RECTIFIED GRADIENT: LAYER-WISE THRESHOLDING FOR SHARP AND COHERENT ATTRIBUTION MAPS

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ABSTRACT

Saliency map, or the gradient of the score function with respect to the input, is the most basic means of interpreting deep neural network decisions. However, saliency maps are often visually noisy. Although several hypotheses were proposed to account for this phenomenon, there is no work that provides a rigorous analysis of noisy saliency maps. This may be a problem as numerous advanced attribution methods were proposed under the assumption that the existing hypotheses are true. In this paper, we identify the cause of noisy saliency maps. Then, we propose **Rectified Gradient**, a simple method that significantly improves saliency maps by alleviating that cause. Experiments showed effectiveness of our method and its superiority to other attribution methods. Codes and examples for the experiments will be released in public.

1 INTRODUCTION

The gradient of the score function with respect to the input, also called the saliency map (Erhan et al., 2009; Baehrens et al., 2010; Simonyan et al., 2014), is the most basic means of interpreting deep neural networks (DNNs). It is also a baseline method for other advanced attribution-based methods. However, our understanding of saliency maps is still poor.

Previous studies such as Springenberg et al. (2015) and Selvaraju et al. (2017) have noted that saliency maps tend to be visually noisy. To explain this phenomenon, Sundararajan et al. (2016) and Smilkov et al. (2017) suggested saturation and discontinuous gradients as the causes (see Section 2.1 for further explanation). There were several studies attempting to improve saliency maps by tackling these hypothesized causes (Bach et al., 2015; Montavon et al., 2017; Sundararajan et al., 2016; Shrikumar et al., 2017; Smilkov et al., 2017; Sundararajan et al., 2017).

Even though such attribution methods generally produce better visualizations, we find troubling that the hypotheses regarding noisy saliency maps have not been rigorously verified (see Section 2.2 for more detail on attribution methods). In other words, numerous attribution methods were built upon unproven claims that gradient discontinuity or saturation truly causes saliency maps to be noisy. This situation gives rise to two major problems. First, if the hypotheses regarding noisy saliency maps are incorrect, current and future works based on those hypotheses will also be erroneous. Second, as we do not know precisely why saliency maps are noisy, we have to rely on heuristics and guessworks to develop better attribution methods.

In this paper, we address these problems by identifying saliency maps are noisy because DNNs do not filter out irrelevant features during forward propagation. We then introduce **Rectified Gradient**, or RectGrad in short, a simple technique that significantly improves the quality of saliency maps by alleviating the cause through layer-wise thresholding during backpropagation. Finally, we demonstrate that Rectified Gradient produces attributions qualitatively superior and quantitatively comparable to other attribution methods. Specifically, we have the following key contributions:

- We explain why saliency maps are noisy. Noise occurs in saliency maps when irrelevant features have positive pre-activation values and consequently pass through ReLU activation functions. This causes gradients to be nonzero at unimportant regions. We perform experiments with networks trained on CIFAR-10 to justify our claims (Section 3).

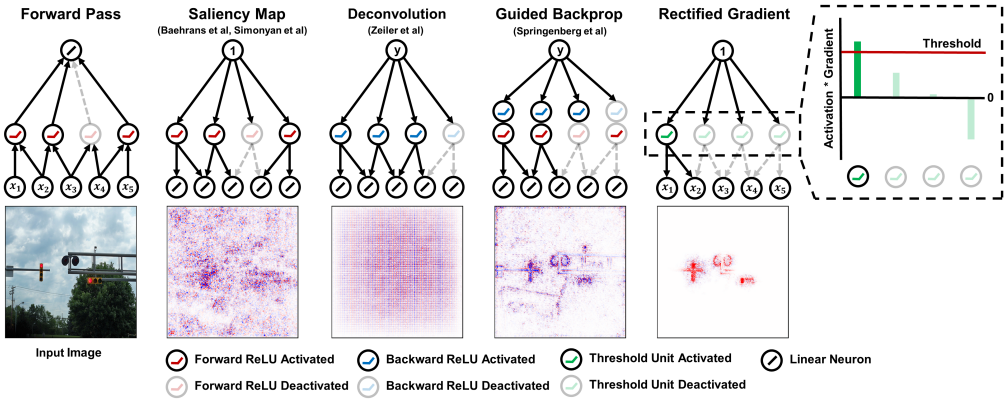


Figure 1: Comparison of attribution methods. See Section 5 for details on the visualization.

- We introduce Rectified Gradient, a method that removes noise from saliency maps by thresholding irrelevant units at ReLU binary gates during backpropagation (Section 4). We then prove that Rectified Gradient generalizes Deconvolution and Guided Backpropagation (Section 4.1). In addition, we discuss two techniques that enhance the visual quality of Rectified Gradient attribution maps (Section 4.2).
- We first investigate the effect of threshold level on attribution maps produced by Rectified Gradient (Section 5.1). Then, we apply Rectified Gradient to networks trained on MNIST, CIFAR-10 and ImageNet to demonstrate that it produces qualitatively superior attribution maps (Section 5.2). We also compare Rectified Gradient with other attribution methods using several quantitative metrics (Section 5.3).

2 Background Overview

Let $S : \mathbb{R}^d \mapsto \mathbb{R}^{|C|}$ be an image classification network, where $x \in \mathbb{R}^d$ is a single image instance and C is the set of image classes. Then, we can define a score function $S_c : \mathbb{R}^d \mapsto \mathbb{R}$ for each class $c \in C$ and the final class of the image x is given by $class(x) = \arg\max_{c \in C} S_c(x)$. A typical score function is constructed by alternately composing affine transformations and nonlinear activation functions. A squashing function such as softmax is applied to the final layer.

Since functions comprising S_c are differentiable or piecewise linear, the score function is also piecewise differentiable. Using this fact, Erhan et al. (2009), Baehrens et al. (2010) and Simonyan et al. (2014) proposed the saliency map, or the gradient of S_c with respect to x, to highlight features within x that the network associates with the given class. In an ideal case, saliency maps highlight objects of interest. However, previous studies such as Springenberg et al. (2015) and Selvaraju et al. (2017) have pointed out that saliency maps tend to be visually noisy, as verified by Figure 1. Three hypotheses were proposed to account for this phenomenon. We describe them in the next section.

2.1 Previous Hypotheses

Saliency Maps are Truthful. Smilkov et al. (2017) suggested that noisy saliency maps are faithful descriptions of what the network is doing. That is, pixels scattered seemingly at random are actually crucial to how the network makes a decision. In short, this hypothesis claims that noise is actually informative.

Discontinuous Gradients. Smilkov et al. (2017) and Shrikumar et al. (2017) proposed that saliency maps are noisy due to the piece-wise linearity of the score function. Specifically, since typical DNNs use ReLU activation functions and max pooling, the derivative of the score function with respect to the input will not be continuously differentiable. Under this hypothesis, noise is caused by meaningless local variations in the gradient.

Saturating Score Function. Shrikumar et al. (2017) and Sundararajan et al. (2017) suggested that important features may have small gradient due to saturation. In other words, the score function can flatten in the proximity of the input and have a small derivative. This hypothesis explains why informative features may not be highlighted in the saliency map even though they contributed significantly to the decision of the DNN.

2.2 Previous Works on Improving Saliency Maps

DNN interpretation methods that assign a signed *attribution* value to each input feature are collectively called *attribution methods*. Attributions are usually visualized as a heatmap by arranging them to have the same shape as the input sample. Such heatmaps are called *attribution maps*. We now describe attribution methods that have been proposed to improve saliency maps.

Attribution Methods Addressing Discontinuity. SmoothGrad (Smilkov et al., 2017) attempts to smooth discontinuous gradient with a Gaussian kernel. Since calculating the local average in a high dimensional space is intractable, the authors proposed a stochastic approximation which takes random samples in a neighborhood of the input x and then averages their gradients.

Attribution Methods Addressing Saturation. Since saliency maps estimate the local importance of each input feature, they are vulnerable to saturation. Therefore, attribution methods such as Gradient * Input (Shrikumar et al., 2017), Layer-wise Relevance Propagation (LRP) (Bach et al., 2015), DeepLIFT (Shrikumar et al., 2017) and Integrated Gradient (Sundararajan et al., 2017) attempt to alleviate saturation by estimating the global importance of each pixel (Ancona et al., 2018). Ancona et al. (2018) has also shown that several global attribution methods are closely related under certain conditions.

Other Attribution Methods. Some attribution methods take a different approach to improving saliency maps. Deconvolution (Zeiler & Fergus, 2014) and Guided Backpropagation (Springenberg et al., 2015) remove negative gradient during backpropagation. Due to this imputation procedure, Deconvolution and Guided Backpropagation yield attribution maps sharper than those of other methods. However, Nie et al. (2018) has recently proven that these methods are actually doing partial image recovery which is unrelated to DNN decisions.

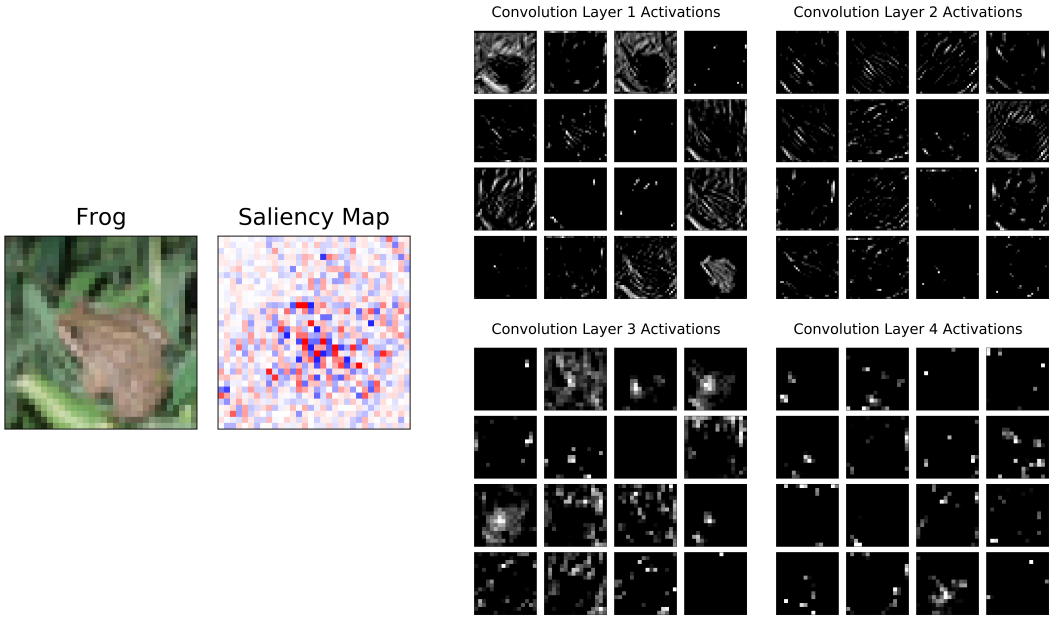
3 Our Explanation for Noisy Saliency Maps

For brevity, we refer to pixels on the background as *background features* and pixels on the object as *object features*. Then, noise in a saliency map corresponds to *background gradient*, or gradient that highlights background features. We assume the DNN uses ReLU activation functions. Under this condition, nonzero background gradient indicates the presence of at least one positive pre-activation in each network layer corresponding to background features.

To verify this, we visualized intermediate layer activations of a convolutional neural network (CNN) trained on CIFAR-10. Figure 2b shows convolutional layer feature maps for an image that produced a noisy saliency map. Since CNN filters act as feature extractors, we expected the CNN to remove most background feature activations through convolutions. However, we found significant amounts of background feature activations in all convolution layers. As the last convolution layer is connected to fully connected layers, the majority of activations in the last convolution layer will have nonzero gradient. Hence, the gradient flowed through background feature activations up to the input. This gradient flow caused background gradient, as shown in Figure 2a. From our perspective, the answer to "why are saliency maps noisy?" is trivial. Saliency maps are noisy because background features pass through ReLU activation functions.

Therefore, rather than asking why saliency maps are noisy, we ask "do activations of background features highlighted by background gradient have nontrivial influence on the decision?" If the answer is *yes*, noise in saliency maps is informative as suggested by Smilkov et al. (2017), and saliency maps do not need any major improvement. However, if the answer is *no*, we should find a way to remove background gradient. We investigated this question through two experiments.

Feature Map Occlusion. We evaluated the significance of background features by occluding activations at intermediate layers. Then, we analyzed the effect of this perturbation on the final decision. Note that this is different from the Sensitivity metric (Bach et al., 2015; Samek et al., 2017). Sensi-



(a) Sample image and its saliency map.

(b) Intermediate layer activations.

Figure 2: Feature map visualization for an image with a noisy saliency map. Lighter pixels indicate higher absolute values.

tivity measures the impact of occlusion in the data space (e.g. pixel occlusion) while we measured the impact of occlusion in each feature space.

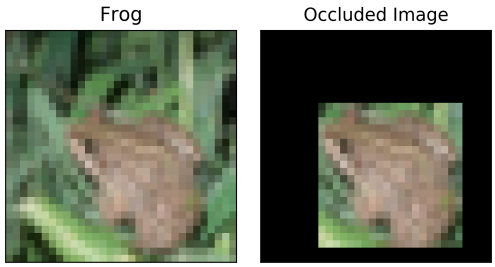
We first created a background mask that covers background features in the images. We then plotted the average class logits as we incrementally occluded intermediate layer activations that fell on the background mask. We carried out occlusion following a random ordering and took the average over 50 trials. Figures 3a and 3b give an example of a background mask and a completely occluded feature map respectively. Figure 3c shows that the final decision did not change throughout the occlusion process for all convolution layers. Moreover, the difference between the top label logit and the next largest logit remained constant. Therefore, background feature activations are irrelevant to the classification task.

Training Dataset Occlusion. Next, we show that gradient can be nonzero for completely uninformative features. We occluded the upper left corner of all images in the training dataset with a 10×10 random patch and trained a randomly initialized CNN on the modified dataset. We used the same patch for all images. Since the test accuracy did not change significantly (79.4% to 79.3%), we expected the CNN to have learned to extract important features and ignore irrelevant ones. However, Figure 4 shows that gradient is nonzero for the patch although it is completely irrelevant to the classification task.

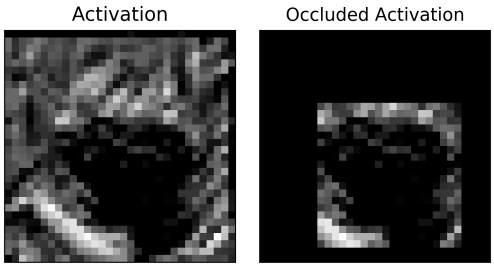
We can draw three conclusions from these experiments:

1. DNNs do not filter out irrelevant features during forward propagation.
2. DNNs are capable of making correct decisions even if we occlude the majority of background feature activations in intermediate layers. This implies that most background feature activations are irrelevant to the classification task.
3. Since DNNs do not remove irrelevant features through ReLU activation functions, zero threshold at ReLU binary gates during backpropagation also allow irrelevant information to flow through the gradient.

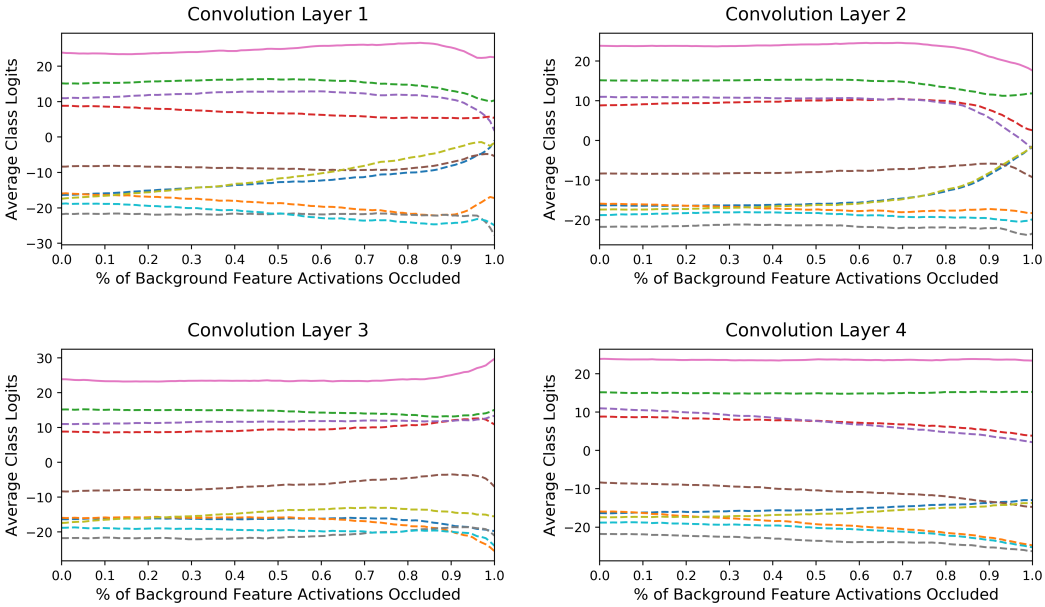
With the conclusions above, we can refute the first of three previous hypotheses. As for the second hypothesis, we can interpret meaningless local variation in the gradient as a side effect of irrelevant features contaminating the gradient. Why the network does not learn to filter out irrelevant features is



(a) Example of a background mask.



(b) Example of an occluded feature map.



(c) Average class logits as background feature activations are incrementally occluded in a random order. The average is taken over 50 trials. Image class is illustrated by a solid line and other classes by dotted lines.

Figure 3: Impact of background feature activation occlusion on the final decision.

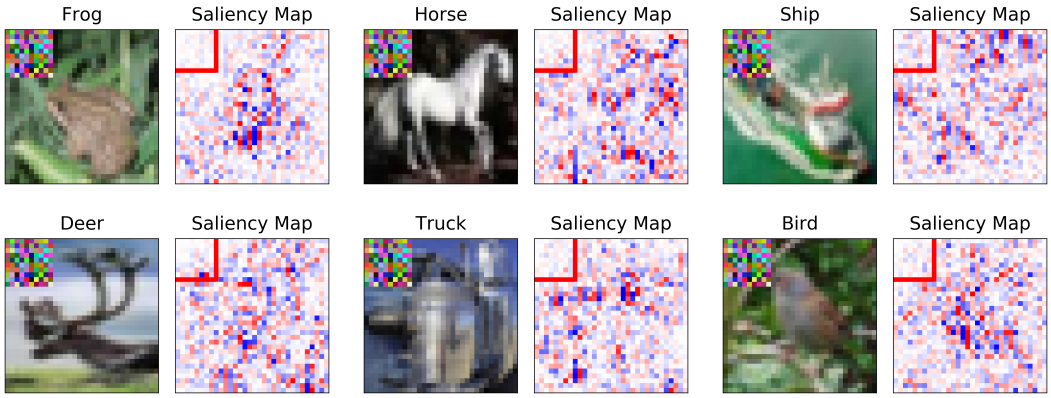


Figure 4: Saliency maps produced from a CNN trained on occluded images. The upper left corner of all the images in the training dataset is replaced with a 10×10 random patch, as shown above. Readers should examine the 8×8 patch enclosed by the red square instead of the entire 10×10 patch due to the receptive field of filters in the first convolution layer (3×3).

a matter of optimization, which is out of scope of this paper. However, we believe it is a phenomenon worth investigating.

4 RECTIFIED GRADIENT

We now introduce our technique to improve saliency maps. As we have shown in Section 3, zero is a poor threshold at ReLU binary gates during backpropagation. This indicates that we need better thresholds at ReLU binary gates in order to remove uninformative gradient from saliency maps. To this end, we propose **Rectified Gradient**, or RectGrad in short, where the gradient propagates only through units whose importance scores exceed some threshold. Importance score for an unit is calculated by multiplying its activation with gradient propagated up to the unit. Formally, Rectified Gradient is given as follows:

Suppose we have a L-layer ReLU DNN. Denote input feature i as x_i, pre-activation of unit i in layer l as $z_i^{(l)}$, its activation as $a_i^{(l)}$ and gradient propagated up to $a_i^{(l)}$ as $R_i^{(l+1)}$. Let $\mathbb{I}(\cdot)$ be the indicator function. Then, the relation between $a_i^{(l)}$ and $z_i^{(l)}$ is given by $a_i^{(l)} = ReLU(z_i^{(l)}) = \max(z_i^{(l)}, 0)$ when $l < L$ and $a_i^{(L)} = softmax(z_i^{(L)})$. By the chain rule, backward pass through the ReLU nonlinearity for vanilla gradient is achieved by $R_i^{(l)} = \mathbb{I}(a_i^{(l)} > 0) \cdot R_i^{(l+1)}$.

We modify this rule such that $R_i^{(l)} = \mathbb{I}(a_i^{(l)} \cdot R_i^{(l+1)} > \tau) \cdot R_i^{(l+1)}$ for some threshold τ. Backward pass through affine transformations and pooling operations is carried out in the same manner as backpropagation. Finally, importance scores for input features are calculated by multiplying gradient propagated up to input layer ($l = 0$) with input features: $x_i \cdot R_i^{(1)}$.

Due to the simplicity of the propagation rule, Rectified Gradient can easily be applied to DNNs in graph computation frameworks such as TensorFlow (Abadi et al., 2016) or PyTorch (Paszke et al., 2017). Listing 1 in Appendix C.1 shows how to implement Rectified Gradient in TensorFlow. Instead of setting τ to a constant value, we use the qth percentile of importance scores at each layer. This prevents the gradient from entirely dying out during the backward pass. Next, we show that Rectified Gradient generalizes Deconvolution and Guided Backpropagation.

4.1 RELATION TO DECONVOLUTION AND GUIDED BACKPROPAGATION

Claim 1. *Deconvolution * Input is equivalent to Rectified Gradient with the propagation rule*

$$R_i^{(l)} = \mathbb{I}\left[\left(a_i^{(l)} + \epsilon\right) \cdot R_i^{(l+1)} > 0\right] \cdot R_i^{(l+1)}$$

for some small $\epsilon > 0$.

Claim 2. *Guided Backpropagation * Input is equivalent to Rectified Gradient when $\tau = 0$:*

$$R_i^{(l)} = \mathbb{I}\left(a_i^{(l)} \cdot R_i^{(l+1)} > 0\right) \cdot R_i^{(l+1)}.$$

The proofs for Claims 1 and 2 are provided in Appendix D.1 and D.2 respectively. These results indicate that Rectified Gradient generalizes Deconvolution and Guided Backpropagation. Figure 1 illustrates the relation between the saliency map, Deconvolution, Guided Backpropagation and Rectified Gradient.

However, Nie et al. (2018) has recently proven that Deconvolution and Guided Backpropagation are actually doing partial image recovery which is unrelated to DNN decisions. Rectified Gradient does *not* suffer from this problem as it does not satisfy the assumptions of the analyses of Nie et al. (2018) for two reasons. First, the threshold criterion is based on the product of activation and gradient which is not Gaussian distributed.[1] Second, we set τ as the qth percentile of importance scores and therefore τ will vary layer by layer. We also show in Section 5.2 with adversarial attacks that attributions produced by Rectified Gradient are class sensitive. Therefore, Rectified Gradient inherits the sharp visualizations of Deconvolution and Guided Backpropagation while amending their disadvantages with layer-wise importance score thresholding.

[1] Product of a half normal random variable and a normal random variable is not Gaussian distributed.

4.2 USEFUL TECHNIQUES

Here, we present two useful techniques that can enhance the visual quality of attribution maps produced by Rectified Gradient.

Padding Trick. Convolution inputs are typically zero padded along the border in order to preserve the spatial dimension of feature maps.[2] This occasionally leads to high activation values along the border if zero is out of input distribution. Since importance scores are calculated by multiplying activation with gradient, outlying border activation can cause Rectified Gradient to be propagated through the border instead of relevant features. To solve this problem, we masked the border of gradient to zero before the backward pass through convolutions with padding. One possible concern with the padding trick is that attributions may be faint for features adjacent to the border of the image. However, we did not find this to be a significantly problem experimentally. Listing 2 in Appendix C.2 shows how to implement the padding trick in TensorFlow.

Proportional Redistribution Rule (PRR) for Pooling Layers. Attribution maps produced by Rectified Gradient tend to be rough due to the discrete nature of thresholding. This discontinuity can be compensated by using the proportional redistribution rule proposed by Montavon et al. (2017) for the backward pass through max-pooling layers. Instead of propagating the gradient through only the most activated unit in the pool, gradient is redistributed proportional to unit activations. Since the redistribution operation is continuous, attribution maps generated with the proportional redistribution rule are smoother. Listing 3 in Appendix C.3 shows how to implement the proportional redistribution rule in TensorFlow.

5 EXPERIMENTS

To evaluate Rectified Gradient, we performed a series of experiments using Inception V4 network (Szegedy et al., 2017) trained on ImageNet (Russakovsky et al., 2015) and CNNs trained on CIFAR-10 (Krizhevsky & Hinton, 2009) and MNIST (LeCun et al., 1998). To visualize the attributions, we summed up the attributions along the color channel and then capped low outlying values to 0.5^{th} percentile and high outlying values to 99.5^{th} percentile for RGB images. We only capped outlying values for grayscale images.

5.1 EFFECT OF THRESHOLD PERCENTILE

Rectified Gradient has one hyper-parameter τ, which is set to q^{th} percentile of importance scores for each layer. Figure 5 shows the effect of threshold percentile for several images from ImageNet. While the attribution maps were incomprehensible for $q = 0$, the visual quality dramatically improved as we incremented q up to 20. There was no significant change up to $q = 80$. Then the attribution maps began to sparse out again as we incremented q further. We also observed that regions of high attributions did not change from $q > 20$.

We speculate that the attributions stay constant between $q = 20$ and 80 because of zero activations. That is, since we use ReLU activation functions, the majority of activations and consequently importance scores will be zero. Hence, $\tau \approx 0$ for $20 \leq q \leq 80$. This causes Rectified Gradient attribution maps to resemble those produced by Guided Backpropagation * Input. It indicates that we have to increment $q > 80$ in order to produce sparser attribution maps that highlight important regions instead of reconstruct input images.

5.2 QUALITATIVE COMPARISON WITH BASELINE METHODS

We used the saliency map, Gradient * Input, Guided Backpropagation, SmoothGrad, Integrated Gradient, Epsilon-LRP and DeepLIFT as baseline methods. As for Rectified Gradient, we used the padding trick and $q = 98$ for all attribution maps. We show attributions both with and without application of the proportional redistribution rule. In this subsection, we compare Rectified Gradient with other attribution methods through three experiments that each focus on different aspect of qualitative evaluation.

[2] This corresponds to convolution with SAME padding in TensorFlow terminology.

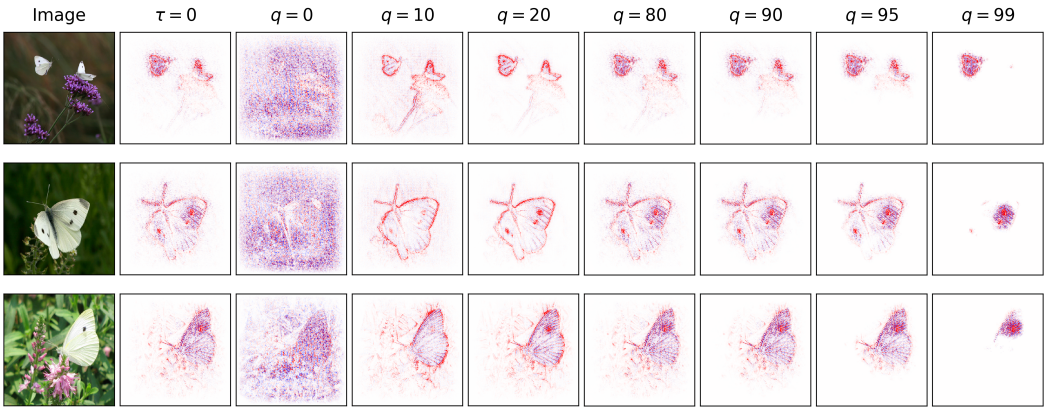


Figure 5: Effect of threshold τ (columns) on Rectified Gradient for 3 images of the cabbage butterfly class in ImageNet (rows). The second column shows attribution maps with $\tau = 0$, which is equivalent to Guided Backpropagation * Input. For the following columns, τ is set to q^{th} percentile of importance scores. The padding trick was used for all attribution maps above.

Training Dataset Occlusion. Just like the training dataset occlusion experiment in Section 3, we occluded the upper left corner of all images in CIFAR-10 training dataset with a 10×10 random patch and trained a randomly initialized CNN on the modified dataset. A reasonable attribution method should not assign any positive or negative values to the patch as it is completely irrelevant to the classification task. Figure 6 compares attribution maps produced by our method and baseline methods for a CNN trained on occluded images. We observed that Rectified Gradient assigned little or no attribution to the random patch. However, all other methods failed to do so. This indicates that baseline methods may not be working in a reasonable manner.

Coherence. Following prior work (Simonyan et al., 2014; Zeiler & Fergus, 2014), we inspected two types of visual coherence. First, the attributions should fall on discriminative features (e.g. the object of interest), not the background. Second, the attributions should highlight similar features for images of the same class.

For the first type of visual coherence, Figure 7 shows a side-by-side comparison between our method and baseline methods. It can clearly be seen that Rectified Gradient produced attribution maps more visually coherent and focused than other methods—background noise was nearly nonexistent.

For the second type of visual coherence, Figure 9 in Appendix A.1 shows attribution maps for two pairs of images with each pair belonging to the same class. Attribution maps generated by Rectified Gradient consistently emphasized similar parts of the object of interest. On the contrary, Saliency map, Gradient * Input and Epsilon-LRP emphasized different regions for each image instance. Attributions for SmoothGrad, Guided Backpropagation, Integrated Gradient and DeepLIFT were generally coherent across images of the same class. Nevertheless, they also highlighted background features and hence failed to satisfy the first type of visual coherence.

Adversarial Attack. We evaluated class sensitivity following prior work by Nie et al. (2018). Specifically, we compared the attributions for an image and its adversarial example. If the attribution method is class sensitive, attribution maps should change significantly since ReLU activations and consequently the predicted class have changed. On the other hand, if the attribution method merely does image reconstruction, attribution maps will not change much since we add an indistinguishable adversarial perturbation to the image. In this experiment, we used the fast gradient sign method (Goodfellow et al., 2015) with $\epsilon = 0.01$ to generate adversarial examples.

Figure 8 shows large changes in attribution maps produced by Rectified Gradient. We observed that only Rectified Gradient attributions were coherent with the class labels. Figure 10 in Appendix A.1 shows some instances where there was no significant change in attribution maps produced by Rectified Gradient. In those cases, attribution maps for other methods also showed little change. Hence, we can conclude that Rectified Gradient is equally or more class sensitive than baseline attribution methods. It is also possible that adversarial attacks only modified a tiny amount of ReLU

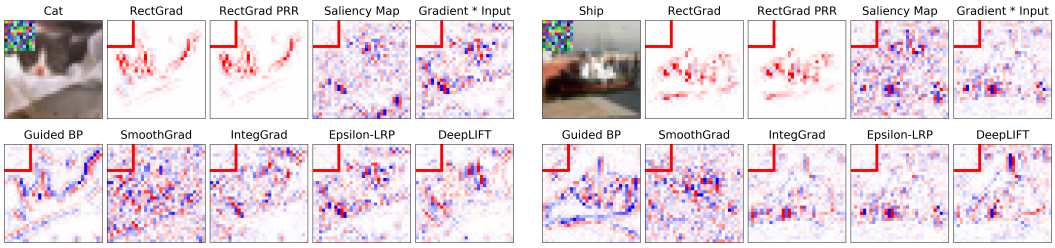


Figure 6: Comparison of attribution maps produced from a CNN trained on occluded images. The upper left corner of all the images in the training dataset was replaced with a 10×10 random patch, as shown above. Readers should compare the 8×8 patch enclosed by the red square instead of the entire 10×10 patch due to the receptive field of filters in the first convolution layer (3×3).

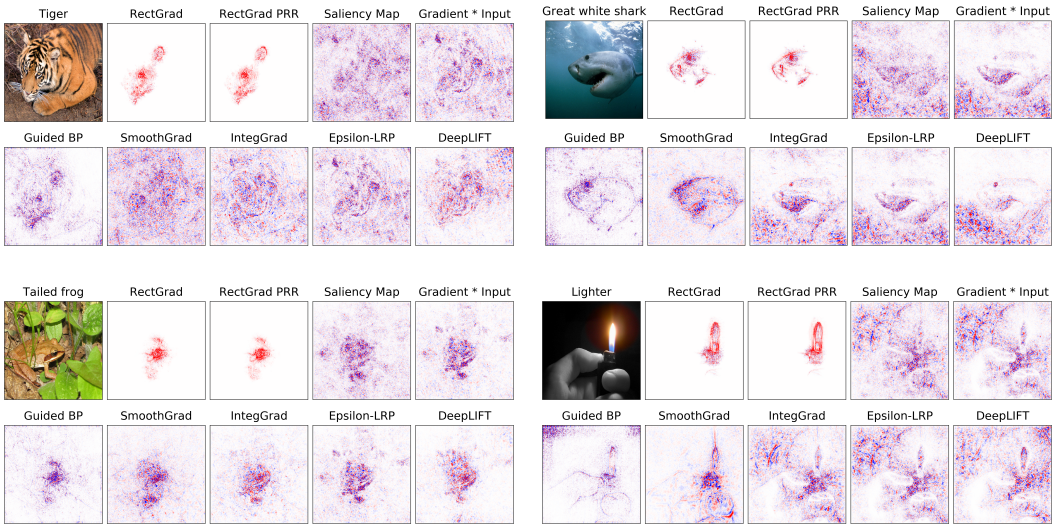


Figure 7: Evaluation of coherence across different classes.

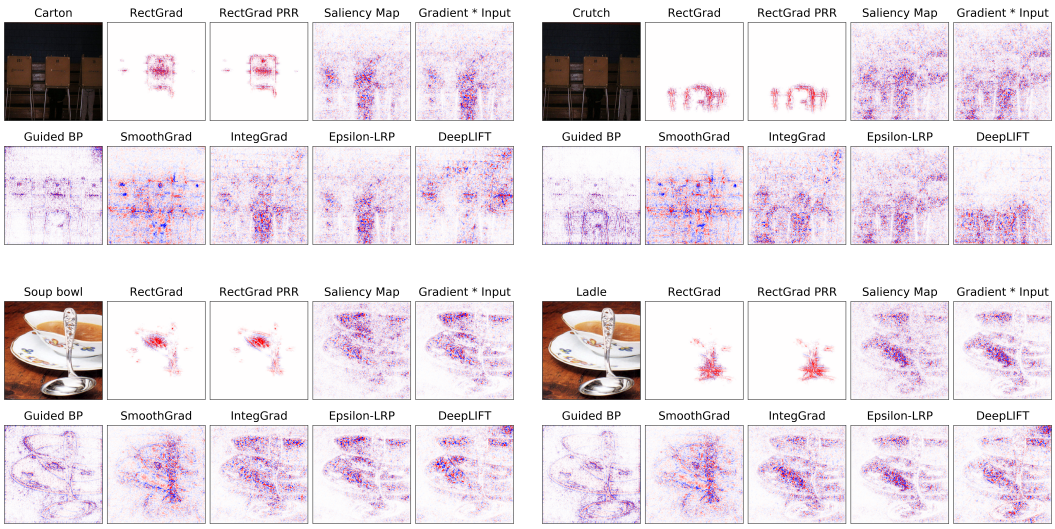


Figure 8: Comparison of attribution maps for images (left column) and their adversarial examples (right column). This figure shows examples where attribution maps produced by Rectified Gradient changed significantly.

activations (i.e. the images were near the decision boundary), causing little change in attribution maps. We also observed similar phenomena with the MNIST dataset. See Figures 11 and 12 in Appendix A.1 for same experiments on MNIST.

5.3 Quantitative Comparison with Baseline Methods

In this section, we quantitatively compare Rectified Gradient with baseline methods using DNNs trained on CIFAR-10. We did not include Epsilon-LRP since it is equivalent to Gradient * Input for ReLU DNNs (Ancona et al., 2018). We divided baseline attribution methods into local and global methods following the criterion proposed by Ancona et al. (2018). All figures for quantitative experiment outcomes are in Appendix A.2.

Sensitivity. We evaluated Rectified Gradient using the Sensitivity metric proposed by Bach et al. (2015) and Samek et al. (2017). Specifically, we measured how the logit for the initial class changed as features were occluded based on the ordering assigned by the attribution method. We split the image into non-overlapping patches of 2×2 pixels. Next, we computed attributions and summed all the values within each patch. We sorted the patches in decreasing order based on the aggregate attribution values. We then incrementally replaced the first 100 patches with per-channel mean computed using the entire training set and measured the change in class logit. We calculated the average across 500 randomly chosen test set images. An attribution method is better if it has a lower sensitivity AUC.

The results are shown in Figure 13. All attribution methods outperformed the random baseline in which we randomly removed patches. We observed that Rectified Gradient performed better than local attribution methods. In comparison with global attribution methods, Rectified Gradient showed similar performance up to approximately 10 patches (red vertical line) but the performance dropped as more patches were removed. In Appendix B.1, we offer an explanation for this behavior.

ROAR and KAR. We evaluated Rectified Gradient using Remove and Retrain (ROAR) and Keep and Retrain (KAR) proposed by Hooker et al. (2018). Specifically, we measured how the performance of the classifier changed as features were occluded based on the ordering assigned by the attribution method. For ROAR, given an attribution method, we replaced a fraction of all CIFAR-10 pixels that were estimated to be *most* important with a constant value. We then retrained a CNN on the modified dataset and measured the change in test accuracy. For KAR, we replaced a fraction of all CIFAR-10 pixels that were estimated to be *least* important. We trained 3 CNNs per estimator for each fraction $\{0.1, 0.3, 0.5, 0.7, 0.9\}$. We measured test accuracy as the average of theses 3 CNNs. An attribution method is better if it has a lower ROAR AUC and a higher KAR AUC.

Figure 14 presents ROAR scores. All attribution methods outperformed the random baseline in which we randomly removed pixels. Rectified Gradient showed similar performance to local attribution methods but performed worse than all global attribution methods. Next, Figure 15 shows KAR scores. Interestingly, all baseline attribution methods failed to exceed even the random baseline. Only Rectified Gradient had similar or better performance than the random baseline. In Appendix B.2, we offer an explanation for why Rectified Gradient performed poorly in ROAR.

6 Conclusions

Saliency map is the most basic means of interpreting deep neural network decisions. However, it is often visually noisy. Although several hypotheses were proposed to account for this phenomenon, there is no work that provides a thorough analysis of noisy saliency maps. Therefore, we first identified saliency maps are noisy because DNNs do not filter out irrelevant features during forward propagation. We then proposed Rectified Gradient which significantly improves saliency maps by alleviating this problem through layer-wise thresholding during backpropagation. We showed that Rectified Gradient generalizes Deconvolution and Guided Backpropagation and moreover, overcomes the class-insensitivity problem. We also demonstrated through extensive experiments that Rectified Gradient outperforms previous attribution methods.

REFERENCES

Martín Abadi, Paul Barham, Jianmin Chen, Zhifeng Chen, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Geoffrey Irving, Michael Isard, Manjunath Kudlur, Josh Levenberg, Rajat Monga, Sherry Moore, Derek G. Murray, Benoit Steiner, Paul Tucker, Vijay Vasudevan, Pete Warden, Martin Wicke, Yuan Yu, and Xiaoqiang Zheng. Tensorflow: A system for large-scale machine learning. In *Proceedings of the 12th USENIX Conference on Operating Systems Design and Implementation*, OSDI'16, pp. 265–283, Berkeley, CA, USA, 2016. USENIX Association. ISBN 978-1-931971-33-1. URL `http://dl.acm.org/citation.cfm?id=3026877.3026899`.

Marco Ancona, Enea Ceolini, Cengiz Öztireli, and Markus Gross. Towards better understanding of gradient-based attribution methods for deep neural networks. In *International Conference on Learning Representations*, 2018.

Sebastian Bach, Alexander Binder, Grégoire Montavon, Frederick Klauschen, Klaus Robert Müller, and Wojciech Samek. On pixel-wise explanations for non-linear classifier decisions by layer-wise relevance propagation. *PLoS ONE*, 10(7):1–46, 2015. ISSN 19326203. doi: 10.1371/journal.pone.0130140.

David Baehrens, Timon Schroeter, Stefan Harmeling, Motoaki Kawanabe, Katja Hansen, and Klaus-Robert Müller. How to explain individual classification decisions. *Journal of Machine Learning Research*, 11(Jun):1803–1831, 2010.

Dumitru Erhan, Yoshua Bengio, Aaron Courville, and Pascal Vincent. Visualizing higher-layer features of a deep network. *University of Montreal 1341.3*, 2009.

Ian J. Goodfellow, Jonathon Shlens, and Christian Szegedy. Striving for simplicity: The all convolutional net. In *International Conference on Learning Representations*, 2015.

Sara Hooker, Dumitru Erhan, Pieter-Jan Kindermans, and Been Kim. Evaluating feature importance estimates. In *ICML Workshop on Human Interpretability in Machine Learning*, 2018.

Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *International Conference on Learning Representations*, 2015.

ALex Krizhevsky and Geoffrey Hinton. Learning multiple layers of features from tiny images. 2009.

Yann LeCun, Corinna Cortes, and Christopher JC Burges. The mnist database of handwritten digits. 1998.

Grégoire Montavon, Sebastian Lapuschkin, Alexander Binder, Wojciech Samek, and Klaus-Robert Müller. Explaining nonlinear classification decisions with deep taylor decomposition. *Pattern Recognition*, 65:211–222, 2017.

Weili Nie, Yang Zhang, and Ankit Patel. A theoretical explanation for perplexing behaviors of backpropagation-based visualizations. In *International Conference on Machine Learning*, 2018.

Adam Paszke, Sam Gross, Soumith Chintala, Gregory Chanan, Edward Yang, Zachary DeVito, Zeming Lin, Alban Desmaison, Luca Antiga, and Adam Lerer. Automatic differentiation in pytorch. In *NIPS Workshop on Autodiff*, 2017.

Olga Russakovsky, Jia Deng, Hao Su, Jonathan Krause, Sanjeev Satheesh, Sean Ma, Zhiheng Huang, Andrej Karpathy, Aditya Khosla, Michael Bernstein, et al. Imagenet large scale visual recognition challenge. *International Journal of Computer Vision*, 115(3):211–252, 2015.

Wojciech Samek, Alexander Binder, Grégoire Montavon, Sebastian Lapuschkin, and Klaus-Robert Müller. Evaluating the visualization of what a deep neural network has learned. *IEEE transactions on neural networks and learning systems*, 28(11):2660–2673, 2017.

Ramprasaath R. Selvaraju, Michael Cogswell, Abhishek Das, Ramakrishna Vedantam, Devi Parikh, and Dhruv Batra. Grad-cam: Visual explanations from deep networks via gradient-based localization. In *The IEEE International Conference on Computer Vision*, Oct 2017.

Avanti Shrikumar, Peyton Greenside, and Anshul Kundaje. Learning important features through propagating activation differences. In *International Conference on Machine Learning*, 2017.

Karen Simonyan, Andrea Vedaldi, and Andrew Zisserman. Deep inside convolutional networks: Visualising image classification models and saliency maps. In *International Conference on Learning Representations Workshop*, 2014.

Daniel Smilkov, Nikhil Thorat, Been Kim, Fernanda Viégas, and Martin Wattenberg. Smoothgrad: removing noise by adding noise. In *ICML Workshop on Visualization for Deep Learning*, 2017.

Jost Tobias Springenberg, Alexey Dosovitskiy, Thomas Brox, and Martin Riedmiller. Striving for simplicity: The all convolutional net. *International Conference on Learning Representations Workshop*, 2015.

Mukund Sundararajan, Ankur Taly, and Qiqi Yan. Gradients of counterfactuals. *arXiv preprint arXiv:1611.02639*, 2016.

Mukund Sundararajan, Ankur Taly, and Qiqi Yan. Axiomatic attribution for deep networks. In *International Conference on Machine Learning*, 2017.

Christian Szegedy, Sergey Ioffe, Vincent Vanhoucke, and Alexander A Alemi. Inception-v4, inception-resnet and the impact of residual connections on learning. In *AAAI Conference on Artificial Intelligence*, 2017.

Matthew D Zeiler and Rob Fergus. Visualizing and understanding convolutional networks. In *European Conference on Computer Vision*, pp. 818–833. Springer, 2014.

A EXPERIMENT RESULTS

A.1 QUALITATIVE EXPERIMENTS

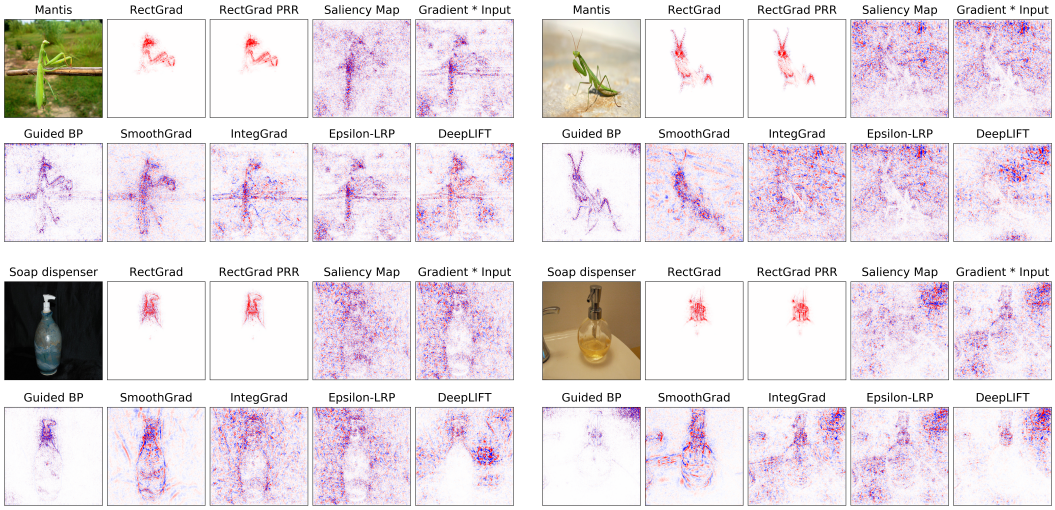


Figure 9: Evaluation of coherence within the same class (rows).

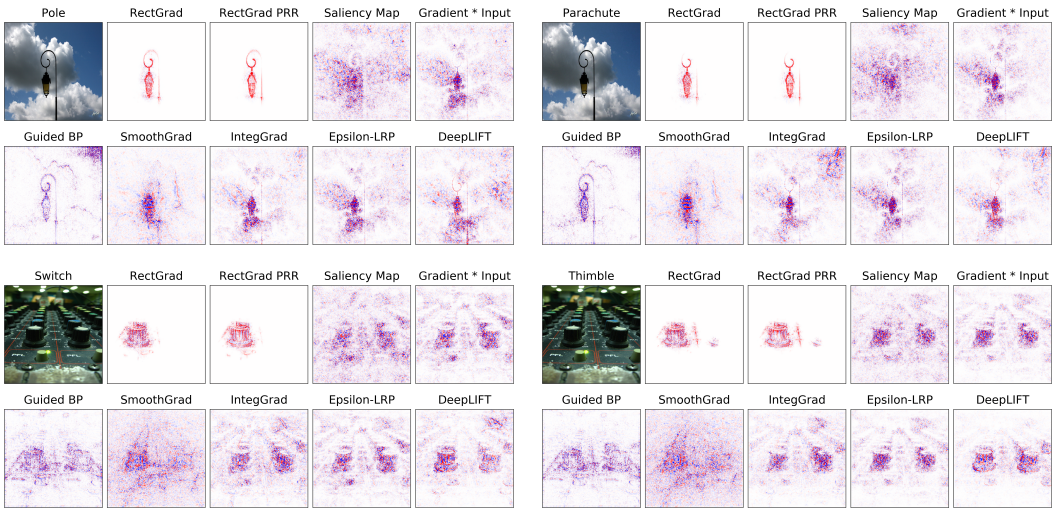


Figure 10: Comparison of attribution maps for images (left column) and their adversarial examples (right column). This figure shows examples where attribution maps produced by Rectified Gradient did not change significantly.

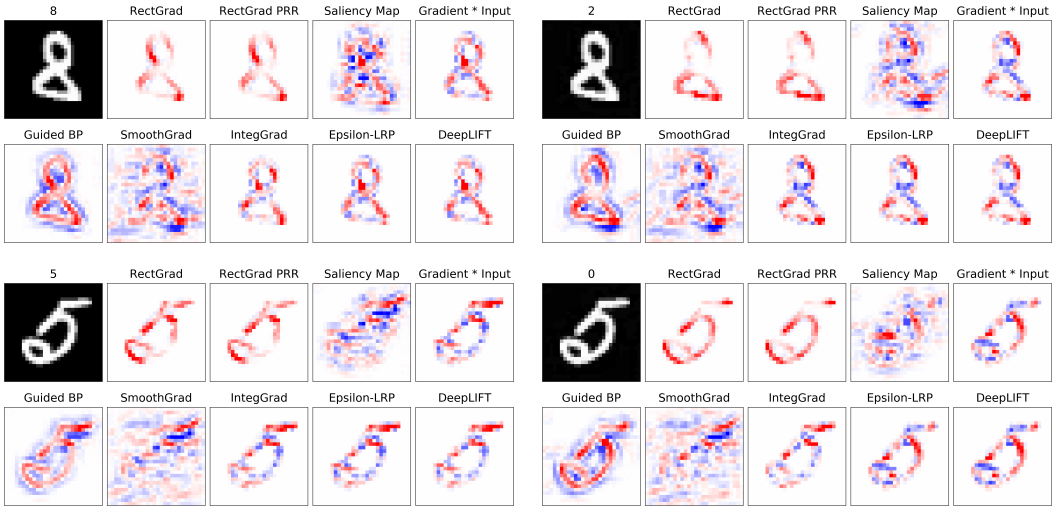


Figure 11: Comparison of attribution maps for images (left column) and their adversarial examples (right column). This figure shows examples where attribution maps produced by Rectified Gradient changed significantly.

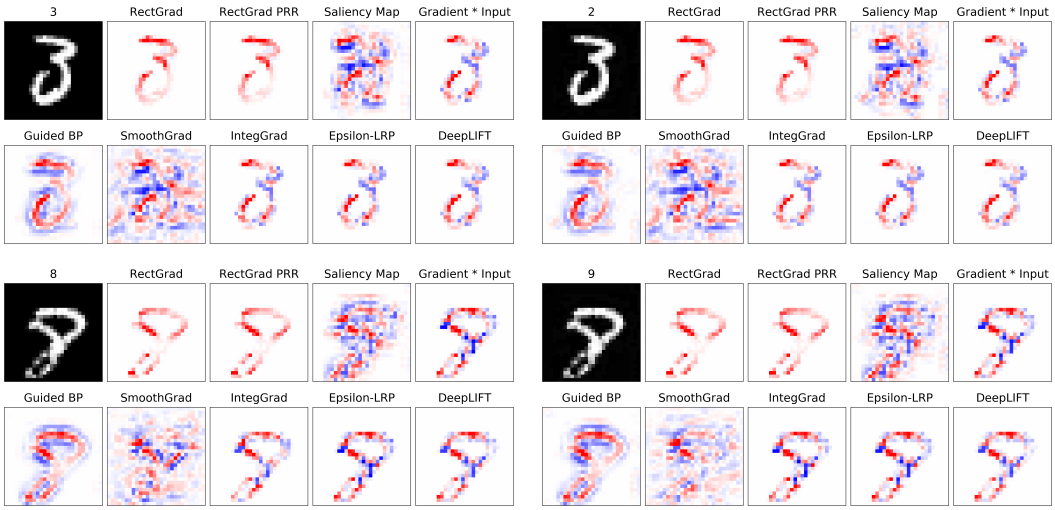


Figure 12: Comparison of attribution maps for images (left column) and their adversarial examples (right column). This figure shows examples where attribution maps produced by Rectified Gradient did not change significantly.

A.2 QUANTITATIVE EXPERIMENTS

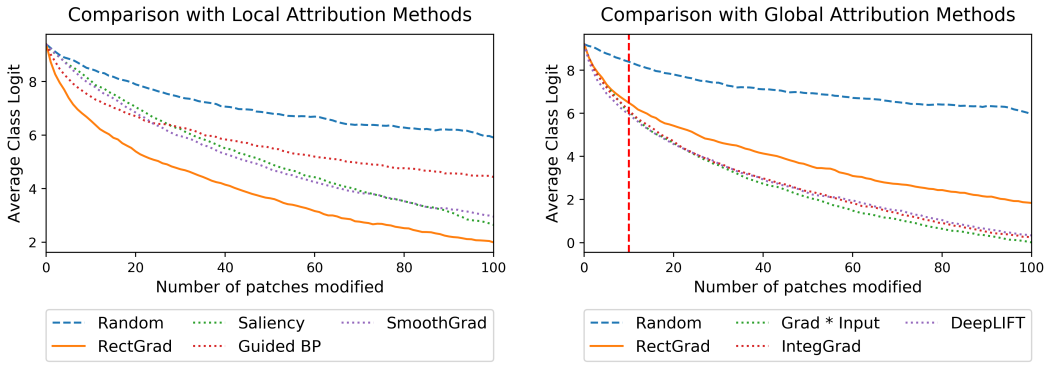


Figure 13: Comparison of Sensitivity. The left plot compares Rectified Gradient with local attribution methods and the right plot with with global attribution methods. We also include the random baseline (patches are randomly removed) for reference. Lower AUC indicates a better attribution method. The red vertical line in the right plot indicates where Rectified Gradient starts to perform worse than baseline global attribution methods (10 patches). We took the average over 500 randomly chosen test set images.

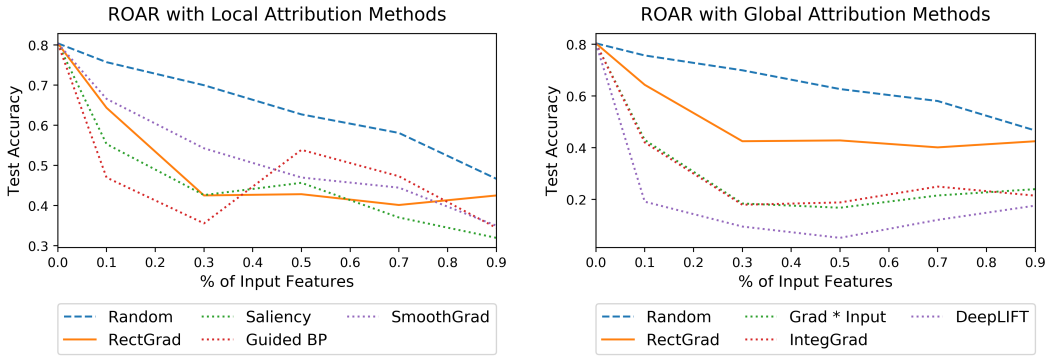


Figure 14: Comparison of ROAR. The left plot compares Rectified Gradient with local attribution methods and the right plot with with global attribution methods. We also include the random baseline (pixels are randomly removed) for reference. Lower AUC indicates a better attribution method.

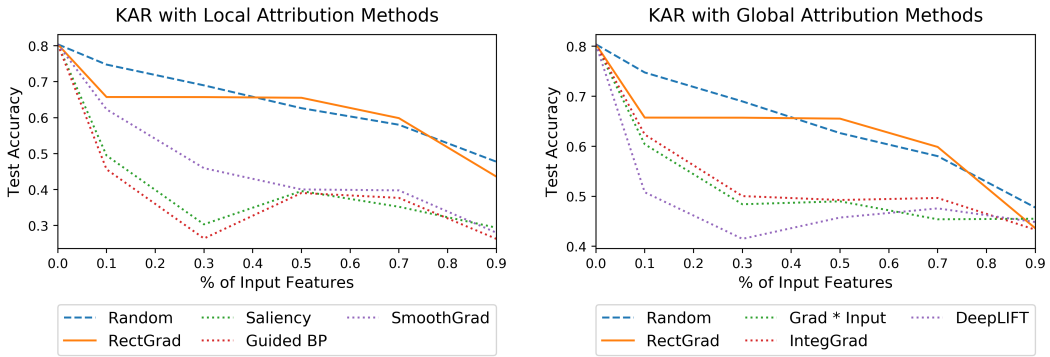


Figure 15: Comparison of KAR. The left plot compares Rectified Gradient with local attribution methods and the right plot with with global attribution methods. We also include the random baseline (pixels are randomly removed) for reference. Higher AUC indicates a better attribution method.

B ADDITIONAL EXPLANATION FOR QUANTITATIVE EXPERIMENTS

B.1 SENSITIVITY

In comparison with global attribution methods, Rectified Gradient showed similar performance up to approximately 10 patches (red vertical line) but the performance dropped as more patches were removed (Figure 13). We speculate this happens due to the sparseness of Rectified Gradient attribution maps. Since Rectified Gradient attribution maps are sparser than those of other methods, occluding approximately 10 features will be enough to remove core features highlighted by Rectified Gradient. Attributions for other features will not be as informative since they have trivial values. Figure 16 shows that it is indeed the case. For Rectified Gradient, after occluding 10 top 2×2 patches, only attributions of small values remained. For Gradient * Input, on the other hand, still had significant amount of nontrivial leftover attributions.

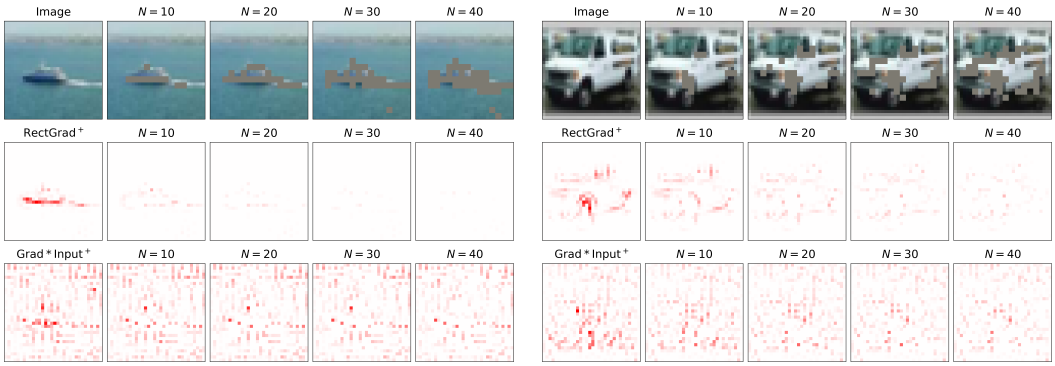


Figure 16: Comparison of attribution methods in sensitivity. The first row shows the image as top N 2×2 patches are occluded according to Rectified Gradient. The second and third rows show the positive parts (indicated by $+$) of Rectified Gradient and Gradient * Input attribution maps as top N 2×2 patches are occluded respectively. We did not cap outlying values in this visualization.

B.2 ROAR

We believe that the poor performance of Rectified Gradient in ROAR is also due its sparseness. Since Rectified Gradient produces visually coherent attribution maps, the occluded regions can act as discriminative features. To verify this, we replaced 10% of all CIFAR-10 pixels that were estimated to be most important with the channel-wise mean. We then trained a CNN on the occluded dataset and visualized Rectified Gradient attribution maps for images whose original and occluded versions were both classified correctly. Figure 17 shows the results. Attribution maps highlighted pixels around the occluded regions and moreover, similar regions were emphasized in the original image. This corroborates our claim that the occluded regions act as discriminative features.

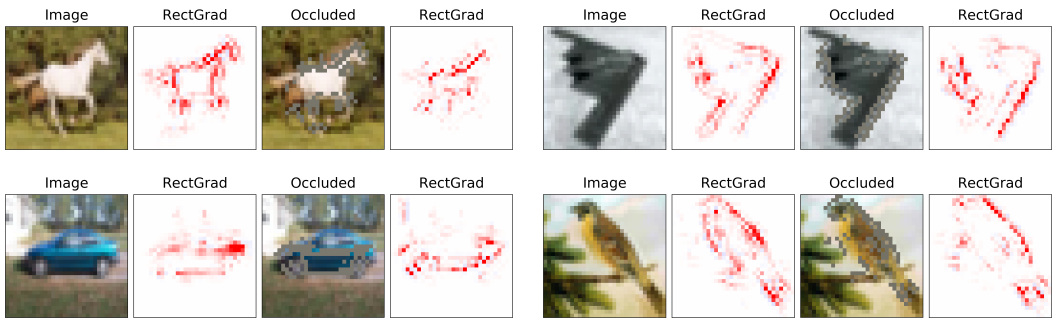


Figure 17: Rectified Gradient attribution maps produced from a CNN trained on images occluded according to Rectified Gradient. We show images whose original and occluded versions were both classified correctly.

C TENSORFLOW CODES

C.1 IMPLEMENTATION OF RECTIFIED GRADIENT

```
import tensorflow as tf

from tensorflow.contrib.distributions import percentile

@tf.RegisterGradient("RectifiedRelu")
def _RectifiedReluGrad(op, grad):

    def threshold(x, q):

        if len(x.shape.as_list()) > 3:
            thresh = percentile(x, q, axis=[1,2,3], keep_dims=True)
        else:
            thresh = percentile(x, q, axis=1, keep_dims=True)

        return thresh

    activation_grad = op.outputs[0] * grad
    thresh = threshold(activation_grad, q)

    return tf.where(thresh < activation_grad, grad, tf.zeros_like(grad))
```

Listing 1: Implementation of Rectified Gradient in TensorFlow. After registering this function as the gradient for ReLU activation functions, call `tf.gradients()` and multiply with inputs to generate attributions.

C.2 IMPLEMENTATION OF THE PADDING TRICK

```
import tensorflow as tf

@tf.RegisterGradient("RectifiedConv2D")
def _RectifiedConv2DGrad(op, grad):

    if op.get_attr('padding') == b'SAME':

        shape = tf.shape(grad)
        mask = tf.ones([shape[0], shape[1] - 2, shape[2] - 2, shape[3]])
        mask = tf.pad(mask, [[0,0],[1,1],[1,1],[0,0]])
        grad = grad * mask

    input_grad = tf.nn.conv2d_backprop_input(tf.shape(op.inputs[0]), op.
    inputs[1], grad, op.get_attr('strides'), op.get_attr('padding'))
    filter_grad = tf.nn.conv2d_backprop_filter(op.inputs[0], tf.shape(op.
    inputs[1]), grad, op.get_attr('strides'), op.get_attr('padding'))

    return input_grad, filter_grad
```

Listing 2: Implementation of the padding trick in TensorFlow. After registering this function as the gradient for convolution operations, call `tf.gradients()` and multiply with inputs to generate attributions.

C.3 Implementation of the Proportional Redistribution Rule

```
import tensorflow as tf

@tf.RegisterGradient("RectifiedMaxPool")
def _RectifiedMaxPoolGrad(op, grad):

    z = tf.nn.avg_pool(op.inputs[0], op.get_attr('ksize'), op.get_attr('strides'), op.get_attr('padding')) + 1e-10
    s = grad / z
    c = gen_nn_ops._avg_pool_grad(tf.shape(op.inputs[0]), s, op.get_attr('ksize'), op.get_attr('strides'), op.get_attr('padding'))

    return op.inputs[0] * c
```

Listing 3: Implementation of the proportional redistribution rule in TensorFlow. After registering this function as the gradient for max-pooling operations, call `tf.gradients()` and multiply with inputs to generate attributions.

D Proof of Claims

D.1 Proof of Claim 1

Proof. Note that the backward propagation rule for Deconvolution through the ReLU nonlinearity is given by

$$R_i^{(l)} = \mathbb{I}\left(R_i^{(l+1)} > 0\right) \cdot R_i^{(l+1)}. \tag{1}$$

Since the DNN uses ReLU activation functions, $a_i^{(l)} + \epsilon > 0$ and therefore

$$\mathbb{I}\left[\left(a_i^{(l)} + \epsilon\right) \cdot R_i^{(l+1)} > 0\right] = \mathbb{I}\left(R_i^{(l+1)} > 0\right) \tag{2}$$

for all l and i. The result follows from Equation 2. □

D.2 Proof of Claim 2

Proof. Note that the backward propagation rule for Guided Backpropagation through the ReLU nonlinearity is given by

$$R_i^{(l)} = \mathbb{I}\left(z_i^{(l)} > 0\right) \cdot \mathbb{I}\left(R_i^{(l+1)} > 0\right) \cdot R_i^{(l+1)}. \tag{3}$$

Since the DNN uses ReLU activation functions, $a_i^{(l)} \geq 0$ and therefore

$$\mathbb{I}\left(a_i^{(l)} \cdot R_i^{(l+1)} > 0\right) = \mathbb{I}\left(z_i^{(l)} > 0\right) \cdot \mathbb{I}\left(R_i^{(l+1)} > 0\right) \tag{4}$$

for all l and i. The result follows from Equation 4. □

E EXPERIMENTS SETUP

E.1 MNIST

We did not use any pre-processing for the MNIST dataset (LeCun et al., 1998). We trained a CNN using ReLU activation functions. The lists of layers for the architecture is listed below. The network was trained using Adam (Kingma & Ba, 2015) for 10 epochs to achieve 99.1% test accuracy. For the adversarial attack, we used the fast gradient sign method (Goodfellow et al., 2015) with $\epsilon = 0.01$.

MNIST CNN
Conv 2D (3×3, 32 kernels)
Conv 2D (3×3, 64 kernels)
Max-pooling (2×2)
Dense (128)
Dense (10)

E.2 CIFAR-10

The CIFAR-10 dataset (Krizhevsky & Hinton, 2009) was pre-processed to normalize the input images into range $[-1; 1]$. We trained a CNN using ReLU activation functions with Adam for 20 epochs to achieve 79.4% test accuracy. For the dataset occluded with the random patch, we used the same settings to achieve 79.3% test accuracy.

CIFAR-10 CNN
Conv 2D (3×3, 32 kernels)
Conv 2D (3×3, 32 kernels)
Max-pooling (2×2)
Dropout (0.25)
Conv 2D (3×3, 64 kernels)
Conv 2D (3×3, 64 kernels)
Max-pooling (2×2)
Dropout (0.25)
Dense (256)
Dropout (0.5)
Dense (10)

E.3 INCEPTION V4

We used a pre-trained Inception V4 network. The details of this architecture can be found in Szegedy et al. (2017). For the adversarial attack, we used the fast gradient sign method with $\epsilon = 0.01$.