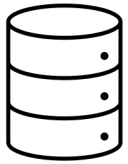
Gradient-based explainability methods

Explainable and Trustworthy AI

Eliana Pastor

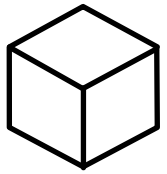
Stages of Explainability

- Explainability involves the entire AI development pipeline



Pre-modelling explainability

Before building the model
- Data exploration
- Data selection
- Feature engineering



Explainable modeling

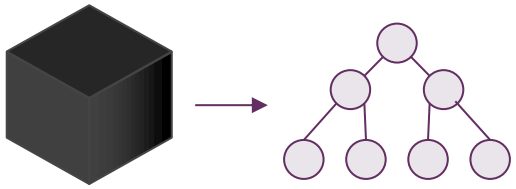
Build inherently interpretable models
- Manage the accuracy and interpretability trade-off

Post-modelling explainability

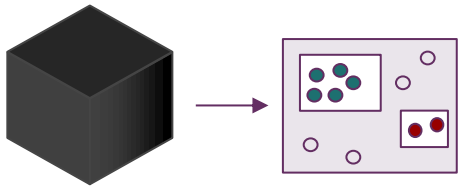
After model development
- Explaining predictions and behavior of trained models

Scope of Explainability

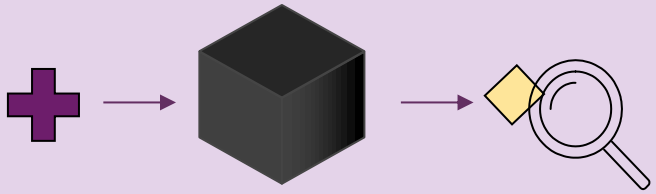
- *What do we explain?*



Global



Subgroup



Individual/local

How the model globally works

How the model behaves in data subgroups

Explaining the reasons behind individual predictions

Gradient-based explainability methods

- Techniques that leverage the **gradient** information **of the model with respect to the input features** to identify which features are most influential in the model's decision-making process.

- Gradient-based methods differ in how the gradient is computed

- Generally, the explanation has the same size as the input
- They assign each part of the input a value that is interpreted as the relevance
  - e.g., for images, importance for each pixel of the image
  - e.g., for text, importance of each toke

Saliency map

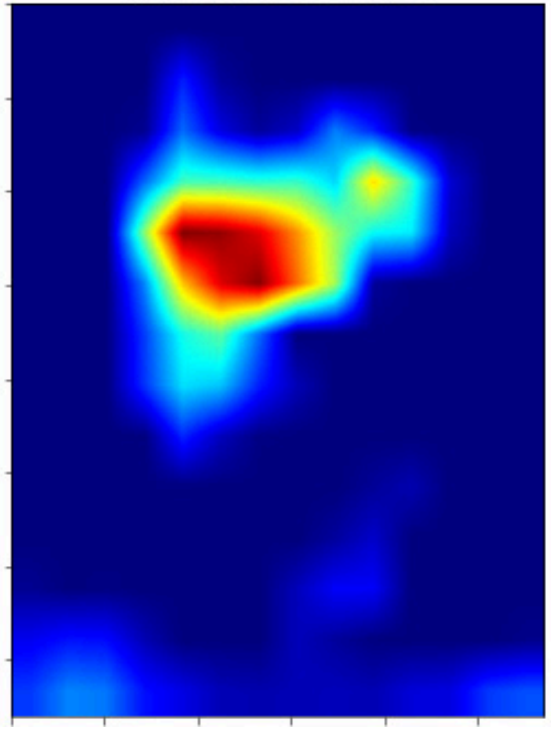


Image from: https://dlhr.de/8

Saliency map

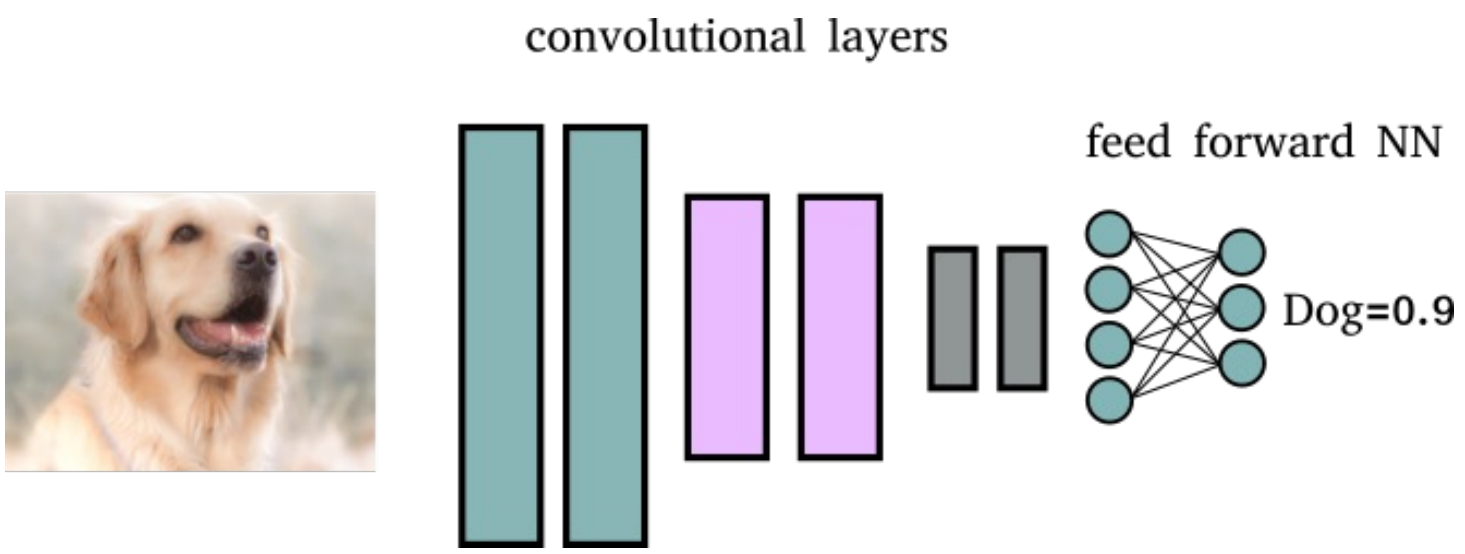
- **Saliency** is a **visualization** technique to highlight the important regions or features in an input data sample
  - It is a way to visualize **feature attributions**, i.e., to represent the attribution scores assigned to each input feature
- Brighter regions in the saliency map indicate higher saliency or importance, highlighting the regions of interest in the input data

I am really happy

Vanilla Gradient

Compute the gradient of the loss function with respect to the input

- Proposed for image data → respect the input pixel



Gradients: from backprogation to saliency

Gradient in the training process.

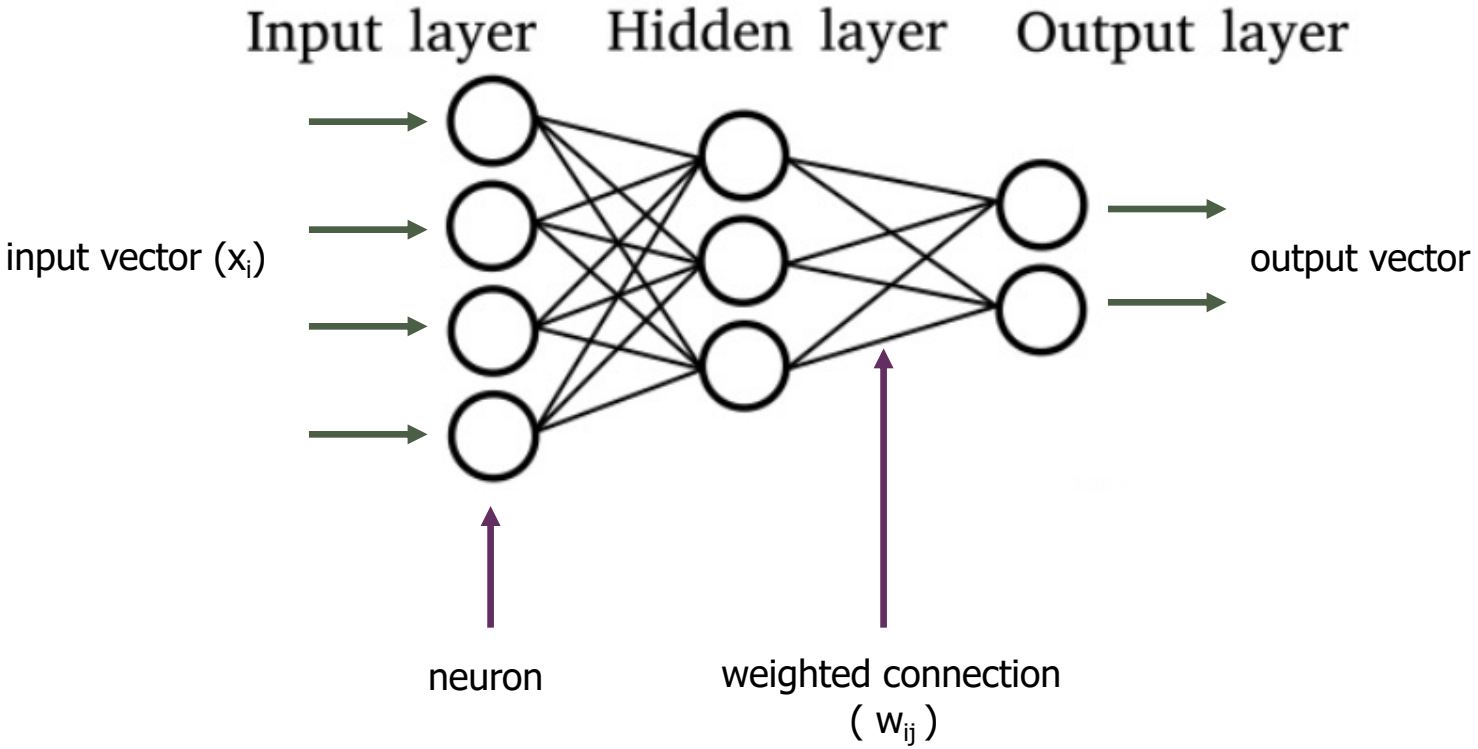
- During the training process, gradients are computed with respect to the model parameters to update them.
  - These gradients indicate how changes in the model parameters affect the loss.

Gradients in explainability.

- In gradient-based explainability methods, instead of computing gradients with respect to the parameters, **we compute gradients with respect to the input features themselves**.
  - We analyze how changes in the input features affect the output directly.

Gradients – at training time

Backpropagation $\frac{\partial L}{\partial w}$



Gradients for explainability - Goal

Given.

- A network trained for C classes. Output of the network for input I is a prediction vector $\mathrm{F}(I) = [F_1(I), \ldots, F_C(I)]$
- For a class c, $F_c(I)$ is the score of the class c

Goal.

- Given an input $\mathrm{I_o}$ with p features and a class c, we want to compute a relevance score for each features for class c

$$R^c = \left[R_1^c, .., R_p^c\right]$$

for the score F_c

For image data, the features can be the pixels of the image with width w and height h, with $\mathrm{p} = w \times h$

Gradients for explainability - How

How.

$F_c(I)$ is the score of the class c and R^c relevance score for each features for class c

We derive R^c by computing the gradient of class score of interest $F_c(I)$ with respect to the input pixels:

$$\left.\frac{\partial F_c}{\partial I}\right|_{I_0}$$

i.e., the derivative of F_c with respect to the input for the given image $\mathrm{I_o}$

Gradients for explainability -

Let F be the model function and $F_c(x)$ the score function for the input x for the class c

We **compute** the **input gradient importance**

$$\nabla_x F_c(x) = [\frac{\partial F_c}{\partial x_1}, \dots, \frac{\partial F_c}{\partial x_p}]$$

where $\nabla_x F_c(x)$denotes the **gradient** of $F_c(x)$ for input x and $\frac{\partial F_c}{\partial x_i}$ is the **partial derivative** of $F_c(x)$ with respect to the i-th input feature.

We typically compute it via backpropagation.

Gradients for explainability

Interpretation of the image-specific class saliency

- Features with **larger gradients** indicate that **small changes in those features will result in more significant changes** in the model's output
  - Magnitude of the derivative indicates **which features need to be changed the least to affect the class score the most**
  - Gradients tell us which features (e.g., pixels) have the steepest local relative to your model's prediction at a given point along your model's prediction function

Gradients for explainability

The idea is to model the score model F_c as a linear function. Since F_c is non-linear, we approximate with the first-order Taylor expansion

$$F_c(I) \approx w^T \cdot I + b = R_c^T \cdot I + b$$

Where the weight vector $w = R_c$ is the derivate of the score and b is the bias of the model.

The weights R_c define the importance of the feature of I for the class c.

From gradient to saliency map

- $F_c(I)$ = score for class c, e.g., logits
- w has size as the input
- For images, $I_0 \in \mathbb{R}^{H \times W \times K}$ (e.g., K=3 for RGB) -→ $w \in \mathbb{R}^{H \times W \times K}$

If we want to plot a saliency map over the image, we need to **aggregate the scores** w to have a saliency map of size $H \times W$

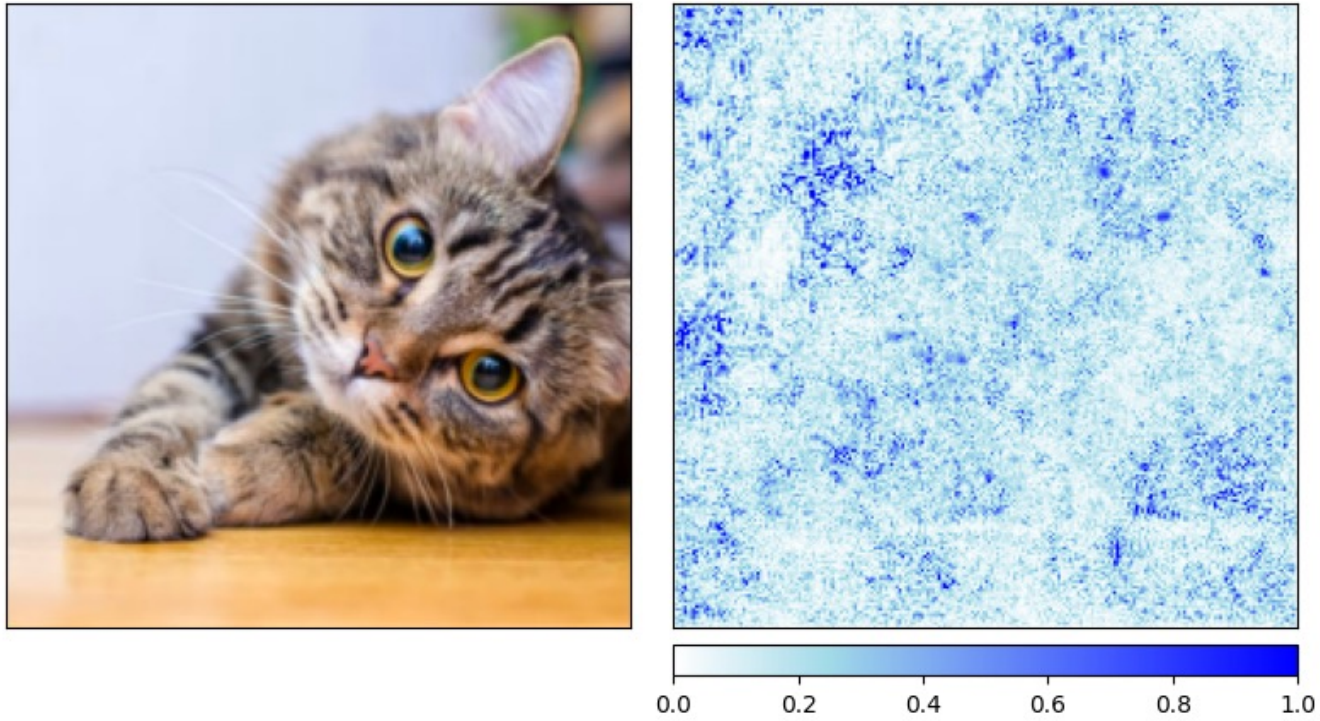
We can derive the **saliency map** $\mathrm{M} \in \mathbb{R}^{H \times W}$ as follows

$$M_{ij} = \max_k |w_{ijk}|$$

i.e., we collapse the challenge dimensions

Vanilla gradient – Limitation

- Noisy!
  - Derivative can fluctuate great at small scales
  - Slight variations to the input data can result in significant changes in the model output (thus in the gradients), resulting in noisy gradients and instability



SmoothGrad

Vanilla Gradient can produce noisy saliency maps, hence difficult to interpret

SmothGrad **averages the gradients** for ‘noisy inputs’

$$\frac{1}{N}\sum_{1}^{N}\nabla_x F_c(x+\epsilon)$$

Where ϵ is Gaussian Noise.

We create a **smoothing effect**. The intuition is that by averaging the gradients over modifications of the input, smooths out fluctuations & average out noise

SmoothGrad

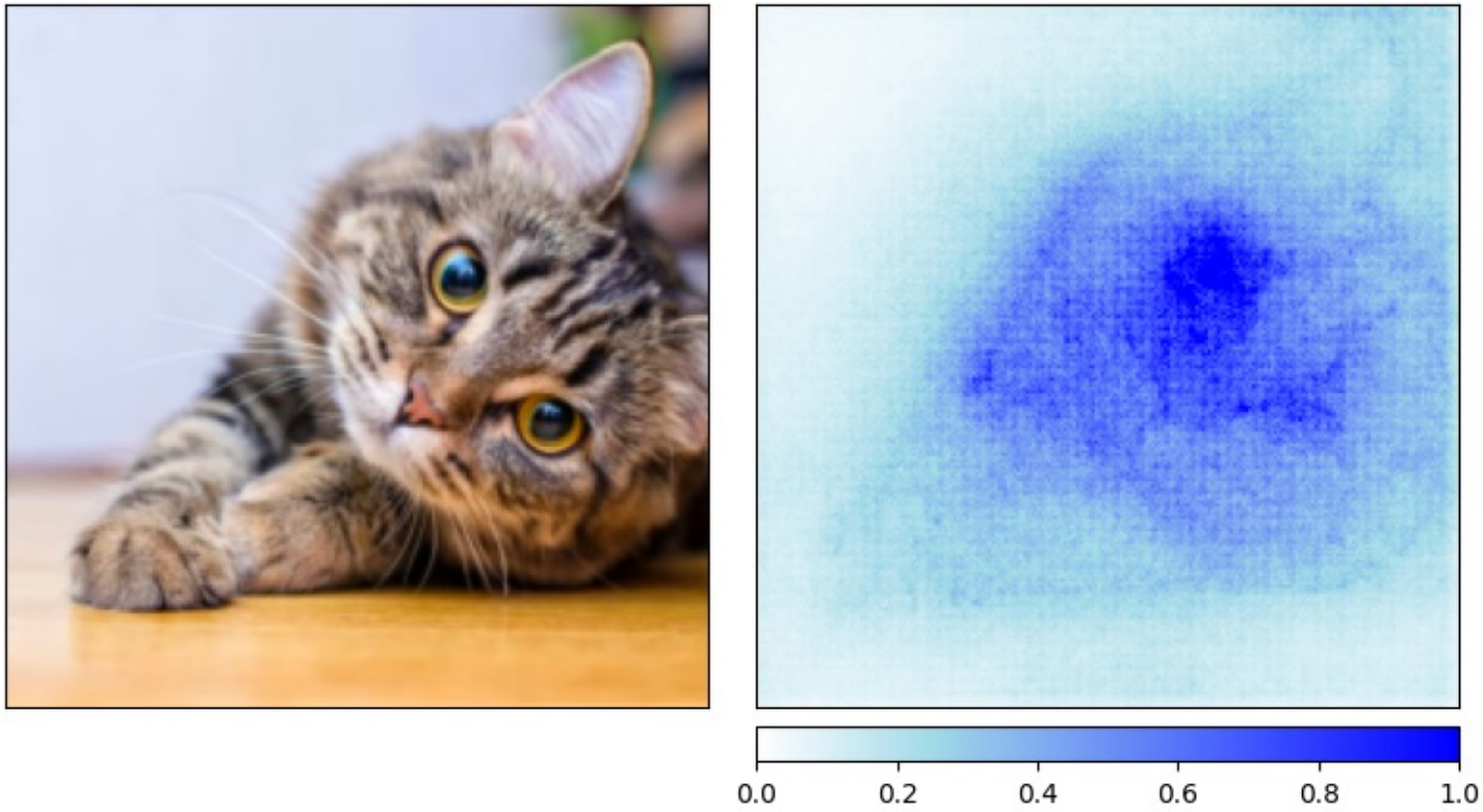
Process.

- Generate N versions of the input by adding noise to it.
- Compute the gradients for the N input, thus generating N relevance scores R_c
- Average the pixel attribution maps

- Parameters
  - Noise level
  - Number of samples

Note that we can generally apply a generic gradient-based explainability approach

Smooth-Grad + Vanilla Gradient - Example



Gradient x Input

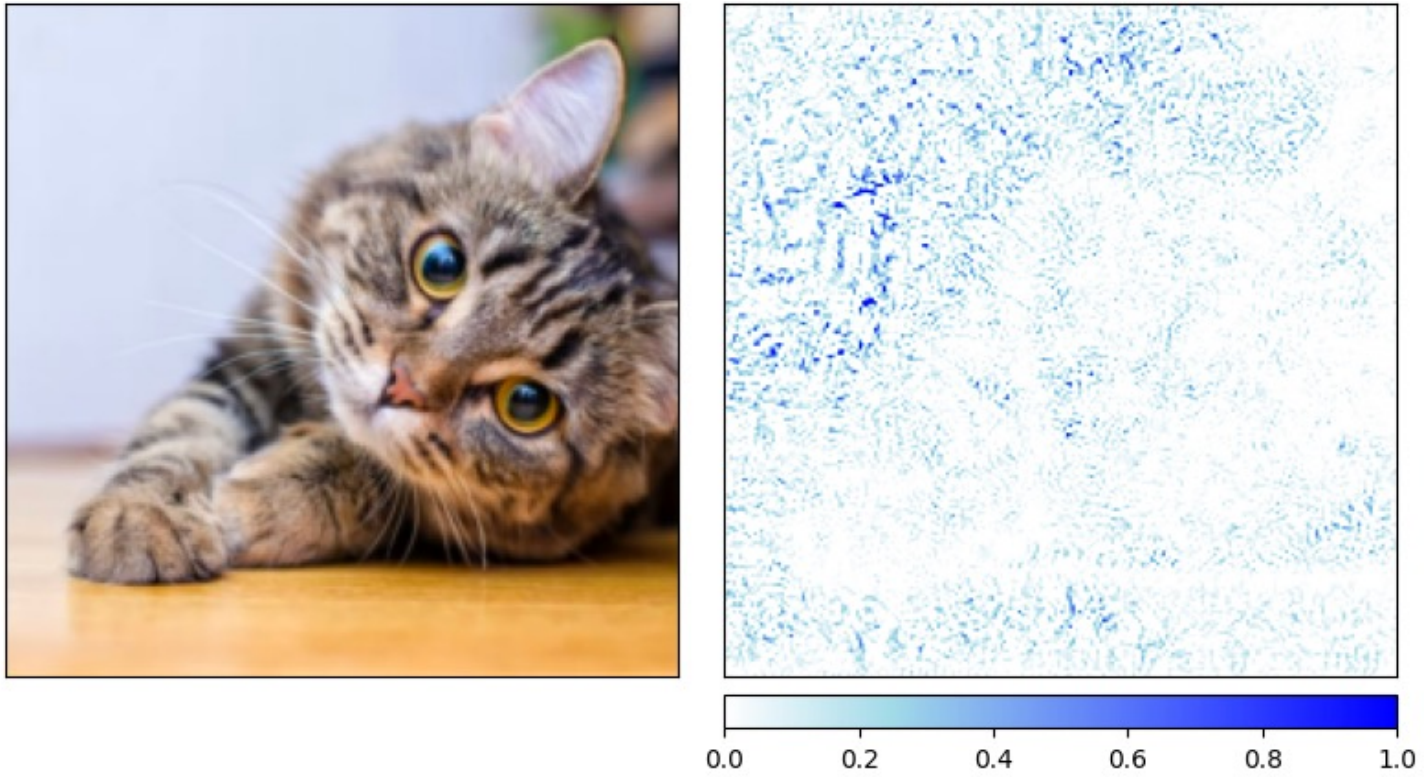
- Small variation of Vanilla Gradient
- The gradients w.r.t. the input are multiplied for the input (element wise product)

$$\nabla_x F_c(x) \odot x$$

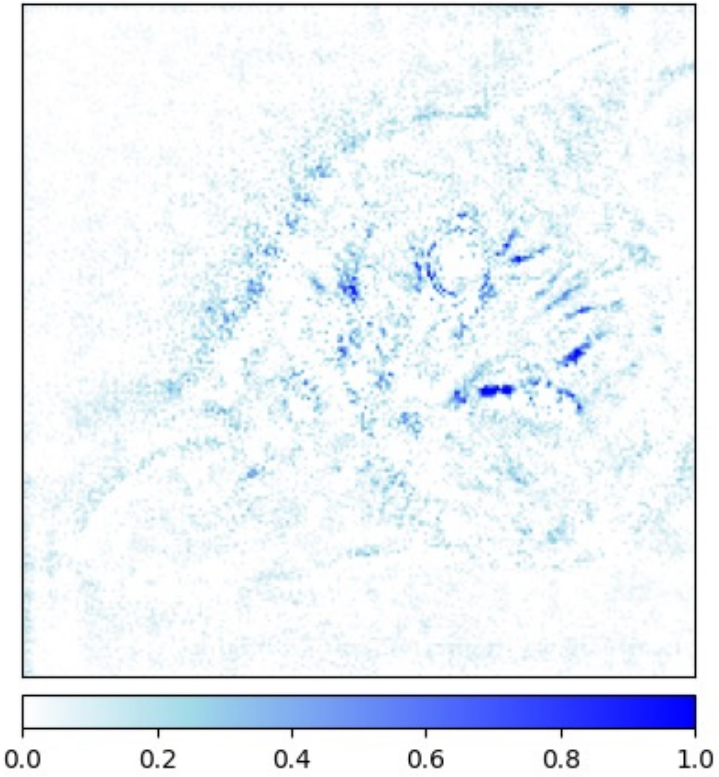
- It generally provides better results

Gradient x Input - Example

Gradient x Input

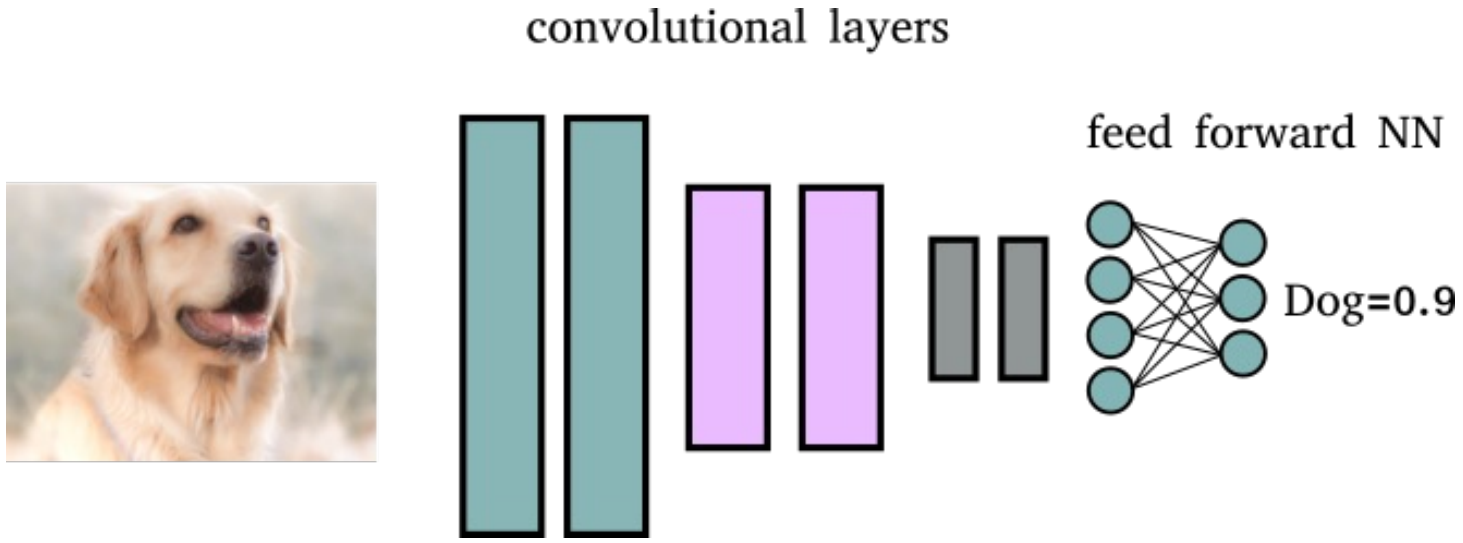


Gradient x Input + SmoothGrad



GradCAM

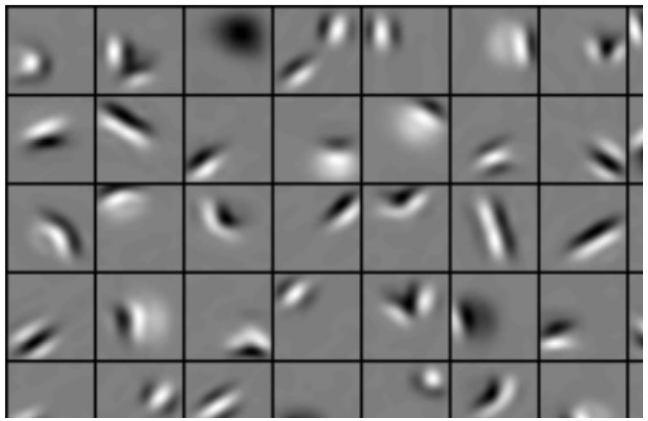
- Gradient-weighted Class Activation Mapping
- Suitable for CNN-based architectures



GradCAM

Intuition.

- Deeper representations in a CNN capture **higher-level visual constructs**



Lee et al, “Convolutional Deep Belief Networks for Scalable Unsupervised Learning of Hierarchical Representations”, ICML 2009.

GradCAM

Intuition.

- Deeper representations in a CNN capture **higher-level visual constructs**
- Convolutional layers naturally retain spatial information which is lost in fully-connected layers, so we can expect the **last convolutional layers** to have the best compromise between **high-level semantics** and detailed spatial information.

- Grad-CAM uses the **gradient** information flowing into the **last convolutional layer** of the CNN to assign importance values to each neuron for a decision.
  - Explain activations in the output layer decisions

GradCAM

Difference→ the gradient is not backpropagated back to the image $\left.\frac{\partial F_c}{\partial I}\right|_{I_0}$

Grad-CAM → **Propagated** (usually) to the **last convolutional layer**

Let $A^k \in \mathbb{R}^{U \times V}$ be feature map activations of a convolutional layer (typically the last). The layer produces K feature maps

- Each element is by i, j. Hence, $A^k_{i,j}$ refers to the activation at location (i, j) of the feature map A_k

Grad-CAM produces a **coarse localization map** that highlights important regions of the image, i.e., **Layer-wise importance**, $Layer\text{-}R^c \in \mathbb{R}^{U \times V}$ for a class c, where U, V is the shape of A_k

$$\frac{\partial F_c}{\partial A^k_{i,j}}$$

GradCAM

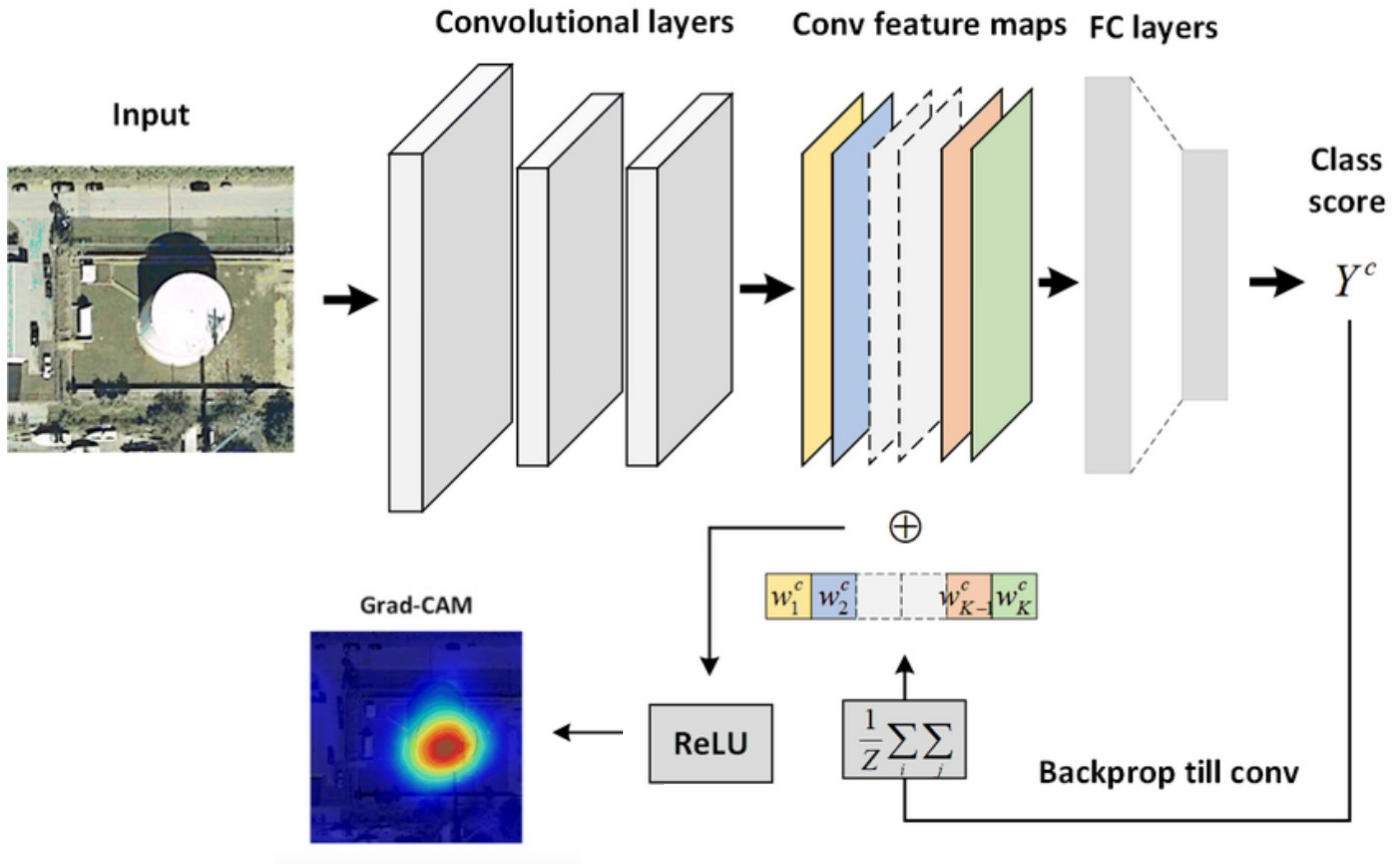


Image from: Guo, Xianpeng et al (2022). Prob-POS: A Framework for Improving Visual Explanations from Convolutional Neural Networks for Remote Sensing Image Classification. Remote Sensing.

GradCAM - Process

a. Compute the **gradient of** the score for class c, F_c, with respect **to feature map activations** A_k of that convolutional layer of interest (usually the last) -- via backpropagation

$$\frac{\partial F_c}{\partial A^k}$$

b. Compute the **average** for each output channel – global average pooling

$$\alpha_{\mathrm{k}}^{\mathrm{c}} = \frac{1}{\mathrm{Z}} \sum_i \sum_j \frac{\partial F_c}{\partial A_{i,j}^k}$$

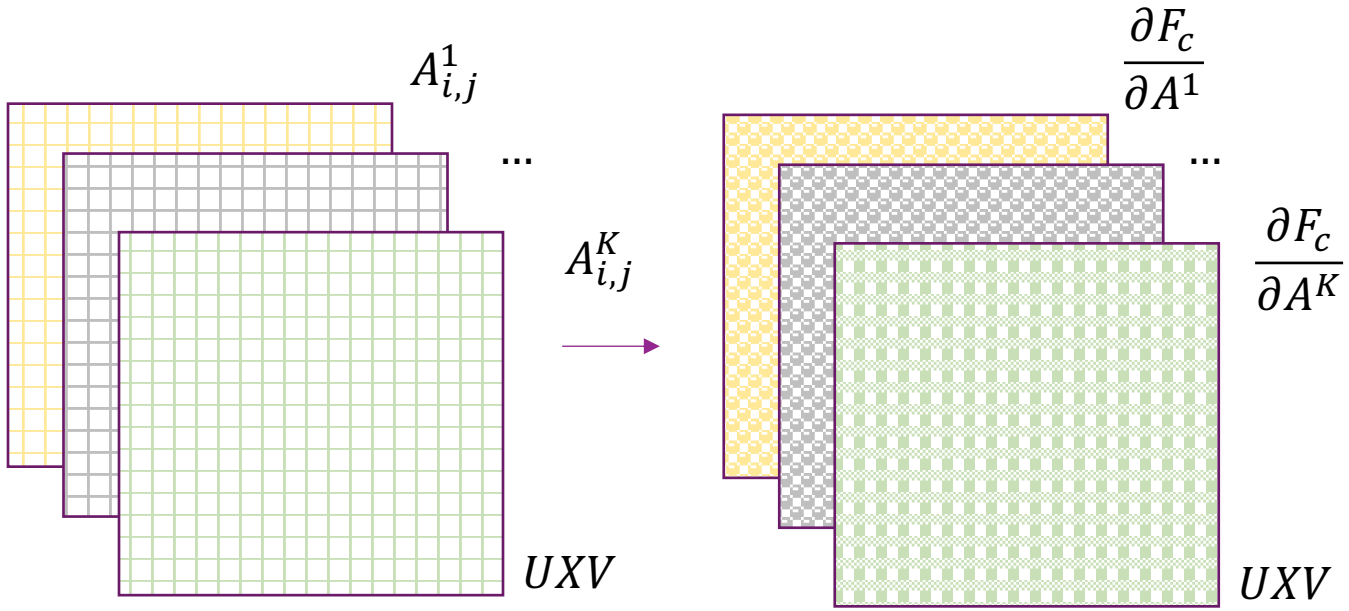
$\alpha_{\mathrm{k}}^{\mathrm{c}}$ captures the ***importance* of feature map k** for a class c

c. Multiply the average gradient for each channel by the **layer activations** and apply a **ReLU**

$$Layer\text{-}R^c = ReLU(\sum_k \alpha_k A^k)$$

ReLU since only interested in the features that have a positive influence on the class, i.e. pixels whose intensity should be increased to increase class c

GradCAM – Activations $A^1_{i,j}$

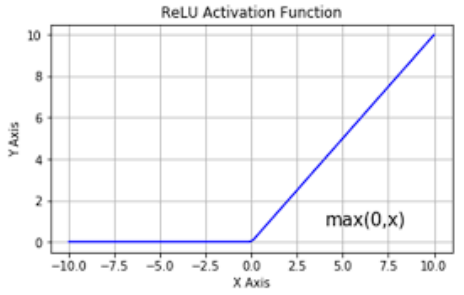


$$\alpha_1^c = \frac{1}{Z}\sum_i\sum_j \frac{\partial F_c}{\partial A^1_{i,j}}$$

...

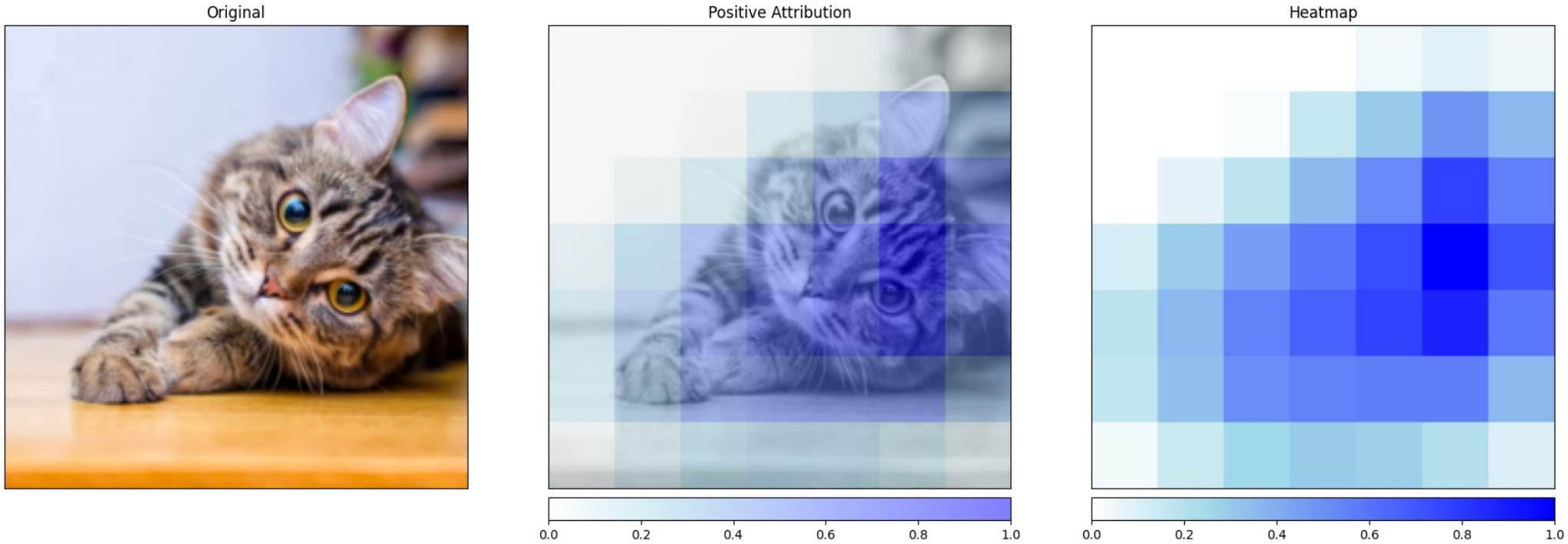
$$\alpha_K^c = \frac{1}{Z}\sum_i\sum_j \frac{\partial F_c}{\partial A^K_{i,j}}$$

$$Layer\text{-}R^c = ReLU\left(\sum_k \alpha_k A^k\right)$$



GradCAM - Relevance - Example

- $Layer -R^c$ in a **coarse heatmap** of the same size as the convolutional feature maps
- Often we upsample it and view as mask to the input



Guided GradCAM

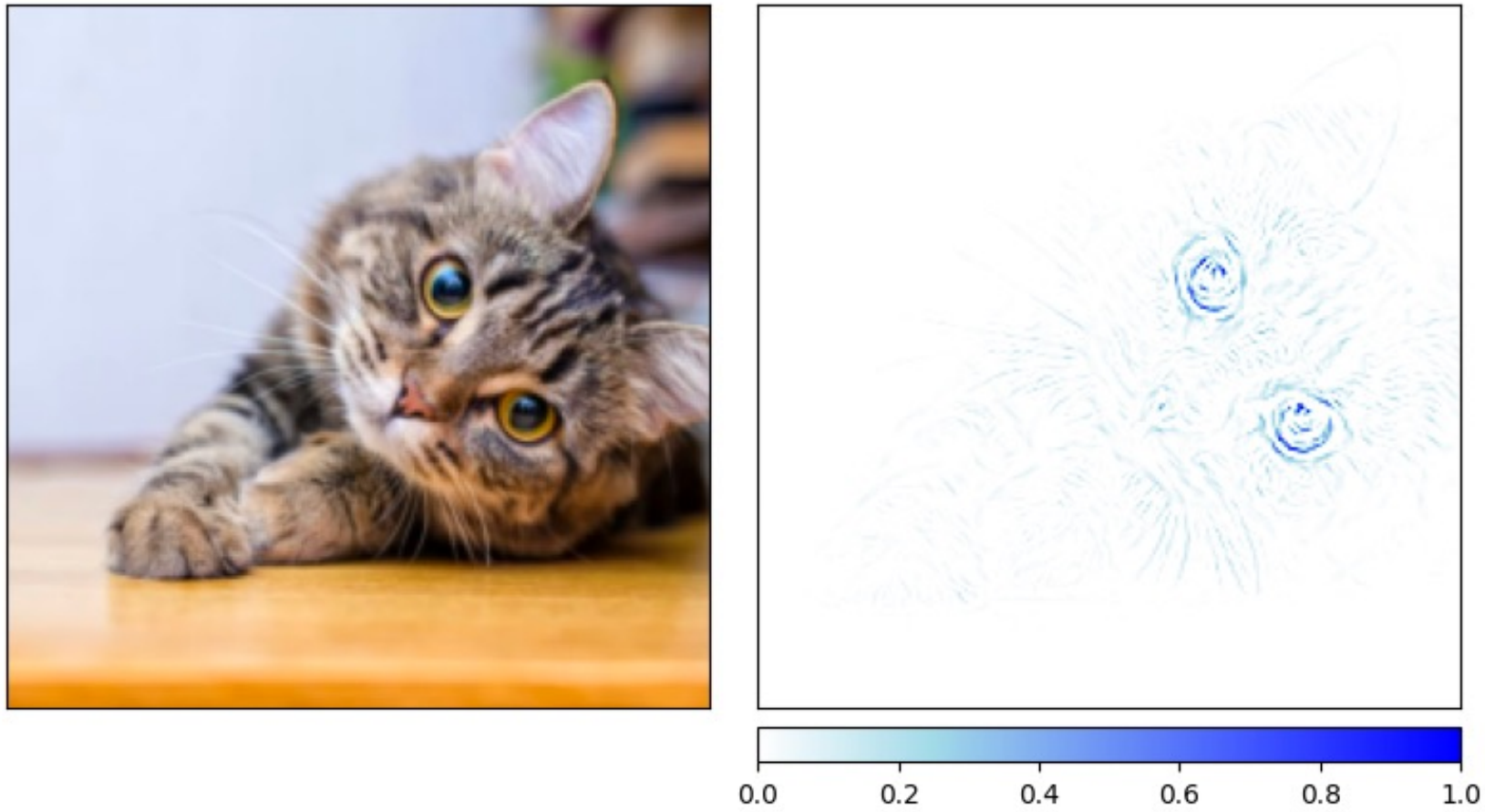
- Grad-CAM produces coarse importance as the last convolutional feature maps have a coarser resolution compared to the input image
- We may want to have a per-pixel importance

- **Idea**

Combine Grad-CAM explanation and the explanation from another attribution method, such as Vanilla Gradient, by multiplying element-wise

$$\text{Guided Grad-CAM} = upsample(Layer - R^c_{GRADCAM}) \odot R^c_{other\ method}$$

Guided GradCAM - Example



Integrated Gradients

Paper proposed two **axioms**: sensitivity and implementation variance

Sensitivity.

If two inputs x and x' differ only in one feature A_i but have different predictions, then the feature A_i should be given a non-zero attribution

Example

x = [1, 0, 1] → f(x) = class 0

x' = [1, 1, 1] → f(x) = class 1

Implemetation invariance.

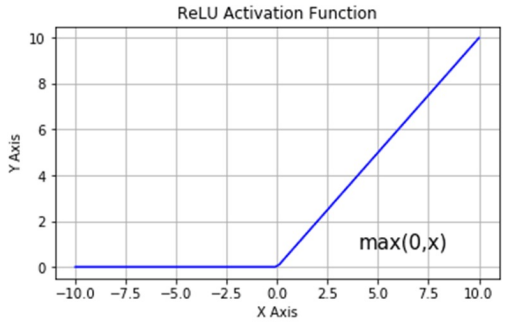
If two models f anf f' have identical input/output behavior, then the attributions for M and M' should be identical.

Sundararajan, Mukund, Ankur Taly, and Qiqi Yan. "Axiomatic attribution for deep networks." *International conference on machine learning*. PMLR, 2017.

Gradients X Input fails sensitivity

- f(x) = 1-ReLU (1-x) = 1-max(0, 1-x)

- Example
  - f(0) = 1-max(0, 1-0) = 0
  - f(2) = 1-max(0, 1-2) = 1



$$\nabla RELU'(x) = \begin{cases} 1 \; if \; x > 0 \\ 0 \; if \; x \leq 0 \end{cases}$$

Since we have different outputs, for the sensitivity axiom, we should have **different attributions**

$$\textbf{InputXGradient}(f, x) = \nabla f(x) \cdot x$$

$$\textbf{InputXGradient}(f, 0) = 1 \cdot 0 = 0$$

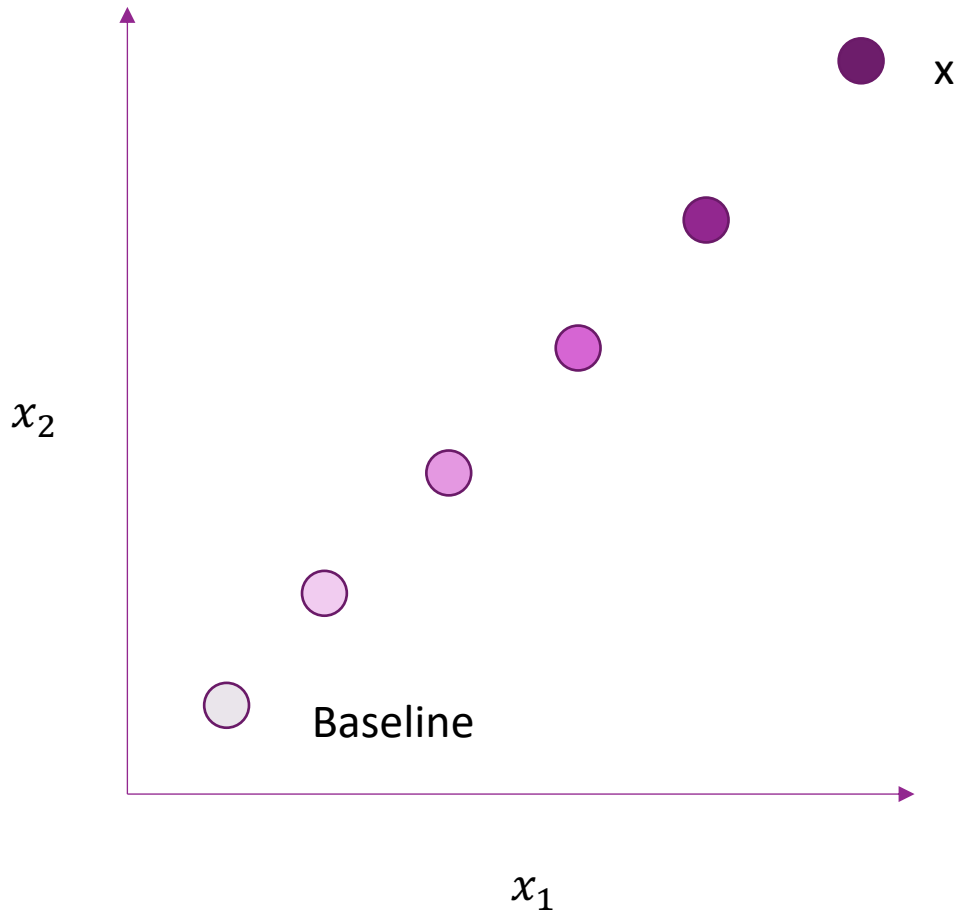
$$\textbf{InputXGradient}(f, 2) = 0 \cdot 2 = 0$$

= → Failed test!

$$\nabla f(x) = \begin{cases} 1 \; if \; x < 1 \\ 0 \; if \; x > 1 \end{cases} = \max(0, sign(1 - x))$$

$$sign(x) = \begin{cases} -1 \; if \; x < 0 \\ 0 \; if \; x = 0 \\ 1 \; if \; x > 0 \end{cases}$$

Integrated Gradients



- **Compare x with a baseline**
  - No information, e.g., zero vector
- **Interpolate** between the point of this baseline and the input x
- Take the gradient with respect to each interpolated input
- Compute the average of these gradients
  - Give us the feature importance

Intuition: total contribution of input features as we move from baseline/nothing to the actual input.

Integrated Gradients

- Let x be the instant to explain and x' a baseline input.
- Let α be interpolation constant to perturb features by

$$IntegratedGrads_i(x) = (x_i - x_i') \times \int_{\alpha=0}^{1} \frac{\partial f\left(x' + \alpha \times (x - x')\right)}{\partial x_i} da$$

Let k be a scaled feature perturbation constant and m the number of steps

$$IntegratedGrads_i^{approx}(x) = (x_i - x_i') \times \sum_{k=1}^{m} \frac{\partial f\left(x' + \frac{k}{m} \times (x - x')\right)}{\partial x_i} \times \frac{1}{m}$$

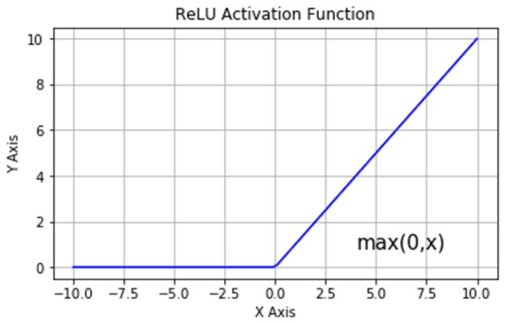
Approx: numerical approximation instead of the integral

Integrated Gradients - steps

$$IntegratedGrads_i^{approx}(x) = \overset{5}{(x_i - x_i')} \times \overset{4}{\frac{1}{m}} \times \overset{3}{\sum_{k=1}^{m}} \overset{2}{\frac{\partial f(x' + \frac{1}{m} \times (x - x'))}{\partial x_i}}$$

1. Consider multiple perturbations
2. Interpolate inputs between baseline x' and the input x
3. Compute the gradients for each interpolated input
4. Compute the average – approximation of the integral
5. Scale to remain in the original space

Integrated gradients and sensitivity



- **Example**
  - f(x) = 1-ReLU (x) = 1-max(0, 1-x)
  - f(0) = 1-max(0, 1-0) = 0
  - f(2) = 1-max(0, 1-2) = 1

$$\nabla RELU'(x) = \begin{cases} 1 \; if \; x > 0 \\ 0 \; if \; x \leq 0 \end{cases}$$

$$\nabla f(x) = \begin{cases} 1 \; if \; x < 1 \\ 0 \; if \; x > 1 \end{cases} = \max(0, sign(1 - x))$$

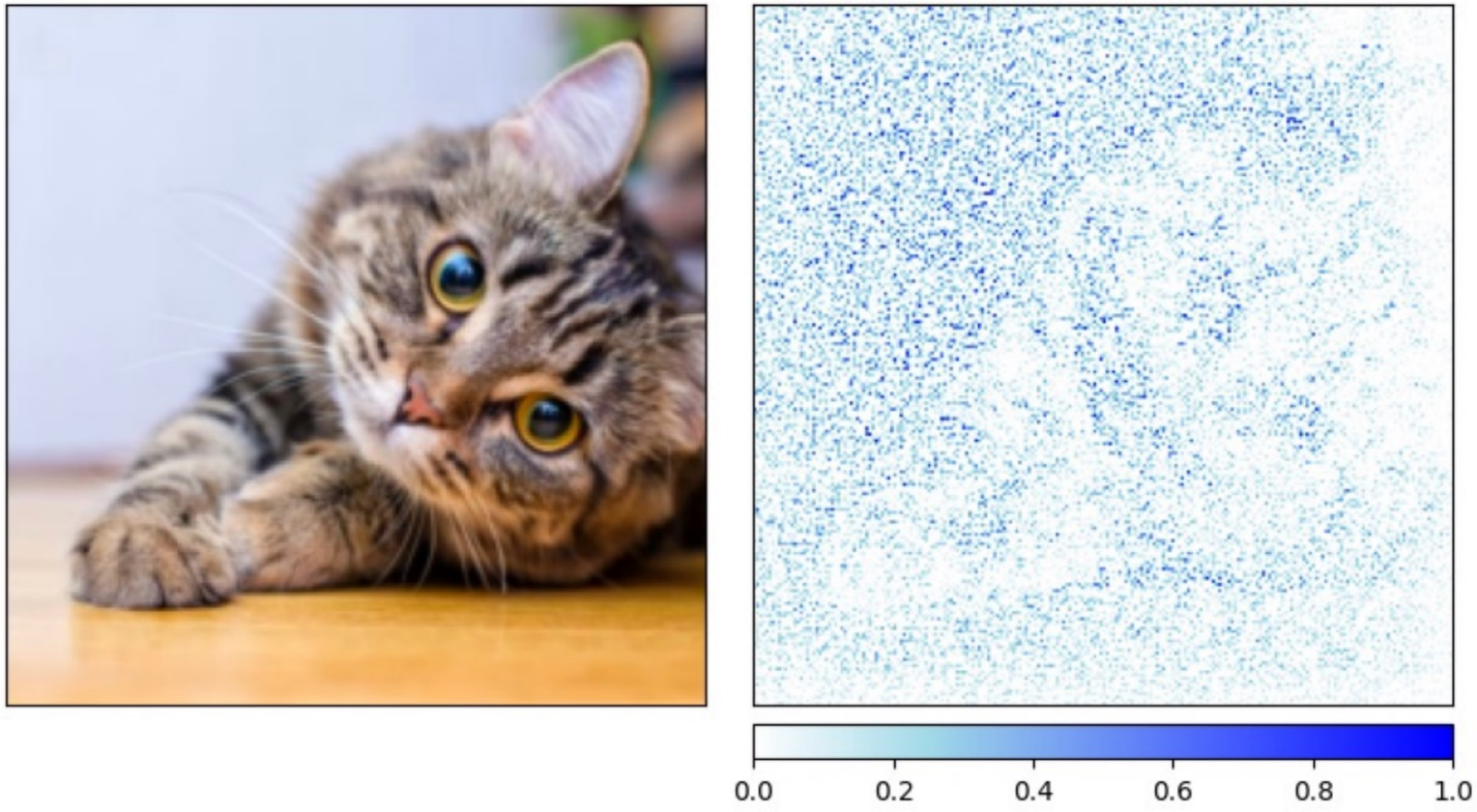
Since we have different outputs, for the sensitivity axiom, we should have **different attributions**

IntegratedGradient$(f, x, x') = (x_i - x_i') \times \sum_{k=1}^{m} \frac{\partial f(x' + \frac{k}{m} \times (x - x'))}{\partial x_i} \times \frac{1}{m}$

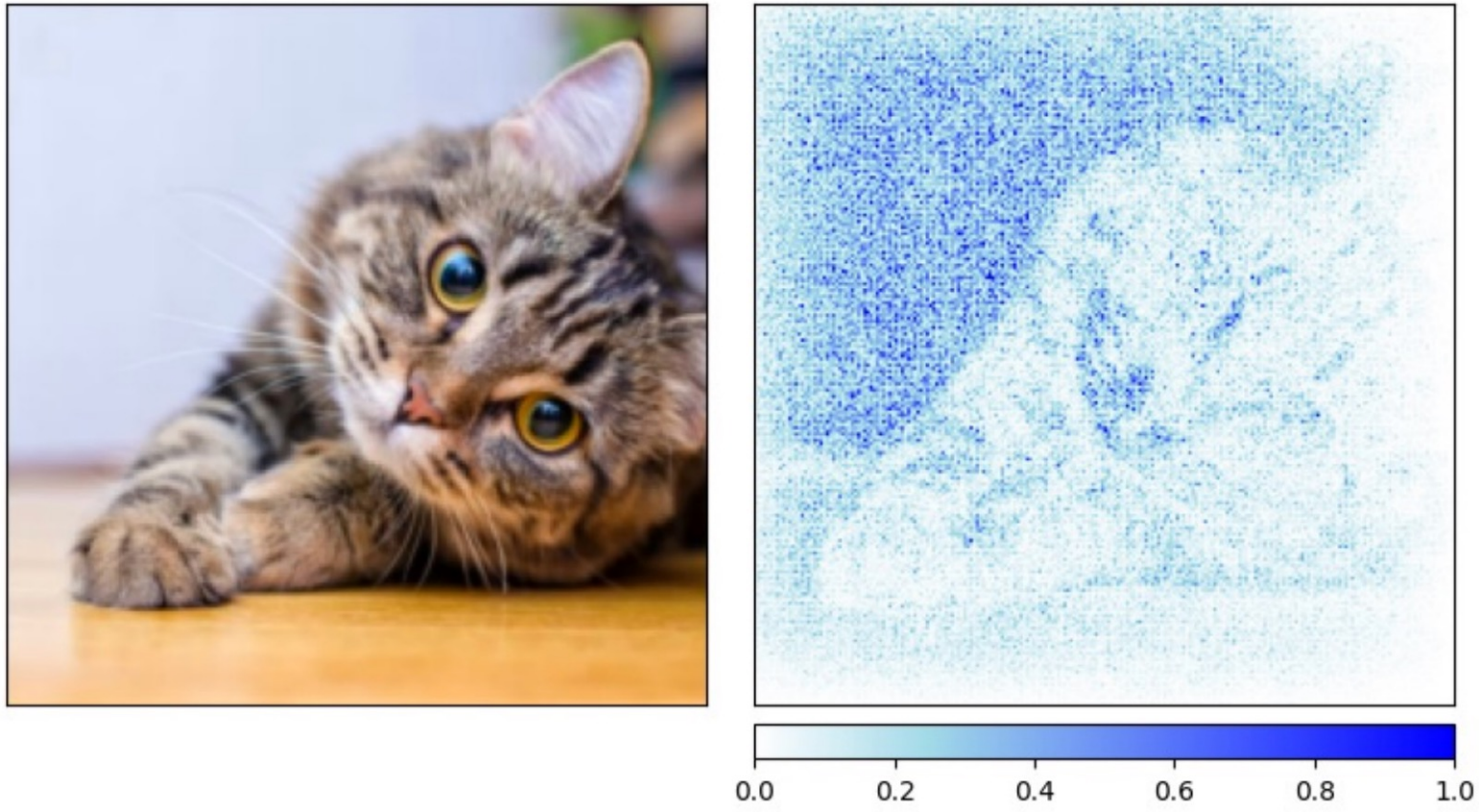
IntegratedGradient$(f, 2, 0) = (2 - 0) \frac{1}{m} \sum (\max(0, sign(1 - 0.00) + \max(0, sign(1 - 0.02)) + .. + \max(0, sign(1 - 2)) \approx 1$

IntegratedGradient $(f, 0,0) \approx 0$

Integrated Gradients - Example



Integrated Gradients + SmoothGrad - Example



It is more computational expensive! Locally only on 5 samples..

Advantages

- Efficiency
- Many gradient-based methods are computationally efficient
- Multiple approaches
- Effective visualization via saliency maps

Limitations

- Some methods do not satisfy the sensitivity axiom
  - Methods insensitive to model and data.
  - Explainers or edge detectors simply highlight color changes in images?

- Sensitivity to Perturbations
  - Methods may be sensitive to small changes in input data, leading to unstable explanations

- Gradient Vanishing/Saturating

- Different approach, different explanations..
  - Which one to trust?
  - Need for evaluation approaches..!