Formatting Instructions for TMLR Journal Submissions

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Abstract

The original paper provides a method for contrastively explaining why a certain class in a neural network image classifier is picked above others. This method consists of using back-propagation-based explanation methods from after the softmax layer rather than before. Our work consists of reproducing the work in the original paper. We also provide extensions to the paper by evaluating the method on XGradCAM and Vision Transformers to evaluate its generalization capabilities. The reproductions show similar results as the original paper, with the only contrast being the visualization of heatmaps which could not be reproduced to look similar. We also show that the original paper suffers from issues such as a lack of detail in the method and an erroneous equation which makes reproducibility difficult. To remedy this we provide an open-source repository containing all code used for this project.

1 Introduction

The original paper *"Why Not Other Classes?": Towards Class-Contrastive Back-Propagation Explanations*, see Wang & Wang (2022), describes how backpropagation-based explanations used in image classification can utilize backpropagation from the softmax-layer to generate contrastive explanations. These explanations signal key parts of the input used in favoring classifying as one class over others, rather than signaling key parts for classification in general.

In the original paper, four different explanation methods are compared, original, mean-, max- and weighted contrast, where weighted contrast is considered the paper's novel contribution. Weighted contrast is formulated as

$$\phi_i^t(\boldsymbol{x})_{\text{weighted}} = \phi_i^t(\boldsymbol{x}) - \sum_{s \neq t} \alpha_s \phi_i^s(\boldsymbol{x}) \tag{1}$$

where ϕ_i is the original explanation for pixel i and the weight α is the softmax activation of the logit vector without the target class t

$$\alpha_s = \frac{\exp y_s}{\sum_{k \neq t} \exp y_k} \tag{2}$$

The paper further shows that the weighted contrast method is equal to taking the explanation directly toward the probability after the softmax layer.

The authors argue that this is a superior contrastive explanation method by performing two forms of adversarial attacks with regard to the different explanations. They show that an adversarial attack on the pixels highlighted by weighted contrast results in a more significant effect on the accuracy of the model, while original methods more accurately impact the logit strength. By performing a blurring and removal attack with explanations extracted from GradCAM and Linear Approximation they show that their method finds more impactful negative and positive regions of interest with regards to the model accuracy.

This document aims to reproduce the main results of the paper as well as provide insights into the general reproducibility and impact of the paper. We also expand upon the paper and attempt applications outside its scope, with

other backpropagation-based explanation methods as well as applying it to Vision Transformers (ViT) as introduced in Dosovitskiy et al. (2020). This was done to see the generalization capabilities of the paper.

2 Scope of reproducibility

To evaluate the reproducibility of the paper we replicated the steps described in section *5 Experiments* of the original paper for a subset of the models and datasets used in the original paper and thus made our own experiments using our own code. The results of these experiments were then compared with those of the paper, in order to find if they are consistent. We furthermore test the generalizability of the paper by applying the contrastive explanation method shown in the original paper using XGradCAM (Fu et al., 2020) and Vision Transformers (Dosovitskiy et al., 2020).

2.1 XGradCAM

As an attempt to test the paper's contrastive method's generalization capability an additional back-propagation method in the form of a modified version of XGradCAM (Fu et al., 2020) was used. This modified version removes ReLU, as in the original paper, and as a consequence uses the absolute values in the feature map sum when normalizing rather than only the sum. This gives the following explanation $\boldsymbol{\phi}^t(\boldsymbol{x})_y$ when backpropagating from the logit y_t with the target feature map layer $\boldsymbol{a}$ with $k \in K$ feature maps:

$$\boldsymbol{\phi}^t(\boldsymbol{x})_y = \sum_k \left(\sum_{i,j} \frac{a_{ij}^k}{\|\boldsymbol{a}^k\|_1} \frac{\partial y_t}{\partial a_{ij}^k} \right) \boldsymbol{a}^k \tag{3}$$

A weighted contrastive version, $\boldsymbol{\phi}^t(\boldsymbol{x})_{\text{weighted}}$ as described in the original paper, of XGradCAM can be obtained by propagating from the softmax neuron p_t and can be proven as follows using notation $[c]$ for all classes:

$$\boldsymbol{\phi}^t(\boldsymbol{x})_p = \sum_k \left(\sum_{i,j} \frac{a_{ij}^k}{\|\boldsymbol{a}^k\|_1} \sum_{s \in [c]} \left(\frac{\partial p_t}{\partial y_s} \frac{\partial y_s}{\partial a_{ij}^k} \right) \right) \boldsymbol{a}^k = \sum_{s \in [c]} \frac{\partial p_t}{\partial y_s} \boldsymbol{\phi}^s(\boldsymbol{x})_y \propto \boldsymbol{\phi}^t(\boldsymbol{x})_{\text{weighted}} \tag{4}$$

2.2 Vision Transformers

In order to test how differences in architecture affect the results we modified two sets of explanation methods and tested them together with the `vit_b_16` model as first described in Dosovitskiy et al. (2020) and implemented in `PyTorch`[1]. This model works by dividing the image into 16x16 squares, assigning each square of the image a token. The information in these layers is then propagated throughout the network using a self-attention mechanism. Unlike standard CNN architectures, spatial coherence is not guaranteed through the network, and information is easily mixed - with some layers containing little to no spatial coherence. The explanation methods we have implemented contrastive methods for are GradCAM and Gradient-weighted attention rollout.

3 Experiments

In this section, we detail the various reproduction experiments and additions to the original paper. They were performed mainly using the `PyTorch` library and the code is available publicly at https://github.com/ArvidEriksson/contrastive-explanations/ under the MIT License. All experiments were performed on a `n2-standard-4` Google Cloud VM with an NVIDIA T4 GPU.

3.1 Reproducing 5.1 Back-Propagation till the Input Space

This section reproduces all experiments from section 5.1 in the original paper. The experiment tests 9 networks with perturb input images where the perturbation uses 4 different methods to select pixels to change. All models use `PyTorch` pre-trained models, with the most up-to-date weights, and are tested on the validation set of ILSVRC2012

[1] See, using the default weights, https://pytorch.org/vision/main/models/generated/torchvision.models.vit_b_16.html.

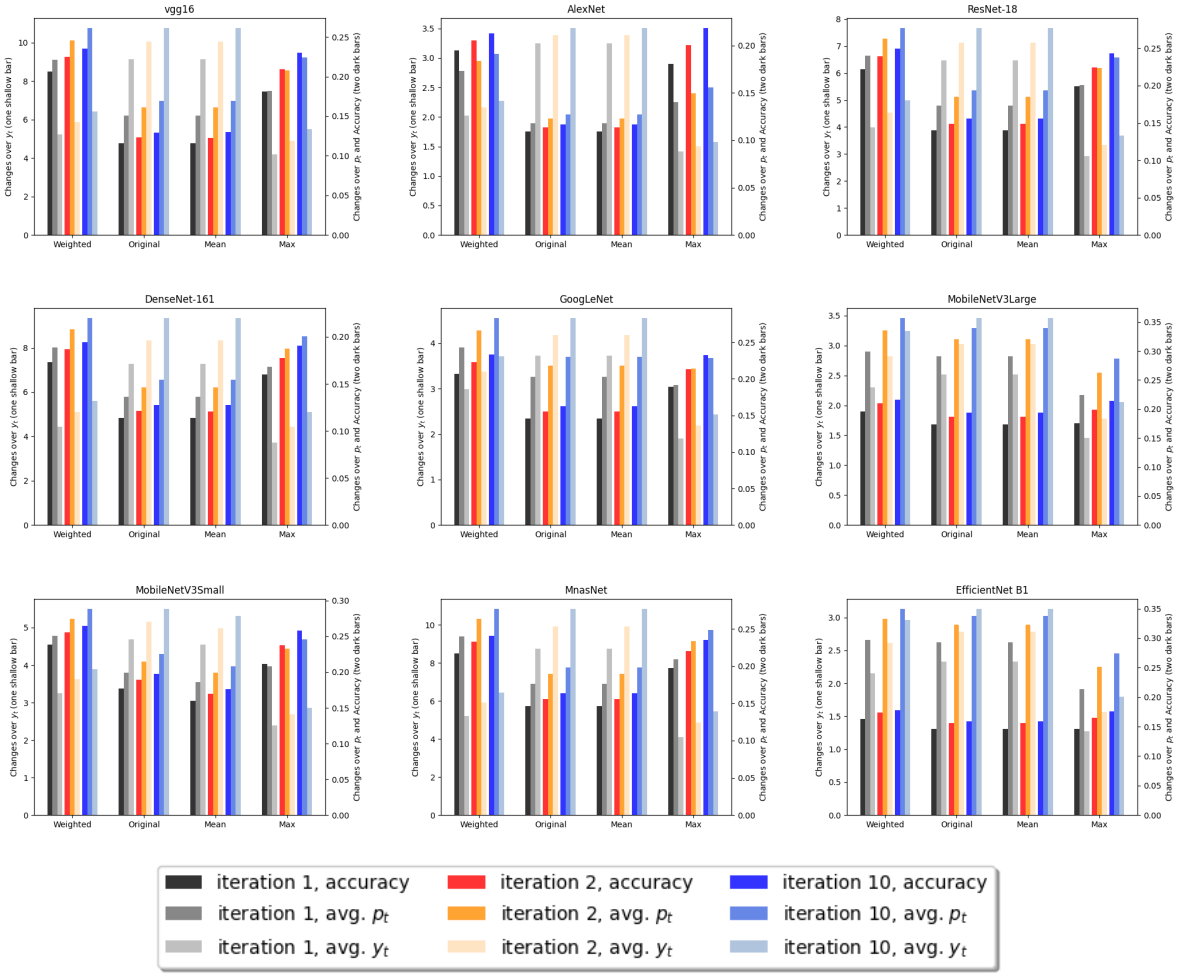


Figure 1: Reproducing of Figure 3 in the original paper with $\epsilon = 10^{-3}$. Changes in accuracy, y_t and p_t (t is the target classification class) when certain input features are perturbed. Perturbed features are selected based on four gradient explanations (original, mean, max and weighted), where original is directly with respect to the gradients of the logits.

Deng et al. (2009). The experiments is repeated with a perturbation limit, ϵ, of 1×10^{-3} and 3×10^{-3}, see Figures 1 and 2. This is because the original paper states that they use $\epsilon = 10^{-3}$, while after being in contact with the original authors we found that $\epsilon = 3 \times 10^{-3}$ had been used.

Furthermore, the equations for the gradient sign perturbation in the original paper turned out to have errors both in the clamping and indexing of the iterations. The correct equations are

$$\boldsymbol{x}^{n+1} \leftarrow \boldsymbol{x}^n + \alpha \operatorname{sign}(\phi^t(\boldsymbol{x}^n)) \tag{5}$$

$$\boldsymbol{x}^{n+1} \leftarrow \operatorname{clamp}(\boldsymbol{x}^{n+1}, \max(\boldsymbol{x} - \epsilon, 0), \min(\boldsymbol{x} + \epsilon, 1)) \tag{6}$$

where n is the number of iterations, ϵ is the perturbation limit, and $\alpha = \frac{\epsilon}{n}$ is the step size.

Our results verify the results of the original paper, mainly that the weighted and max explanation methods yield an increase to p_t and accuracy, while the original and mean explanation methods yield an increase to y_t.

Although the results are similar to those of the original paper there are some numerical differences in Figure 2 which is probably due to different weights in the models and hence also different original performance.

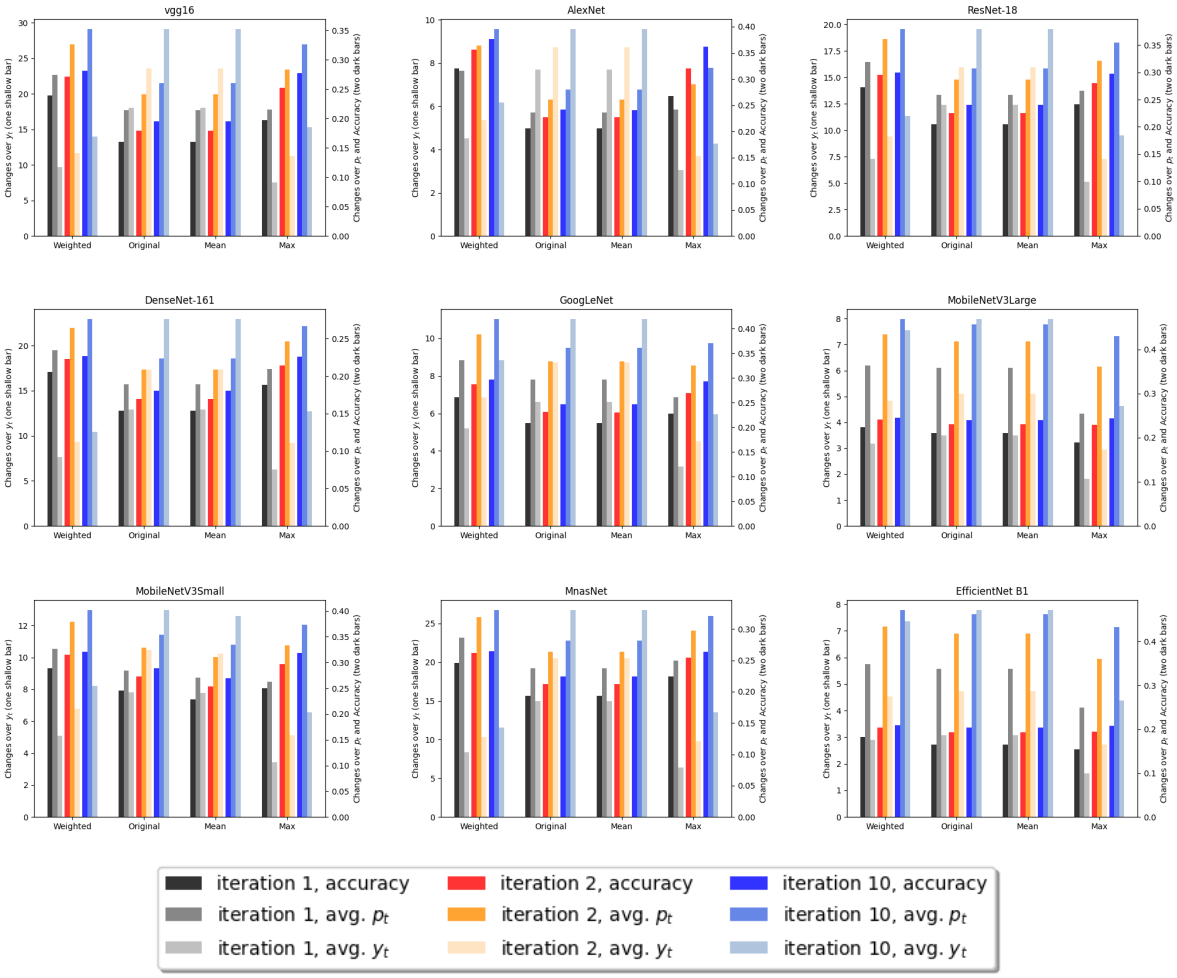


Figure 2: Reproducing of Figure 3 in the original paper with $\epsilon = 3 \times 10^{-3}$. Changes in accuracy, y_t and p_t (t is the target classification class) when certain input features are perturbed. Perturbed features are selected based on four gradient explanations (original, mean, max and weighted), where original is directly with respect to the gradients of the logits.

3.2 Reproducing 5.2 Back-Propagation till the Activation Space

This section reproduces section 5.2 in the original paper by performing the same experiments of both visualization and effects of blurring and masking. These experiments were all performed on VGG-16 with batch normalization (Simonyan & Zisserman, 2014) fine-tuned on the CUB-200 dataset (Wah et al., 2011). The fine-tuning was done with an SGD optimizer with momentum using a batch size of 128, learning rate of 10^{-3}, momentum of 0.9, and weight decay of 5×10^{-4}. The model was trained for 200 epochs on the training set as defined by the dataset. For an exact implementation or to reproduce the model, see our repository.

3.2.1 Visualizations

Reproduction of the visualizations of three different back-propagation-based methods can be seen in Figure 3. Here we compare GradCAM and Linear Approximation, as described in the original paper, and XGradCAM, as described in section 2.1, to their contrastive weighted counterpart, which was obtained by back-propagating from the softmax neuron p_t of the target class t rather than its logit y_t. The visualization was done by overlapping the bilinearly interpolated relevance map on top of the original image with an alpha of 0.5. A centered norm was applied on the heatmap before visualizing using the `bwr` colormap in `Matplotlib`. The images were picked such that $p_2 > 0.1$ and were selected at random to prevent bias from only selecting good samples. Observe that the samples picked are different from those in the original paper as those samples did not have a probability for the second most probable class over the threshold.

The results are partly in line with what the original paper suggests. Firstly, one can note that the original explanation method is quite consistent among the two classes with differences being mostly the intensity of the positive and negative areas. Secondly, one can also see that the weighted methods produce almost complementary heatmaps for the two classes, which makes sense as they are mostly dominant over all other classes. Lastly, we see a large difference in the size of the negative and positive areas visualized compared to the original paper. This is presumably due to different methods of visualization, but as the procedure of visualization of the original paper was not detailed this cannot be confirmed. Observe that the large negative areas in some images, especially seen when comparing our GradCAM to other implementations, are due to the omission of ReLU as described in the original paper. Our results therefore also conflict with the claim in the original paper in appendix G, where the authors claim that non-contrastive methods have much larger positive than negative areas. In Figure 3 one can see that the original GradCAM has much larger negative areas than positive for all selected images.

3.2.2 Blurring and masking

Reproduction of the blurring and masking experiment seen in Table 1 of the original paper can be seen in Table 1. Here we also added an additional row with results using XGradCAM. This gave similar results to GradCAM and Linear Approximation although performed slightly better on the negative features and for positive features for the second most probable class t_2. Here we use the same baselines as the original paper with the motivation of them having slightly different results without a generally accepted standard (Sturmfels et al., 2020). The values in the table are the average relative probability of the most and second most probable classes for each image. This relative probability is defined as $\bar{p}_{t_i} = \mathbb{E}\left[e^{y_{t_i}} / (e^{y_{t_1}} + e^{y_{t_2}}\right], i = 1,2$ where $t_i \in [c]$ represents the i-th most possible class. These expectations are, like in the article, only calculated over samples that fulfill the threshold criteria $p_2 > 0.1$.

The results are very similar to those of the original paper, although not identical, and show the same patterns. We decided to use equal blurring and masking here to prevent bias where one method might yield larger or smaller negative areas to guarantee that the original and weighted methods both modify an equal number of pixels. This was also suggested in the original paper in appendix G and seems to have a minor impact on the results while negating some bias. We want to emphasize, however, that these results are expected since the weighted method back-propagates from the softmax neuron p_t, and therefore blurring using that method will impact the resulting activation of the very same neuron more than back-propagating from the preceding logit y_t.

3.3 Reproducing 5.3 Comparison with Mean/Max Contrast

We perform the same experiments as in section 5.3 of the original article. Here we reuse the same VGG-16 model used in section 3.2 and implement mean and max contrast as described in the original paper. The used method

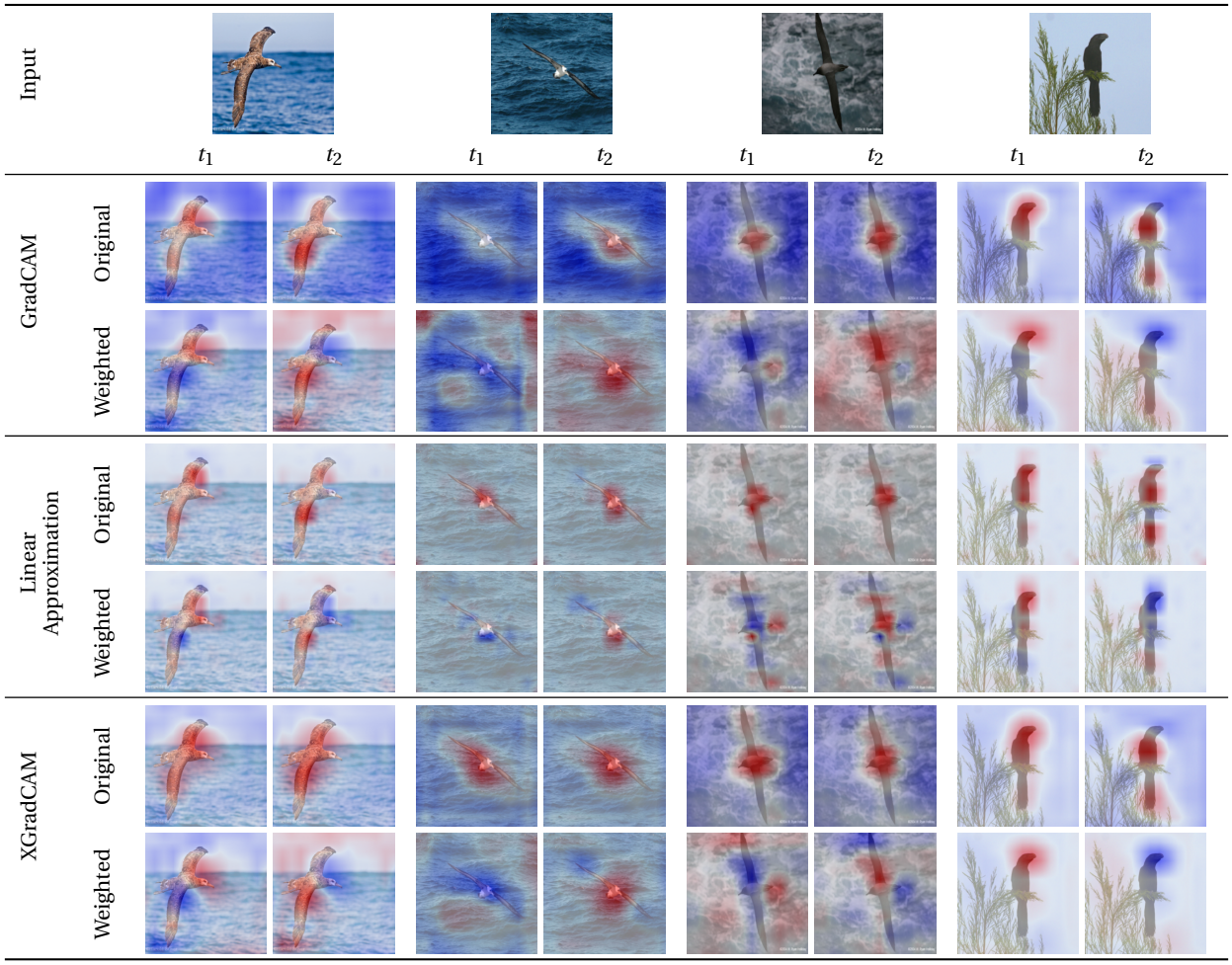


Figure 3: Reproduction of Figure 4 in the original paper. Comparison between the back-propagation from logits y_t (Original) and weighted contrastive back-propagation from p_t (Weighted) for GradCAM, Linear Approximation, and XGradCAM. The columns for each image signify the most possible and second possible class, respectively. Red and blue signal positive and negative activations respectively.

Table 1: Reproduction of Table 1 in the original paper using equal blurring. Comparisons between weighted contrastive method (wtd.) and original method (ori.) when blurring and masking. Using baselines Gaussian Blur, Zeros, and Channel-wise Mean and the methods Linear Approximation (LA), GradCAM (GC), and XGradCAM (XC). t1 and t2 are the classes with the highest and second highest probability respectively. Each line shows how the average relative probability changes among each image's top two classes. Pos. and Neg. Features mean that only positive and negative features are kept with respect to the corresponding target class. It is expected that when the positive or negative features corresponding to the target are kept, the expected relative probability is expected to increase or decrease respectively.

				Gaussian Blur				Zeros				Channel-wise Mean			
			p_t	Pos. Features		Neg. Features		Pos. Features		Neg. Features		Pos. Features		Neg. Features	
				ori.	wtd.	ori.	wtd.	ori.	wtd.	ori.	wtd.	ori.	wtd.	ori.	wtd.
CUB-200	LA	t_1	0.712	0.695	**0.789**	0.419	**0.274**	0.663	**0.754**	0.428	**0.292**	0.676	**0.766**	0.426	**0.281**
		t_2	0.288	0.560	**0.738**	0.390	**0.211**	0.563	**0.717**	0.398	**0.253**	0.558	**0.729**	0.391	**0.235**
	GC	t_1	0.712	0.747	**0.858**	0.428	**0.271**	0.731	**0.850**	0.432	**0.286**	0.745	**0.857**	0.426	**0.277**
		t_2	0.288	0.461	**0.759**	0.402	**0.199**	0.469	**0.761**	0.414	**0.226**	0.468	**0.759**	0.406	**0.214**
	XC	t_1	0.712	0.733	**0.847**	0.422	**0.248**	0.711	**0.838**	0.426	**0.266**	0.719	**0.844**	0.419	**0.253**
		t_2	0.288	0.504	**0.785**	0.393	**0.169**	0.515	**0.777**	0.402	**0.184**	0.511	**0.784**	0.395	**0.177**

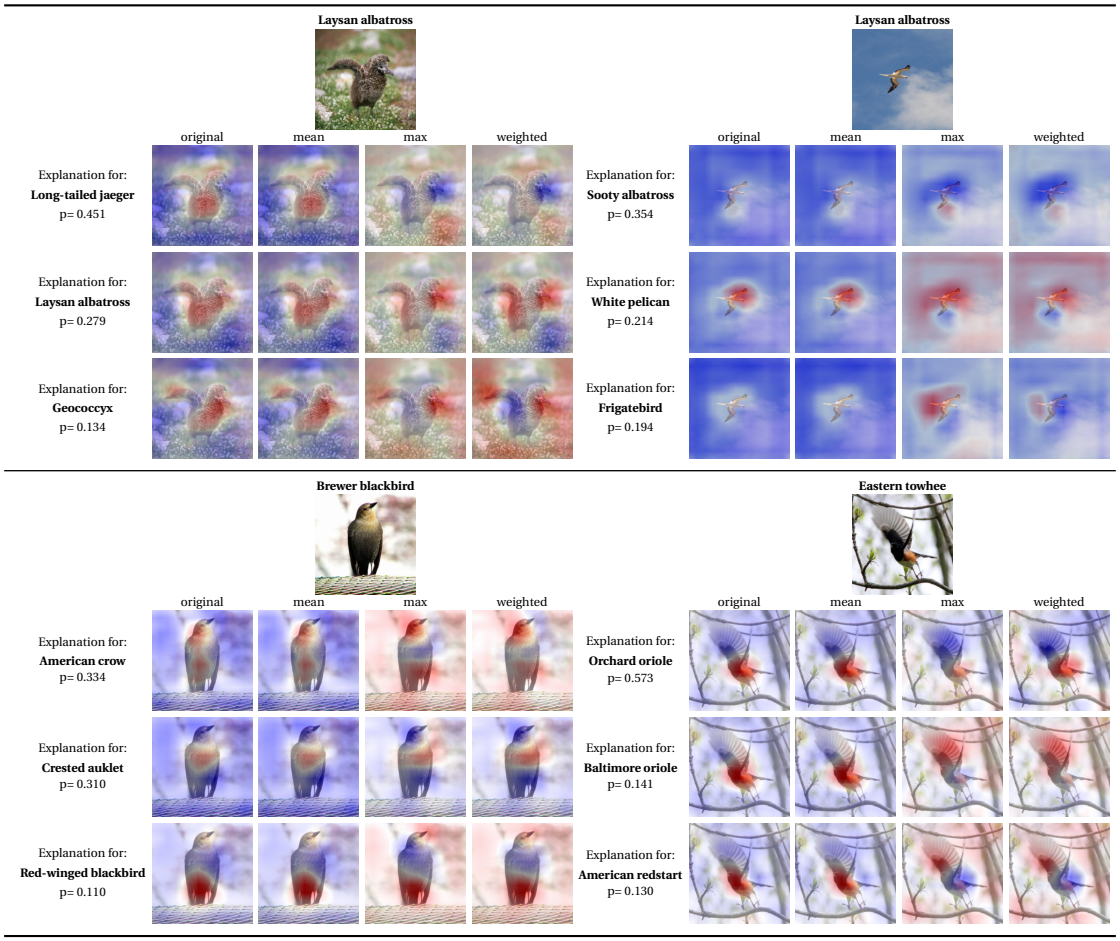


Figure 4: Reproduction of Figure 5 in the original paper. Comparison between mean, max, and weighted contrast for 4 images from CUB-200. In each column, we present explanations for the three most probable classes for GradCAM using the original image and the three contrastive methods.

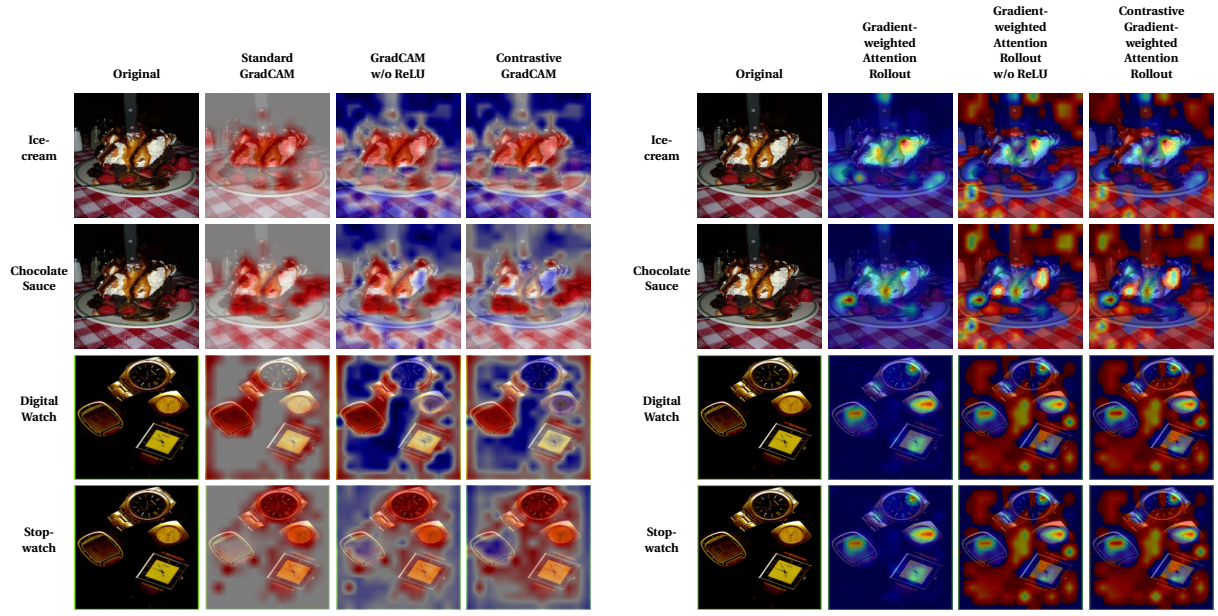
for visualization is also the same as in section 3.2 and a threshold of $p_3 > 0.1$ is used. The results are similar to the original paper, especially the observation that original and mean methods yield extremely similar results due to the tiny scaling factor used when subtracting by the other classes in the mean method. We also note that max similarity for the two most probable classes is each other's inverse and that the weighted method gives a similar but more detailed comparison that includes several classes simultaneously. Like in section 3.2 we also observe that the negative areas are much larger than in the compared article, presumably due to different visualization methods.

3.4 Vision Transformers and contrastive GradCAM

In order to adapt GradCAM to Vision Transformer models, tokens are reimagined as the spatially coherent nodes in standard CNN models, with the tokens' features as channels. This results in a 16x16 explanation map after taking the mean of the channels in standard GradCAM fashion, these explanations are later upsampled to the original image's size. This method has been proposed and implemented in Gildenblat & contributors (2021).

In order to adapt the method to the contrastive version all ReLU operations have been removed and the gradients are calculated from the softmax output instead of the logits.

Due to the mixing of information during self-attention, most explanation maps produce qualitatively bad results, not highlighting the important parts of the image to our eyes. The layers in Figure 5a have been explicitly selected because they gave good results, explanations in regard to other layers do not produce spatially coherent results.



(a) (b)

Figure 5: Comparision between proposed explanations, in (a) a comparison between GradCAM, GradCAM w/o ReLU, and Contrastive GradCAM is considered, in (b) a comparison between Gradient-weighted Attention rollout of the standard, without ReLU and contrastive variant is considered. Red sections are considered areas with high explainability. $p_{\text{ice cream}} = 0.30$, $p_{\text{chocolate sauce}} = 0.30$, $p_{\text{digital watch}} = 0.32$, $p_{\text{stopwatch}} = 0.32$

We find that the contrastive explanations with regards to the softmax do not have a significant effect on the results. We also observe that the explanation is often dominated by the explanation of the dominating class, if images are not selected to have similar probabilities for the top elements then there is usually no visual difference between doing a softmax GradCAM and a standard GradCAM without ReLU.

3.5 Vision Transformer: Contrastive Gradient-weighted Attention Rollout

Attention rollout is an explanation method proposed by the authors of Dosovitskiy et al. (2020) and further researched in Abnar & Zuidema (2020). Here, attention is propagated throughout the network from layer to layer towards the input neurons by multiplying the attention. This method has later been further developed in order to weight explanations with regards to their gradients (Gildenblat, 2020) (Chefer et al., 2020).

In order to adapt the method to the corresponding contrastive method, all ReLU operations have been removed and the gradient is calculated from the softmax output instead of the logits.

This explanation is significantly more accurate to the perceived localization of the image. However, the contrastive method with regards to the softmax does not seem to significantly impact the explanation compared to the contrastive one.

4 Scientific considerations

4.1 Reproducibility

As seen in the checklist of the original paper no large efforts were made toward the reproducibility of the paper. For example, no links to working code or details on the fine-tuned model training were provided. This heavily impacted our work as we had to make many assumptions about the process. We did find, however, a repository at https://github.com/yipei-wang/ClassContrastiveExplanations/ that contained some code regarding the fine-tuning

of VGG-16 on CUB-200. This helped in specifying hyperparameters that would reflect those of the original paper. This also showed that they used VGG-16 with batch normalization, which was not specified in the original paper and the difference compared to the non-batch normalized variant will yield different results.

Lack of code or detailed method also led to difficulties reproducing some results, as seen in section 3 especially coupled with some errors. For example, the very inaccurate equation in section 5.1 in the original paper coupled with the wrong epsilon led to many difficulties in reproducing and understanding that section. It is also not specified as to which data the fine-tuned models are trained. There are also some minor mistakes such as the bird in Figure 1 of the original paper having the wrong input label.

We also did not understand for our first readthroughs of the article that the authors' weighted contrastive method should ideally be implemented by back-propagating from the p neuron and the performance gains that this gives. In general, the presentation of their weighted contrastive method as novel led us to ignore the conclusion that it was proportional to back-propagating from the p neuron. We, therefore, find their presentation of the method to be slightly misleading especially as back-propagating from the p neuron is not something novel, even if they show why it can be useful.

4.2 Scientific contribution

The original paper provides an intuitive and efficient way of generating contrastive explanations that can take multiple classes into account. They also show that these outperform generally non-contrastive methods regarding the strength of the probability for the target class. They do not, however, make any large comparisons to state-of-the-art baselines in contrastive explanations. They defend this in peer reviews by claiming that many other contrastive methods ask the question of "how to change the instance to other classes?" while the authors aim to answer "why the instance is classified into this class, but not others?". Furthermore, many other contrastive methods are only suitable for preliminary data such as MNIST rather than the high-resolution images used here. Therefore we deem this lack of comparisons to other methods as valid.

Another concern is that all results rely on the class probability p as a metric for the relevance of the explainability method. While this is intuitive it also seems obvious that the contrastive weighted method presented which back-propagates from the p_t neuron will outperform the same method based on the preceding y_t neuron. This makes the results very expected, especially the ones shown in Figures 1 and 2 and Table 1. The visualizations show, however, that this method yields a clear explanation as to which areas of the image are especially important for a certain class, and in the end, this is perhaps the greatest contribution.

We also find that the authors' work is more of an explanatory nature than inventing something novel, as back-propagating from the p neuron has been commonly done before and even mentioned in the original GradCAM paper (Selvaraju et al., 2019). The value is therefore in showing what effects back-propagating from p_t yields compared to back-propagating from y_t.

4.3 Dominating classes

The authors have explicitly chosen not to do experiments on images where there exist dominating classes where $p_1 \gg p_2$. This is not motivated in the paper but is likely because the method becomes worse or is reduced to the original explanation under such circumstances. This is easy to make note of during testing when looking at randomly selected images or images that are not selected for their prediction uniformity. We have been unable to fully explain this behavior, as the formulation of the weighted contrast should weigh the target class and the weighted sum of all other classes equally.

Our reasoning for this behavior is explained by the observed relationship that explanation weights seem to increase with logit strength or output probability. This is exemplified in Figure 6. Due to this, we can expect an explanation with regards to the dominating value to be weighted significantly higher, around 3 to 4 times, than all other features. For future work, normalizing the explanation before weighing should be considered.

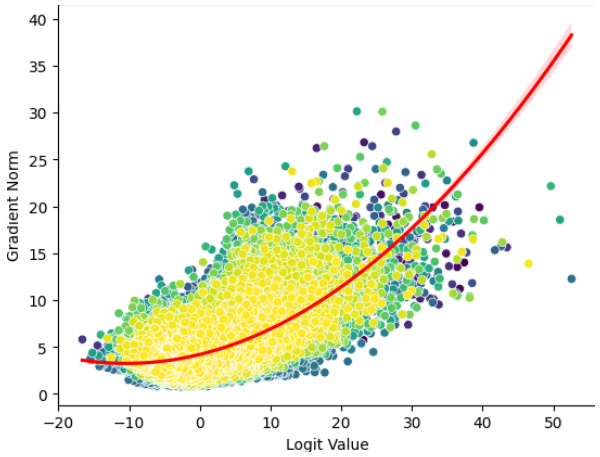


Figure 6: Relationship between the explanation weight $\|\phi_y\|$ and logit value y, using $\phi_y = \nabla_x y$ as explanation. A clear upwards trend is observed.

The behaviour of $\frac{\partial p_i}{\partial y_j}$ should also be considered. Here we observe that if the softmax output is dominated by a single value the gradient goes to zero. That if there exists a $p_t \to 1$ then it implicates $\frac{\partial p_i}{\partial y_j} \to 0$, this is easily observed in the Jacobian.

5 Conclusion

Overall the paper provides a clear argument as to how back-propagating from the softmax prediction instead of the logits gives improved connectivity to the actual prediction and thus a more relevant contrastive explanation. They propose a simple way of implementing this, which is applicable to many models and methods, and it shows a clear connection to accuracy using removal and blurring metrics. Their method also answers why a sample is predicted to belong to a certain class above others. It is somewhat problematic, however, that the paper relies on results that can generally be seen as different types of adversarial attacks with regards to p instead of y and that this bias is not mentioned in the paper.

We have reimplemented their work, made some corrections to their method, and have further been able to apply their method to other similar tasks using vision transformer architectures and the XGradCAM explanation method with reasonable results. Due to the simple nature of their contrastive method, one can also easily reproduce it by simply using back-propagating explanation methods from after the softmax layer which makes it generally reproducible. Their results in general, however, suffered from some reproducibility issues mainly caused by a lack of code and detail.

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