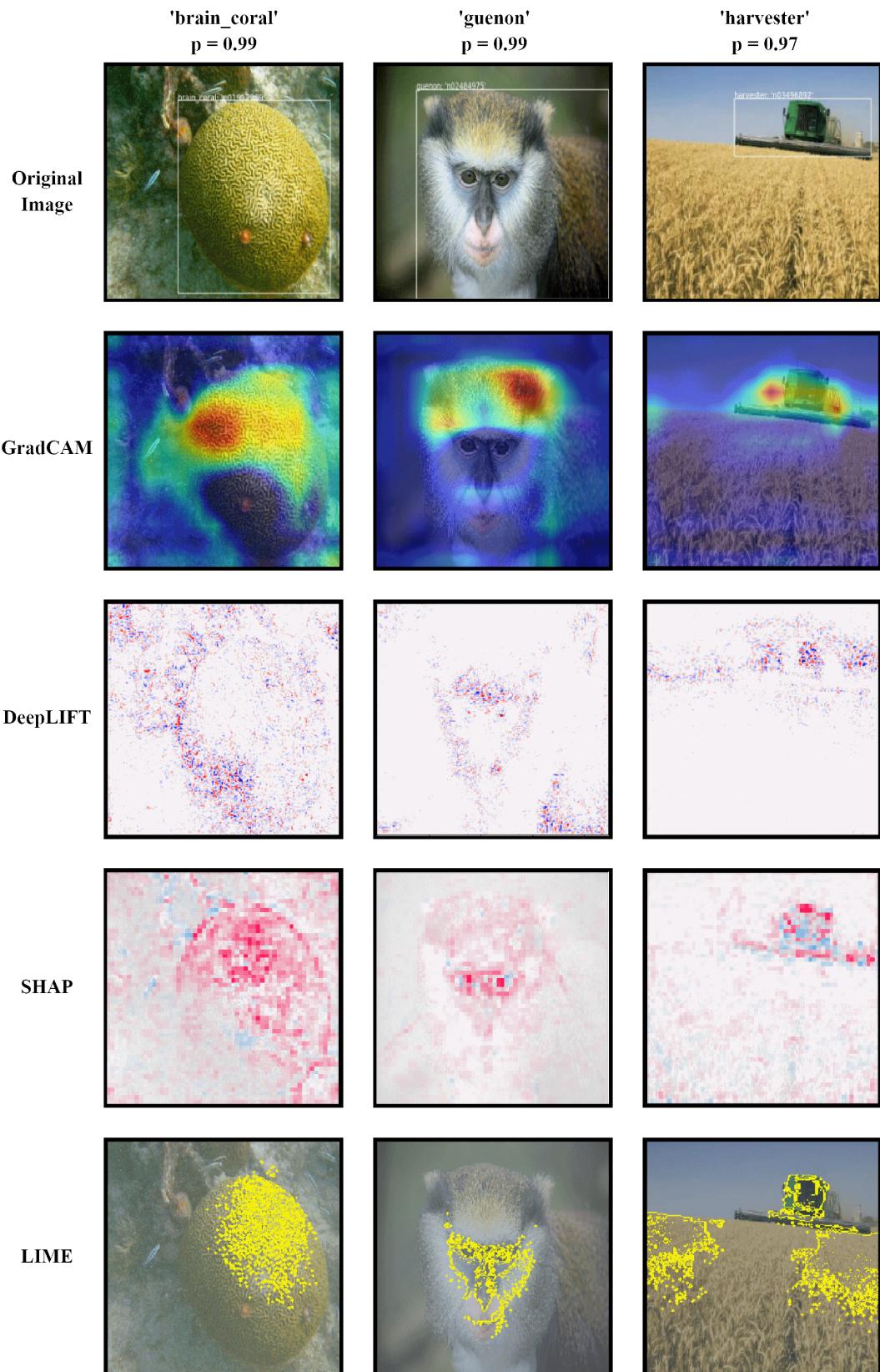


Figure 3.2: Default attributions for methods applied to high-confidence VGG16 predictions (class label and softmax output at top). Original image is resized with annotation drawn for reference.

## 3.7 Adapting Methods for Compatibility

Some methods had higher level implementations than others (SHAP and DeepLIFT) in the code. For example, the output representation of SHAP was generated in internal methods that made it necessary to implement modified functions that overrode method internals. Others did not hide internal logic and were easier to adapt.

Visual examples of the methods made compatible for evaluation are shown in Figures 3.4 and 3.5. Some brief comments about work necessary for each method and the insights gained:

- **GradCAM:** Guided GradCAM required very little adaption, since the attributions were already in the shape of the input feature space. Support for specifying the final conv. layer (target for each model architecture) was added.
- **DeepLIFT:** Similar to GradCAM, the only changes made for DeepLIFT were to change the colour map function and extract logic into the *Attributer* class.
- **SHAP:** These attributions had to be resized into the shape of the input feature space. Initially the smaller dimensions were dealt with by scaling them up and using an interpolation method from the OpenCV library. However, this led to biased results from the ‘blur’ effect of the interpolation. To replace that workaround, the attribution was multiplied with a Guided Backpropagation output following the Guided GradCAM approach.

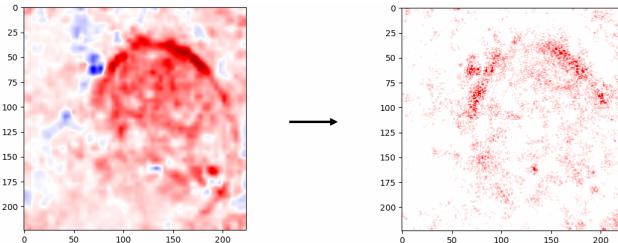


Figure 3.3: Blurred workaround for SHAP versus the improved approach.

- **LIME:** To obtain per-pixel attributions from the super pixel regions, the linear model weights on each super pixel (output by an internal LIME method) were applied to a mask over the region bounded by each super pixel. This is a change in the interpretation of the authors’ method, though it was necessary to obtain attribution weights.

Importantly, support for thresholding the attributions in terms of standard deviations was added at this point. An optional parameter was also implemented to have attributions returned with the absolute value taken, to take positive and negative evidence together as simply evidence.

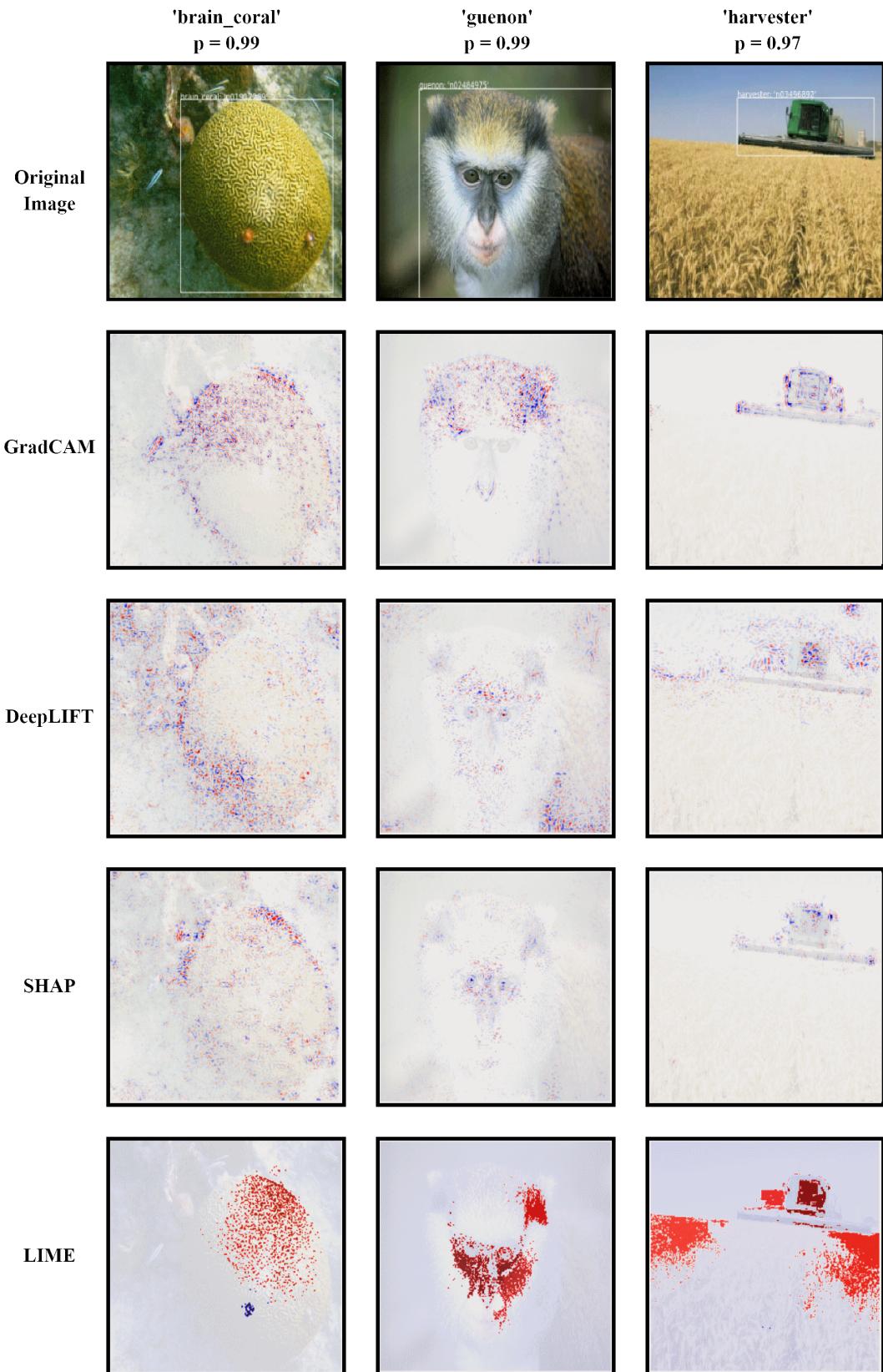


Figure 3.4: Adapted attributions for methods applied to high-confidence VGG16 predictions (original image faintly imposed). Each is a 2D, input-space-sized Numpy array that is normalised between -1 and 1 for the pixel attribution weights / entries in the array. Positive evidence/weights are in red and negative evidence is in blue, and darker colours indicate larger weights / ‘stronger’ evidence.

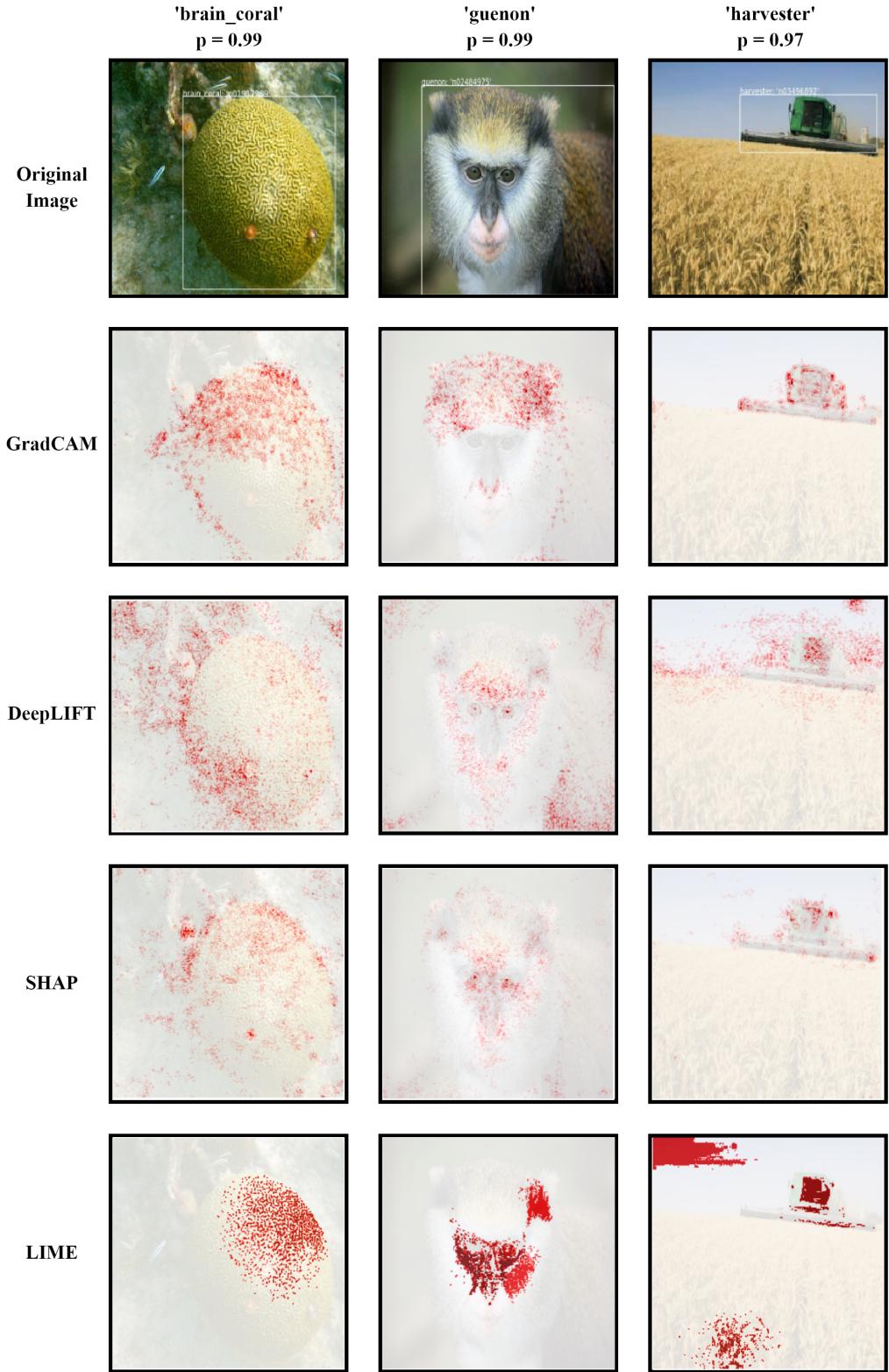


Figure 3.5: Adapted attributions with absolute value taken and a threshold of one standard deviation applied.

## 3.8 Evaluation Metric Design

In Section 2.5.2 it was argued that existing saliency metrics in the literature do not account for pixel-level saliency via feature weights, and the approach to generate bounding boxes via single-component segmentation can unfairly punish perforated-looking saliency maps. Figures 3.4 and 3.5 also show that the adapted method outputs are discriminatory and fine-grained, rather than localising and coarse-grained, which adds a further motivation for a more suitable metric than the connected-component approach for WSOL. The two metrics designed were both based on intersection-over-union though calculated over individual pixels rather than bounding boxes:

1. **Pixel-wise IOU:** A mask of the instance’s ground truth bounding box is compared with the 2D array of each method’s saliency map (example in Figure 3.6). Weights are ignored and pixels are counted as intersecting if they have a value in both arrays. The intersection array’s area is divided by the union array’s area to generate the result.
2. **Pixel-wise IOU\*:** A variant to account for intensity of attribution / weights on each pixel. Instead of 1s in the intersection array the attribution weight is directly stored (with absolute value taken). The union array (denominator) is unchanged. This was a purely intuitive measure to crudely reward intensity of attribution and punish methods that provide uncertain or ‘non-committal’ explanations with low attribution weights.

This approach to explanation quality is different from the localisation performance approach of others and results in much lower IOU (though this is not as concerning since there is consistency across the panel). Related work introducing *individual* methods did care about IOU magnitude to be able to use ILSVRC object localisation competitors as benchmarks for evaluating their own method.

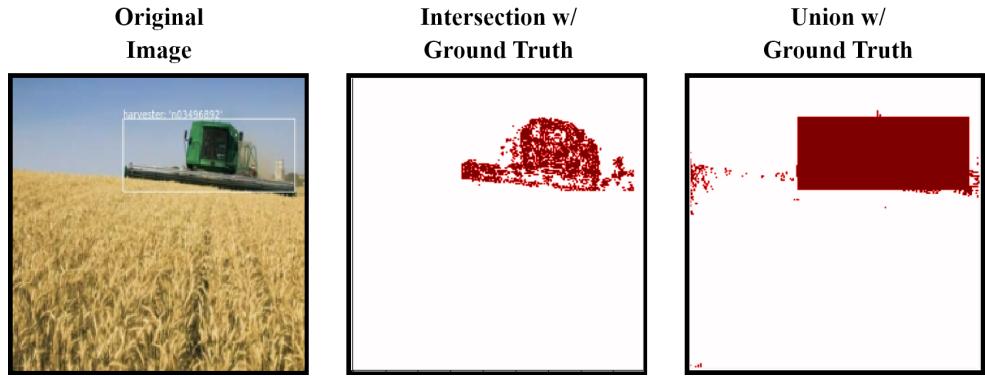


Figure 3.6: Example IOU calculation for a GradCAM attribution ( $=0.33$ ). Threshold of one standard deviation is applied to the attribution before calculation.

The design of a proxy metric was meant to provide only some objective basis for evaluating methods in the image classification context. Other analysis was also performed for testing methods on higher level criteria than only IOU saliency (Results chapter).

## 3.9 Software Abstraction III

To collect IOU and IOU\* evaluations over many instances an *Evaluator* class was developed that implements the following functions:

1. Collect annotation mask for an instance, and a method’s output attribution
2. Calculate IOU and IOU\* for a given annotation mask and attribution
3. Append results to a dataframe and periodically write to a CSV file
4. Perform the above for batches of instances and for the full method panel

The class can potentially implement other saliency metrics, as IOU and IOU\* are modularised functions.

img_no	deeplift	gradcam	lime	shap
1	0.00987	0.02161	0.0661	0.01876
2	0.00394	0.01049	0.01741	0.00697
3	0.00582	0.00571	0.03523	0.00479
4	0.0118	0.01316	0.10822	0.00989
5	0.01853	0.00909	0.05108	0.0041

Figure 3.7: CSV excerpt of a results batch file for IOU metric data.

Finally an *Analyser* class was created to read the collected CSV data, calculate statistics (means and standard deviations), and generate graphs for any subset of methods or metrics. Example graphs are shown in the Results chapter.

The descriptions in Sections 3.4, 3.6 and this section of the developed testing framework are summarised in Figure 3.8. The *Attributer* and *Evaluator* classes are included in **Appendices A and B** respectively.

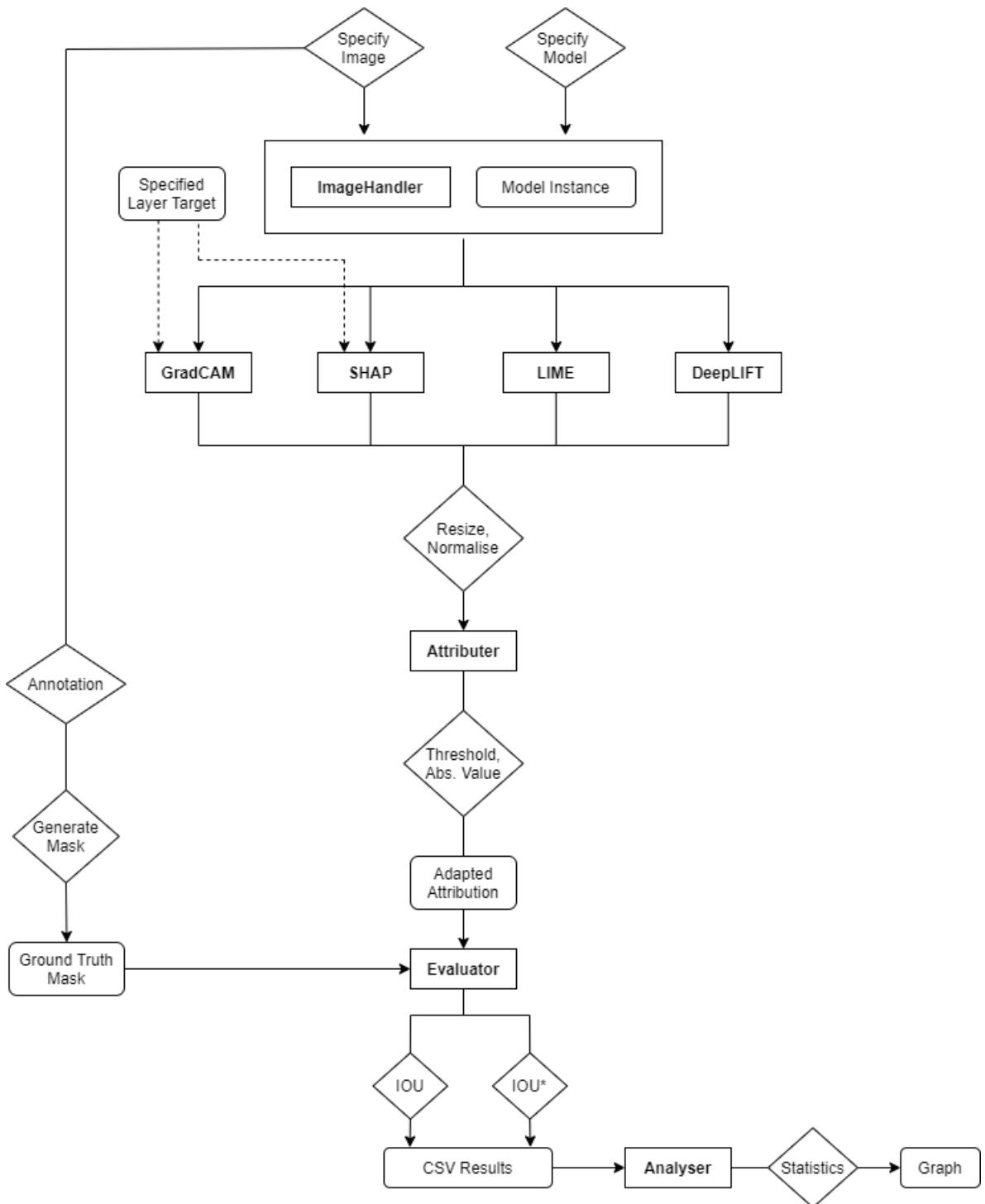


Figure 3.8: High-level flow diagram of testing software.

# Chapter 4

## Results & Insights

This chapter includes the saliency metric and qualitative results from testing the method panel on ImageNet data and pre-trained CNN models. Insights on each method are compared with existing insights in the literature and summarised at the end of the chapter.

### 4.1 Results Overview

#### 4.1.1 Sample Sizes

A set of 300 attributions for the full method panel took around 10 hours to collect and evaluate using a Nvidia GTX-1080 GPU. LIME was thought to be a key bottleneck due to its perturbation-based approach, but analysis in Section 4.3.1 showed GradCAM was also slow in attribution. After several hundred attributions the process also became very slow and would have to be restarted from that point (possibly due to a GPU memory leak in method internals). These performance considerations meant only 1000 instances out of 50,000 available in the validation set were used for evaluation. This was at least the same 1000 instances for all methods, and different dimensions were added to generate insights regardless: different attribution thresholds, and subsetting the results for high confidence ( $p > 0.9$ ) vs low confidence model predictions.

#### 4.1.2 Software Availability

Code for the project is available on GitHub and is intended to be made public after improving the existing model agnosticity for practitioners as well as cleaning up dependencies and file structures. The framework has modular support for attribution methods provided they are compatible with image data and return an input-space representation of their explanation, and modular support for other saliency metrics

as mentioned in Section 3.9.

### 4.1.3 Other Model Testing

Some limitations were encountered on SHAP for ResNet50 and InceptionV3 architectures. Other methods were successfully tested on other models with results below, though the bug in SHAP was not resolved in time for project completion. The impact of this obstacle is discussed.

## 4.2 Saliency Metric Results

### 4.2.1 VGG-16

Figure 4.1 shows IOU and IOU\* statistics for a 1000-instance sample explaining VGG-16 model predictions. The 1000 instances are broken up into high confidence (top row) and low confidence predictions (bottom row), where high confidence refers to a model output of  $p > 0.9$ . Error bars indicate one standard deviation from the mean result displayed by bar height, and can be used a proxy of method consistency. For this setup a threshold of 0.5 standard deviations was applied to the attribution output for IOU and 1 standard deviation for IOU\*.

Some observations on Figure 4.1 (other insights in Section 4.2.4):

- Results are similar for high vs low confidence predictions, with LIME’s variance being one noticeable difference.
- SHAP and DeepLift perform similarly on IOU but not IOU\*
- GradCAM scores lower on these metrics though is visually less noisy than DeepLIFT and SHAP

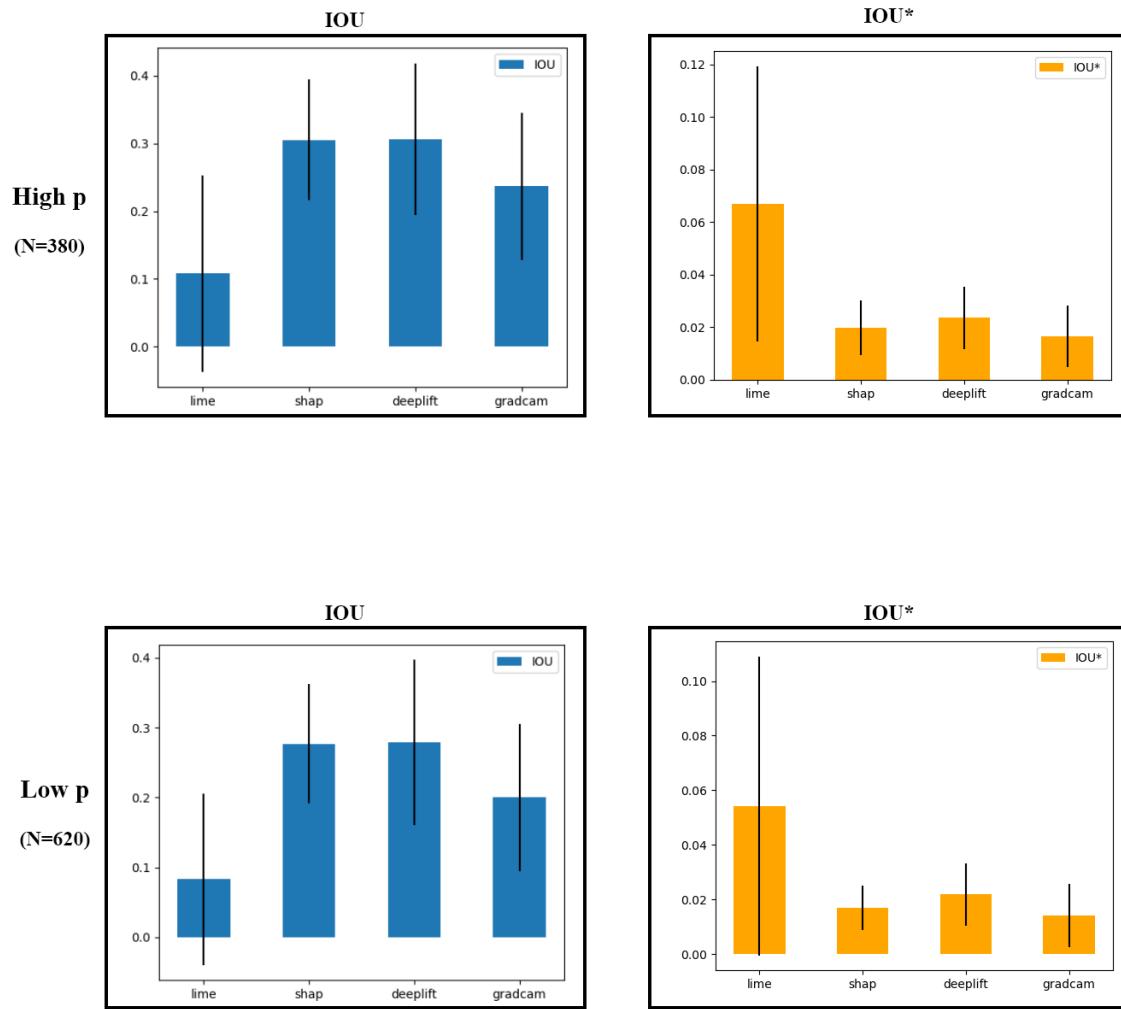


Figure 4.1: IOU, IOU\* statistics for a 1000-instance attribution sample of VGG-16.

In Appendix C, Figure X shows comparatively identical results for a smaller sample ( $N=300$ ) with a different threshold set: 1 for IOU and 2 for IOU\*.

### 4.2.2 InceptionV3

### 4.2.3 ResNet50

#### 4.2.4 Insights from Saliency Metrics

##### VGG16

Some results from the saliency metrics contradict visual observations from each method, however. This is explored in For example, DeepLIFT's attributions were visually much noisier than others. Even with thresholds applied, it performed well on IOU possibly because of this noise across the input space.

LIME outperformed others on IOU\*, but since super pixel regions are broadly brushed with the same attribution score,

What is it about the attribution weights that made IOU\* high for DeepLIFT??  
Why is GradCAM's variance higher??

##### ResNet50 & Inception V3

DeepLIFT performed strongly on VGG16 but poorly on more complex architectures. The reason may be due to the implementation: DeepLIFT requires an architecture modification that has to be done for each layer type. The modification is to implement the custom backward function incorporating reference activations. For this project, the implementation relied upon may not have been able to handle ResNet's residual layers or Inception's use of layer modules. Full neural network 'compatibility' may be a true claim by the authors but these implementation difficulties are a genuine drawback for practitioners and researchers

## 4.3 Other Criteria

### 4.3.1 Performance

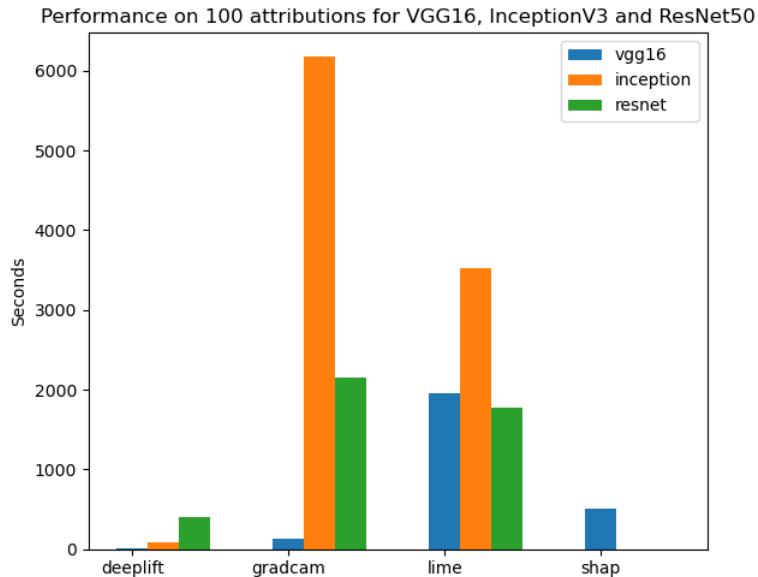


Figure 4.2: Performance/speed in seconds for VGG-16, InceptionV3, and ResNet50.

Some insights from performance measurements in Figure 4.2 are described here. Note SHAP’s incomplete results due to the note in Section 4.1.3.

These results are correlated with the time the underlying model takes to calculate a prediction, which is itself a function of the number of model layers and parameters. This is controlled across the panel at least, so the relative performance of each method can still be highlighted (and to some extent performance correlation with model complexity). For example, DeepLIFT’s claims of fast performance due to requiring only a single backwards pass are supported by these results. It was also extremely fast for InceptionV3 and much slower on ResNet50, which cannot be explained easily, though two possible reasons are the denser convolutional layers in ResNet50 or a method internal bug.

A surprising insight is that GradCAM performed much worse than LIME for a 100-instance sample. A standard assumption in the literature is that perturbation techniques are necessarily much slower than other approaches. Further analysis however with Guided Backpropagation removed from the Guided GradCAM method used here saw its performance on InceptionV3 reduce from over 6000 seconds (Figure 4.2) to roughly 200 for the same sample size. This shows that the discriminative version of GradCAM comes at a significant performance cost for architectures with many layers, and similar or worse results would have been seen for SHAP for this project’s methodology to apply Guided Backpropagation to its outputs as well.

### 4.3.2 Consistency

Some analysis is provided below on consistency across attributions. Table 4.1 lists standard deviations for the method panel from the 1000-instance experiment (error bars in Figure 4.1):

	IOU		IOU*	
	High p	Low p	High p	Low p
<b>LIME</b>	0.145	0.122	0.052	0.055
<b>SHAP</b>	0.089	0.085	0.010	0.008
<b>DeepLIFT</b>	0.112	0.118	0.012	0.011
<b>GradCAM</b>	0.109	0.105	0.012	0.012

Table 4.1: Standard deviations on 1000-instance saliency metrics.

### ANALYSIS

For consistency across models, it was noted in Section 4.2.4 that DeepLIFT performed strongly on VGG16 and very poorly on more complex architectures. This was therefore a strength of SHAP and GradCAM that performed slightly worse on IOU but better on more complicated architectures. LIME’s attributions were also less consistent

### 4.3.3 Visual Observations

Localisation vs Pattern Discrimination

Impact of Thresholding

### 4.3.4 Model Compatibility & Ease of Adaption

Some insights from comparing each method's formulation approach are described in this section: i.e. gradient, perturbation and backpropagation. Reference is made to their hyperparameter complexity and model compatibility which together can be summarised as ease of adaption.

#### SHAP

The difficulty of applying SHAP to other model architectures than simpler convolutional ones like VGG16 indicates that other practitioners may have similar difficulties. Two reasons can be thought of for the problems encountered:

- SHAP is more a higher level ‘specification’ of an explanation method () than a particular formulation, which makes it somewhat difficult to evaluate independent of its model-specific approximations of other modified methods like Integrated Gradients.

In these results, the Integrated Gradients approximation which underpins the SHAP implementation observed almost identical results to DeepLIFT (i.e saliency in 4.2.1 and consistency in ). With SHAP’s lower performance for VGG16 than DeepLIFT, this supports the observation in related work that DeepLIFT is a more practical version of Integrated Gradients (Section 2.5.1).

Though it couldn’t be practically evaluated on other architectures, its visual saliency on VGG16 was appealing and notably different features were highlighted than other methods for the same prediction (e.g. Figure 3.4).

#### GradCAM

A note on GradCAM made in 4.3.1 was that its performance significantly deteriorates for replacing its localisation ‘heatmap’ formulation with the discriminative upgrade proposed by the authors (i.e. multiplied with Guided Backpropagation). This is a compromise that a practitioners can be aware of: for individual explanations, it may be more desirable to see a higher resolution explanation since scale is not a concern. For explaining many model predictions, or where localisation is more important to the use case than individual patterns or edges, the variant without Guided Backpropagation would be preferred.

Other insights about GradCAM’s use cases:

- GradCAM’s explanations were consistently visually salient, and also more consistent in the saliency metrics. This could be because it is inherently designed for CNN architectures: the target of the final convolutional layer where the

features are intuitively represented in the most abstract sense seems to lead to the most visually appealing explanations for model behaviour.

**DeepLIFT**

DeepLIFT’s performance on architectures with fewer convolutional layers was not noticeably worse, which possibly indicates it is suited for ‘network in network’ architectures like InceptionV3. For solely convolutional architectures, it is arguably not the best in the panel (based on visual saliency and the saliency metrics). SHAP

**LIME**

## 4.4 Summary of Insights

### 4.4.1 Quantitative

	Saliency (IOU)	Consistency (Variance)	Performance (Seconds)
LIME	saliency text LIME more text more text	consistency text LIME more text more text	performance text LIME more text more text
SHAP			
DeepLIFT			
GradCAM			

### 4.4.2 Qualitative

Discuss developed software novelty

# Chapter 5

## Discussion

### 5.1 Strengths & Limitations of Metric-based Evaluation

There are a plethora of considerations around the design of proxy metrics for explanation quality. Some of these observations, ranging from obvious to more subtle, have been made in the prior art and were empirically confirmed:

- Human perception of explanation quality is difficult to quantify and is an active area of research (??).
- Errors of the method are not easy to distinguish from errors of the model (**cite**).

Other novel conclusions were made however:

Method evaluation should account for localisation vs discriminative abilities of the method - a single localisation metric and a single pixel-wise metric are not . A more refined saliency metric may be able to account for connected components, edges and pixel-wise attribution intensity.

A set of higher level criteria, including Adebayo's randomisation-based sanity checks, implementation invariance as well as lower level, functionally-grounded saliency metrics, would be the fairest way to compensate for the subjectivity of a single measure of explanation quality.

In a context where the underlying model predictions are constant for a panel of methods, as in this project, this can be somewhat controlled for.

### 5.2 Comparing Approaches

Backpropagation techniques require custom backward functions that override activation functions and gradient operators. This gives them implementation complexities

for models with many *types* of layer: this was previously mentioned as an explanation for DeepLIFT’s poor performance on InceptionV3 and ResNet50 (Section ??).

For GradCAM on the other hand, targeting only the final convolutional layer gives it a strength over others: it does not depend on complexity in earlier layers. Its limitation is that it can only be implemented for convolutional neural networks, therefore solely dominant in image-based tasks or other applications of that architecture. Other less implementation-dependent methods in the gradient class include Gradient \* Input and SmoothGrad.

Perturbation techniques, including LIME but also those proposed by Fong & Vedaldi [30] (‘mask generation’) and Zeiler & Fergus (2014) [13] (‘Occlusion’) have a very clear interpretation in what they iteratively reveal. However, the requirement to test a large number of small, progressively increasing occlusion patches was shown to suffer bad performance even on “simpler” architectures like VGG16. For modern, more complex architectures, perhaps those trained on higher resolution images or taking longer to compute a single prediction, the performance may make the method completely unviable, unless a very small number of explanations are required. The strength of LIME and the perturbation approach generally is its ‘off the shelf’ ease of adoption, which is true for practitioners and researchers working on *any* classification task.

### 5.3 Obstacles & Methodology Limitations

There was some disappointment around the bugs in SHAP’s implementation that meant it couldn’t be applied to more complicated model architectures than VGG16. Other practitioners and researchers have noted similar difficulties in its GitHub issue list [35].

There was also some regret around saliency metrics being limited to the intuition based on pixel-wise attribution. The implicit procedure in the project’s methodology was to “massage” attribution method outputs into a discriminative common form. This may have compromised or misrepresented the methods where a divergence from the authors’ intent occurred (i.e. super-pixels for LIME, heatmaps for GradCAM). It would have been fairer analysis to critique them on their own criteria (i.e. localisation of bounding boxes for GradCAM) *as well as* the saliency metrics and qualitative criteria used in this project. This would also have formed a positive contribution towards reproducibility.

## 5.4 Software Framework

Existing software packages combine only gradient-based methods, or single methods. This extra explanation firepower can be largely redundant when some method outputs are so strikingly similar (e.g. Figure 2.10 in Related Work). A strong contribution of this project was to combine different approaches and offer a more diverse set of explanations for image data, to overall offer a better explanation for any one instance. For example, Figures 3.3 and 3.4 in the Methodology highlight very different input space features for even a single model's prediction.

Modular support for attribution methods and evaluation metrics was achieved through the object-oriented approach to the testing framework (Figure 3.8 in the Methodology).

The original project aims have been successfully met:

1. **Examine and evaluate** a panel of feature attribution methods using proxy metrics of explanation quality supported by analysis on performance, use cases and other qualitative criteria.
2. **Develop** an attribution software package for testing methods at scale with modular support for different metrics, methods and models, to make it easier for researchers to collect explanations and build more adoptable models.

Testing of the modular model support was not fully achieved due to obstacles described in the Discussion. However, this was only for two of four methods, and the difficulty of adapting methods for models (even using high-level public implementations) in a sense highlights a strength of the model-agnostic approach.

This project was not a theoretical contribution to unifying methods available in any one class, but provided novel insights from comparing the diversity in approach to saliency:

- model-specific methods are not necessarily more discriminative, though may be much more performant.
- Methods developed for neural network architectures can perform as well as CNN-specific methods; and with easier therefore easier adaption;

# **Chapter 6**

## **Conclusions**

### **6.1 Contribution**

Project aims

### **6.2 Future work**

increasing the breadth of supported methods, adding higher level support for adding new saliency metrics,

New datasets,



# **Appendix A**

## **Software Documentation**

# **Appendix B**

## **Software Descriptions**

### **B.1 Attributer Class**

Text

### **B.2 Evaluator Class**

## **Appendix C**

### **Software Repository Link**



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