Explainability of Neural Networks (XAI)

CPSC680: Trustworthy Deep Learning

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Readings

- Readings are updated on the website (syllabus page)
- **Lecture 4 readings**:
  - https://arxiv.org/abs/1703.01365

Content

- Introduction to Explainability
- Explainability Settings
- Explainable Models
- Gradient-based Methods
- Methods using Surrogate Models
- Perturbation Methods

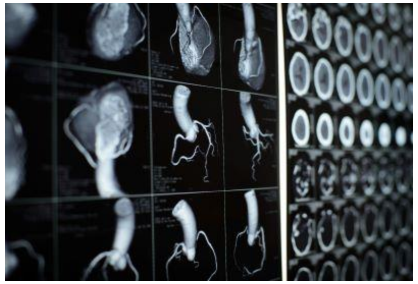
Content

Explainability

- The **black-box** nature of deep learning makes it a **major challenge** to:
  - Understand what is learned by the ML model
  - Extract insights of the underlying data we are trying to model
- Explainable Artificial Intelligence (XAI) is an umbrella term for any research trying to solve the **black-box problem for AI**
- Why is it useful?
  - Enable users to **understand the decision-making** of the model
  - **Gain trust from human users** of the deep learning system
- Simple-to-read guide: 2004.14545.pdf (arxiv.org)

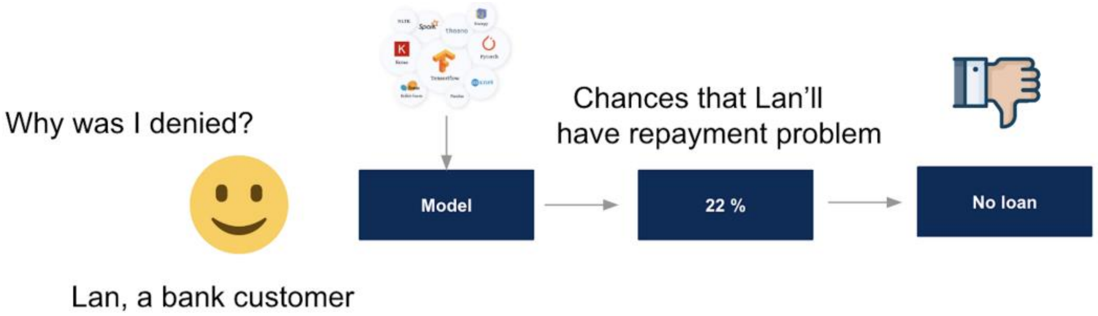
Goal of Explainability

- Model’s behavior might be different from the underlying phenomenon
- **Explaining ground truth phenomenon**



What are the characteristics of certain diseases in terms of imaging?

- **Explaining model predictions**



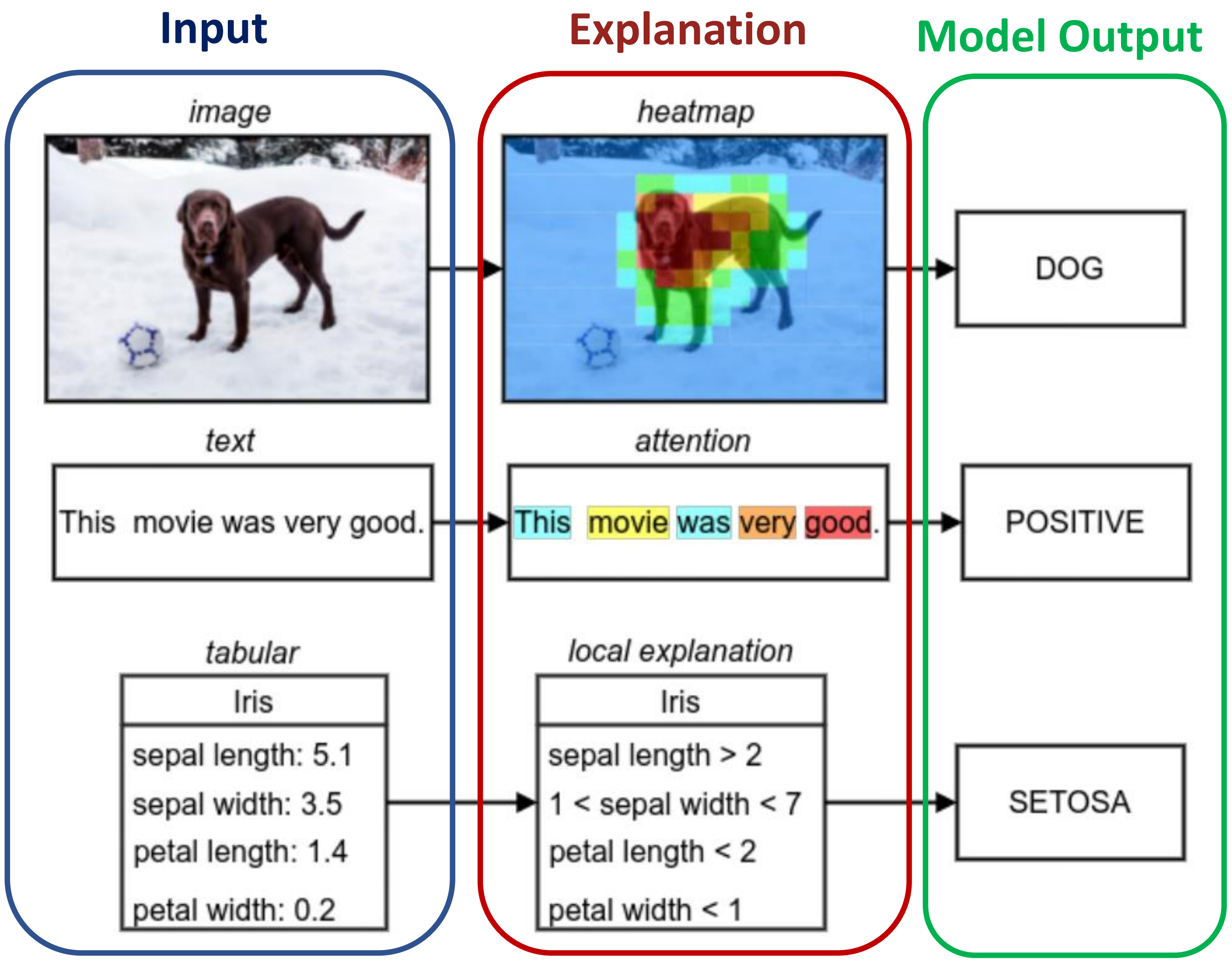
Why does the model recommend no loan for Person X?

Forms of Explanation

example of image data:

example of text data:

example of tabular data:

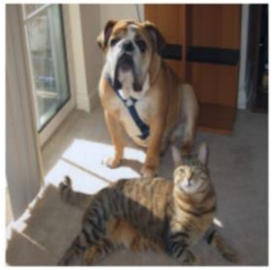


Example: Computer Vision

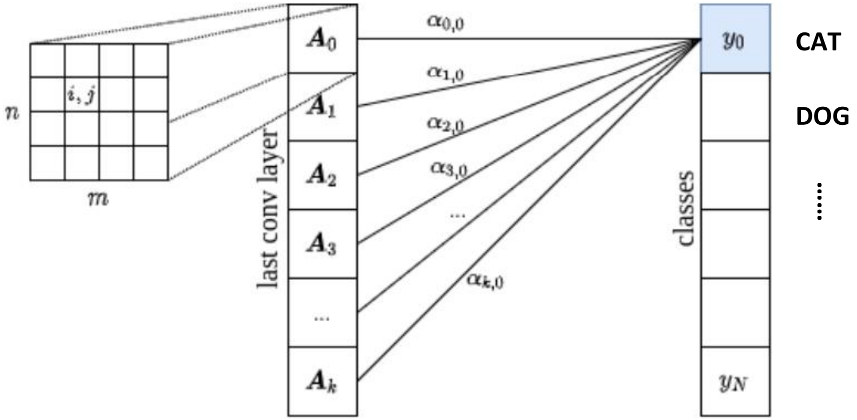
Explanation in Computer Vision:

A particular region of the image **displays the predicted class of objects** (cat / dog in this example)

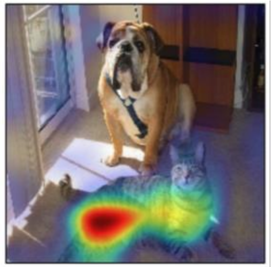
Importance scores on pixels



original graph

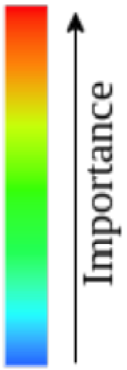


computation process of **CNN** and the prediction



explanation of “cat”

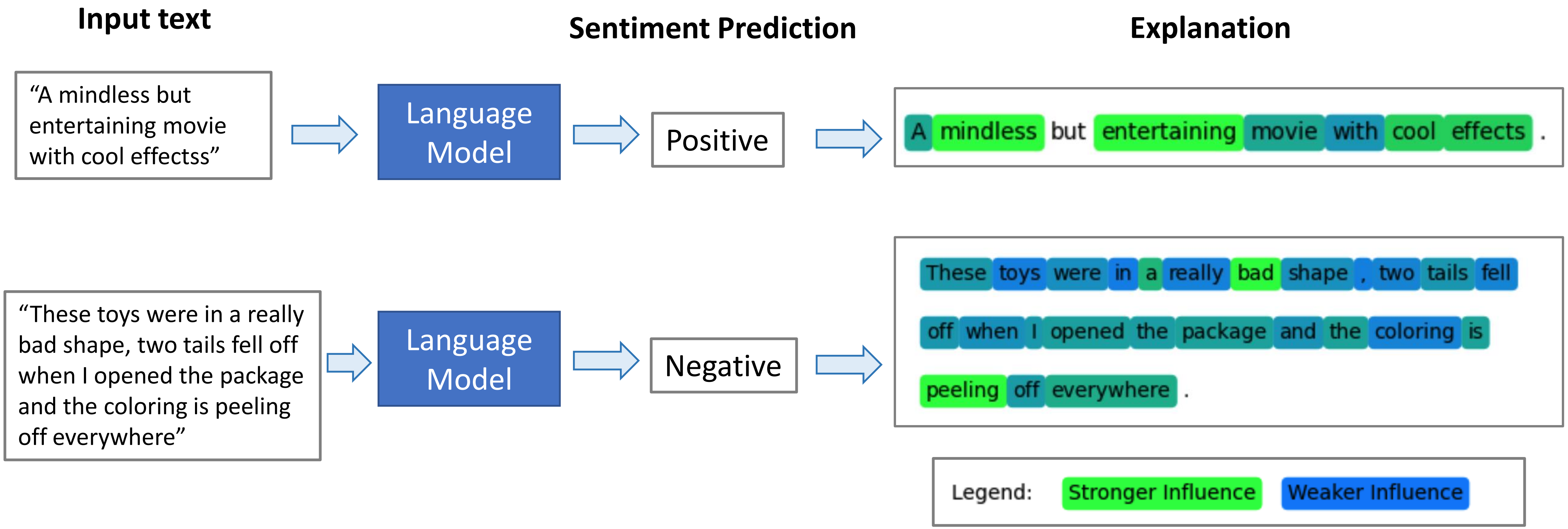
explanation of “dog”



Selvaraju, Ramprasaath R., et al. "Grad-cam: Visual explanations from deep networks via gradient-based localization."

Example: Natural Language Processing

Explanation in Natural Language Processing: **important tokens** that lead to the prediction



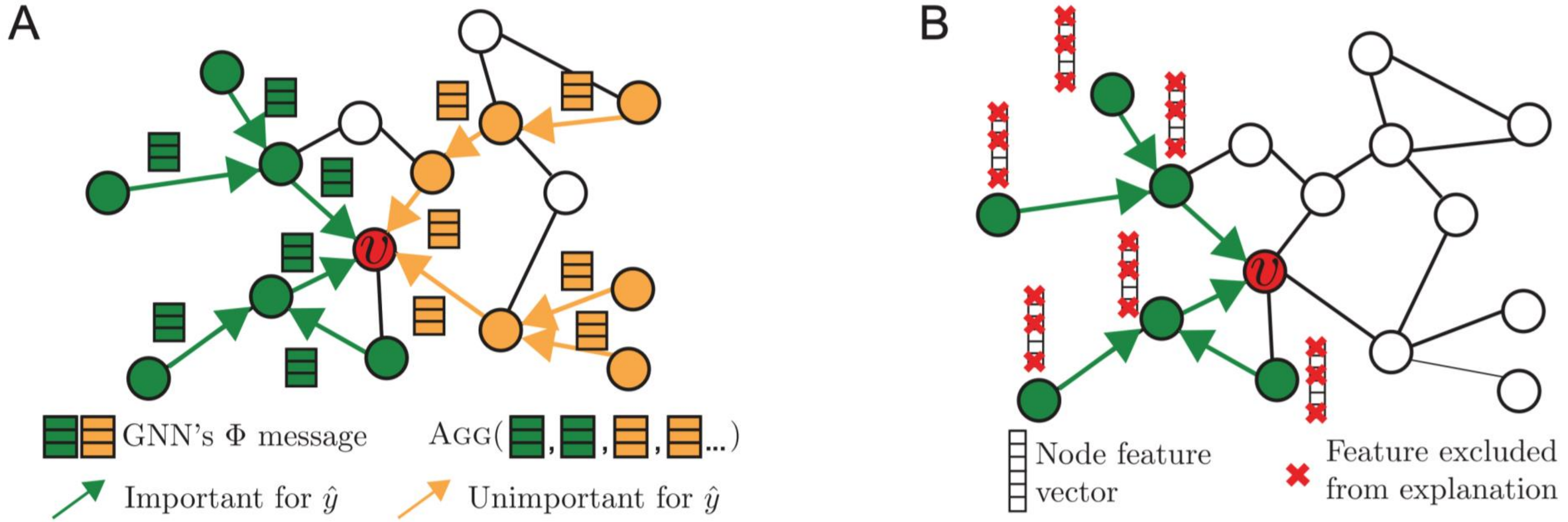
Dunn, Andrew, Diana Inkpen, and Răzvan Andonie. "Context-Sensitive Visualization of Deep Learning Natural Language Processing Models."

Example: Graph Learning

Explanation in Graph Learning: an important **subgraph structure** and a small **subset of node features** that play a crucial role in GNNs prediction

Explanations for prediction at **node v**

A: Import subgraph structure **B: important subset of features**



Ying, et al. "Gnnexplainer: Generating explanations for graph neural networks."

Reasons for Explainability

Why do we need Explainability?

- **Trust**: Explainability is a prerequisite for humans to **trust and accept** the model's prediction.
- **Causality**: Explainability (e.g. attribute importance) conveys **causality** to the system's target prediction: attribute X causes the data to be Y
- **Transferability**: The model needs to convey an understanding of decision-making for humans before it can be **safely deployed to unseen data**.
- **Fair and Ethical Decision Making**: Knowing the reasons for a certain decision is a societal need, in order to perceive if the prediction **conforms to ethical standards.**

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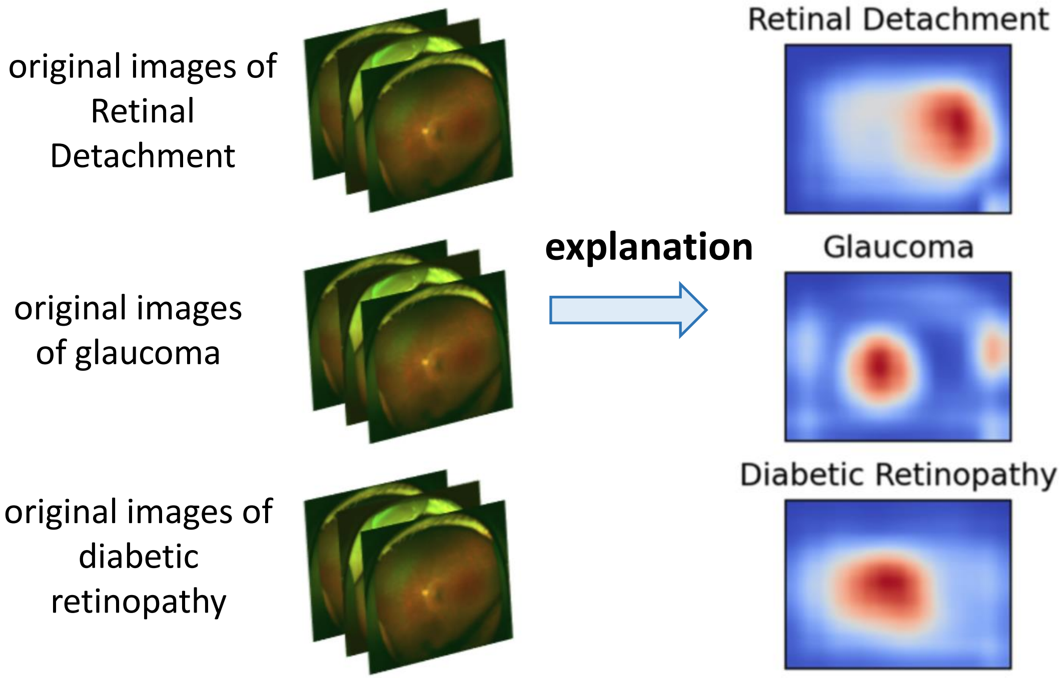
Explainability Settings (1)

By target:

- **Instance-level:** a **local** explanation for a single input x and the prediction $\hat{y}$
  - identify the important components of individual instances
- **Model-level:** a **global** explanation for a specific dataset D or classes of D
  - provide **high-level insights** into the model's decision-making behaviors



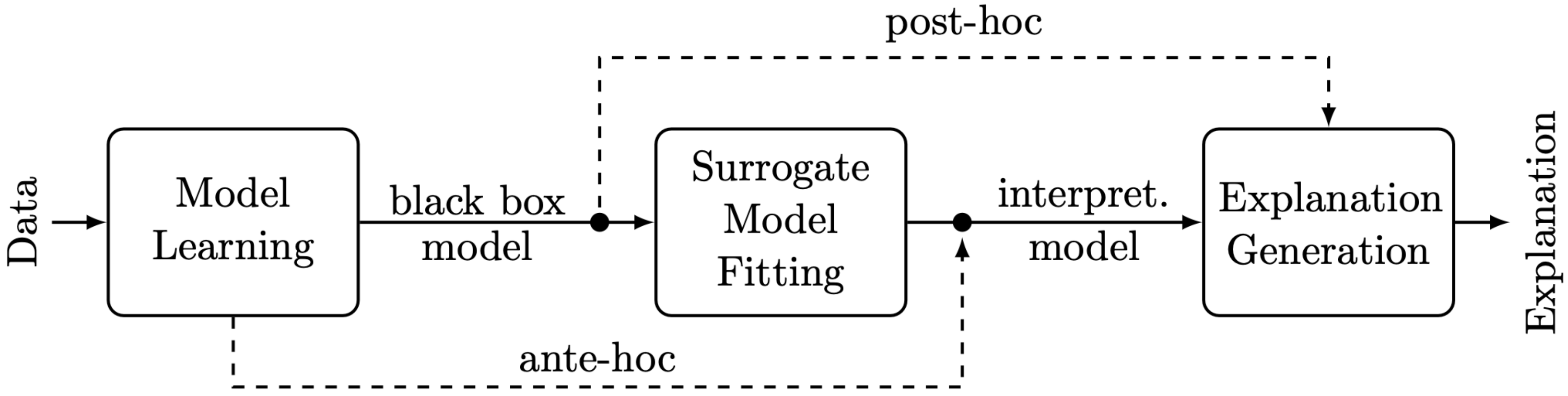
Example: model-level explanations for each class

Engelmann, Justin, Amos Storkey, and Miguel O. Bernabeu. "Global explainability in aligned image modalities."

Explainability Settings (2)

By stages:

post-hoc: Explainability is created after model creation **(for black-box models)**



ante-hoc: Explainability is **built-in** from the beginning of the model creation **(for intrinsically interpretable / white-box models)**

By applicability of the method:

model-specific: the machanism for generating explanation is **model-dependent** and works only for a specific model.

model-agnostic: the machanism for generating explnation is **applicable** for many or even all model classes

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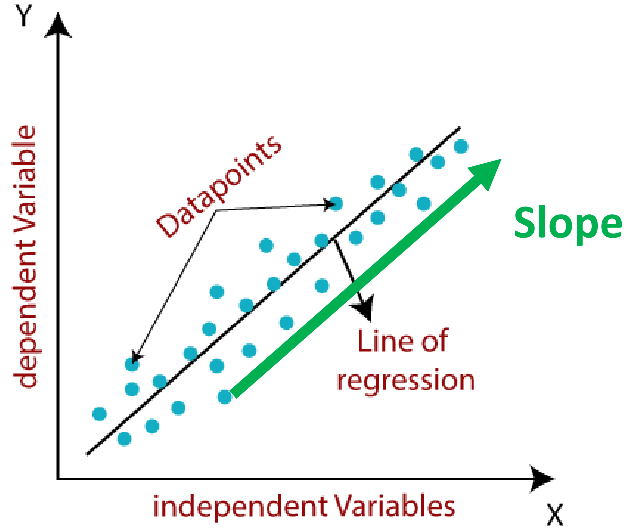
Explainable Models: Linear regression

- **Linear regression**
  - **Slope is explainable** (how much does one variable affects a prediction)
  - $y = w_1x_1 + w_2x_2 + w_3x_3 + \cdots$

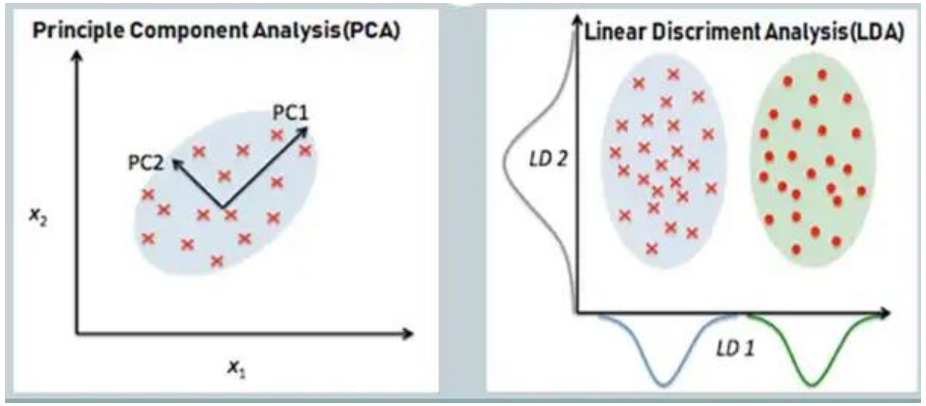
prediction weights features



- Each feature has an associated **weights**, indicating its **importance**
  - "A change of Δx amount to feature x_1 will result in increase of prediction by Δy

Explainable Models: Dimension Reduction

- **Dimension reduction**
  - Dimension reduction allows us to visualize the training data distribution



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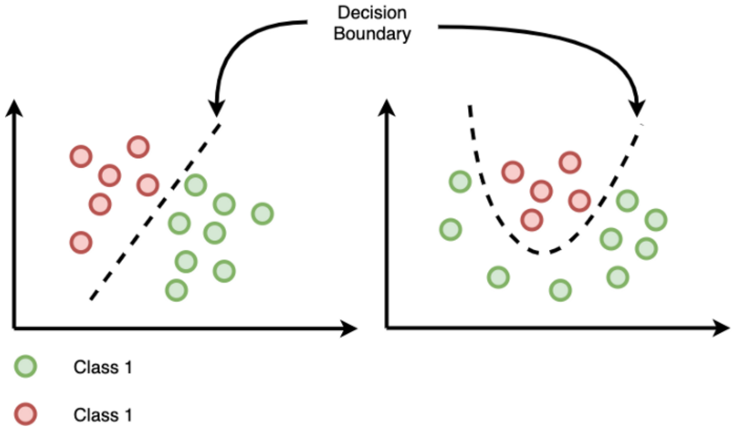
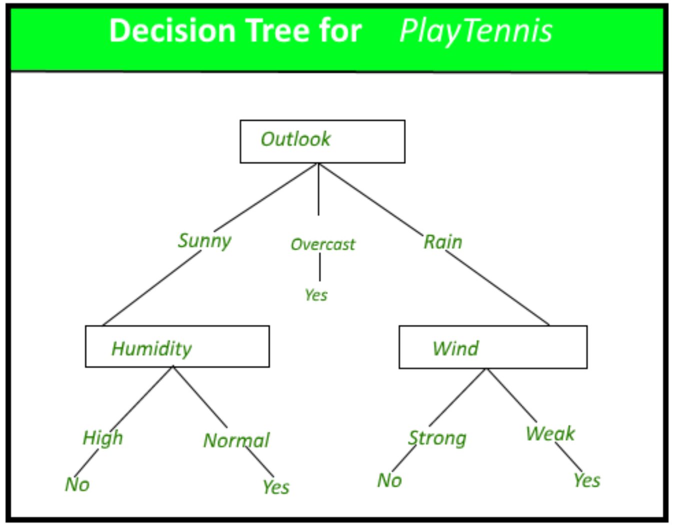


Source

- Decision boundary can be visualized and understood
  - Instances at the boundary characterizes how different classes are different

Explainable Models: Decision Tree

- **Decision trees** are very explainable!
- On every node of the decision tree, we understand a criteria for prediction
- We can perform statistics for each decision node
  - E.g. if the condition of the node is met, **80% of the instances will be classified as being positive**



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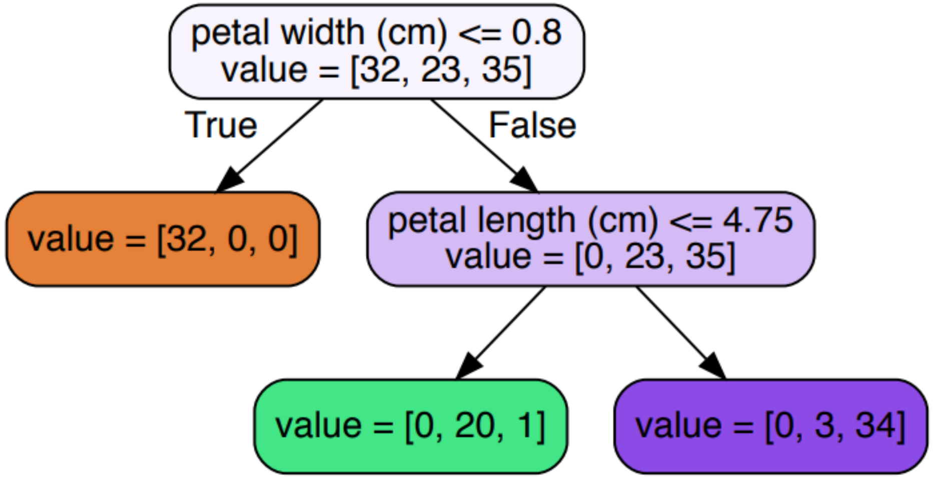

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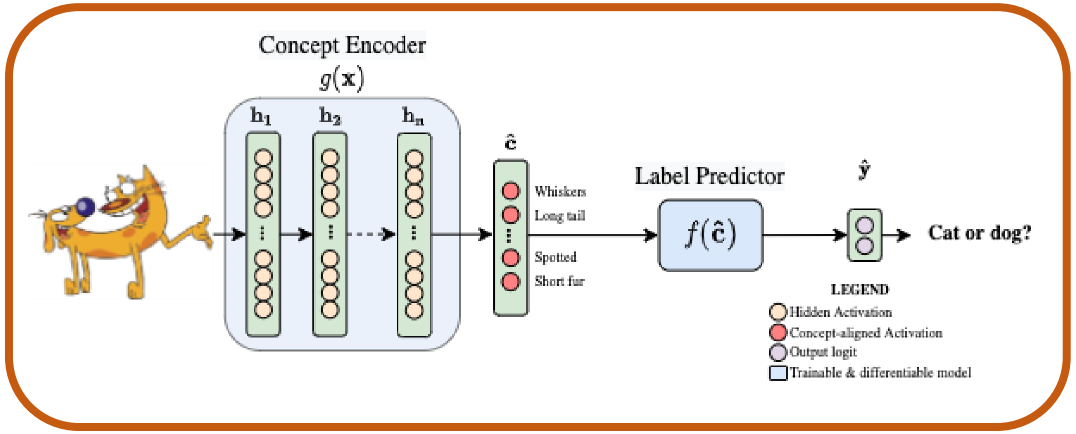
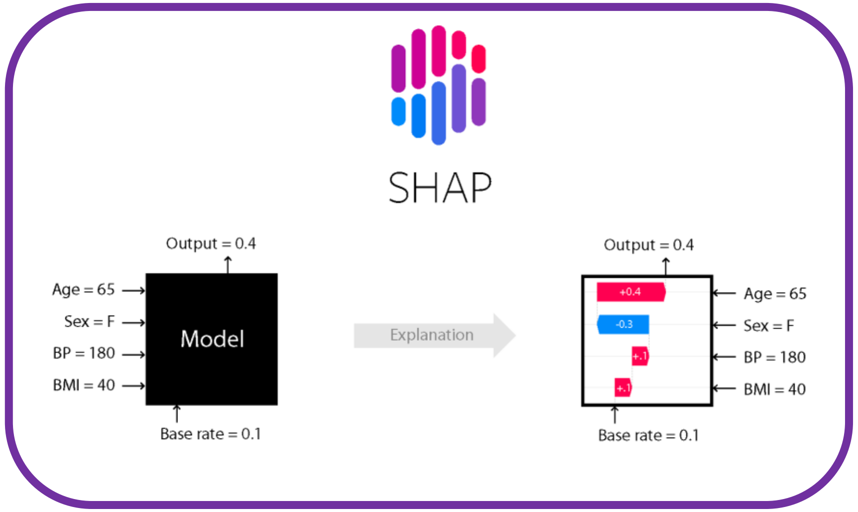
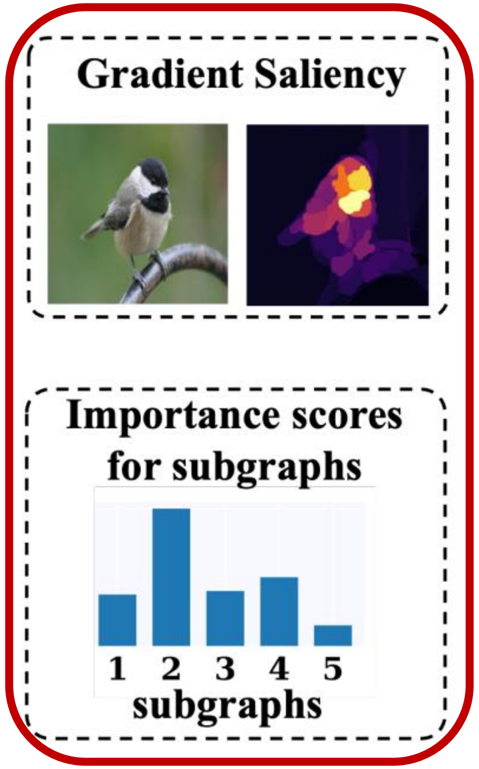
Explainable Characteristics

- What makes model explainable?
  - **Importance** values (for pixels, features, words, nodes in graphs …)
  - **Attributions**: straightforward relationships between prediction and input features
  - Encourage **concepts** and prototypes







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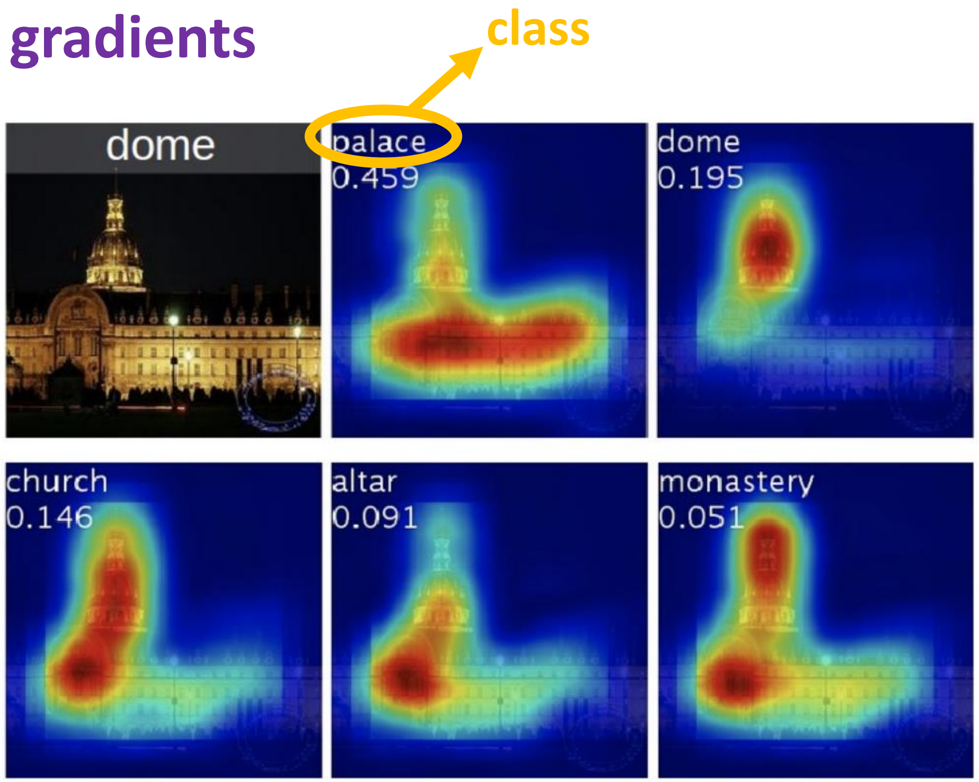
Gradient-based Explanation

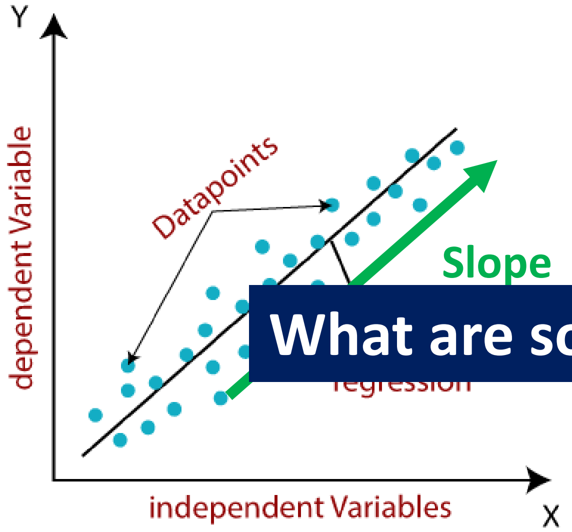
- **Gradient-based methods** identify the **saliency of input features** based on gradient signals passed from output to **input features**
- **Intuition: important features tend to have high gradients**
- **We typically care about magnitude**

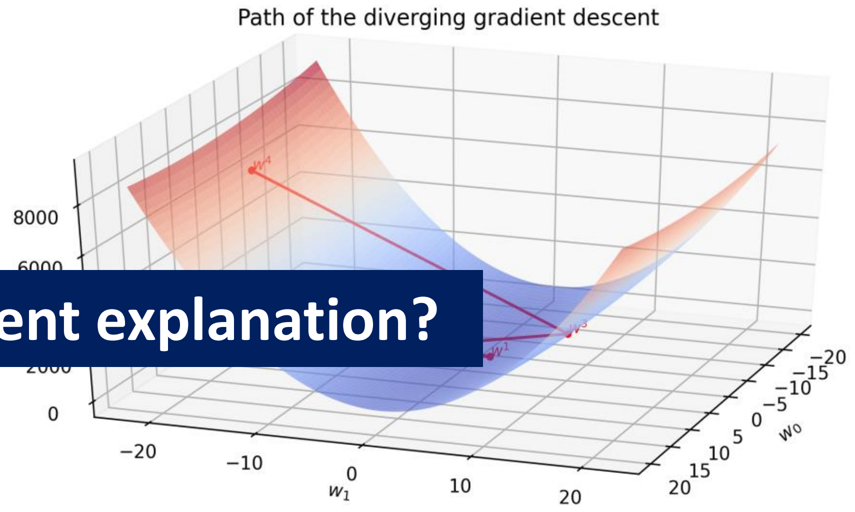


Saliency Map (in the form of a heatmap) highlights the discriminative regions, revealing model's decision-making logic

Zhou, Bolei, et al. "Learning deep features for discriminative localization."

Why Gradients?





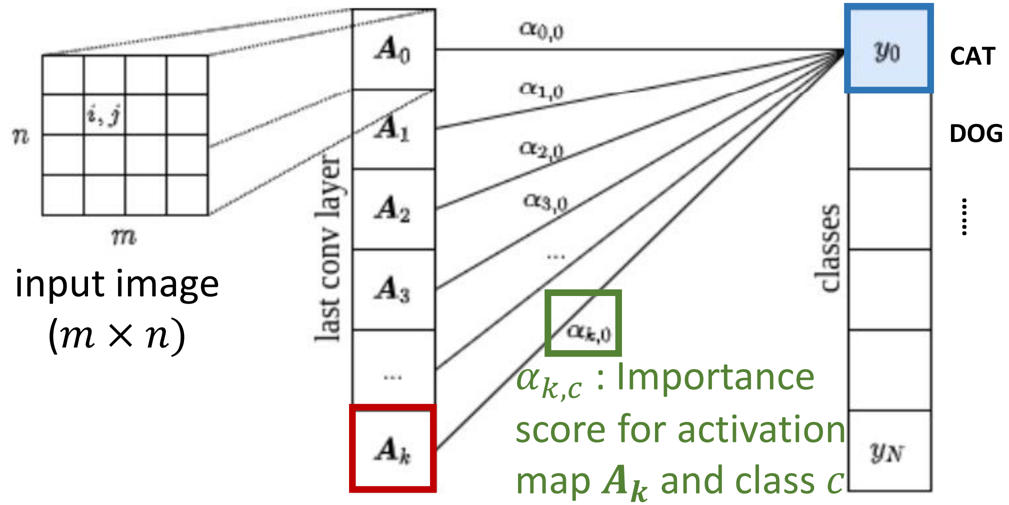
What are some problems with Gradient explanation?

- **The optimization landscape** of deep networks is very complex and a global scope is no longer possible
- Gradient is a **local approximation** of the slope
- Each **dimension** of the gradient vector can indicate how much the prediction is impacted by the input

Grad-CAM (1)

- **Gradient-weighted Class Activation Map (Grad-CAM):**

y_c :the score for class c (before the softmax)



input image ($m \times n$)

$\alpha_{k,c}$: Importance score for activation map A_k and class c

A_k: feature activation map with size $m \times n$

Architecture of CNN

gradients of the output w.r.t. the last convolutional layer

Importance score $\alpha_{k,c}$ for activation map A_k and class c:

$$\alpha_{k,c} = \frac{1}{m \cdot n} \sum_{i=1}^{m} \sum_{j=1}^{n} \boxed{\frac{\partial y_c}{\partial A_{k,i,j}}}$$

$A_{k,i,j}$: value at (i, j) in the $m \times n$ feature map A_k

Saliency map for class c:

$$map_c = \mathrm{ReLU}\Big(\sum_k \alpha_{k,c} A_k\Big)$$

map_c has **the same dimension as the input image**

Why ReLU?

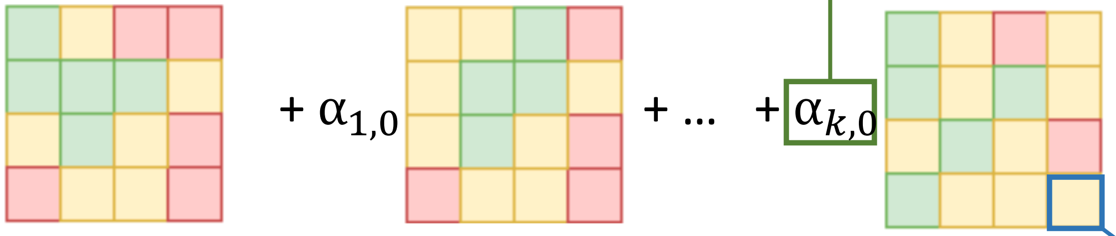
Grad-CAM (2)

Example: class 0 is "cat"

Important score $\alpha_{k,0} = \frac{1}{m \cdot n} \sum_{i=1}^{m} \sum_{j=1}^{n} \frac{\partial y_0}{\partial A_{k,i,j}}$

Saliency map of "cat" :
(of the same size as the original image)

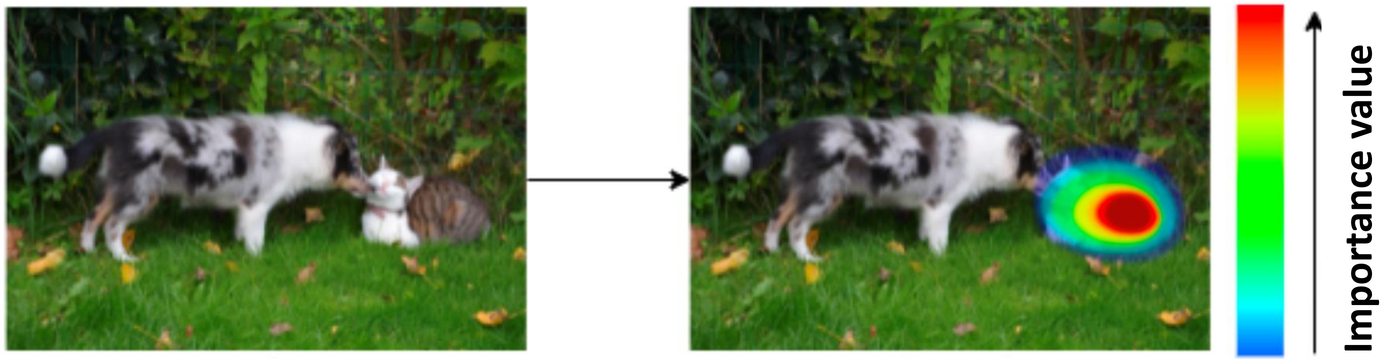
$$map_0 = \mathrm{ReLU}(\alpha_{0,0} A_0 + \alpha_{1,0} A_1 + \ldots + \boxed{\alpha_{k,0}} A_k)$$



A_k: feature activation map with size $m \times n$

corresponds to a **pixel** on the original image

Visualization of the
Saliency map of "cat" :



Original Image **Grad-CAM Importance**

Grad-CAM: Evaluation

- **Localization Evaluation:**
  - Given an image, first obtain class **predictions from the network**
  - Generate Grad-CAM **maps** for **each of the predicted classes**
  - **Binarize** with **threshold of 15% of max intensity**

Localize the flying kites (despite their small sizes)

A group of people flying kites on a beach

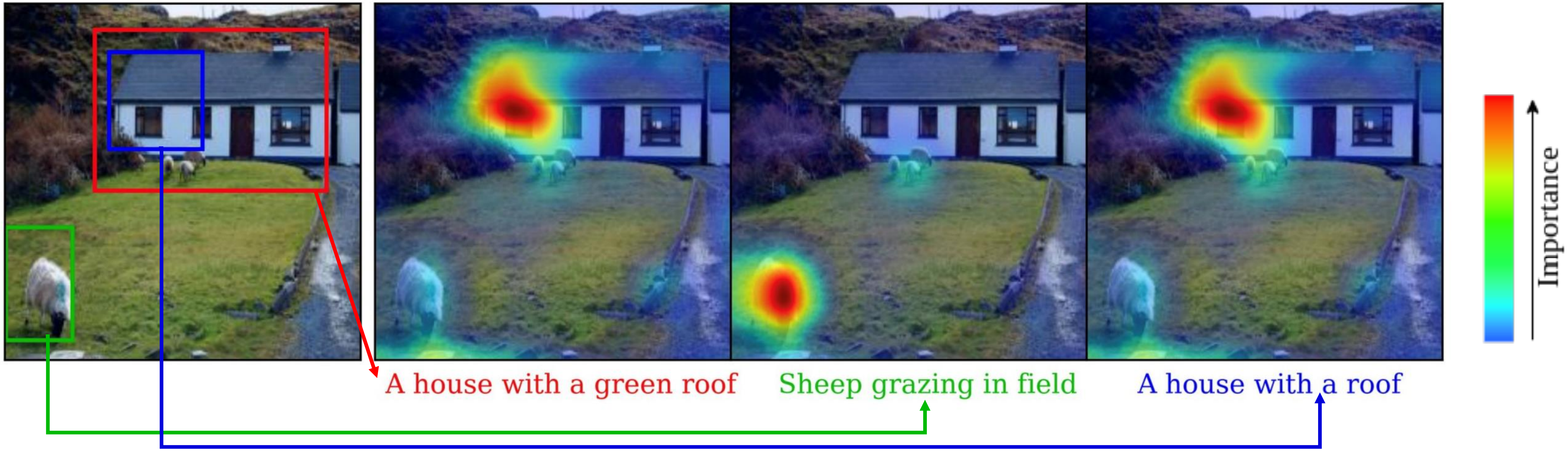
A man is sitting at a table with a pizza

Visual Explanations highlight image regions that are important for producing the captions

Localize the man and the pizza (ignoring the woman)

Grad-CAM:Comparison to DenseCap

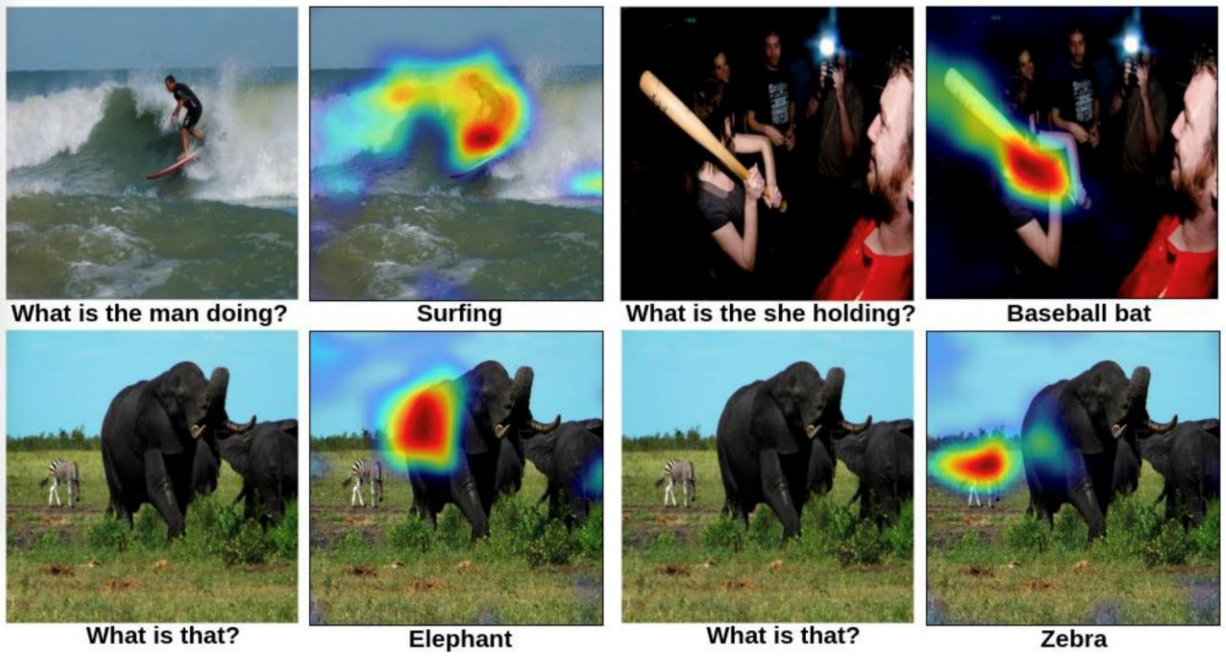
Localizations of a global caption generated by Grad-CAM:



DenseCap: jointly localizes and generates captions for salient regions in each image.
Localization of DenseCap: **bounding boxes** for regions of interest
Localization of Grad-CAM: more **fine-grained** details **with importance values**

Grad-CAM: VQA Evaluation

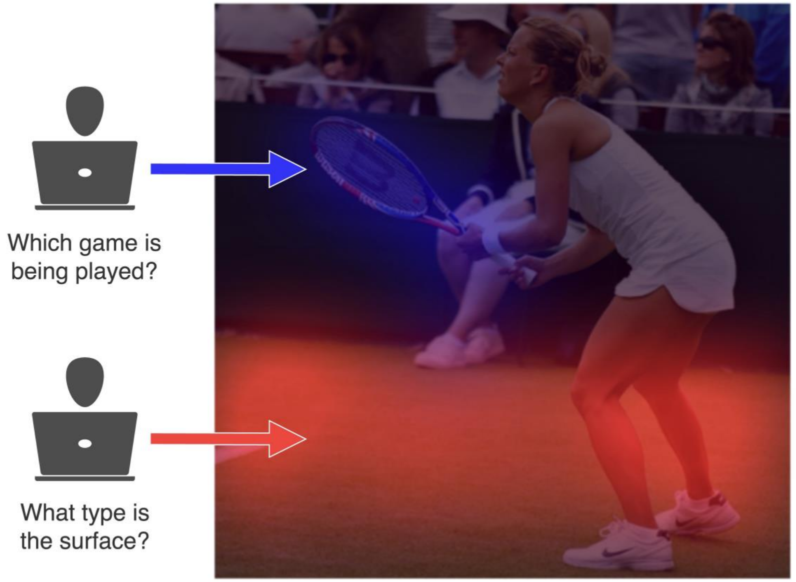
- **Visual Question Answering (VQA):** VQA pipelines consist of **a CNN to process images** and **a language model for questions**. The model will predict the answer to the question.
- Grad-CAM: **visualize salient regions** over the image the **explain the answer**



Grad-CAM: Comparison to Human Attention

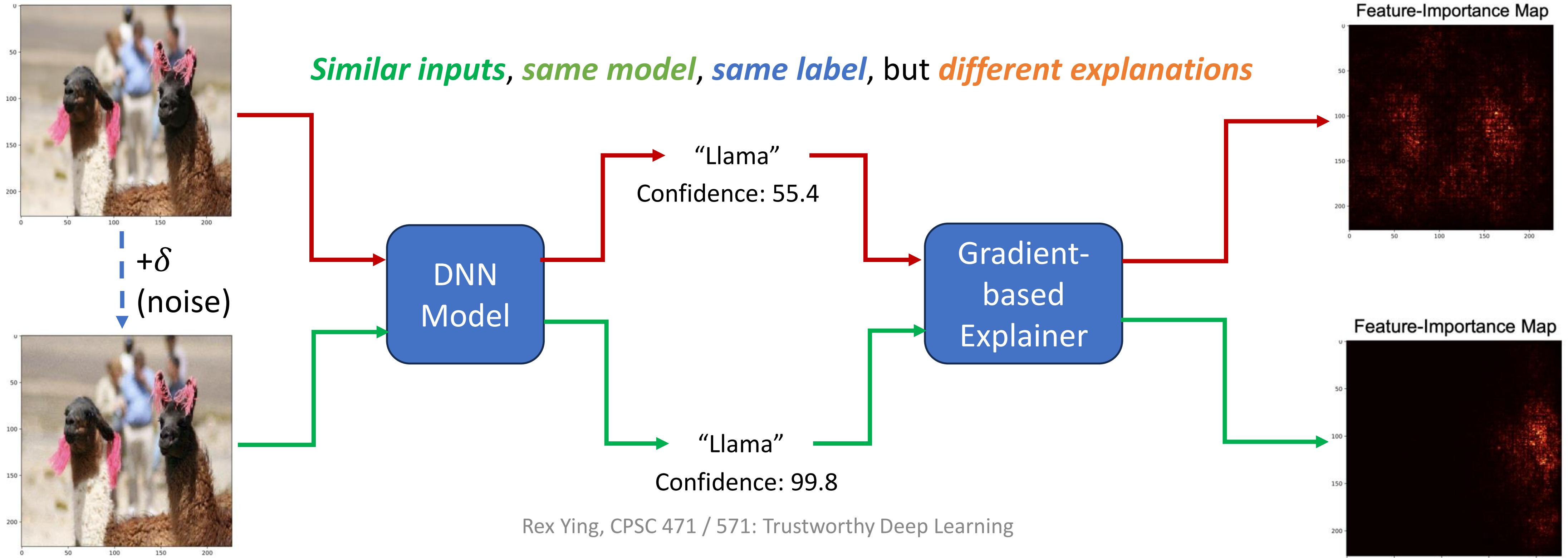
- Use the **rank correlation** to compare the **Grad-CAM visualizations** and **Human attention maps** over visual question answering pairs
- **Correlation: 0.136**
- statistically higher than chance or random attention maps (**zero correlation**)

Human Attention:
Das et. al collected human attention maps for a subset of VQA dataset.
These maps have **high intensity** where **humans looked** in the image in order to answer a visual question.



Sensitivity of Gradients

- Saliency maps using a vanilla gradient are sensitive to small perturbations in the input instance.
  - Adding a small perturbation may change the interpretation significantly, even though the prediction is unchanged.



Integrated Gradients (1)

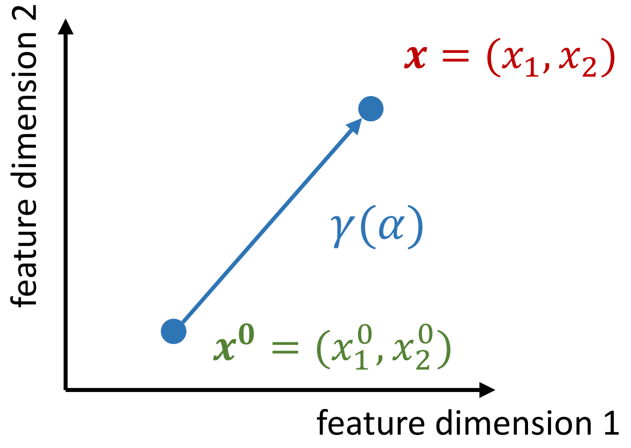
- **Integrated Gradients (IG):** given a **reference (baseline)** input $\boldsymbol{x}^{\mathbf{0}}$, the integrated gradient of the model f w.r.t. the i-th feature x_i for an input $\boldsymbol{x}$:

$$IG_i(\boldsymbol{x}) = \left(x_i - x_i^0\right)\int_0^1 \frac{\partial f\left(\boldsymbol{x}^0 + \alpha(\boldsymbol{x} - \boldsymbol{x}^0)\right)}{\partial x_i} d\alpha$$

  - $\boldsymbol{x}$: input; $\boldsymbol{x}^{\mathbf{0}}$: baseline input; x_i: i-th feature of $\boldsymbol{x}$; x_i^0: i-th feature of $\boldsymbol{x}^{\mathbf{0}}$
  - **Integral path:** $\gamma(\alpha) = \boldsymbol{x}^{\mathbf{0}} + \alpha \times (\boldsymbol{x} - \boldsymbol{x}^{\mathbf{0}}), \alpha \in [0,1]$
- The reference (baseline) input: **Comparison to saliency?**
  - a black image or a zero embedding vector

IG_i: sensitivity of f to changes in the i-th feature from x^0 to x along $\gamma(\alpha)$ in direction i
Higher IG_i $\Longleftrightarrow$ Higher importance of the i-th feature

Example of 2-dimensional features



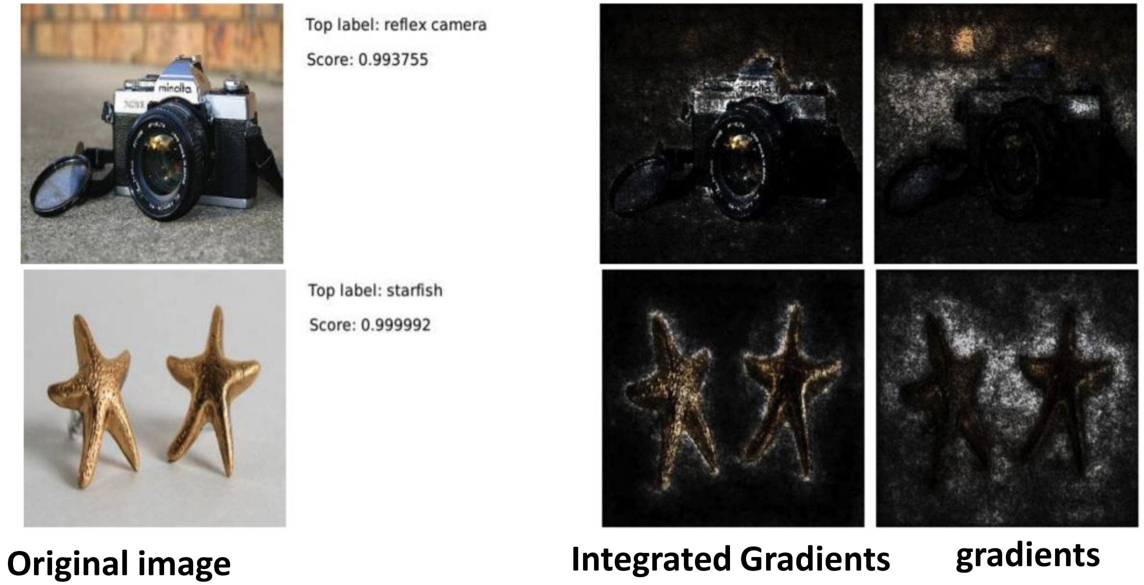
Integrated Gradients (2)

- IG can be **approximated** by a Riemann summation of the integral

$$IG_i(\boldsymbol{x}) \approx (x_i - x_i^0)\frac{1}{M}\sum_{k=1}^{M} \frac{\partial f\left(\boldsymbol{x}^0 + \frac{k}{M}(\boldsymbol{x} - \boldsymbol{x}^0)\right)}{\partial x_i}$$

  - M is the number of steps in the Riemann approximation of this integral (recommended M: 20 to 300 steps)

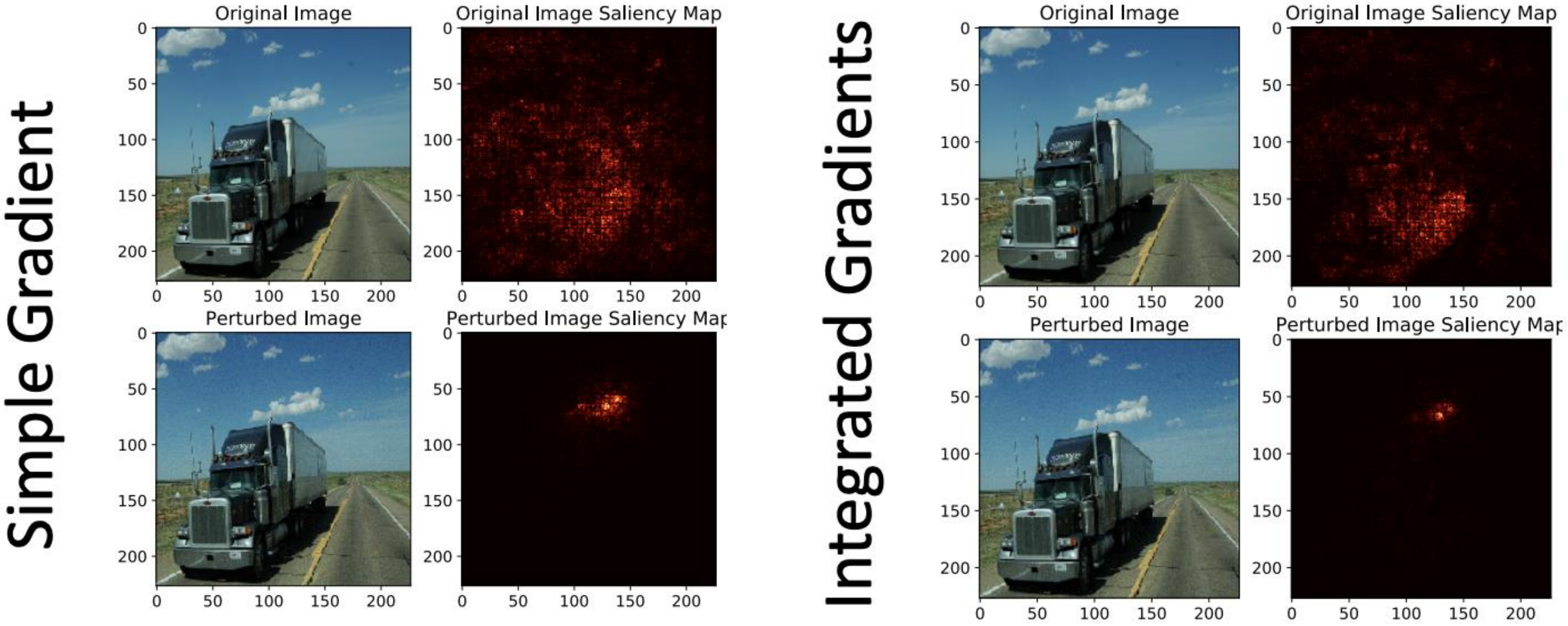
Observation: Integrated Gradients can better reflect distinctive features of the input image



Sundararajan, Mukund, Ankur Taly, and Qiqi Yan. "Axiomatic attribution for deep networks."

Sensitivity of Integrated Gradients

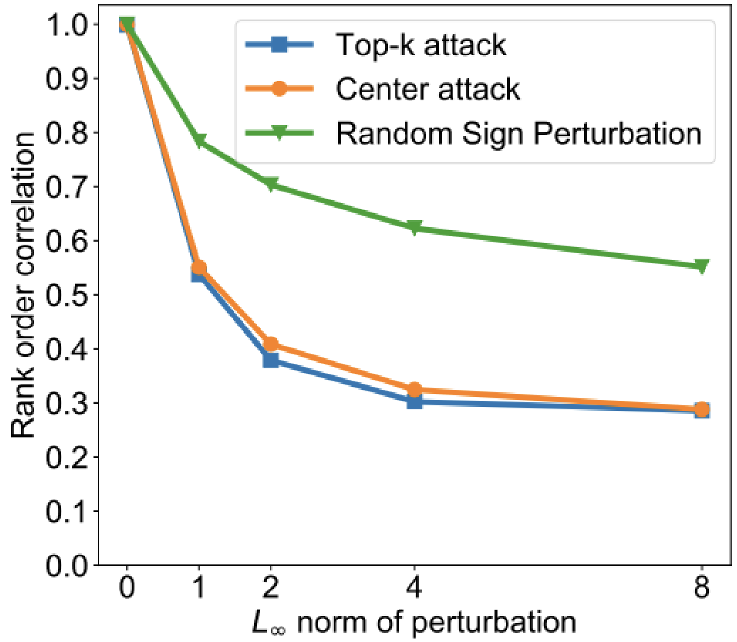
- Integrated Gradients is still vulnerable to adversarial noise.



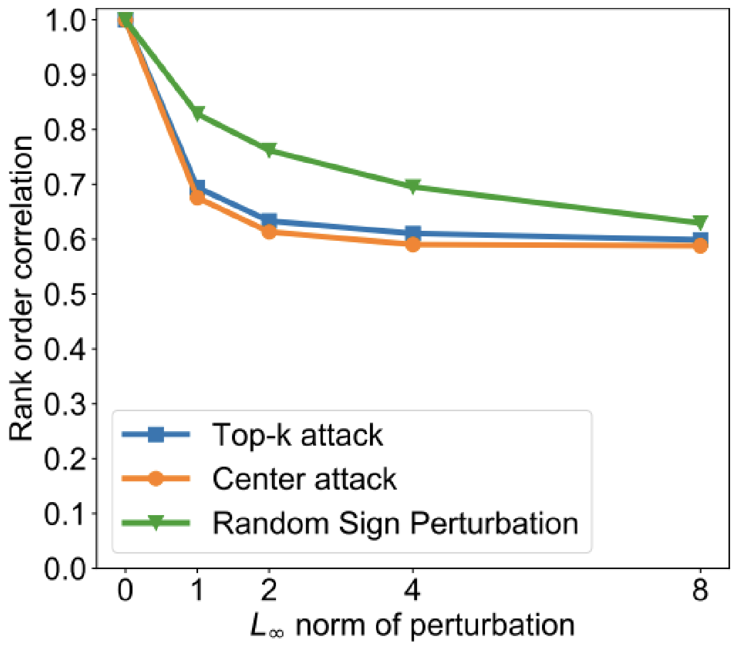
Sensitivity of Integrated Gradients

- Integrated Gradients is still vulnerable to adversarial noise.
- However, Integrated Gradients is **more robust** than Vanilla Gradient-based methods

Simple Gradients



Integrated Gradients



The y-axis is the correlation of the Saliency map at x_0 and at perturbed input $x_0 + \delta$

Comparison of IG and Grad-CAM

- IG is more **flexible** in the setting than Grad-CAM
  - Adjustable parameters: baseline input, number of steps M, etc.
- IG satisfies the **"sensitivity" atom** by introducing a baseline input
  - **"sensitivity" atom:** if input $\boldsymbol{x}$ differs from $\boldsymbol{x}'$ along feature x_i only, and the prediction $f(\boldsymbol{x}) \neq f(\boldsymbol{x}')$. Then x_i should have a **non-zero importance score**.
  - Grad-CAM might generate the same saliency maps for $\boldsymbol{x}$ and $\boldsymbol{x}'$
- IG is **more robust** to noise / small perturbations on the input
  - The saliency maps of Grad-CAM might change drastically due to small variation of input (e.g., for input $\boldsymbol{x}$ and perturbed input $\boldsymbol{x}'$, the prediction $f(\boldsymbol{x}) = f(\boldsymbol{x}')$, the saliency maps differ greatly)
- IG has **larger computation complexity**.

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- **When do we need black-box explainability?**
- **How should we tackle black-box explainability?**

Perturbation-based Explanation

- **Perturbation methods**
  - **Post-hoc, model-agnostic** explanation for **black-box models**
  - Use perturbation (altering or removing the input features) to identify features that can greatly influence predictions
  - **Intuition:** the model's performance **decreases dramatically** when the model does not have access to **the most relevant information**.
  - The performance drop can be used to create a **sensitivity heatmap** to visualize the **importance of each portion**

Discussion: How are these techniques related to adversarial attacks?

Principle of Perturbation-based Explanation

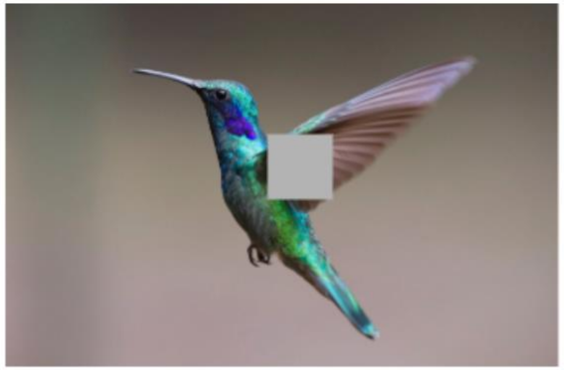
original performance

"Hummingbird" = 0.93

drop: 0.93-0.56=0.37

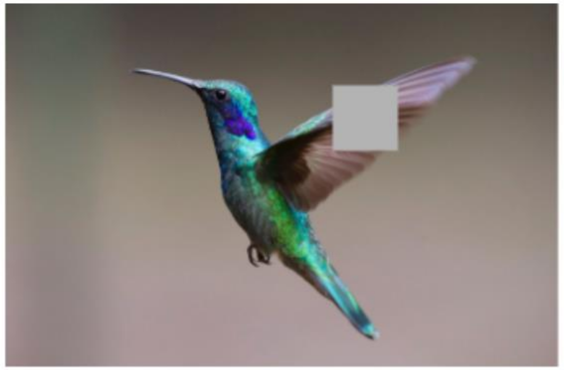
"Hummingbird" = 0.56

drop: 0.93-0.79=0.14



"Hummingbird" = 0.79

drop: 0.93-0.91=0.02



"Hummingbird" = 0.91

Highest performance drop indicates the **highest importance** of this portion

small performance drop indicates a **lower importance**

Use **grey patch** to occlude a portion of input instance

Occlusion Sensitivity

- **Occlusion Sensitivity:** measure the **sensitivity** of the model's output to **occlusion** in different regions by a small grey patch

Strongest feature map: the feature map with the largest values in the top convolution layer

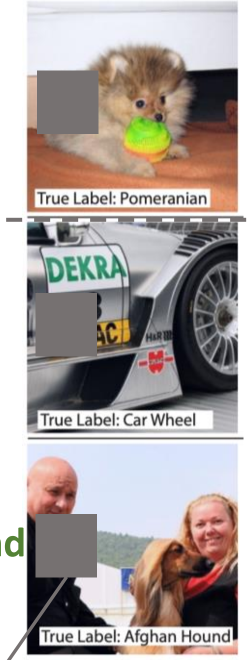
Sensitivity: the change of the value to the occlusion

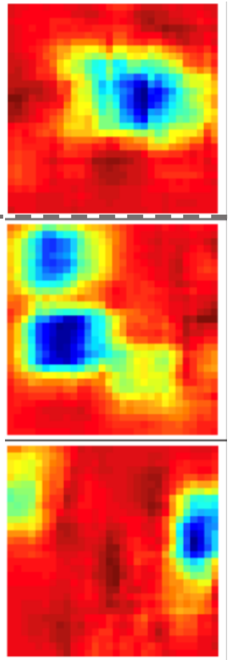
Label	Input image	Sensitivity of the Strongest feature map to the occlusion		Sensitivity of the probability of correct class

Pomeranian

Car Wheel

Afghan Hound

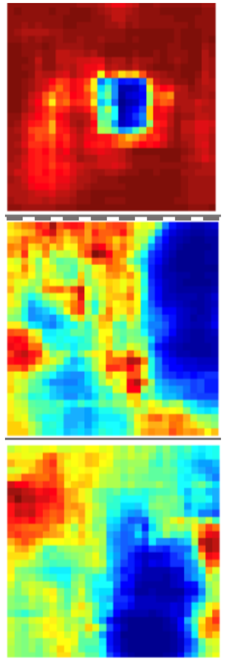




Consistently corresponds to the **dog's face**

Why different blue areas: the final prediction relies on multiple feature maps

A woman's face ⇒ the strongest feature map
The dog ⇒ the final prediciton



weak sensitivity

strong sensitivity

occlude different portions of the input image with **a grey patch**

Zeiler, Matthew D., and Rob Fergus. "Visualizing and understanding convolutional networks."

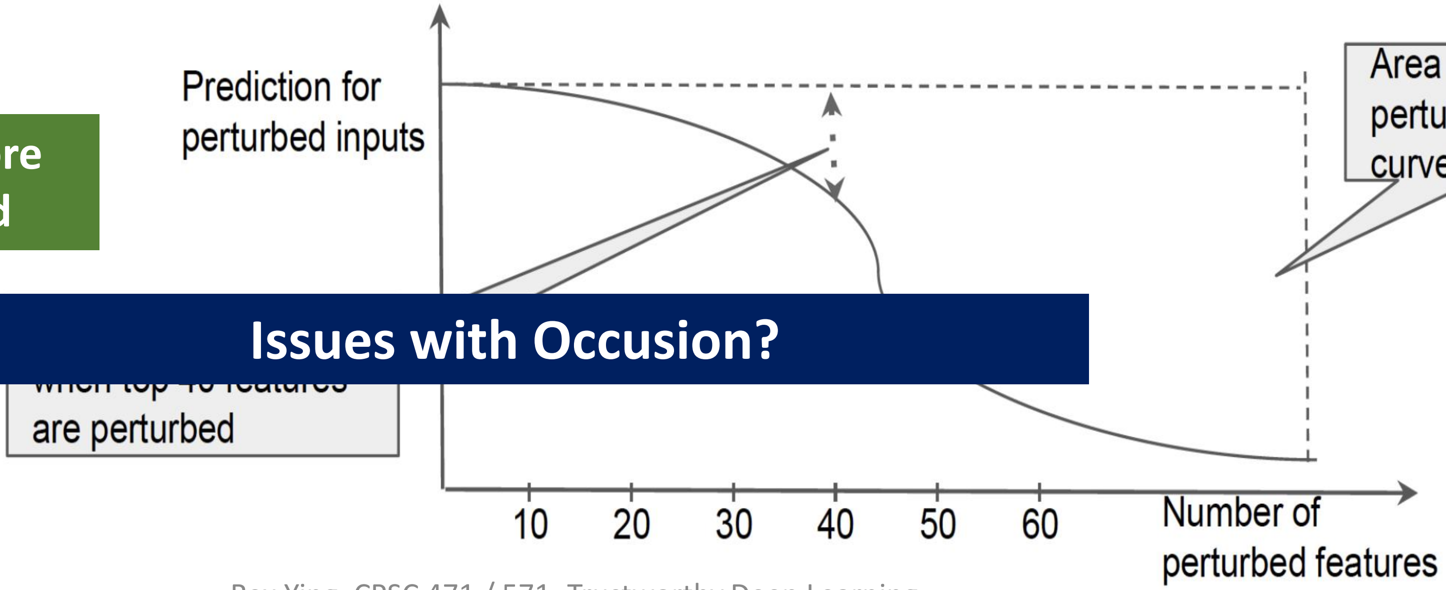
Meaningful Perturbation and Evaluation

- Other types of **perturbation** [1]:
  - **Blur:** blurring the region area
  - **Constant:** replacing with a constant value
  - **Noise:** adding noise to the region

[1] Fong, Ruth C., and Andrea Vedaldi. "Interpretable explanations of black boxes by meaningful perturbation."

- **Area over Perturbation Curve (AOPC):** to evaluate the perturbation methods

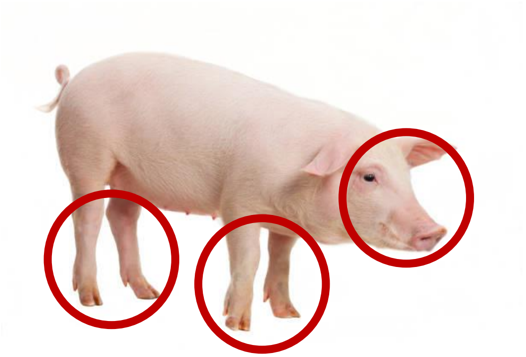
A higher AOPC indicates a more efficient perturbation method



Issues with Occusion?

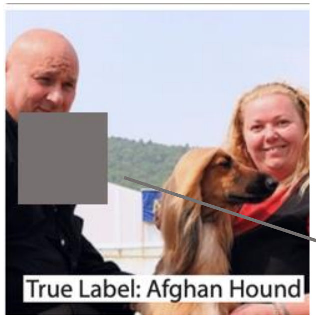
Issues with Occlusion and Perturbation

- Efficiency: occlusion at token / pixel level is very time-consuming
  - Too many forward propagations are needed
- Correlation is not modeled well
  - *E.g.* Presence of Part A "or" part B results in prediction of a class



Removing one of the patch may not have much effect on the logits

- The shape of the occluding patch is pre-defined



The size of the **grey patch** is always the same – **same granularity**

Explanation as Masks

- The learnable mask consists of values between 0 and 1
- $\text{argmin}_M \, \underbrace{f(\phi(\boldsymbol{x}))}_{\text{Masked prediction}} + \underbrace{g(M)}_{\text{Regularization}}$

Original input

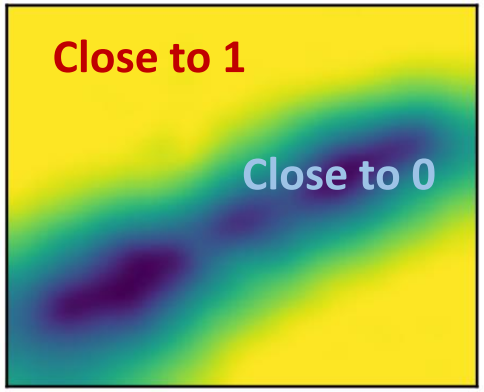
flute: 0.9973

Decrease in model confidence after masking

flute: 0.0007

Explanation of "flute" class in this instance

Learned Mask



Explanation as Masks

- The learnable mask consists of values between 0 and 1
- $\text{argmin}_M \, f\big(\phi(\boldsymbol{x})\big) + g(M), \quad 0 \le M \le 1$

  Mask $\boldsymbol{M}$ is randomly initialized

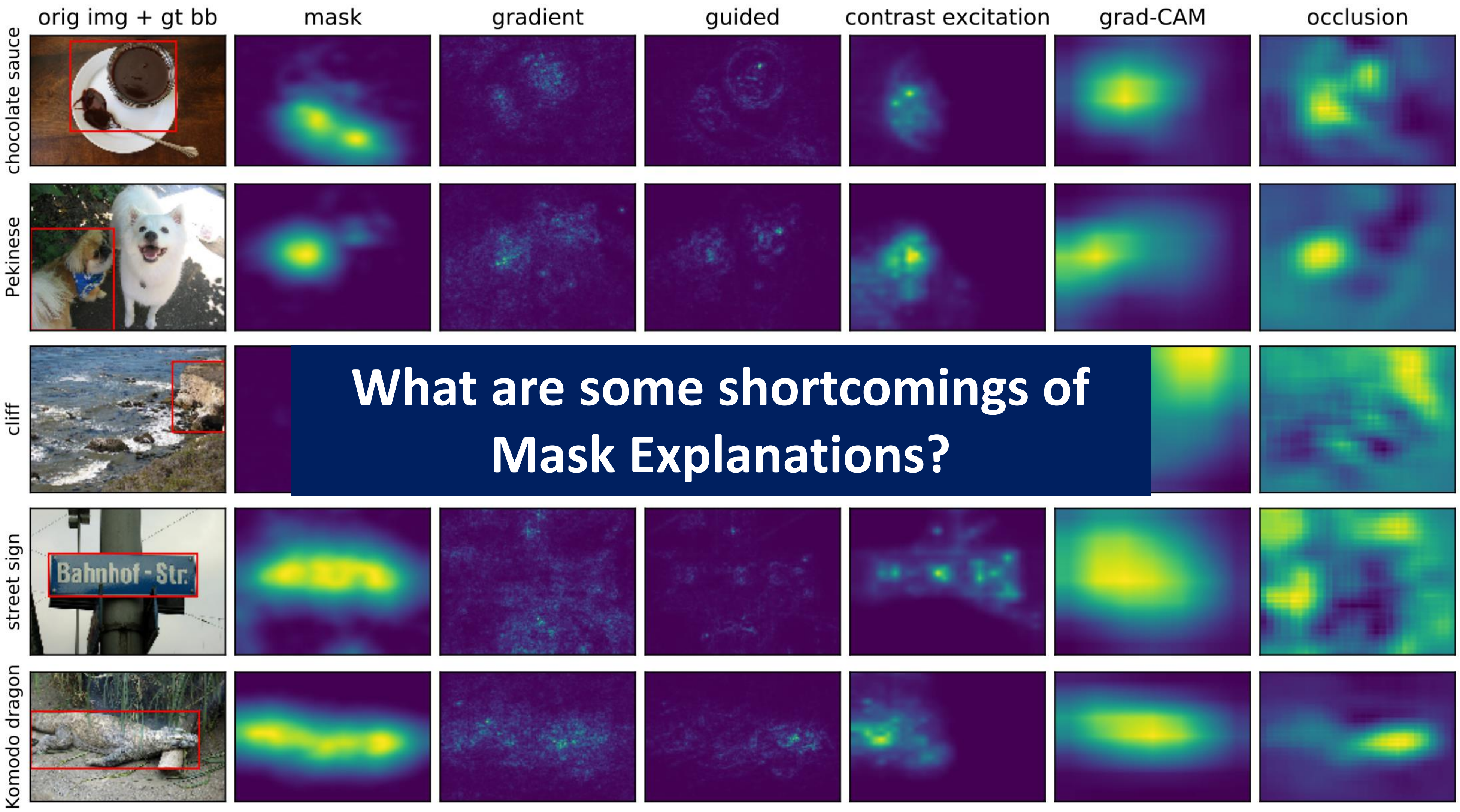
  Masked prediction **Regularization**

- Replace the masked portion of the input
  - $\phi(\boldsymbol{x}) = \boldsymbol{x} \odot M + \boldsymbol{x}^0 \odot (\boldsymbol{1} - M)$
- Control the desirable properties of the mask
  - $g(M) = \lambda_1 \|1 - M\| + \sum_u \nabla M(u)$

Image gradient (difference between adjacent pixels)

What's the rationale behind $g(M)$?

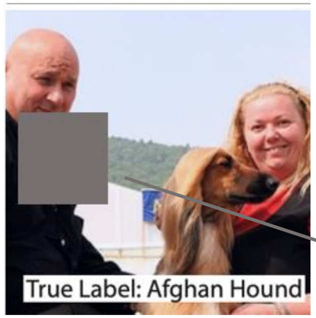
Comparison with Other Methods



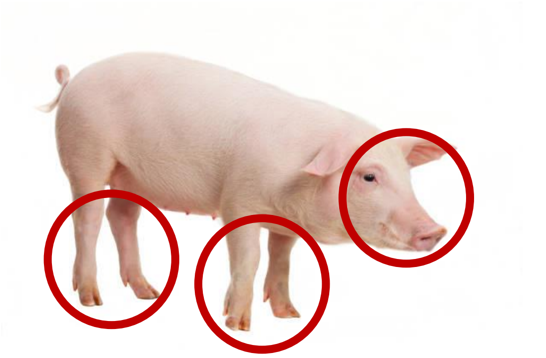
What are some shortcomings of Mask Explanations?

Does Masking Solve These Challenges?

- **Efficiency**: occlusion at token / pixel level is very time-consuming
  - Too many forward propagations are needed
- **Correlation** is not modeled well
  - *E.g.* Presence of Part A "or" part B results in prediction of a class
- The **shape** of the occluding patch is pre-defined



The size of the **grey patch** is always the same – **same granularity**



Removing one of the patch may not have much effect on the logits

What are more issues of masking-based methods?

Problems with Mask Explanations

- **Efficiency**
  - Also slow when the input is large (too many pixels, tokens, nodes etc.)
  - Requires **optimization** for generating explanation for every instance
- **Stability**
  - Explanation can vary across different runs depending on **random seed** of the optimization
  - Mask can get stuck in **local optimum** instead of global optimum
- **Robustness**
  - The process is analogous to the problem of finding **adversarial examples**
  - Explanations might not provide the true insight!

Summary

- The goal of XAI is to enable users to **understand the decision-making** of the model and **gain the trust** of human users of the deep learning system.
- The explanation for a DL system can be categorized as being **model-level or instance-level**; **ante-hoc or post-hoc**; **model-specific or model-agnostic**.
- **Explainable Models** include decision trees, linear models, etc.
- **Gradient-based Explanation**: Saliency, Grad-CAM, Integral gradient
- The change of prediction to **perturbation** over individual regions reveals the importance of the specific region
  - Occlusion and mask-based optimization
- All methods introduced today are instance-level explainability methods

Q & A