Fidelity of Interpretability Methods and Perturbation Artifacts in Neural Networks

Abstract

Despite excellent performance of deep neural networks (DNNs) in image classification, detection, and prediction, characterizing how DNNs make a given decision remains an open problem, resulting in a number of interpretability methods. Post-hoc interpretability methods primarily aim to quantify the importance of input features with respect to the class probabilities. However, due to the lack of ground truth and the existence of interpretability methods with diverse operating characteristics, evaluating these methods is a crucial challenge. A popular approach to evaluate interpretability methods is to perturb input features deemed important for a given prediction and observe the decrease in accuracy. However, perturbation itself may introduce artifacts. We demonstrate that, while perturbation artifacts indeed exist, we can minimize and characterize their impact on *fidelity* estimation by utilizing model accuracy curves from perturbing input features according to the Most Import First (MIF) and Least Import First (LIF) orders. Using the ResNet-50 trained on the ImageNet, we demonstrate the proposed fidelity estimation of four popular post-hoc interpretability methods.

1 Introduction

Deep learning has recently demonstrated state-of-the-art performance in computer vision tasks. However, their decision (detection, classification, and prediction) is difficult to interpret and explain. One of the major approaches to interpretability is to quantify the importance of input features with respect to the model's prediction. However, rigorous evaluation of those feature importance estimators is problematic due to the complexity of DNNs and the lack of ground truth. We investigate challenges arising from perturbation-based evaluation and estimate the *fidelity* of importance estimators using the Most Import First (MIF) and the Least Import First (LIF) perturbation curves.

In DNNs, back-propagation and its variations are often used to quantify importance scores of input features, which are also called saliency maps and pixel attribution (Baehrens et al., 2010; Simonyan et al., 2014). Developments of importance estimators are often justified with human-centered arguments (Kim et al., 2019; Springenberg et al., 2015), such as regions of interest (ROI) (Saporta et al., 2022; Brocki et al., 2022) and sparsity (Chalasani et al., 2020). An objective evaluation of interpretability methods often is challenging due to the introduction of artifacts. One of the most established approaches is to mask input features with high importance scores and to measure the degradation of prediction accuracy of the model (Samek et al., 2016; Zeiler & Fergus, 2014; Kindermans et al., 2017; Petsiuk et al., 2018). However, in such perturbation-based evaluation, it has been unclear whether the observed accuracy degradation stems from information removal or perturbation artifacts. Unnatural perturbations introduce artifacts such that the test set consisted of perturbed images deviates substantially from the training set.

In this study, we characterize perturbation artifacts and estimate the fidelity of importance estimators, focusing on disentangling the sources of decrease of model accuracy. To quantify the influence that perturbation and removal of features have on the model accuracy, we conduct a series of computational experiments, based on measuring the change in model accuracy after feature perturbation in the Most Import First (MIF) or the Least Import First (LIF) order. Particularly, we proposes to use the area above the MIF and LIF accuracy curves to characterize the fidelity of post-hoc importance estimators. The proposed method is showcased on four popular importance estimators on the ResNet-50 (He et al., 2016) trained on the ImageNet.

2 METHODS

Perturbing images may introduce artifacts and create test samples in evaluation that are problematically out-of-distribution (OOD) compared to the training data (Dabkowski & Gal, 2017; Nalisnick et al., 2018; Qiu et al., 2021). However, the impact of perturbation was rarely measured empirically. Using ResNet-50 (He et al., 2016) trained on the ImageNet, we apply $\text{Uniform}(0, 1)$, $\text{Constant}(\overline{\mathbf{X}^i})$, and $\text{Blur}(\sigma)$ perturbation techniques to an increasing proportion of each sample in the validation data. We measure and compare the decrease in prediction accuracy (Supplementary Methods A.1).

For a given importance estimator, accuracy curves after feature perturbation for an image $\mathbf{X^i}$ are obtained by first masking an increasing fraction n of input pixels according to $\mathbf{M^i}(n)$ in either MIF or LIF order, and then measuring the resulting model accuracy (Samek et al., 2016). We quantify the MIF and LIF accuracy curves by the areas above the respective curves up to a fraction n of perturbed pixels (fig. 1). When considering multiple importance estimators, under certain assumptions (spatiality of and interaction among perturbed pixels), the minimal LIF area (U in fig. 1) is a conservative estimate of a contribution due to perturbation artifacts. With n proportion of LIF pixels perturbed, the accuracy degradation is due to both information removal and artifacts. An additional experiment and rationale for this is provided in A.1.3.

We applied the proposed method (Algorithm 1) to four importance estimators, namely vanilla gradient (VG) (Baehrens et al., 2010; Simonyan et al., 2014), Integrated Gradient (IG) (Sundararajan et al., 2017), Smoothgrad (SG) (Smilkov et al., 2017), and Squared SmoothGrad (SQ-SG) (Hooker et al., 2019). See details in A.1.4.

Figure 1: Diagram of the proposed *fidelity* evaluation method.

3 RESULTS AND CONCLUSIONS

First, using SQ-SG (Smilkov et al., 2017), we applied blurring with different radii of a Gaussian filter on the ImageNet samples. The model accuracy drops to nearly zero when the whole images are perturbed with a radius of $\sigma = 14$ (fig. S2). Second, we compared Blur ($\sigma = 14$), Uniform, and Constant perturbation (fig. S4). The choice of perturbation has a substantial influence. For the uniform perturbation, the accuracy drops the fastest for both MIF and LIF. In comparison, perturbing pixels with blurring degrades the model accuracy more gradually.

Table 1: Fidelity of importance estimators measured by F for $n = 0.2$

ESTIMATOR	$F \times 10^2$	$\delta \times 10^2$
VG	3.8	0.4
IG	4.8	0.3
SG	6.0	0.2
SQ-SG	5.7	0.2
RANDOM	2.1	0.8

The proposed fidelity and error are functions of n, which must be chosen. We evaluated the fidelity using $n = 0.2$ and $n = 0.4$, using four importance estimators. The final results for the fidelity of importance estimators are given in table 1 for $n = 0.2$ and in table S1 for $n = 0.4$, whose rankings agree. Importantly, the systematic error due to perturbation artifacts are small enough so that a meaningful evaluation of importance estimators can be established. At $n = 0.4$ the bulk of the model accuracy is already gone (table S1). Table 1 (additionally the estimated intervals for F_I equation 10), all estimators outperform a random ranking. The SG estimator performs the best. In the case of $n = 0.4$, performance of SG is on par with that of SQ-SG within δ term. Our results happen to align with human intuition since SG and SQ-SG focus closely on ROIs (e.g., figure S1).

Our results that four importance estimators are outperforming the random baseline are in conflict with ROAR (Hooker et al., 2019), which re-trains the model on perturbed images and measured the accuracy decrease on that re-trained model. In contrast, we attempt to better understand perturbation artifacts that arises during post-hoc interpretability methods that doesn't require modifying the model under evaluation. Overall, the proposed *fidelity* estimation method for post-hoc interpretability methods is intuitive and straightforward to apply without retraining or cropping.

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A APPENDIX

A.1 SUPPLEMENTARY METHODS

A.1.1 PERTURBATION METHODS

We investigate how different perturbation methods affect model accuracy. Perturbing parts of images may introduce artifacts and create samples in evaluation that are not in the original distribution (Dabkowski & Gal, 2017; Nalisnick et al., 2018; Qiu et al., 2021). However, the impact of perturbation was rarely measured directly. In order to empirically disentangle the removal of information and introduction of artifacts, we run an experiment to quantify perturbation artifacts.

The pre-trained Tensorflow-Keras implementation of ResNet-50 (He et al., 2016), with an input dimension of 224×224 pixels is used with the ImageNet validation dataset (Deng et al., 2009). For each sample $\mathbf{X}^i$, we apply the following perturbation methods:

- Uniform$(0, 1)$: replaces pixel values with a value sampled from an uniform distribution between 0 and 1 (where pixel values are scaled to 1).
- Constant$(\overline{\mathbf{X}^i})$: replaces pixel values by the average pixel value of a given image.
- Blur(σ): replaces pixel values with the corresponding values obtained by blurring the image with a Gaussian filter with radius σ.

The perturbed image $\mathbf{P}^i$ is obtained from the original image $\mathbf{X}^i$ as follows

$$\mathbf{P}^i = \mathbf{X}^i \odot \mathbf{M}^i + \mathbf{A}^i \odot (\mathbf{1} - \mathbf{M}^i), \tag{1}$$

where $\odot$ is the element-wise multiplication and $\mathbf{A}^i$ is an alternative image obtained through one of the perturbation methods. $\mathbf{M}^i$ is a mask with the same dimensions as $\mathbf{X}^i$ with value 0 for pixels to be replaced and 1 for pixels to be left invariant. When clear in context, the superscript i for the sample is omitted.

When considering an importance estimator, the mask $\mathbf{M}^i(n)$ is obtained by ranking the features (e.g., input pixels) according to their estimated importance scores $\mathbf{I}_{i,j}$ and selecting a fraction n of features in either the Most Import First (MIF) or Least Import First (LIF) order. These masks are used to construct accuracy curves (see the next subsection) with an increasing amount of perturbed features.

When choosing a perturbation method, one faces a trade-off between effectively removing information and introducing artifacts. This can be clearly demonstrated for a blurring method. A slight blurring of an image (with a small σ) will introduce almost no artifacts but at the same time barely removes any information. Increasing the radius σ of the Gaussian filter will remove more information but is also more likely to create artifacts. With a very large σ, a blurred image resembles a constant colored image. In order to select σ, we applied blurring with different radii of a Gaussian filter on the ImageNet samples and measured the model accuracy.

A.1.2 QUANTIFICATION OF MIF AND LIF ACCURACY CURVES

Accuracy curves after feature perturbation for an image $\mathbf{X^i}$ are obtained by first masking an increasing fraction n of input pixels according to $\mathbf{M^i}(n)$ in either MIF or LIF order, and then measuring the resulting model accuracy (Samek et al., 2016). This is equivalent to plotting $\mathbf{a}$ with $N = 1.0$ in algorithm 1 with $\mathbf{I}^i$ sorted in either a descending order (MIF) or an ascending order (LIF). See examples in figs. 1 and S4. The mask $\mathbf{M^i}(n)$ depends on the importance estimator under evaluation. For a given importance estimator, we create MIF and LIF curves for all samples in the validation set which was held out during training ($\mathbf{X^i}$ for i $= 1, \ldots, V$). We quantify the MIF and LIF accuracy curves by the areas above the respective curves up to a fraction n of perturbed pixels, which are denoted by $F^{p,e}(n)$ and $U^{p,e}(n)$ (illustrated in fig. S4), where p denotes the perturbation method and e the importance estimator.

Note that $\mathbf{O}$ is a matrix of DNN classifications, where $\mathbf{o}_{(n')}$ is a vector of length V consisted of predicted classes for samples with n' perturbation level. $\mathbf{a}$ is a vector of model accuracies at varying levels perturbation (n'), which are plotted as MIF/LIF accuracy curves.

Algorithm 1 Fidelity Estimation from MIF and LIF accuracy curves

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Input: DNN $f(\mathbf{X})$; n maximum fraction of perturbed pixels;
    Samples $\mathbf{X}^i_{W \times H \times C}$; Importance scores $\mathbf{I}^i_{W \times H}$ $(i = 1, \dots, V)$
    for $n' \leftarrow 0$ to n with a set increment of the sequence
        for $i \leftarrow 0$ to V
            $\mathbf{M}^i(n') = \mathbf{1}_{W \times H \times C}$
            $\mathbf{k}^i \leftarrow \text{sort}(\text{flatten}(\mathbf{I}^i))$
            (i.e. sort in descending order for MIF or ascending order for LIF)
            for $j \leftarrow 0$ to WH
                if $j < n'WH$ **then**
                    $x, y \leftarrow$ pixel position of $\mathbf{k}^i_j$
                    $\mathbf{M}^i(n')_{x,y} \leftarrow 0$
            $\mathbf{P}^i = \mathbf{X}^i \odot \mathbf{M}^i(n') + \mathbf{A}^i \odot (\mathbf{1} - \mathbf{M}^i(n'))$
            Apply DNN $f(\mathbf{P}^i)$, save classifications in $\mathbf{o}_{(n')}$
        Calculate the model accuracy using $\mathbf{o}_{(n')}$, $a_{(n')} = \frac{\text{\# Correct Predictions}}{\text{\# Total Predictions}}$
    F = Area above the MIF accuracy curve traced by $\mathbf{a}$
    U = Area above the LIF accuracy curve traced by $\mathbf{a}$
        (e.g., visualized in fig. S4)

We decompose F and U as follows

$$F^{p,e}(n) = F^{p,e}_I(n) + F^{p,e}_A(n)$$
$$U^{p,e}(n) = U^{p,e}_I(n) + U^{p,e}_A(n),$$

where the subscript I refers to the information removal component (F_I and U_I) and the subscript A refers to the perturbation artifact component (F_A and U_A). When clear in context, n, e, or p may be omitted for brevity. The components F_A and U_A, by definition, capture any decrease in model accuracy that is not due to the removal of information relevant to the model. In general, only F and U can be directly measured, and the decomposition into the information and artifact contribution is in general unknown. Details on obtaining F and U are provided in algorithm 1. This decomposition is motivated by the fact that even the masking of non-informative pixels can lead to a drastic decrease in accuracy (Fong & Vedaldi, 2017), which is also leveraged in adversarial attacks (Kurakin et al., 2018).

We assume that an information removal is non-negative, $F_I \geq 0$ and $U_I \geq 0$, such that

$$F_A \leq F$$
$$U_A \leq U. \tag{2}$$

A.1.3 ESTIMATION OF PERTURBATION ARTIFACTS

The decomposition of F into F_A and F_I is unknown, and therefore needs to be estimated. Consider the following expression for a certain proportion of perturbed features n and a given perturbation method p,

$$\Delta^e = F^e - U^e$$
$$= F^e_A + F^e_I - U^e_A - U^e_I, \tag{3}$$

where e can be any importance estimator.

To demonstrate the basic idea of our method of obtaining an estimate for F_A, let us consider the case where $\mathbf{M}(\mathbf{X})$ is obtained from randomly assigned importance scores. Since the order in which pixels are masked is completely random we can assume that $F^r_I = U^r_I$ from which it follows that

$$\Delta^r = F^r_A - U^r_A, \tag{4}$$

where the superscript r indicates random ranking of pixels. Solving equation 4 for U^r_A and using equation 2, we find

$$F^r_A \leq \Delta^r + U^r. \tag{5}$$

Since the quantities on the right hand side can readily be determined, this provides for us an upper bound for F_A^r.

While the artifact contribution for a random baseline can be easier to analyze, we are interested in F_A^e, where $F_I^e \neq U_I^e$. Since the cancellation of F_I^e and U_I^e in the expression for Δ^e is crucial, the proposition 4 can not be applied to a meaningful importance estimator. To remedy this situation, we perform an experiment in which we are perturbing images $\mathbf{X}$ with a non-informative mask $\mathbf{M}^s(\mathbf{X}')$. $\mathbf{M}^s(\mathbf{X}')$ is a mask that belongs to a randomly chosen $\mathbf{X}' \neq \mathbf{X}$ and is further shifted horizontally and vertically by random amounts between 10 and 100 pixels. Shifting removes a bias in the ImageNet dataset in which labeled objects tends to be in the center. Thus, we can expect that the importance ranking in $\mathbf{M}^s(\mathbf{X}')$ is random and $F_I^{s,e} \approx U_I^{s,e}$, where the superscript s in F_I and U_I indicates that $\mathbf{M}^s(\mathbf{X}')$ have been used.

We now define a new delta

$$\tilde{\Delta}^e = F^{s,e} - U^{s,SQ-SG}, \tag{6}$$

where $SQ - SG$ refers to squared SmoothGrad. We choose $U^{s,SQ-SG}$ because U^{SQ-SG} is the smallest value among the considered importance estimators (figure S2, right side), which allows us to constrain our estimate of the strength of perturbation artifacts (F_A^e) more strongly, see eq. (8) below. Using $F_I^{s,e} \approx U_I^{s,e}$ we can write equation 6 approximately as

$$\tilde{\Delta}^e \approx F_A^{s,e} - U_A^{s,SQ-SG}$$
$$\approx F_A^e - U_A^{SQ-SG}, \tag{7}$$

where in the second line we have assumed that $F_A^{s,e} \approx F_A^e$ and $U_A^{s,SQ-SG} \approx U_A^{SQ-SG}$. The rationale behind this assumption is that the introduced artifacts are not specific to the image as compared to, for example, the adversarial artifacts found in (Szegedy et al., 2013) which are obtained through optimization. We, therefore, expect that any artifact-inducing patterns present in the masks $\mathbf{M}(\mathbf{X})$ are, on average, preserved when using $\mathbf{M}^s(\mathbf{X}')$ instead.

Solving equation 7 for U_A^{SQ-SG} and substituting in equation 2, with $e = SQ - SG$, we finally obtain

$$F_A^e \leq \max(\tilde{\Delta}^e, 0) + U^{SQ-SG}, \tag{8}$$

where we additionally ignore negative $\tilde{\Delta}^e$ to obtain a more conservative estimate. The estimated upper limit equation 8 is understood as a conservative estimate of systematic error due to artifacts

$$\delta^e(n) = U^{SQ-SG}(n) + \max(\tilde{\Delta}^e(n), 0). \tag{9}$$

Thus, we estimate F_I^e, which to compare importance estimators, to be in the interval

$$F^e - \delta^e \leq F_I^e \leq F^e. \tag{10}$$

A.1.4 IMPORTANCE ESTIMATORS

We apply the proposed method of calculating fidelity and estimating artifacts to four importance estimators. The estimators under comparison are:

- **Vanilla gradient (VG)** (Baehrens et al., 2010; Simonyan et al., 2014): Gradients of the class score S_c[1] with respect to input pixels x

$$\mathbf{e} = \frac{\partial S_c}{\partial x}$$

- **Integrated gradient (IG)** (Sundararajan et al., 2017): Average over gradients obtained from inputs interpolated between a reference input x' and x

$$\mathbf{e} = \left(x - x^0\right) \times \sum_{k=1}^{m} \frac{\partial S_c\left(x^0 + \frac{k}{m}\left(x - x^0\right)\right)}{\partial x} \times \frac{1}{m},$$

  where x' is chosen to be a black image and $m = 25$.

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[1]The class score S_c is the activation of the neuron in the prediction vector that corresponds to the class c

- **Smoothgrad (SG)** (Smilkov et al., 2017): Average over gradients obtained from inputs with injected noise

$$\mathbf{e} = \frac{1}{n} \sum_1^n \hat{\mathbf{e}} \left(x + \mathcal{N} \left(0, \sigma^2 \right) \right),$$

where $\mathcal{N} \left(0, \sigma^2 \right)$ represents Gaussian noise with standard deviation σ, $\hat{\mathbf{e}}$ is obtained using vanilla gradient and $n = 15$.

- **Squared SmoothGrad (SQ-SG)** (Hooker et al., 2019): Variant of SmoothGrad that squares $\hat{\mathbf{e}}$ before averaging

$$\mathbf{e} = \frac{1}{n} \sum_1^n \hat{\mathbf{e}} \left(x + \mathcal{N} \left(0, \sigma^2 \right) \right)^2.$$

To obtain two-dimensional saliency maps, we sum up the absolute value of the color channels.

B   SUPPLEMENTARY FIGURES AND TABLES

Figure S1: Examples for masks $\mathbf{M}$ obtained using different importance estimators. For $n = 0.2$, 20% of pixels are perturbed in MIF or LIF orders. See the section A.1.4 for definitions of the importance estimators.

Figure S2: Comparison of decrease in model accuracy when pixels are masked in MIF (*left*) or LIF (*right*) order, according to different importance estimators (same color labels). The ResNet-50 trained on the ImageNet validation dataset are used to obtain the prediction and accuracy.

Figure S3: Average model accuracy of ResNet-50 on the ImageNet, with an increasing strength (radii σ) of blurring used for the whole input images.

Figure S4: Comparison of decrease in model accuracy over the fraction of masked pixels when MIF (*left*) or LIF (*right*) pixels are perturbed using different methods. The ranking of the importance of the pixels is according to the squared SmoothGrad estimator. Area $F(n)$ and $U(n)$ quantify the accumulated decrease in model accuracy when some fraction n of MIF and LIF pixels is perturbed, respectively. In blue, $F(0.3)$ and $U(0.3)$ are shown.

Table S1: Fidelity of importance estimators measured by F for $n = 0.4$ with a systematic error δ determined by the right-hand side of equation 8 and using blur as perturbation method.

ESTIMATOR	$F \times 10^2$	$\delta \times 10^2$
VG	12.6	1.7
IG	14.8	1.6
SG	17.3	1.0
SQ-SG	16.8	1.0
RANDOM	8.1	3.0