iML: Post-hoc Methods for Neural Networks

Motivation

Marius Lindauer and Avishek Anand

Winter Term 2021

Neural Networks as Complex ML models

Neural Networks as Complex ML models

- Neural networks are over parameterised
  - Vision models and Language models routinely have > millions of params
  - Sometimes #parameters > #input instances
  - Which and how do the features, parameters, training instances contribute towards the final decision ?

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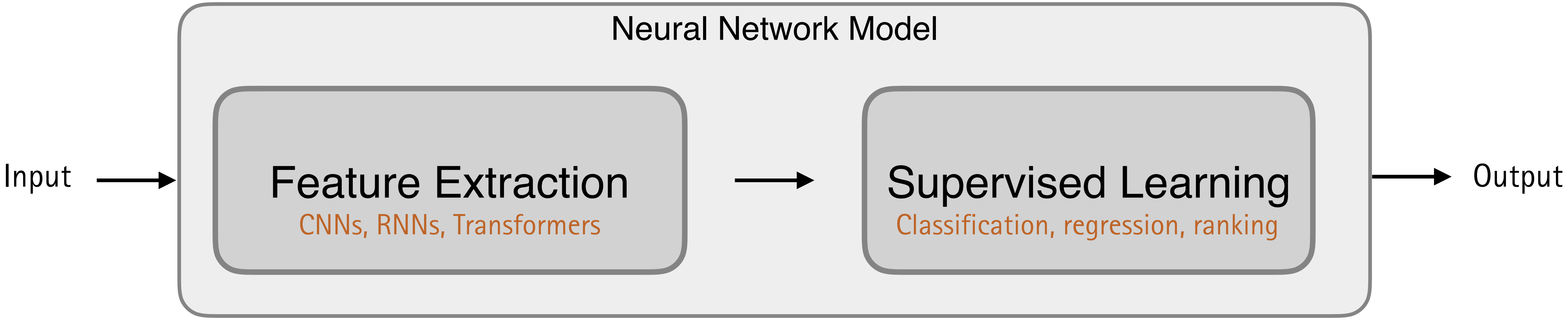
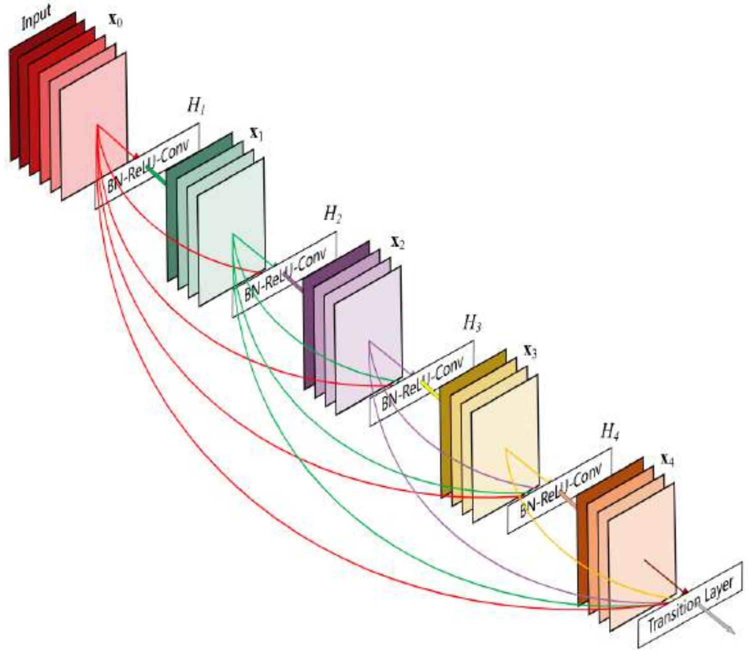


Neural Networks as Complex ML models

- Neural networks are compositional and non-linear systems
  - The success of neural networks is due to their **depth**
    - Depth results in compositional behaviour
  - Non-linearity between layers helps capture non-linear relationships

- Depth and non-linearity leads to lack of interpretability

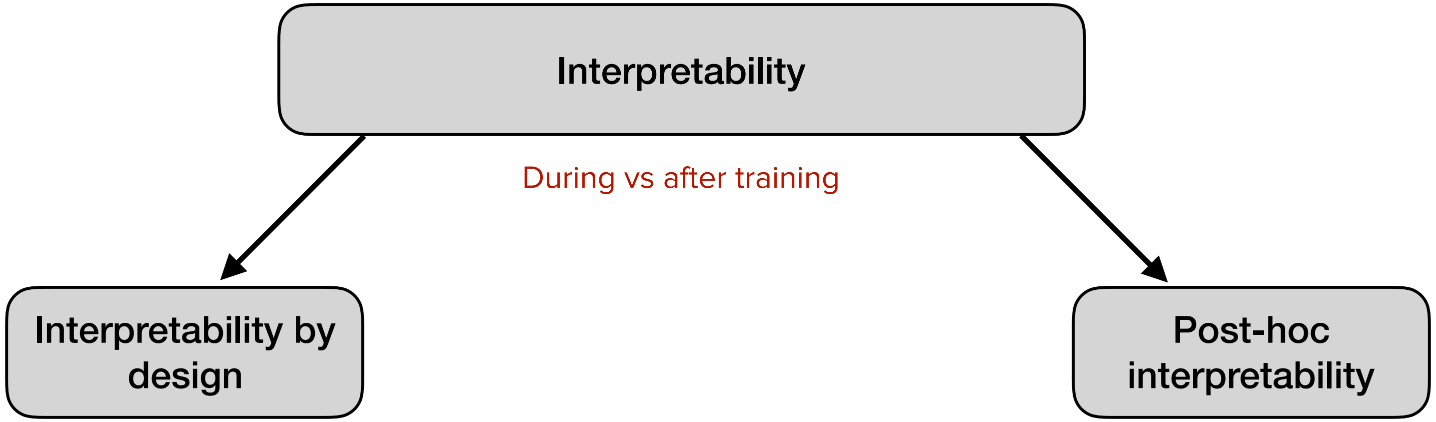


Model-specific interpretability

- What types of neural models are out there ?
  - **For vision:** Convolutional Neural Nets
  - **For language, speech:** Recurrent Neural Nets, Transformer Models
  - **For recommendation systems, ranking:** Factorization-based Models, Embeddings models

- Each of the domains have their challenges and have developed specific approaches for interpretability
  - We will focus on first principles that can be applied to most models
  - We will discuss adaptations to each data modality as and when required

Interpretability landscape in Neural Networks



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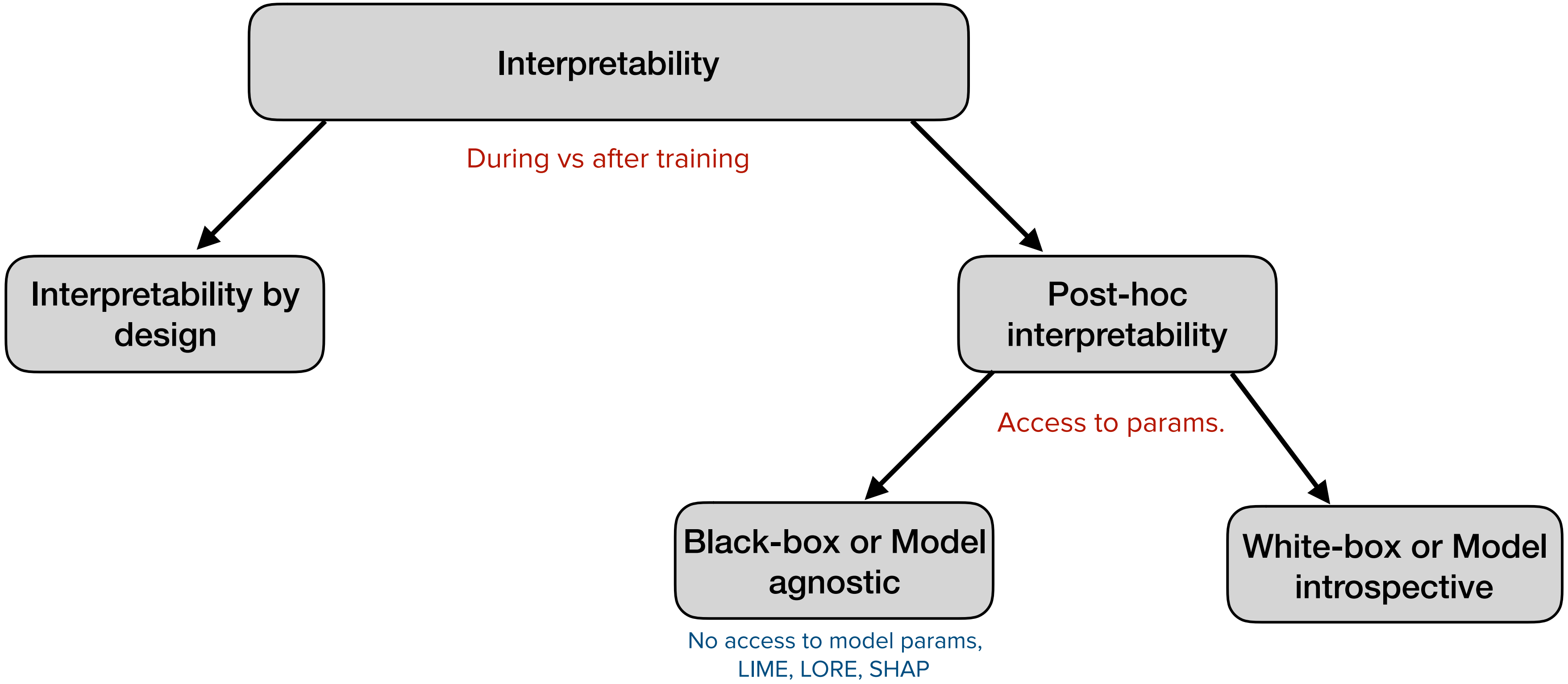

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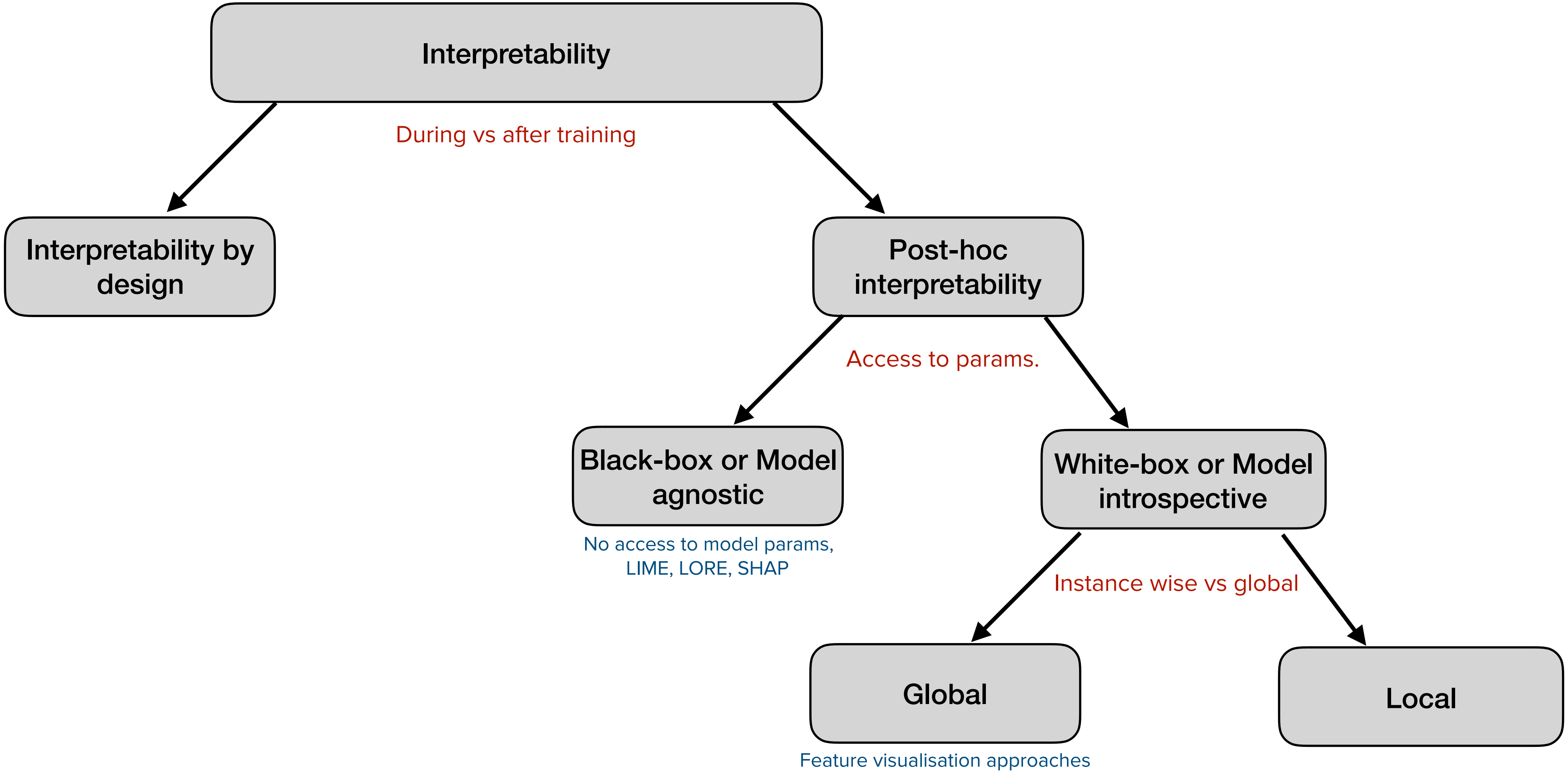

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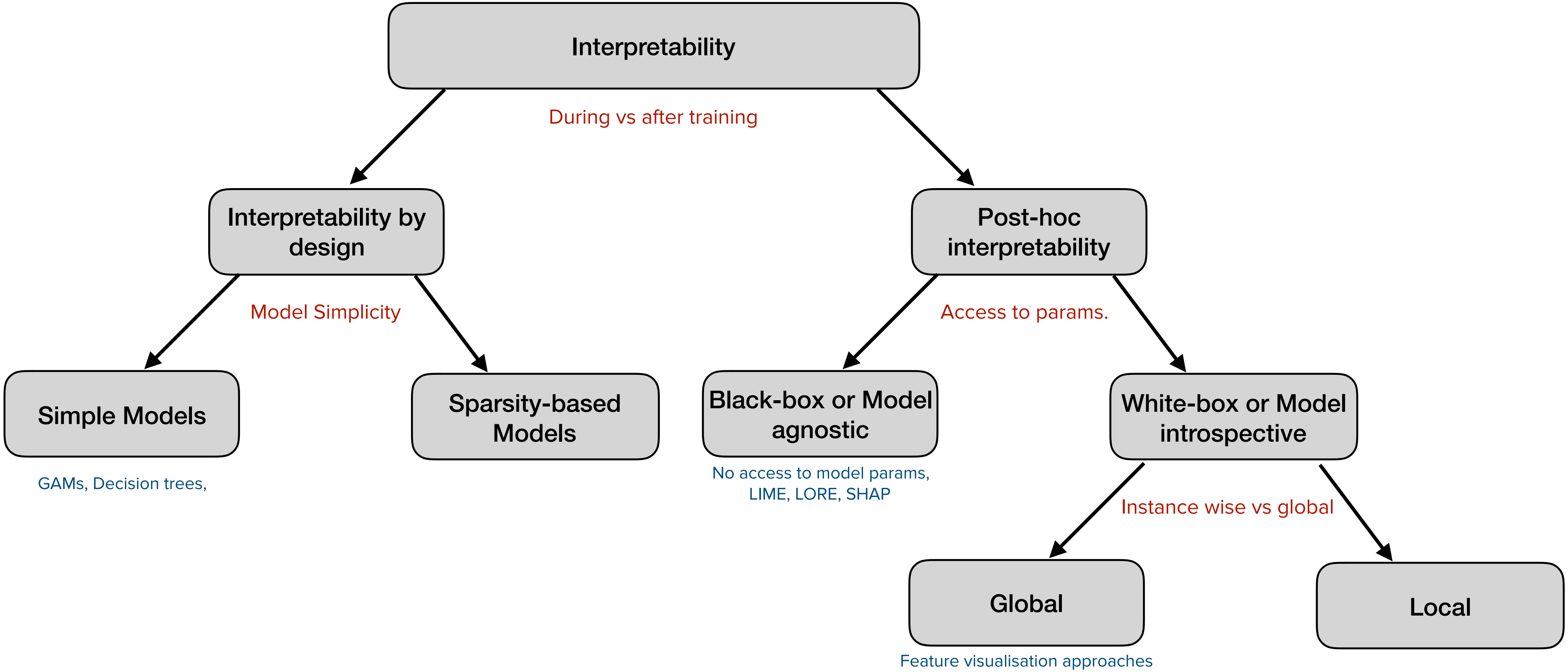

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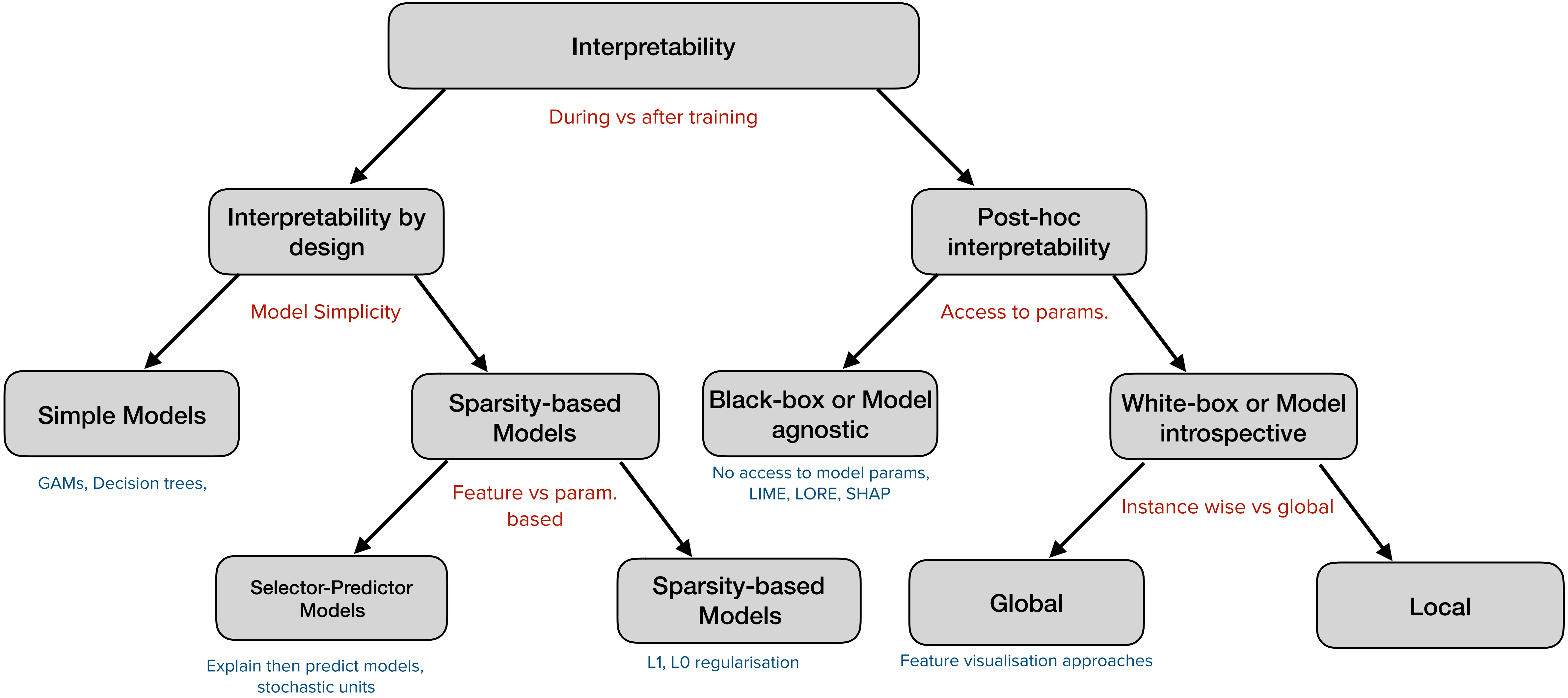


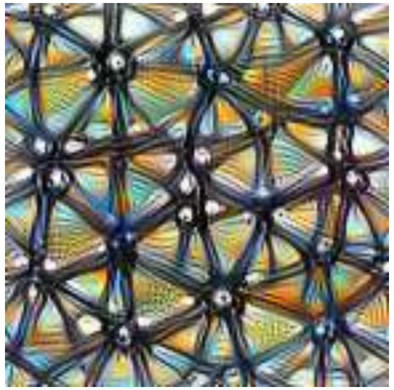
How can we interpret Neural Models ?

- **Feature visualization:** Visualizing components of the neural networks
  - Activations of neurons
  - Attention values
  - Gradient flow

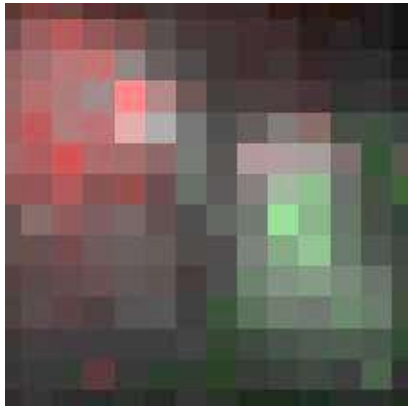
- **Feature attributions:** relevant input features
  - Which input features are responsible for the given decision ?
  - Sensitivity analysis using gradient-based methods
  - Using black-box methods like LIME, SHAP, etc.

How can we interpret Neural Models ?

- **Feature visualization:** Visualizing components of the neural networks



- **Feature attributions:** relevant input features



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Visualizing Neural Networks

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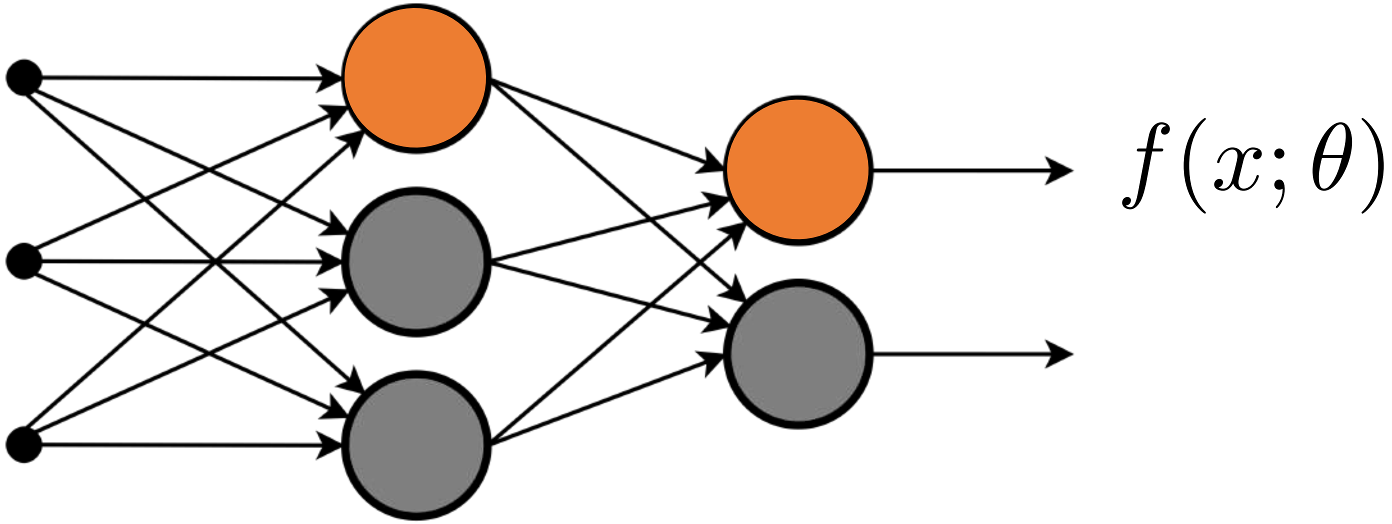
Winter Term 2021

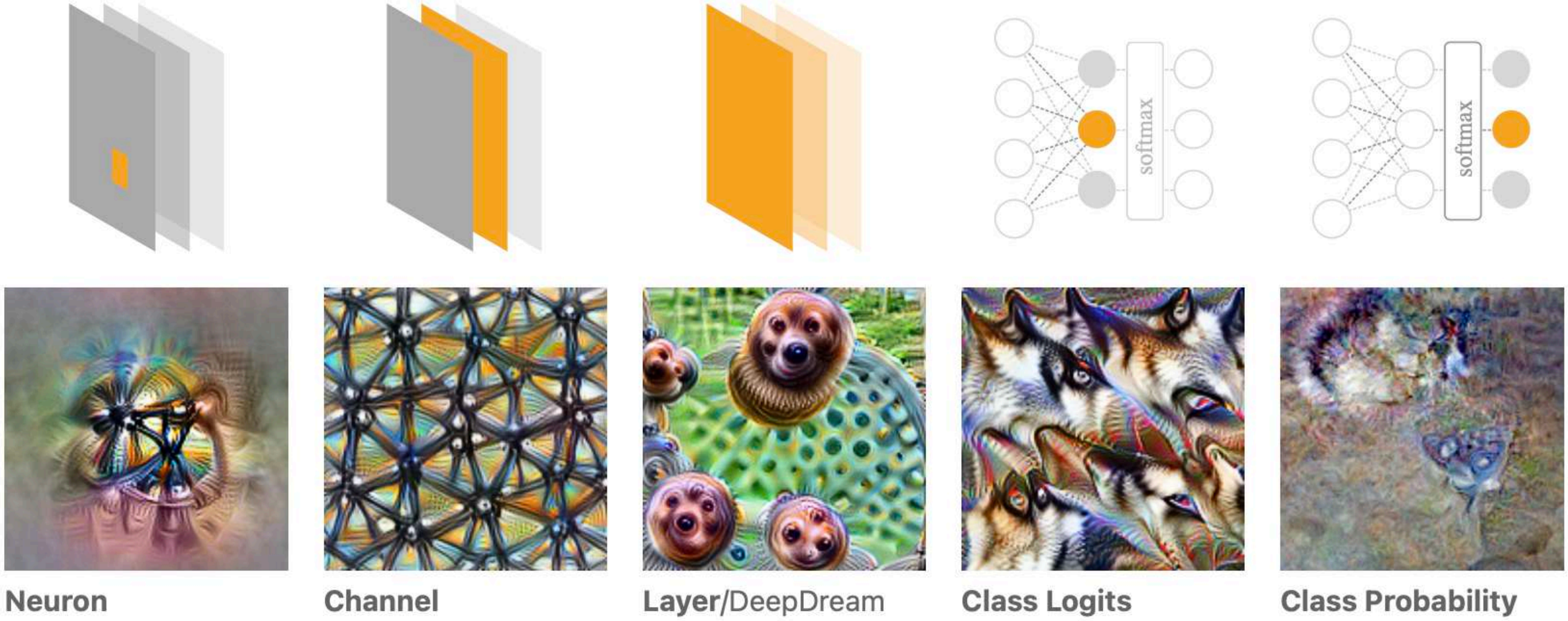
Inspecting the Model units

- Neural Networks architectural units can be inspected to provide insights
- What happens to the input signal as it travels through the network ?
  - **Activations:** Activation in neural networks are sparse
  - **Attention units:** Encode the importance of input representation units



Visualizing Neural Network Architectural Units

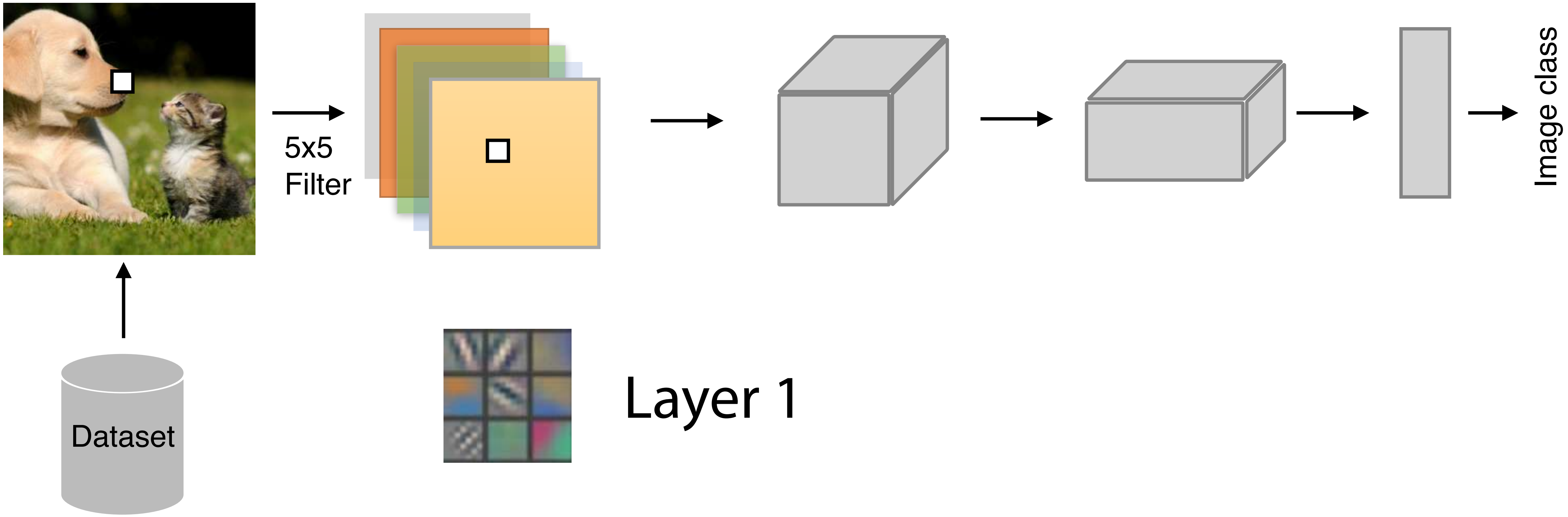
- Search for examples where individual features have high values –
  - Either for a neuron at an individual position, or for an entire channel



https://distill.pub/2017/feature-visualization/

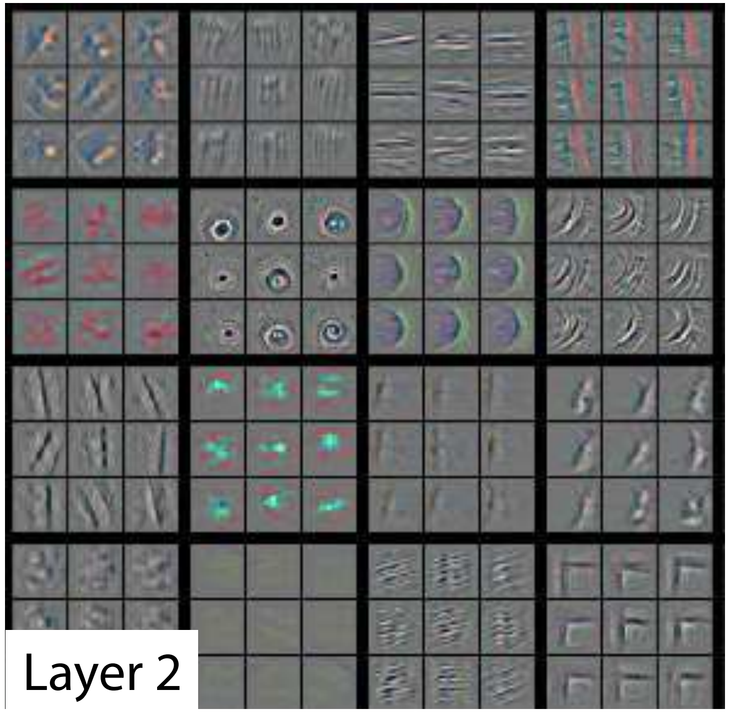
Visualizing Filters in a CNN

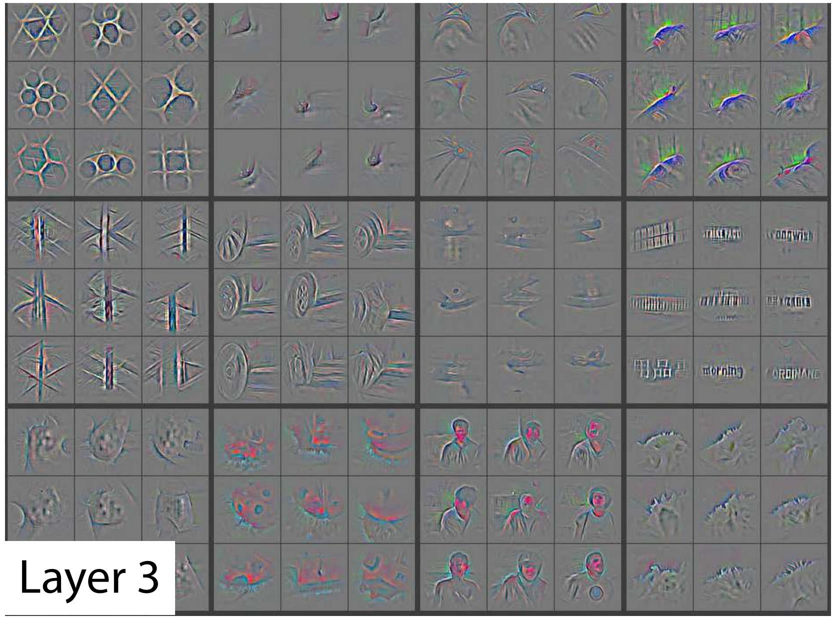
- Most of the aggregated values at neurons do not result in activations
- Find image patches in dataset that maximally activate/excite a unit

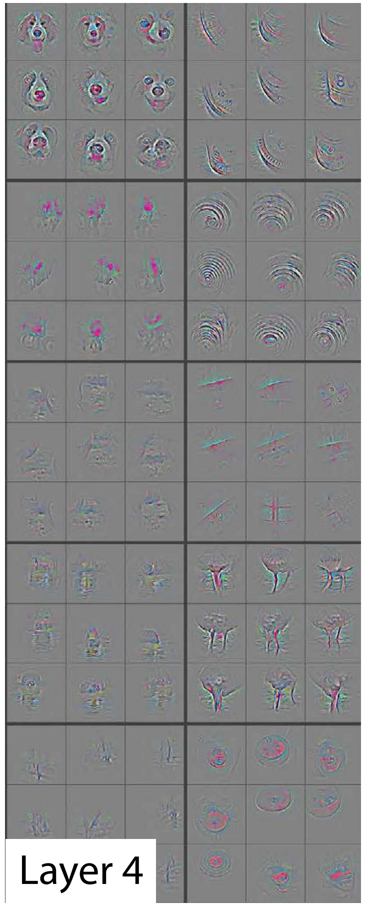


Feature extraction evolution

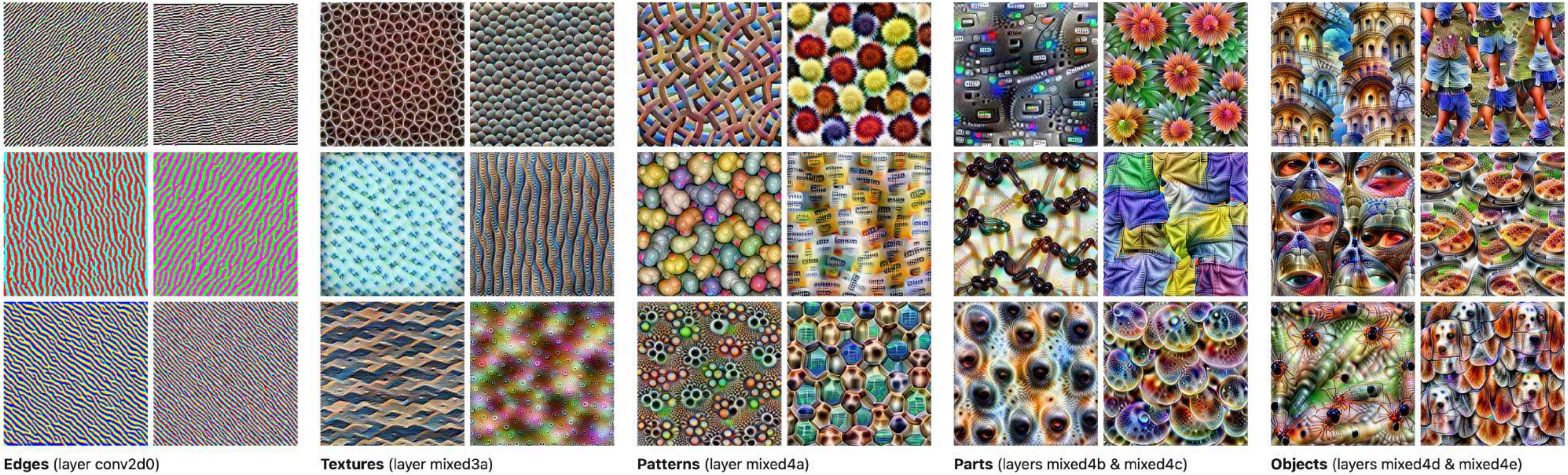
- Lower layers extract lower-level features
- Higher layers compose extracted features to compose high-level features





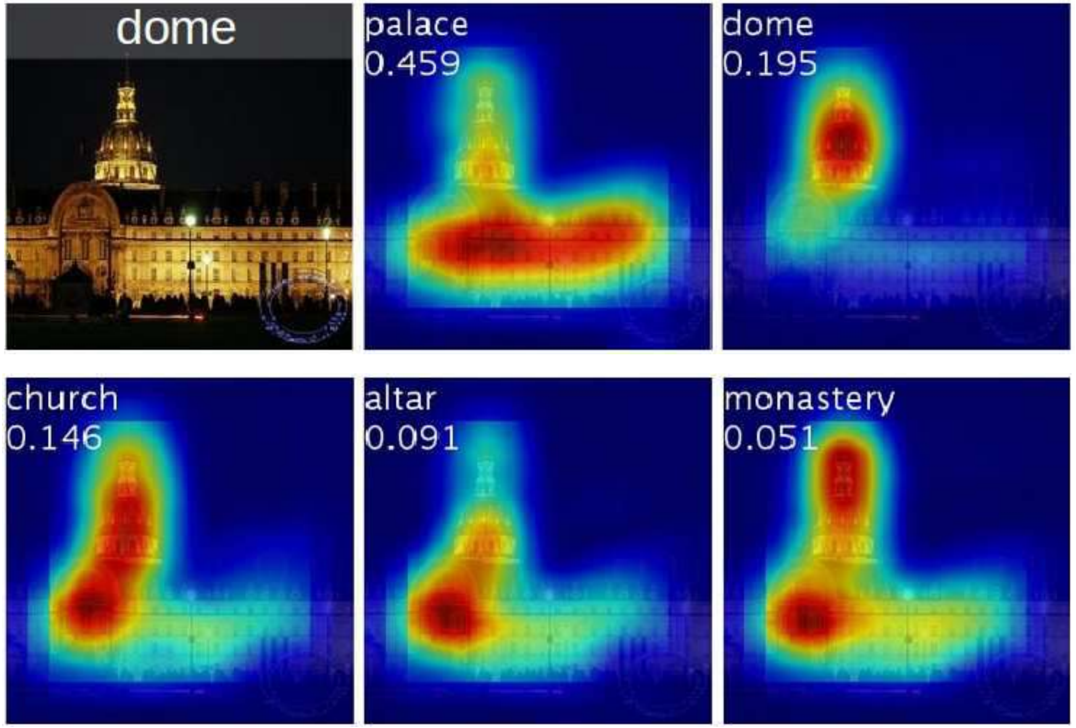


Layerwise Visualisation of CNNs



Class Activation Maps

- CAMs are specific to CNNs
- Class activation map or CAM highlights class-specific discriminative regions
    - Different classes induce different activations

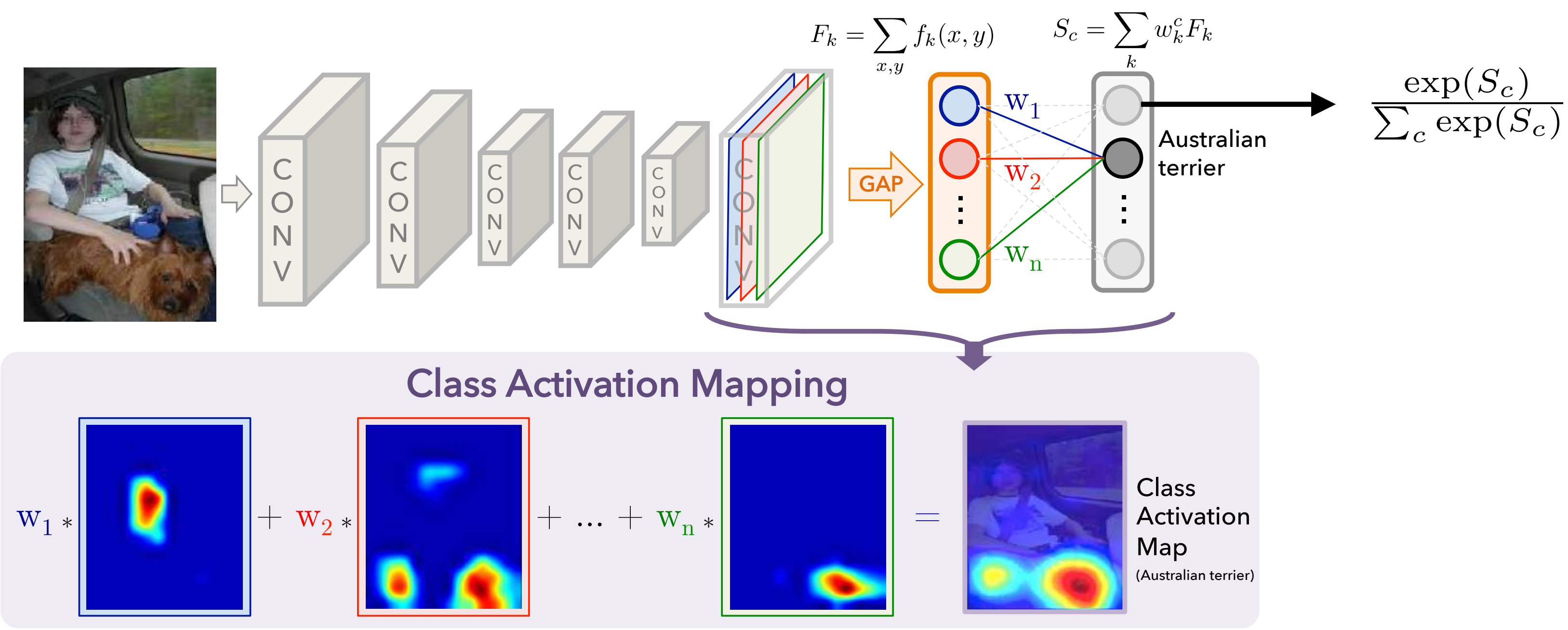


[Zhou et al. CVPR '16] https://arxiv.org/pdf/1512.04150.pdf

Class Activation Maps

- Let the activation at unit k, at the location (x, y) in the last layer $-f_k(x, y)$
- Global avg. pooling at unit k – $F_k = \sum_{x,y} f_k(x, y)$
- For a given class

$$P_c = \frac{\exp(S_c)}{\sum_c \exp(S_c)}, \quad S_c = \sum_k w_k^c F_k$$



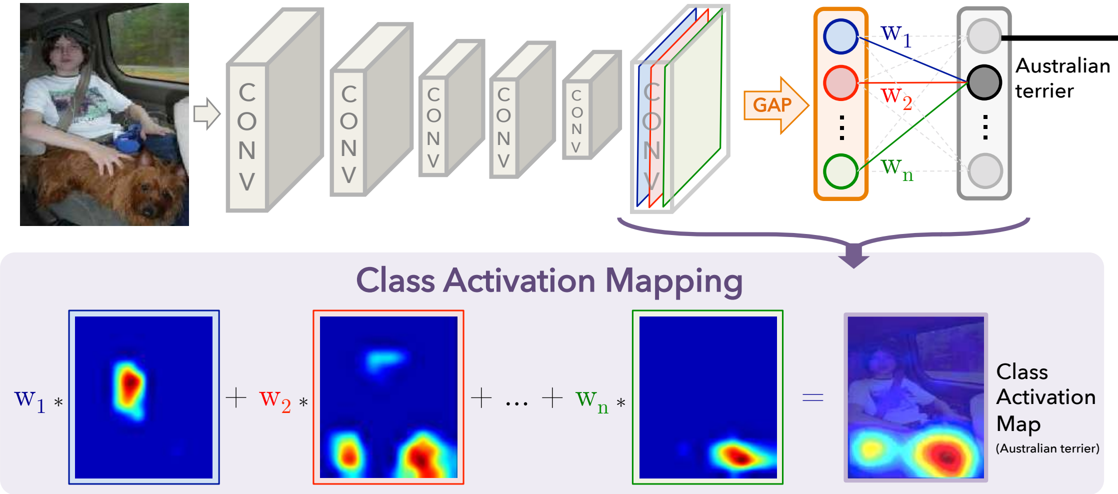
[Zhou et al. CVPR '16] https://arxiv.org/pdf/1512.04150.pdf

Class Activation Maps

- **Input:** Take a pre-trained CNN model
- **Output:** weight vectors for each classes
- How do we learn the weights ?
  - Average pooling of the feature maps in the last layer $S_c = \sum_k w_k^c F_k$
  - Weights learned using simple logistic regression

$$f_k(x,y)$$

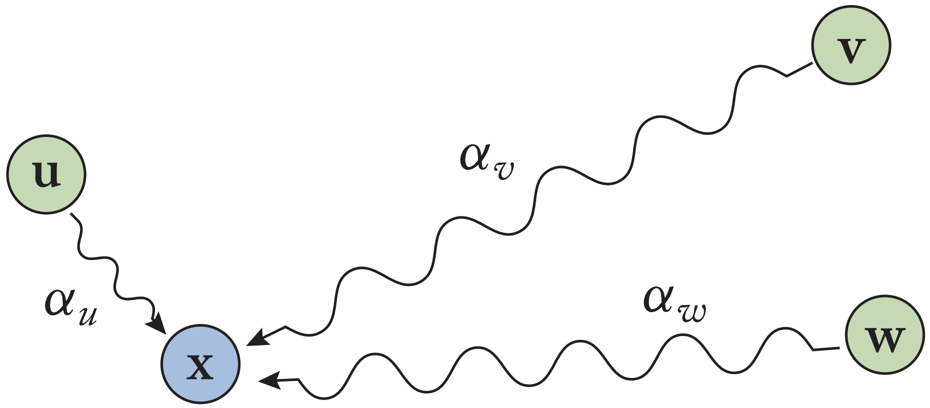
$$\sum_{x,y} f_k(x,y)$$



$$\frac{\exp(S_c)}{\sum_c \exp(S_c)}$$

Attention in Language

- Attention mechanism in neural language models is crucial for extracting latent features
- Self attention in language is aimed at re-representing the initial representation based on the context
- Neural models consume non-contextual token-level representations and output contextual token-level representation



New contextual representation $\mathbf{x}' = \alpha_u\,\mathbf{u} + \alpha_v\,\mathbf{v} + \alpha_w\,\mathbf{w}$

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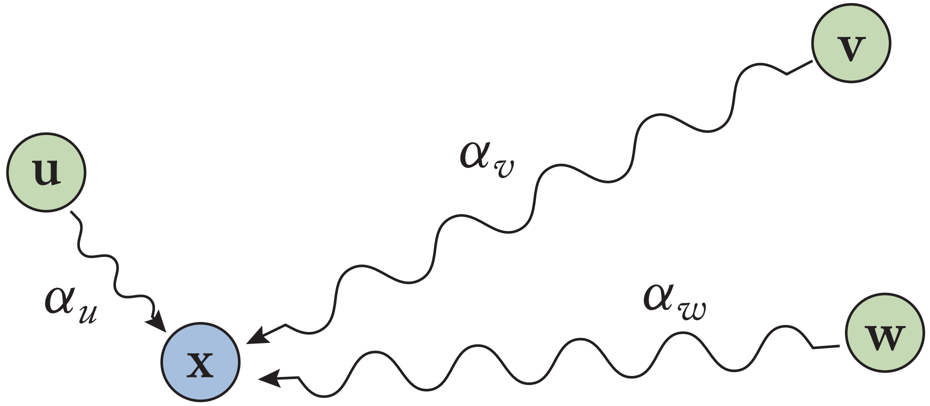
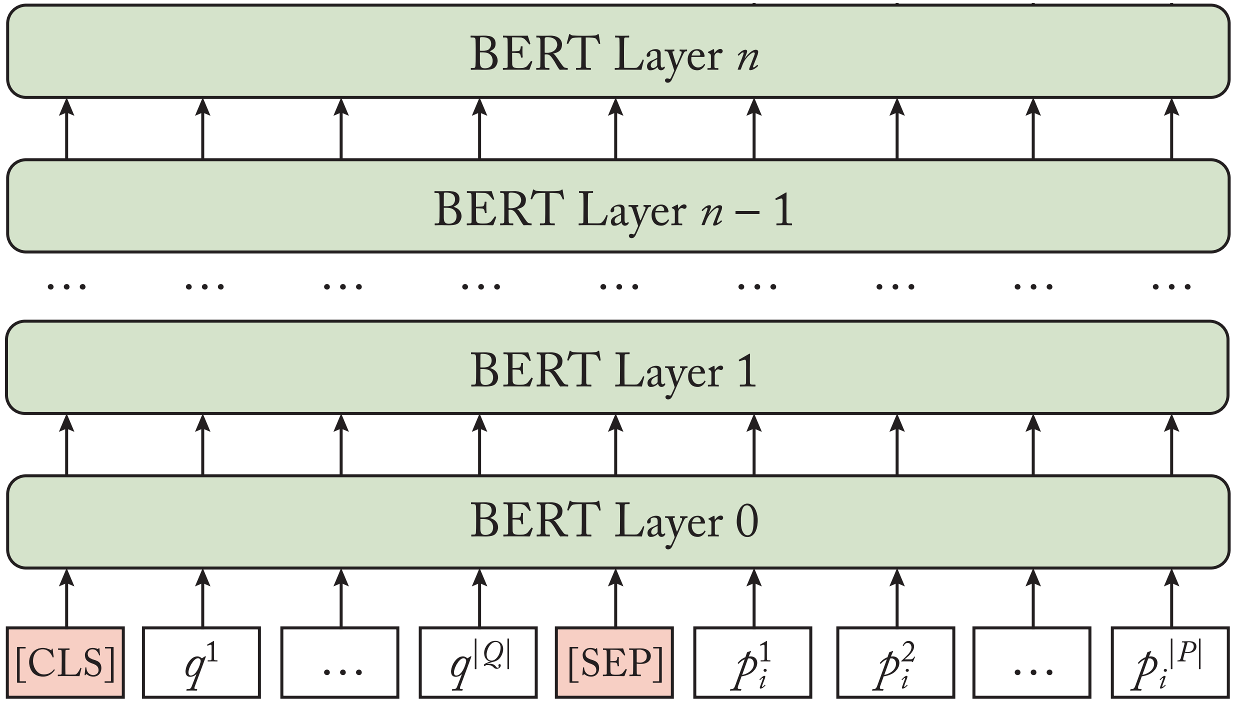
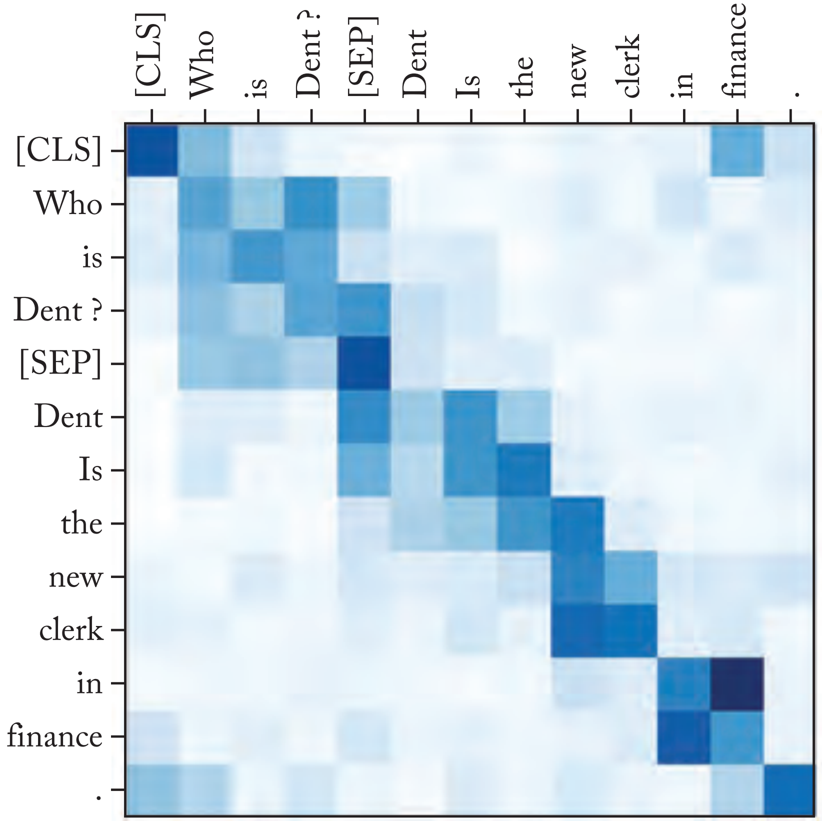


New contextual representation $\mathbf{x}' = \alpha_u \mathbf{u} + \alpha_v \mathbf{v} + \alpha_w \mathbf{w}$

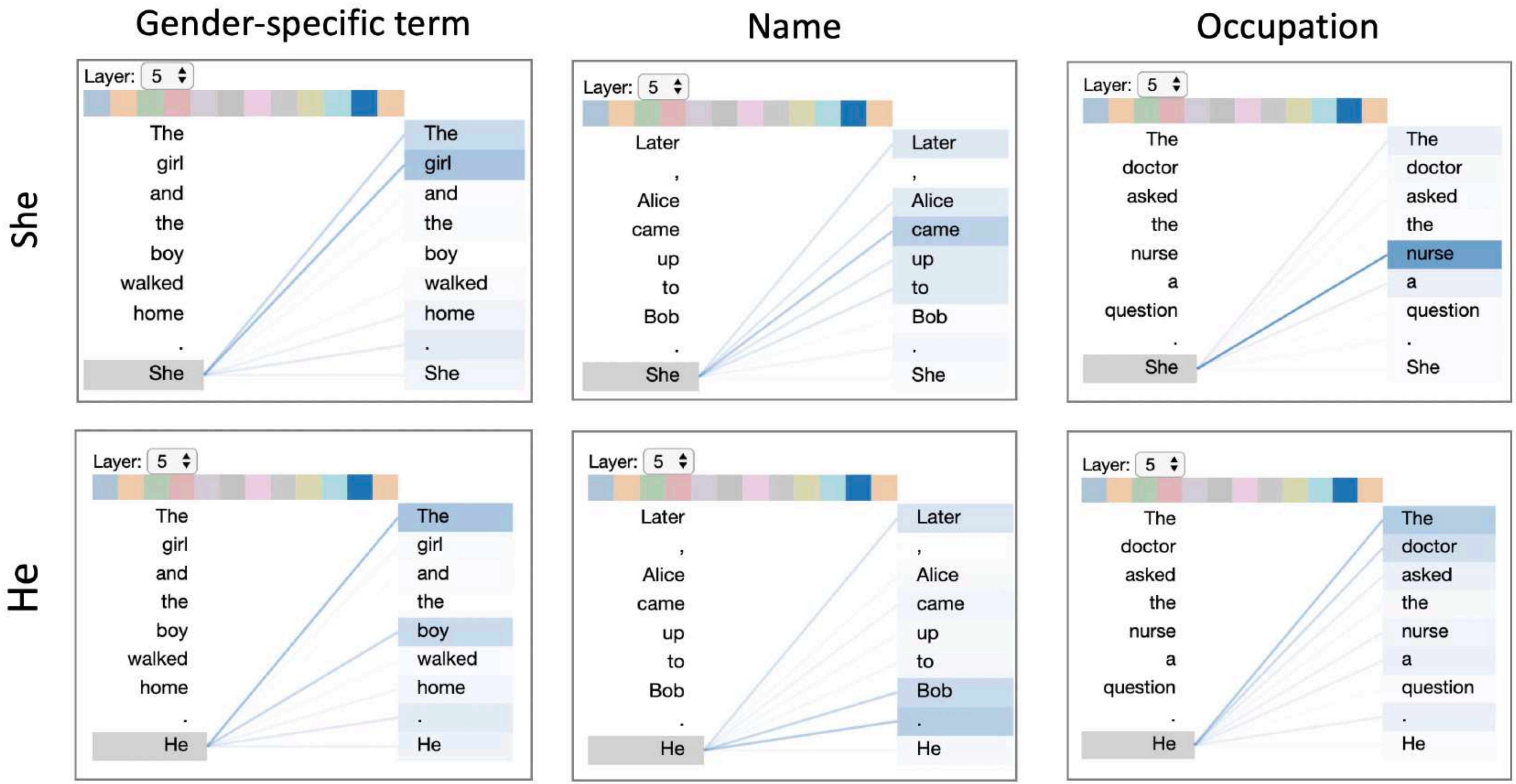
$$\alpha_u = \frac{e^{\mathrm{sim}(\mathbf{u},\mathbf{x})}}{e^{\mathrm{sim}(\mathbf{u},\mathbf{x})} + e^{\mathrm{sim}(\mathbf{v},\mathbf{x})} + e^{\mathrm{sim}(\mathbf{w},\mathbf{x})}}; \quad \mathrm{sim}(\mathbf{u},\mathbf{x}) = \mathbf{x} \cdot \mathbf{W}\mathbf{u}$$

Attention Maps in Transformers





Visualizing Attention Units



Other Interactive visualisations

- Interactive visualisation by Chris Olah: **https://distill.pub/2018/building-blocks/**
- https://distill.pub/2017/feature-visualization/
- Deep Dream
- De-Convolution
- Visualizations in Language: https://github.com/jessevig/bertviz
- ...

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Simple gradients, Integrated gradients

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Winter Term 2021

Sensitivity Analysis

- Neural Networks are differentiable machines
  - The output can be written as a function of the parameters and input
  - One can differentiate the output function w.r.t parameters
  - The underlying idea is used for training Neural Nets using gradient descent

$$f(x;\theta) \qquad\qquad \frac{\partial f(x;\theta)}{\partial \theta}$$

- **Sensitivity Analysis:** How sensitive is the output $f()$ w.r.t to a small change in the input ?

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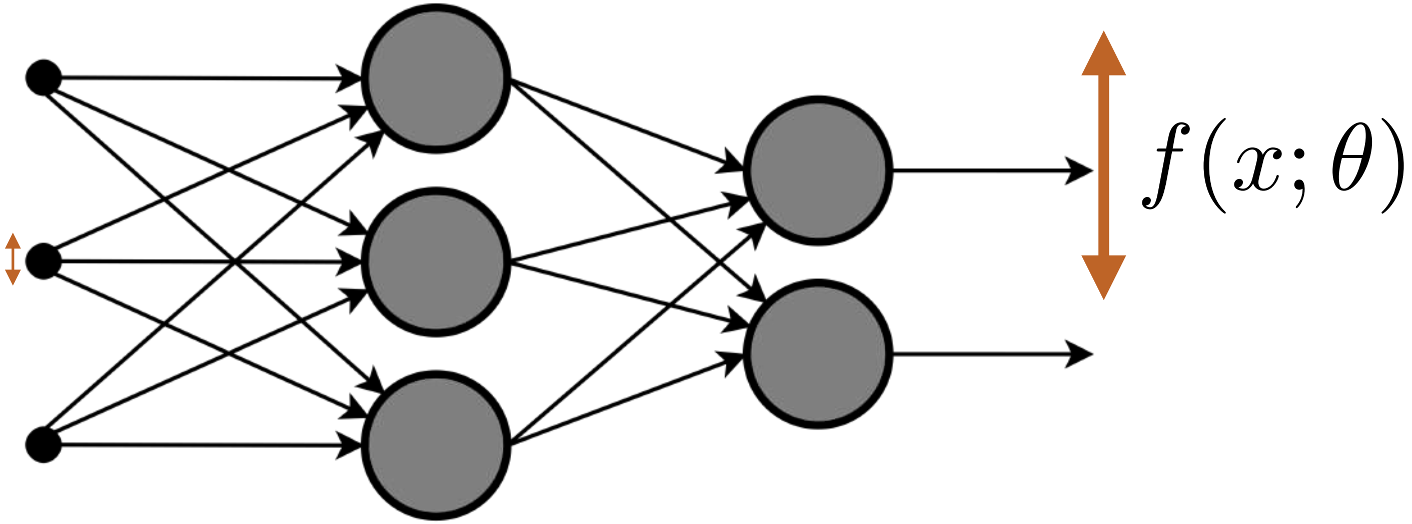
$$\frac{\partial f(x;\theta)}{\partial x}$$

Sensitivity Analysis

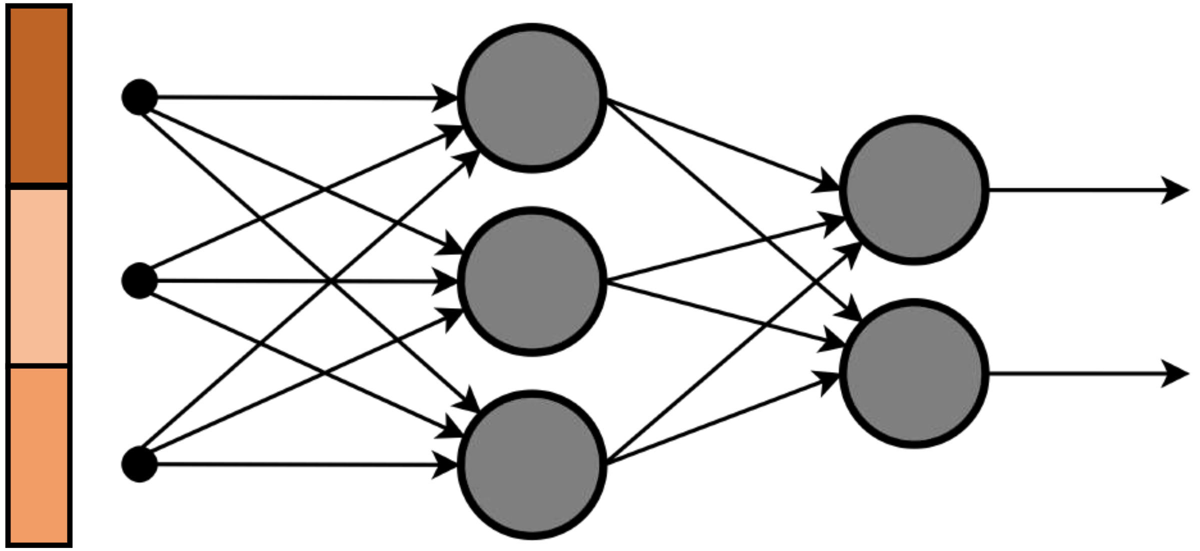
- How sensitive is the output $f()$ w.r.t to a small change in the input ?
  - If a small change in the input feature causes a large change in output, then that feature is **responsible** for the prediction
  - Back-propagation into the input: instead of computing $\frac{\partial f(x;\theta)}{\partial \theta}$

$$\frac{\partial f(x;\theta)}{\partial x}$$



Saliency Maps

- Visualize the gradients over each feature
  - as a heat map or Saliency Maps
  - Saliency maps are feature attribution methods that are based on gradients



$$f(x;\theta)$$

[Simonyan, Vedaldi, Zisserman '14]

Saliency Maps for Images

- Images have multiple channels where each channel is a 2-D matrix

$$M_{ij} = \max_c |\nabla_x S_c(X)|_{(i,j,c)}$$

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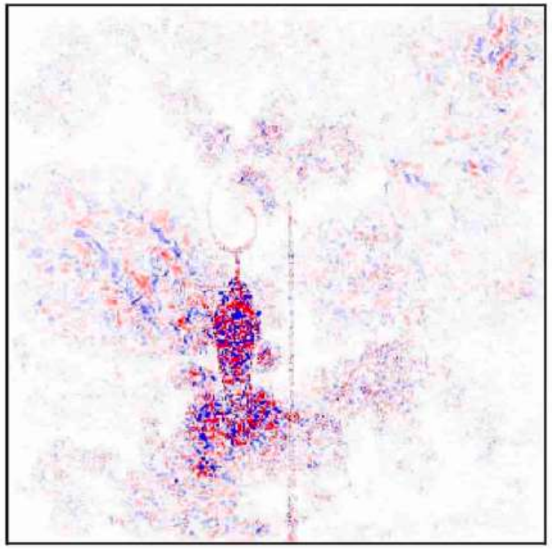
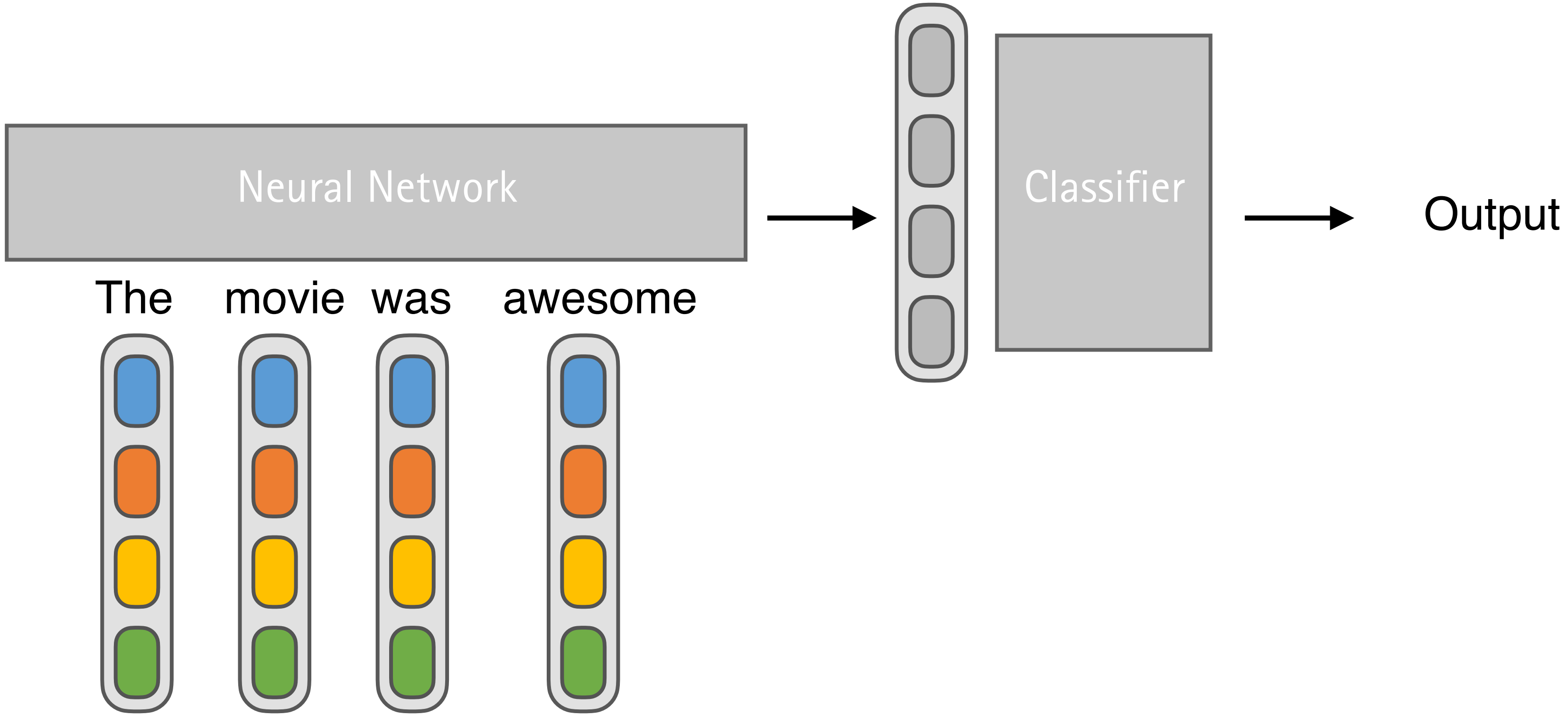


[Simonyan, Vedaldi, Zisserman '14]

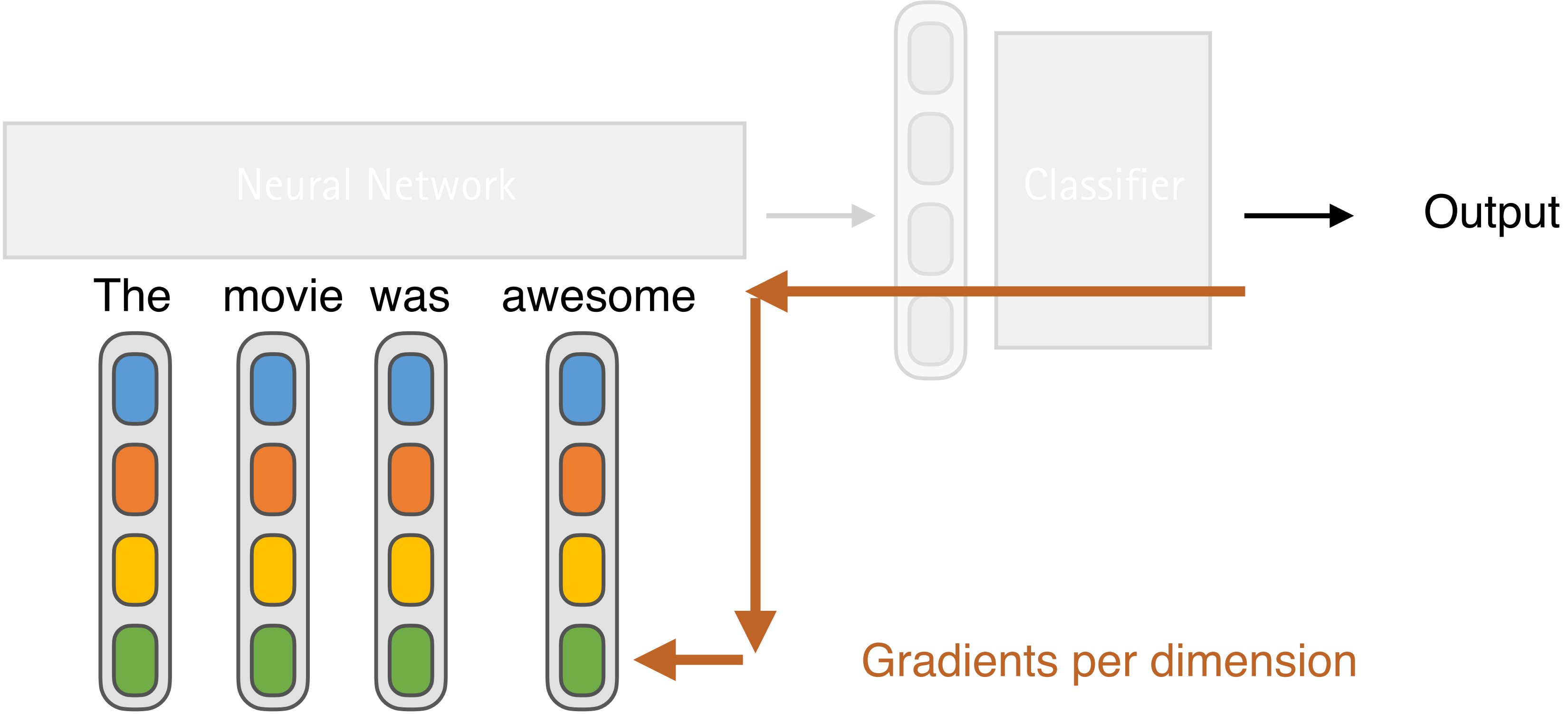
Saliency Maps for Language

- Words are associated with an embedding
- Computing gradients back to the inputs is different in comparison to images



Saliency Maps for Language

- We obtain gradients per dimension but we want attributions or importance scores at the level of world
- **Idea:** Simple aggregations of dimension-level gradients like sum, average, etc.



[Simonyan, Vedaldi, Zisserman '14]

Saliency Maps – Setting

Which features are responsible for the decision given..

A trained model **M**	Post-hoc interpretability
An instance **x**	Local interpretability
Access to model parameters	White-box interpretability

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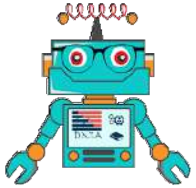
A trained model M — Post-hoc interpretability

An instance x — Local interpretability

Access to model parameters — White-box interpretability

Input



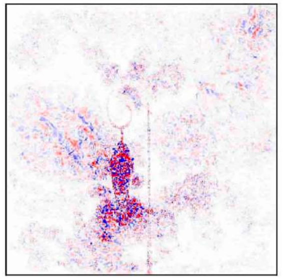
"Pole"

Output

Saliency Maps

Heatmaps

Feature Attributions



Saliency Maps – Setting

Which features are responsible for the decision given..

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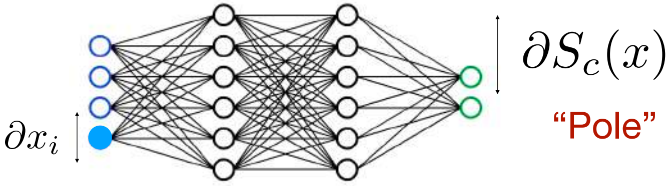
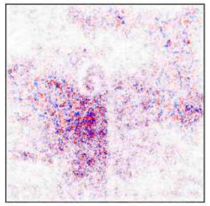


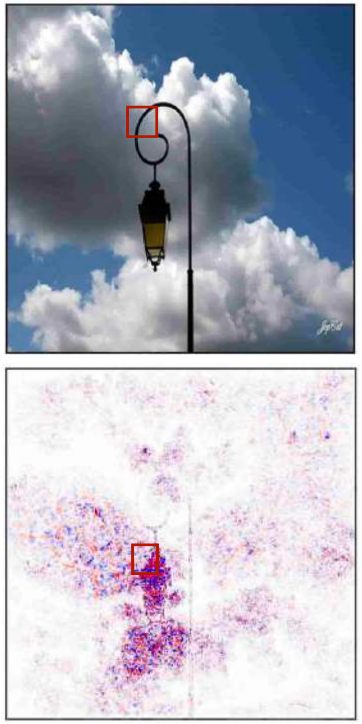
A feature is more relevant if a small perturbation causes large change in the output



Saliency Map

$$R_i^c(x) = \frac{\partial S_c(x)}{\partial x_i}$$

Problems with Deep Nets



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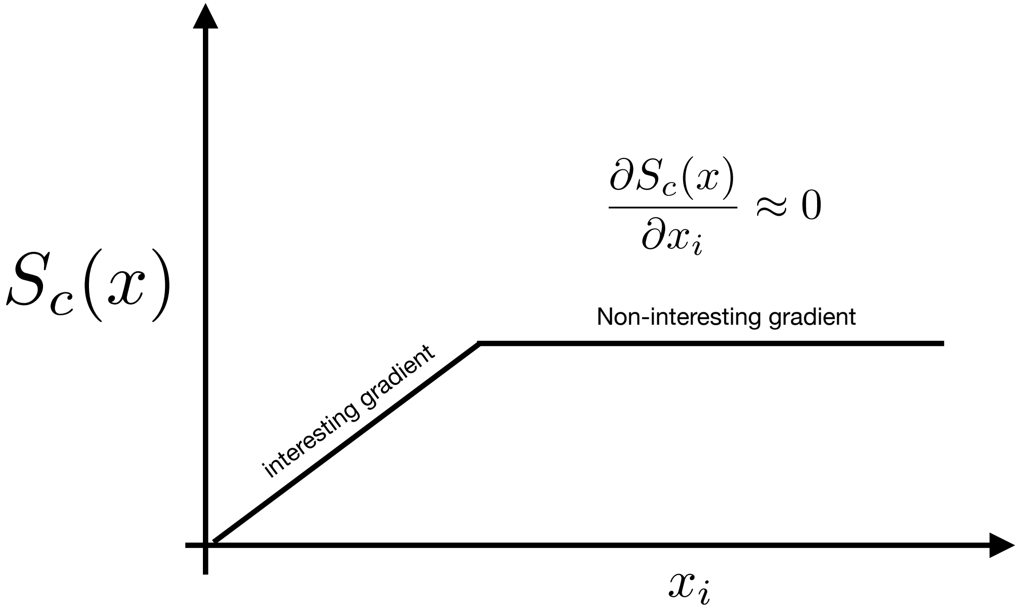
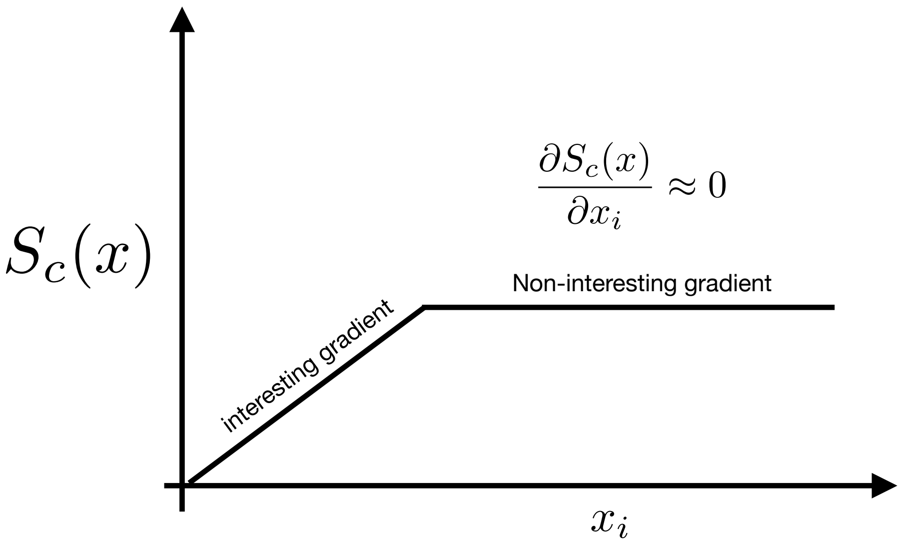


Deep Neural Networks are usually trained till "Saturation"

Perturbing Inputs

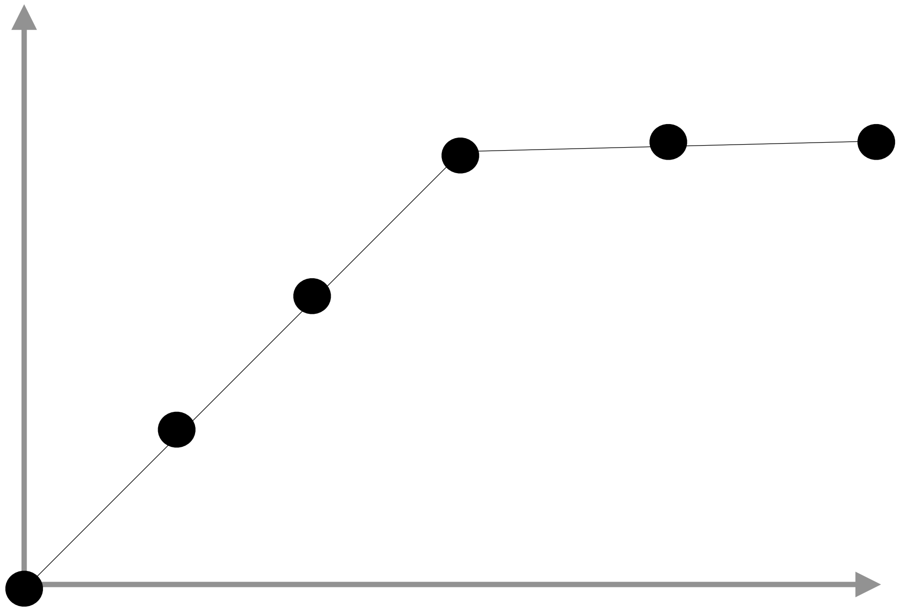
- **Small perturbations** at the saturation point do not give us interesting gradients
- Extreme perturbation (to say a baseline image) can give us interesting gradients

$$R_i^c(x) = \frac{\partial S_c(x)}{\partial x_i}$$



Integrated Gradients

Compute gradient estimate based on gradients over a path of specific perturbations



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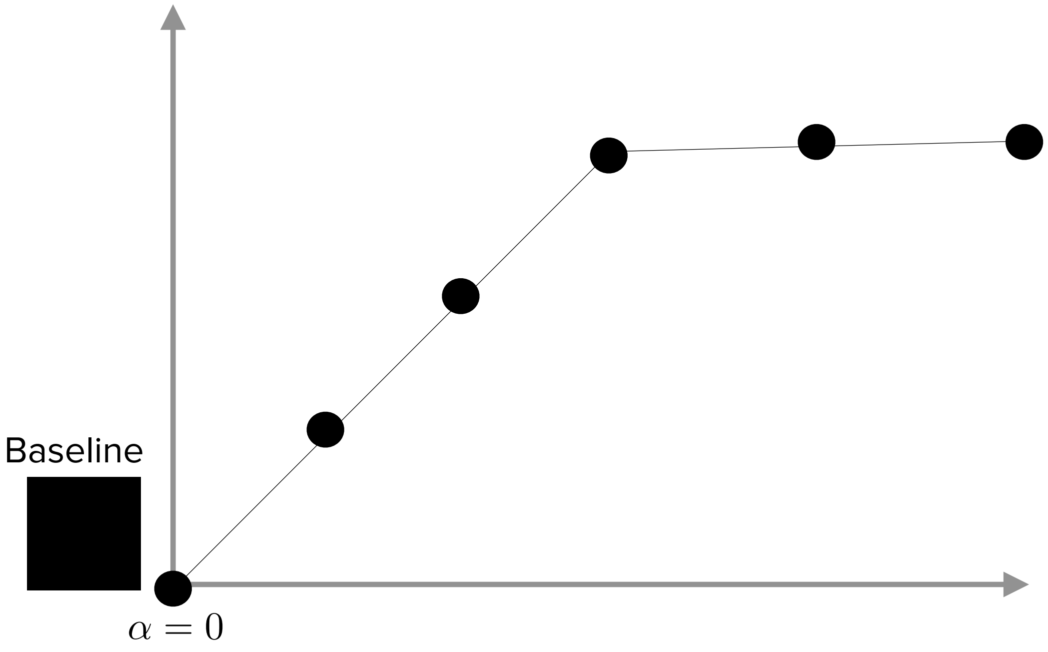

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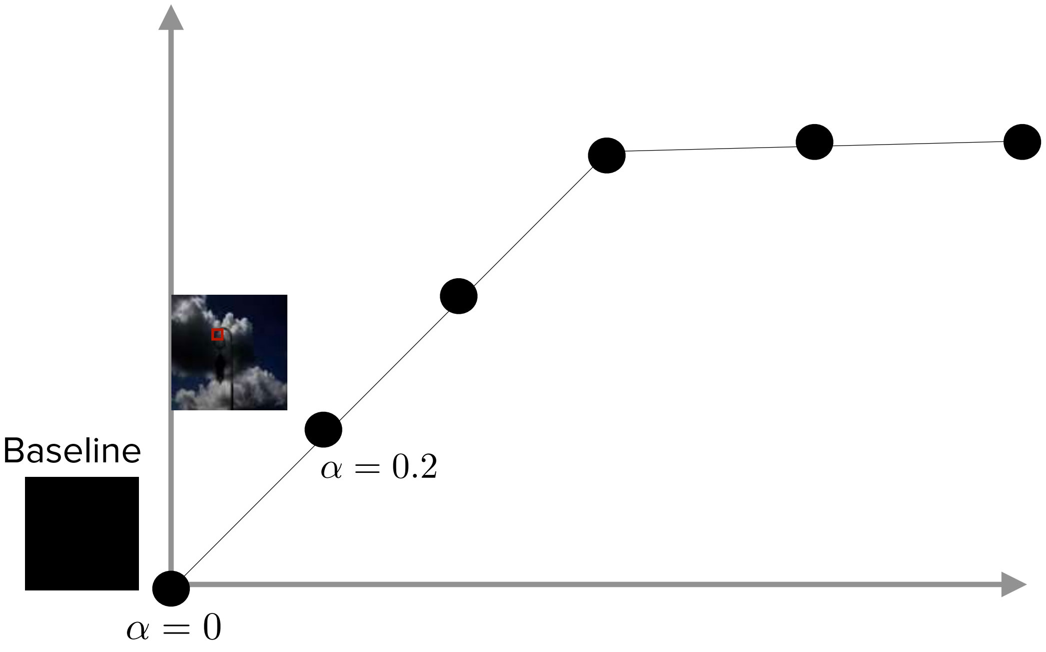

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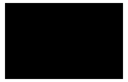
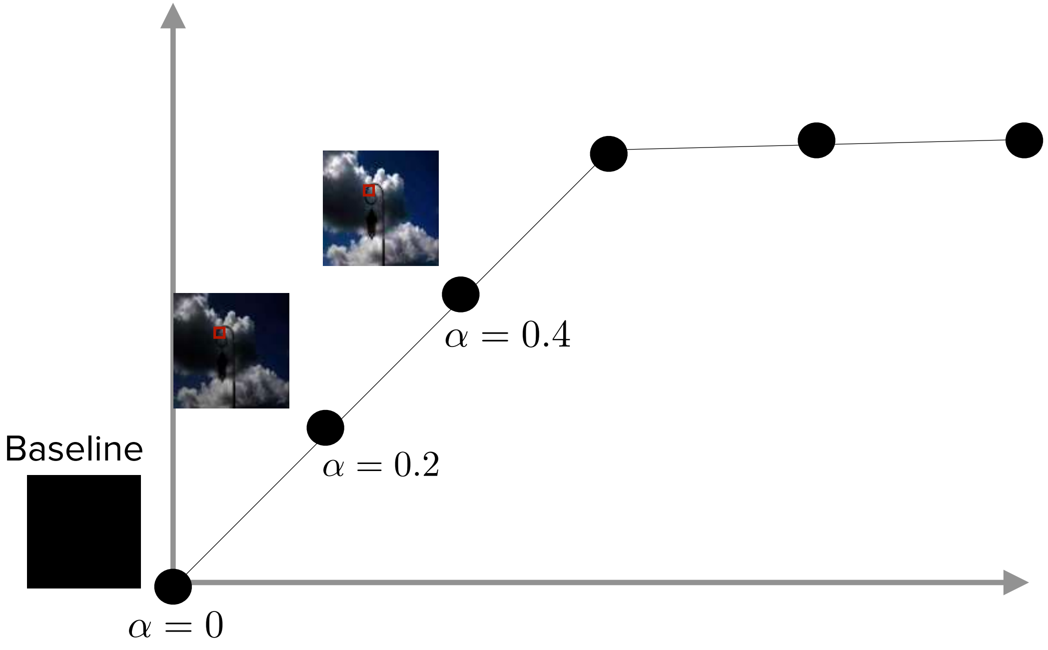
Choose a Baseline to contrast 



[Sundarajan et al. ’16]

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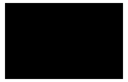
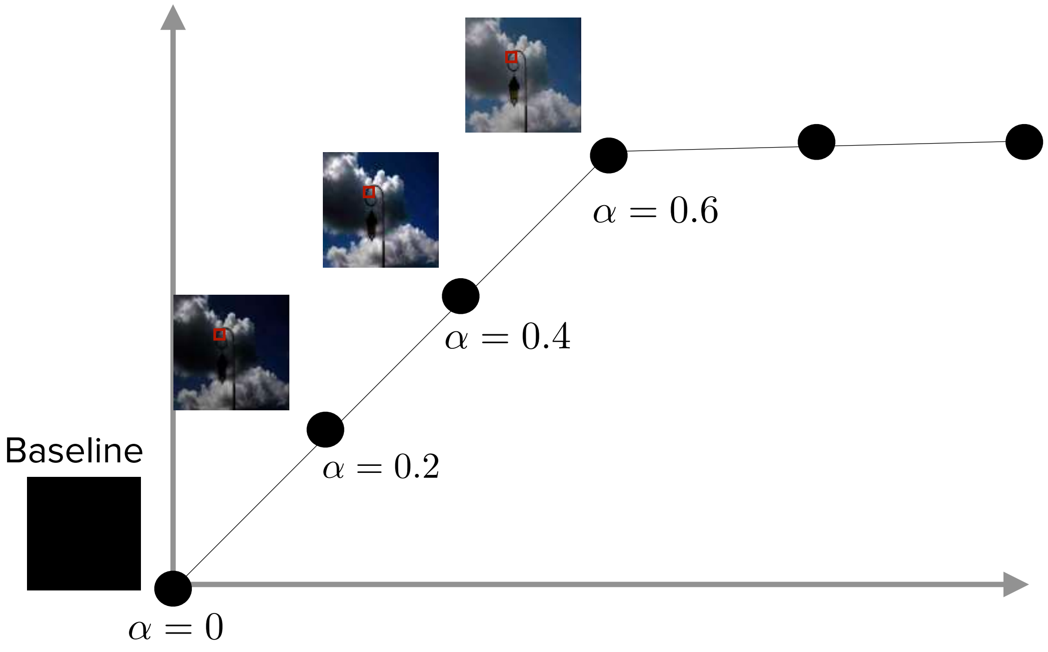
Choose a Baseline to contrast 



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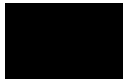
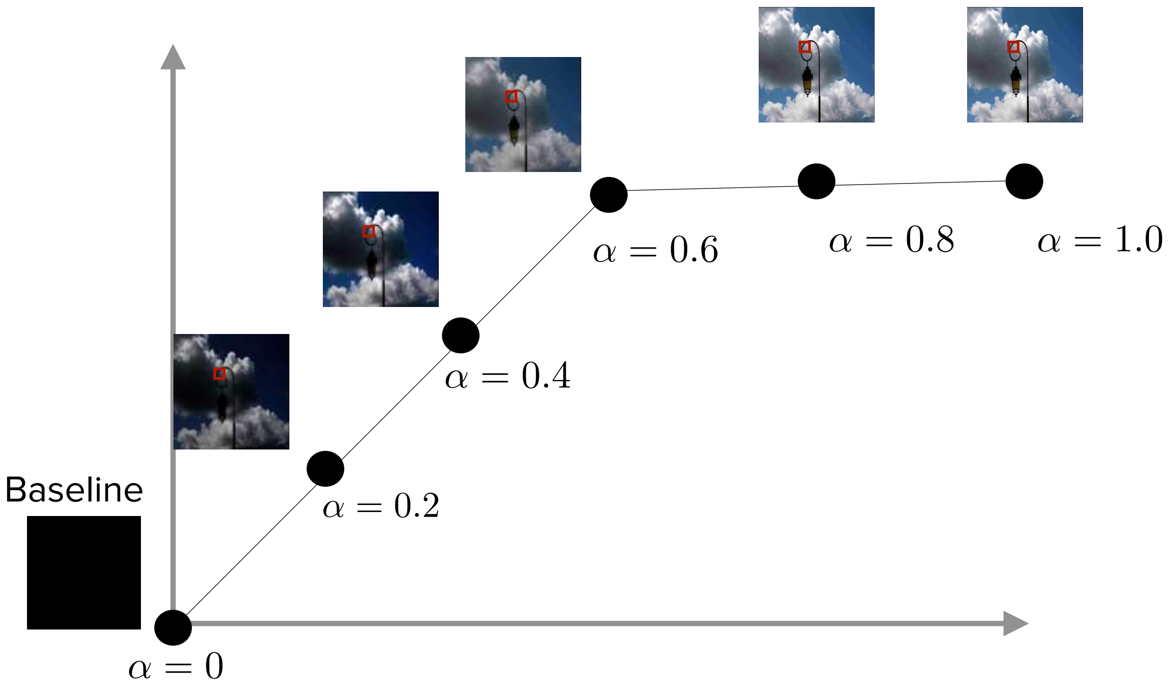
Choose a Baseline to contrast 



Integrated Gradients

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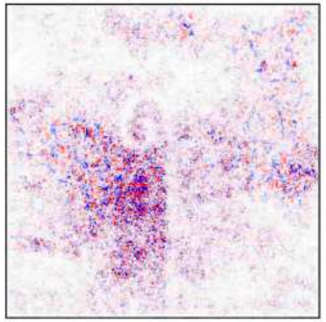
1. Choose a Baseline to contrast
2. Compute gradients at different mask values
3. Attribution = Aggregation over gradients computed for a certain set of perturbations

$$R_i^c(x) = x_i \cdot \int_{\alpha=0}^{1} \frac{\partial S_c(\tilde{x})}{\partial\left(\tilde{x}_i\right)} \bigg|_{\tilde{x}=\underbrace{\bar{x}}_{\text{Baseline}}+\alpha(\underbrace{x}_{\text{Original}}-\bar{x})} d\alpha$$

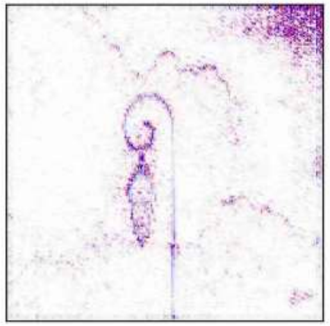
Integrated Gradients monitors how the network changes from a zero signal input to actual input through the use of gradients

Baseline

- Baseline is an information less input
- The choice of baselines matters a lot and is typically domain dependent
    - Black or gray images
    - Zero embedding in language
    - Random document in retrieval



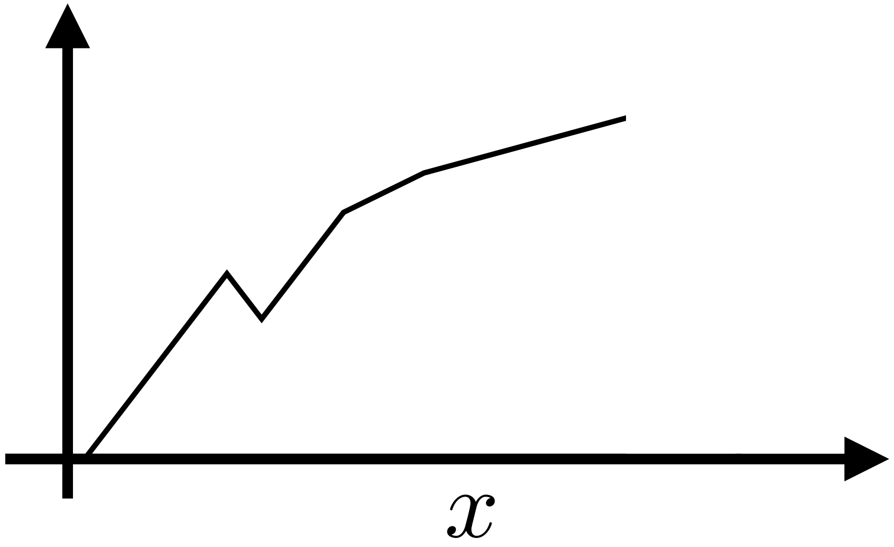
Simple Gradient



Integrated Gradients

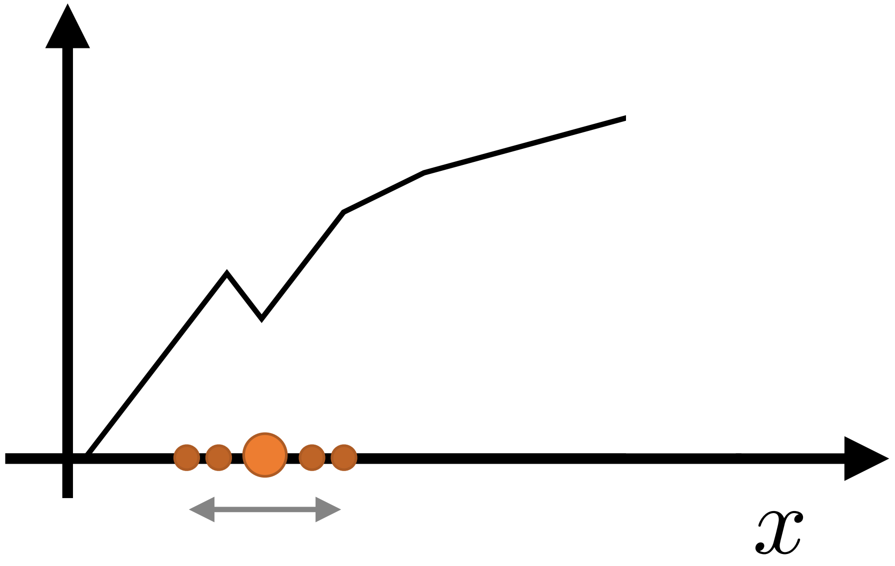
SmoothGrad

- Gradients are local ways to measure sensitivity
- In highly nonlinear loss surfaces you obtain quite noisy gradients
  - In this figure, majority of the neighbourhood gives positive gradient



SmoothGrad

- Calculate multiple copies of the input with a small noise (usually gaussian noise)
- Actual gradient is the average of the gradients of each of the copies



Conclusion

- Gradients are central in computing feature attributions and are visualised using saliency maps
- Simple gradient-based approaches for neural networks attribute the importance back to the input features
- Deep learning models suffer from critical problems for gradient-based methods
  - Models are trained to saturation given near-zero gradients – Integrated Gradients
  - Gradients are unstable due to highly non-linear loss surface – SmoothGrad
- Tons of other approaches proposed in the literature
- Caution that explanations might disagree with each other
- Caution that gradient-based approaches need to be adapted depending on the input style