Vision Transformer Interpretability via Prediction of Image Reflected Relevance Among Tokens

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Abstract: The Vision Transformer (ViT) has a complex structure. To use it effectively in a place of critical decision-making, it is necessary to visualize an area that affects the model’s predictions so that people can understand. In this paper, we propose a new visualization method based on Transformer Attribution which is widely used for visualizing the area for ViT’s predictions. This method estimates the influences of each token on predictions by considering the predictions of images reflected relevance among tokens, and produces saliency maps. Our method increased the accuracy by about 1.28\%, 1.61\% for deletion and insertion and about 3.01\%, 0.94\% for average drop and average increase on ILSVRC2012 validation data in comparison with conventional methods.

1 INTRODUCTION

The Vision Transformer (ViT) (Dosovitskiy et al., 2021) is effective for tasks such as image classification (Wang et al., 2021; Liu et al., 2022) and object detection (Carion et al., 2020; Caron et al., 2021; Liu et al., 2023), semantic segmentation (Zheng et al., 2021; Xie et al., 2021). ViT has a complex structure, and in order to use it effectively in a place of critical decision-making, it is necessary to visualize an area that affects model’s prediction so that people can understand (Zhou et al., 2016; Selvaraju et al., 2017; Petsiuk et al., 2018; Wang et al., 2020). Visualization of an area that affects model’s prediction allows us to understand the trend in predictions, and allows the model for the improvement of performance. Therefore, we considered that interpreting the model is the important task.

In this paper, we pay attention to Transformer Attribution (Chefer et al., 2021) widely used to interpret the ViTs. Although this method visualizes the important area by the relevance scores calculated from a Hadamard product of Attention scores and gradients of the model, the relevance scores tend to be locally larger in objects that occupy the most of the image, and only parts of them are highlighted while the rests are not highlighted as shown in Figure 1.

In Transformer Attribution, it did not leverage the relevance among image tokens. On the other hand, our method focused on leveraging that abandoned relevance. Specifically, the proposed method again predicts multiple images calculated from a Hadamard products of relevance scores produced from Transformer Attribution and input images with the model, and the method calculates a saliency map from the model’s outputs.

In the qualitative experiments, we used validation set in the ILSVRC2012 dataset. We evaluated our method by four measures; the insertion and deletion, average drop, and average increase. Our method increased the accuracy by about 1.28\%, 1.61\% for deletion and insertion and about 3.01\%, 0.94\% for average drop and average increase on ILSVRC2012 validation data in comparison with conventional methods.

Figure 1: Visualization results by our proposed method and Transformer Attribution. Our method highlighted the predicted class object better than the Transformer Attribution.
Figure 2: Overview of Transformer Attribution. Gradients and relevances are propagated through the network, and calculated a matrix product of them to produce the final relevancy scores.

\[ R = R^{(1)} \cdot R^{(2)} \cdots \cdot R^{(B)} \]

Input → Transformer Block(1) → ... → Transformer Block(B) → Output

Gradients

Relevance

\[ R^{(1)} = \mathbb{E}_{\text{head}} (\nabla A \odot A) \]

2 RELATED WORKS

2.1 ViTs Interpretability

The Grad-CAM (Selvaraju et al., 2017), a method for interpreting Convolutional Neural Networks (CNNs), computes saliency maps from the deepest feature maps and gradients of the model. Furthermore, various methods were proposed to interpret CNNs (Chattopadhay et al., 2018; Ramaswamy et al., 2020; Jiang et al., 2021), and some of those methods can also interpret ViTs. Subsequently, a method utilizing the Attention Score (Abnar and Zuidema, 2020) was proposed to interpret ViT because it is considered that the attention scores indicate the areas that affect the ViT predictions.

However, there was a challenge to need effectively combine scores from different layers. For example, if we simply average the attention scores for each token, the signal is often attenuated. Attention Rollout (Abnar and Zuidema, 2020) that computes the matrix product of the attention scores of all layers was proposed to remedy this problem. This method showed an improvement over using a single attention layer, however, often highlighted irrelevant tokens. Furthermore Transformer Attribution (Chefer et al., 2021) using gradient is widely used to interpret the ViT. In this paper, Transformer Attribution is used as a baseline method.

2.2 Transformer Attribution

In Transformer Attribution shown in Figure 2, first, we feed an input image into ViT, and the gradients are computed from the output value through all Transformer blocks to the input image. In order to calculate a relevance score \( R \in \mathbb{R}^{N \times N} \), the method calculates a Hadamard product of each transformer block’s attention score \( A \in \mathbb{R}^{N \times N} \) that represented by the green matrix in the Figure, and gradients \( \nabla A \in \mathbb{R}^{N \times N} \) that represented by the orange matrix in the Figure, and averages those products across all heads. Note that \( N \) represents the number of the token fed into the Transformer block. Only the positive values should contribute to the prediction. Moreover, it calculates the relevance scores from a matrix products of these products. The component \( (i, j) \) of \( R \) is the magnitude of the influence of the pair of the \( i-1 \)-th token and the \( j-1 \)-th token on the prediction, and this is called “relevance”. Furthermore, the component \( (0, 0) \) of \( R \) is the relevance of the class token and itself. The method visualizes the areas that affect the predictions by producing the saliency map from the relevance of the class token and all other image tokens because it is considered that the class token has a high capacity for the interpretability. However, the relevance scores tend to be locally larger, in objects that occupy the most of the image, and only parts of them are highlighted while the rests are not highlighted as shown in Figure 1.

3 PROPOSED METHOD

In the proposed method shown in Figure 3, first, the relevance score obtained by Transformer Attribution. In Figure 3, the blue column in the relevance score indicates the relevance among class token and image tokens, while the orange matrix indicates the relevance score among image tokens. For the orange matrix \( R \in \mathbb{R}^{N \times N} \), the method calculates
Figure 3: Overview of our proposed method. The orange matrix is the relevance score between image tokens obtained by Transformer Attribution, and we cut the diagonal components of those relevance scores. Moreover, we reshape each column to a matrix and interpolate it to the same size as the input image. The image by Hadamard product between the input image and those relevance score is fed into ViT, and we obtain the logits $h w \times C$ (Green and Yellow vectors in the Figure) from ViT. We add the value corresponding to the predicted class of the logits (Yellow vector in the Figure) to the relevance among class token and image tokens (Blue vector in the Figure), and the saliency map is obtained by interpolating the sum result to a matrix to the same size as the input image.

$$R^{(N-1)\times(N-1)} \text{ and identity matrix } I \in R^{(N-1)\times(N-1)},$$

Hadamard product $\odot$, the proposed method corrects the magnitude of the relevance score as

$$R' = R \odot (1 - I),$$

$$R'' = R' + \max_{i,j} R'_{(i,j)} \times I.$$  

When we normalize relevance scores to reflect them into the input image, the diagonal components has a larger value than the other components. Thus, if it is normalized as is, the diagonal components will have a value close to 1 and the other components will have a value close to 0, and the only relevance among each token and itself will be reflected into the input image. We consider that it is better suited to measure the influence each token on the prediction if not only the relevance to itself but also the relevance to itself and others is reflected into the image, so we replaced the diagonal component with the maximum of the other components and then normalized them.

When the relevance scores are simply normalized by the maximum and minimum values of the total relevance scores, if the maximum value is much larger than the other values, the relevance scores of some columns after normalization may be almost the same value, and it may be more difficult to understand the magnitude relationship of the column. We consider that it would be easier to understand which tokens are highly relevance to a particular token if the relevance scores between the columns could be normalized without changing the magnitude relationship within the columns. Therefore, we normalized the relevance scores as shown in Figure 4.

In Figure 4, we calculate the maximum relevance score $R_{(i,j)}$ along the i-axis, and normalize those maximum values along j-axis (Green vector in the Figure). Moreover, we normalize the relevance score along the i-axis (Red matrix in the Figure), and we calculate the Hadamard product of those relevance score represented as the red matrix and the maximum relevance score represented as the green vector. Therefore, we considered that the relevance scores between the columns could be normalized without changing the magnitude relationship within the columns, and it would be easier to understand which tokens are highly
For the input image \( X \in \mathbb{R}^{1 \times 3 \times H \times W} \), we obtain \( N - 1 \) images that reflect the relevance among the image tokens as

\[
X' = X \odot \text{interp(mat}(R'))
\]

(3)

\[
X' = X \odot \text{interp(reshape}(R'))
\]

(4)

where \( \text{reshape}(\cdot) \) represents the process to convert relevance of all tokens to each token from a vector to a matrix, as in \( \mathbb{R}^{(N-1) \times (N-1)} \rightarrow \mathbb{R}^{N \times 1 \times \sqrt{N-1} \times \sqrt{N-1}} \), and \( \text{interp}(\cdot) \) represents the operation of nearest neighbor interpolation to the same size as the input image, so the first image of \( X' \) is the image that reflects the relevance of all the tokens to the first token. After that, the predictions \( L \in \mathbb{R}^{(N-1) \times C} \) is output by classifying the image reflected the relevance among the tokens into \( C \) classes. \( L \) represents a magnitude of the influence of each token on the prediction, and indicate the important areas that affect the predictions. Thus, we calculate the saliency map by bilinear interpolation of the value \( i \in \mathbb{R}^{(N-1)} \) corresponding to the predicted class of \( L \). We also consider that class tokens and other tokens have different areas of gazing, and we add the relevance score obtained by Transformer Attribution to \( L \).

From an example of the images reflected the relevance scores shown in Figure 5, if the relevance of other tokens to one’s own token is high, the image will reflect not only one’s own tokens but also tokens that are highly relevant to one’s own tokens, and we considered to assist in subsequent classifications. Our method estimates from the prediction of the image whether the relevance scores obtained by Transformer Attribution correctly indicate the areas that affect the prediction. If the relevance score for an object in the predicted class has even a small value, the prediction of the image is considered to be larger, and it is expected to improve the problem of the Transformer Attribution, where only parts of them are highlighted.

\[
\text{AverageDrop} = \frac{\sum_{i=1}^{N} \max(0, Y_i^c - O_i^c)}{N}, \quad \text{(5)}
\]

Figure 5: The example of images reflected the relevance scores.

4 EXPERIMENTAL SETTINGS

4.1 Dataset

In the following experiments, we evaluated our proposed method with all images in the validation set of the ILSVRC 2012 (Deng et al., 2009) that consists of 50,000 images from 1,000 classes.

4.2 Baseline

In the following experiments, we used pretrained ViT-B/16, as in (Chefer et al., 2021). We also used ViT-B/32 pretrained with Contrastive Language-Image Pretraining(CLIP)(Radford et al., 2021) as in (Chen et al., 2022). CLIP published by OpenAI is consists of an image encoder and a text encode, and be widely used in zero-shot classification by training on very large data sets.

In the comparison experiment, Grad-CAM computes the saliency map from the gradients and attention scores of the classtoken in the last Transformer Block as in (Chefer et al., 2021). Furthermore, Attention Rollout, Transformer Attribution, and our method compute the saliency map from the gradients and attention scores of the all Transformer Block as in (Chefer et al., 2021).

4.3 Evaluation Metrics

We evaluated our method with deletion and insertion, average drop, average increase widely used in evaluation metrics for interpretability.

The Deletion measures a decrease in the probability of the predicted class when important pixels are deleted, where the importance is obtained from the saliency map. The Deletion is the area of the probability curve with the number of deleted pixels, so the lower is the better. The Insertion measures a increase in the probability of the predicted class when important pixels are inserted, where the importance is obtained from the saliency map. The Insertion is the area of the probability curve with the number of inserted pixels, so the higher is the better.

Average Drop is computed as follows, and the lower is the better.

\[
\text{AverageDrop} = \frac{\sum_{i=1}^{N} \max(0, Y_i^c - O_i^c)}{N}. \quad \text{(5)}
\]
Average Increase is computed as follows, and the higher is the better.

$$Average Increase = \frac{\sum_{i=1}^{N} \text{Sign}(Y_{i}^{c} < O_{i}^{c})}{N}$$  \hspace{1cm} (6)

where $Y_{i}^{c}$ is the predicted probability of the class $c$ in the image $i$ among $N$, and $O_{i}^{c}$ is the predicted probability of the class $c$ in the image $i$ inserted only the top 50% of pixels in the saliency map. $\text{Sign}(\cdot)$ is the function that returns 1 if true and 0 if false.

5 EXPERIMENTAL RESULTS

5.1 ViT Results

Table 1 shows the Deletion, Insertion, Average drop, and Average increase by our method, Grad-CAM, Attention Rollout, and Transformer Attribution. Our method has the best in all metrics. Especially, in the comparison with Transformer Attribution, Deletion, Insertion, Average Drop, and Average Increase was improved by about 1.28%, 1.61%, 3.01%, and 0.94%.

Figure 6 show qualitative comparison results of the saliency maps. The first column shows the input image. The second column shows the model’s predic-
Table 1: Comparison of the proposed method and baseline on the ILSVRC2012 validation dataset.

<table>
<thead>
<tr>
<th>Method</th>
<th>Deletion</th>
<th>Insertion</th>
<th>Average Drop</th>
<th>Average Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grad-CAM</td>
<td>26.48</td>
<td>34.89</td>
<td>62.53</td>
<td>9.52</td>
</tr>
<tr>
<td>Attention Rollout</td>
<td>16.80</td>
<td>44.70</td>
<td>45.18</td>
<td>14.80</td>
</tr>
<tr>
<td>Transformer Attribution</td>
<td>15.49</td>
<td>46.64</td>
<td>40.86</td>
<td>18.68</td>
</tr>
<tr>
<td>Ours</td>
<td><strong>14.21</strong></td>
<td><strong>48.25</strong></td>
<td><strong>37.85</strong></td>
<td><strong>19.62</strong></td>
</tr>
</tbody>
</table>

Table 2: Comparison of the proposed method and baseline for Clip-ViT on the ILSVRC2012 validation set.

<table>
<thead>
<tr>
<th>Method</th>
<th>Deletion</th>
<th>Insertion</th>
<th>Average Drop</th>
<th>Average Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transformer Attribution</td>
<td>11.07</td>
<td>31.21</td>
<td>50.51</td>
<td>15.87</td>
</tr>
<tr>
<td>Ours</td>
<td><strong>10.19</strong></td>
<td><strong>32.55</strong></td>
<td><strong>48.41</strong></td>
<td><strong>16.92</strong></td>
</tr>
</tbody>
</table>

In comparison with our method and other methods, the images predicted to be a Solar Dish and Pizza show more highlighted in our method. This is because that the relevance scores among the tokens corresponding to the object are large, and the model can predict correctly the images that reflect those relevance scores. Except for the Gold Dish image, Grad-CAM, Attention Rollout, and Transformer Attribution highlighted only one part of the object, and we can interpret as if the rest of the object does not contribute to the prediction. We considered that this phenomenon occurs because the relevance scores tend to be locally larger. In contrast, our method further highlights one part of the object while highlighting the whole of the object, and we can interpret as if the whole of the object contributes to the prediction.

In the case of Gold Dish, Indigo Bunting, Samoyed, and Echidna, our method highlighted the background such as branches, trees, and sand. One of the factors is that the relevance scores between the background and object have a value. If the model can predict correctly the images reflected the relevance scores that have the relation between object and background, the saliency map contains noise on background.

Our method is not perfect but Table 1 and Figure 6 demonstrated that our method is superior to Grad-CAM, Attention Rollout, and Transformer Attribution in various indicators.

5.2 CLIP-ViT Results

Table 2 shows the Deletion, Insertion, Average drop, and Average increase by our method and Transformer Attribution for CLIP-ViT. In comparison with Transformer Attribution, our method improved the accuracy by approximately 0.88%, 1.34%, 2.1%, and 1.05% respectively.

Figure 7 shows qualitative comparison results for the CLIP-ViT obtained by our method and Transformer Attribution. In the proposed method, the image predicted to be "Tank" is highlighted the caterpillar portion. The images predicted to be "Abacus" and "Vestment" are more highlighted the object portion in comparison with Transformer Attribution.

6 CONCLUSIONS

In this paper, we improved the Transformer Attribution which is a method for interpreting the Vision Transformer. We calculate saliency maps by estimating whether the relevance score calculated from the predictions of images reflecting the relevance score correctly indicates the important areas affected the ViT’s prediction. Transformer Attribution has a prob-
lem that it fails to highlight objects of the prediction class, however, the proposed method improved the problem. Quantitative and qualitative evaluations demonstrated the effectiveness of the proposed method.

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REFERENCES


