# Interpretable Deep Learning

2019.2.20

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Part I – Introduction to Interpretability

Part 2 – Interpreting Deep Neural Networks

Part 3 – Evaluating Attribution Methods

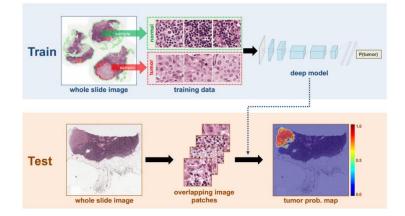
Part I – Introduction to Interpretability

### What is Interpretability?

AlphaGo vs. Lee Sedol



Disease Diagnosis



ImageNet Challenge



Neural Machine Translation



Self-driving Cars

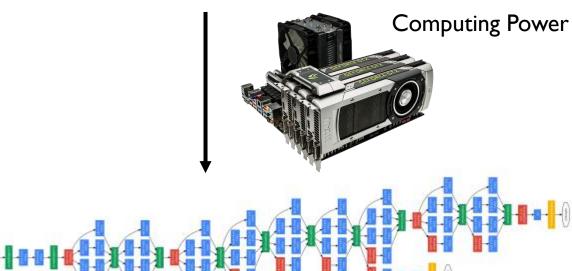


& More to Come!

### What is Interpretability?

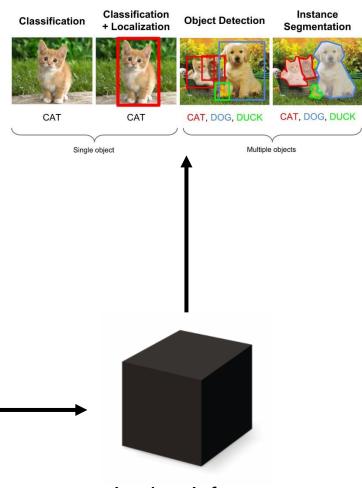
### Large Dataset



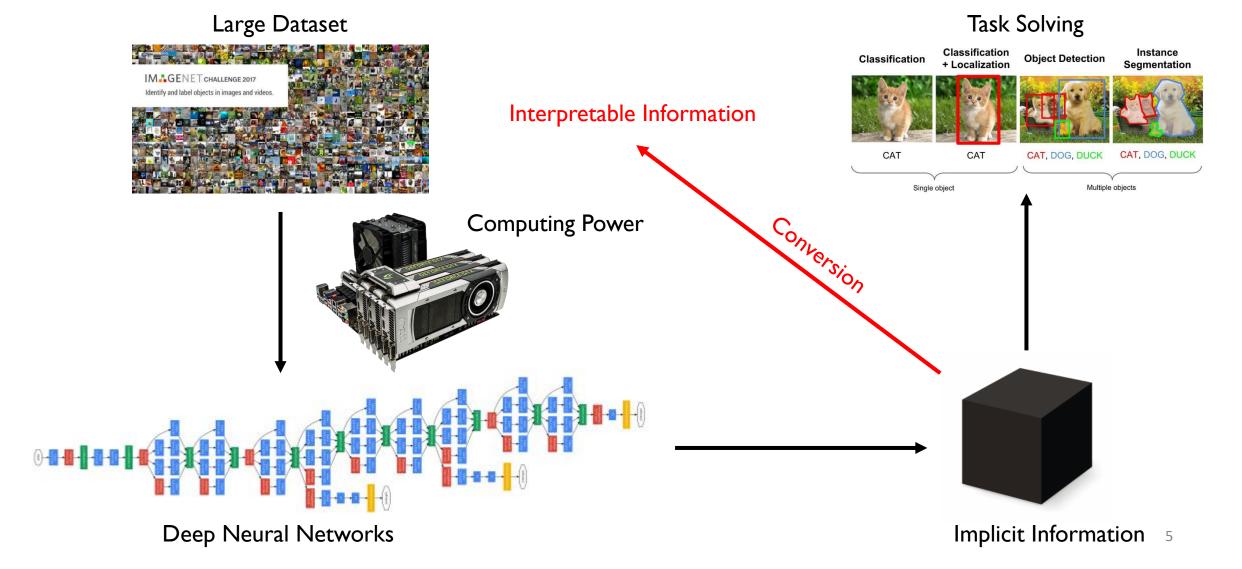




#### Task Solving



### What is Interpretability?

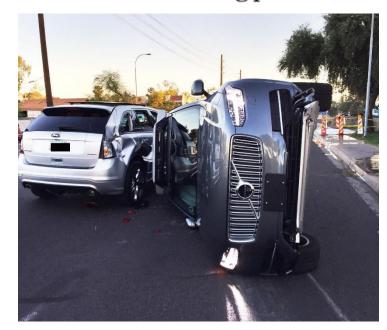


...So What?

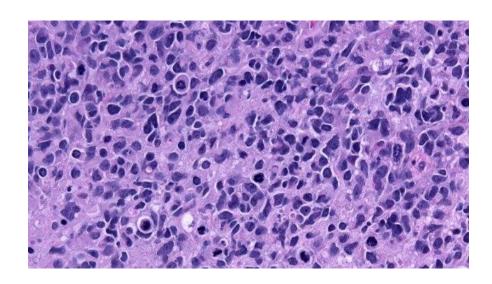
### I. Verify that model works as expected

Wrong decisions can be costly and dangerous

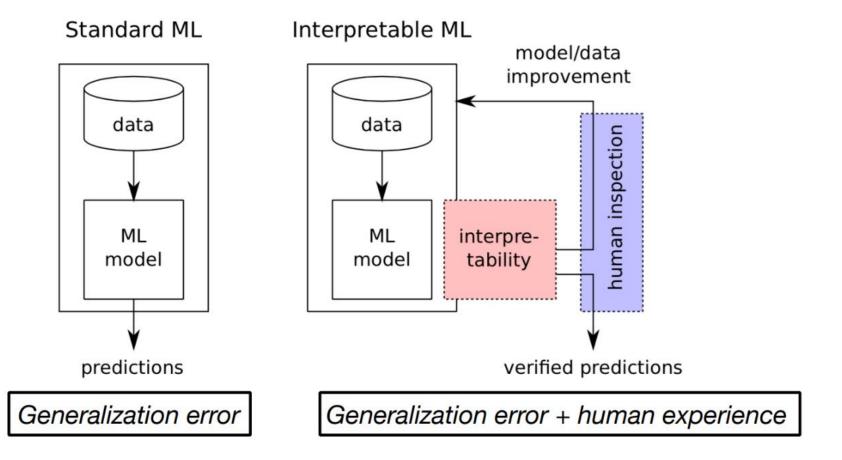
Self-driving Uber kills Arizona woman in first fatal crash involving pedestrian



Disease Misclassification



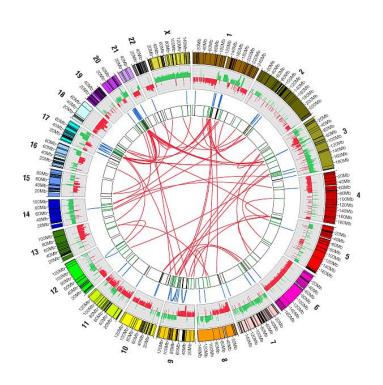
### 2. Improve / Debug classifier

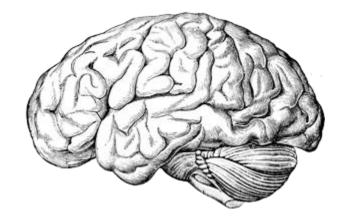


### 3. Make new discoveries

Learn about the physical / biological / chemical mechanisms

Learn about the human brain





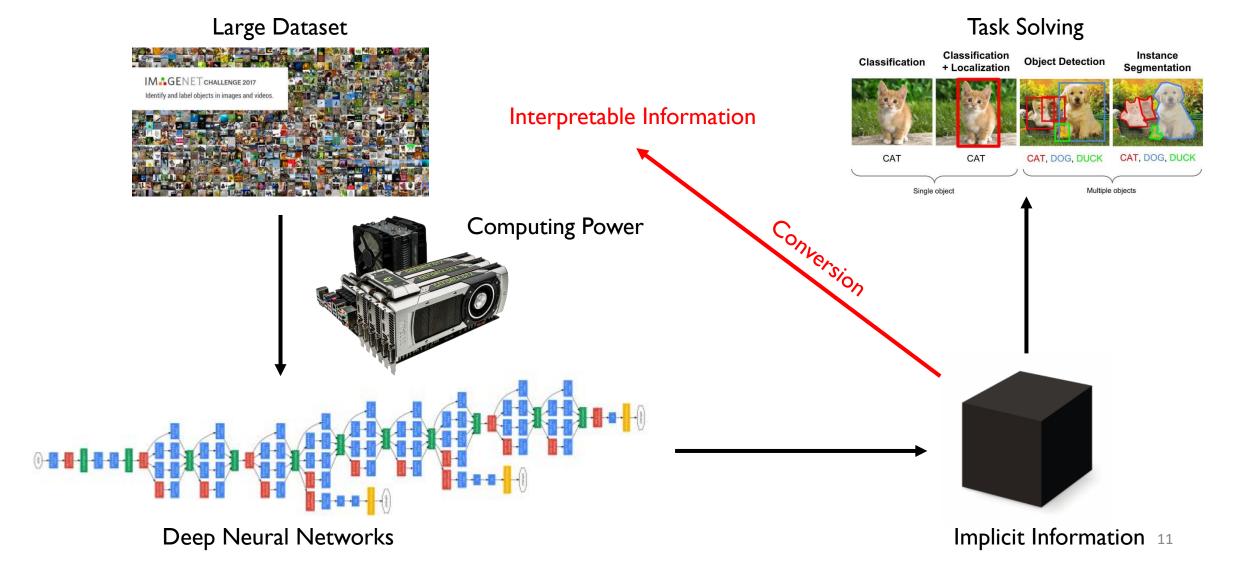
### 4. Right to explanation

"Right to be given an explanation for an output of the algorithm"

#### Ex.

- US Equal Credit Opportunity Act
- The European Union General Data Protection Regulation
- France Digital Republic Act

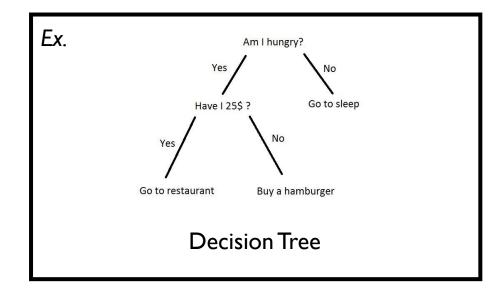
### Back to Interpretability!



### Types of Interpretability in ML

#### **Ante-hoc Interpretability**

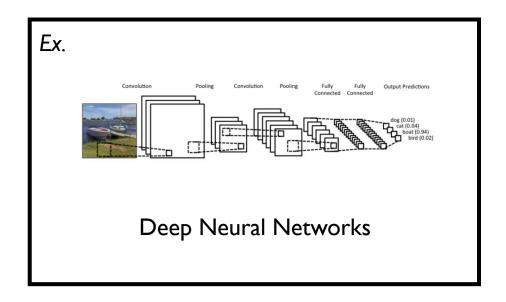
Choose an interpretable model and train it.



**Problem.** Is the model expressive enough to predict the data?

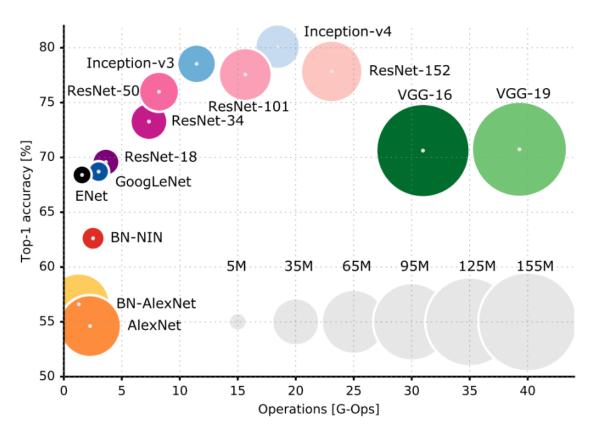
#### **Post-hoc Interpretability**

Choose a complex model and develop a special technique to interpret it.



**Problem.** How to interpret millions of parameters?

### Types of Interpretability in ML

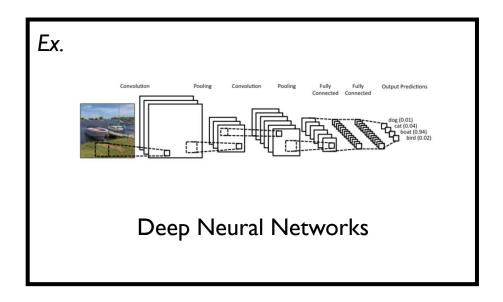


At least 5 million parameters! (오백만)

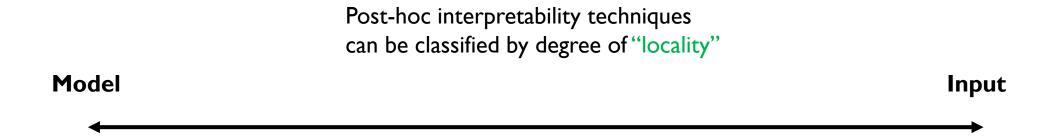
### Types of Interpretability in ML

#### **Post-hoc Interpretability**

Choose a complex model and develop a special technique to interpret it.



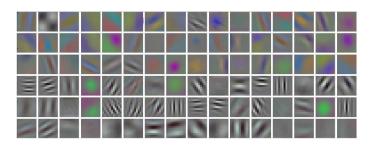
**Problem.** How to interpret millions of parameters?



Post-hoc interpretability techniques can be classified by degree of "locality"

Model Input

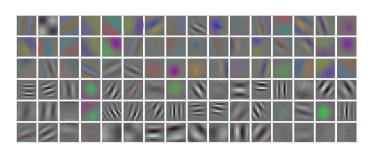
What representations have the DNN learned?



Post-hoc interpretability techniques can be classified by degree of "locality"

Model Input

What representations have the DNN learned?



What pattern / image maximally activates a particular neuron?

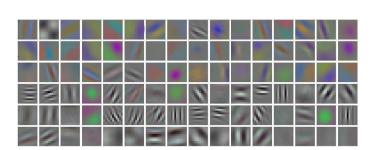


dumbbell

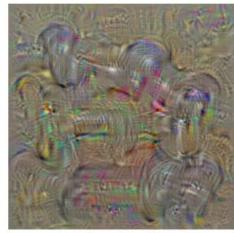
Post-hoc interpretability techniques can be classified by degree of "locality"

Model Input

What representations have the DNN learned?

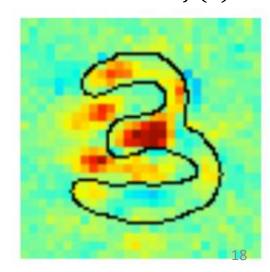


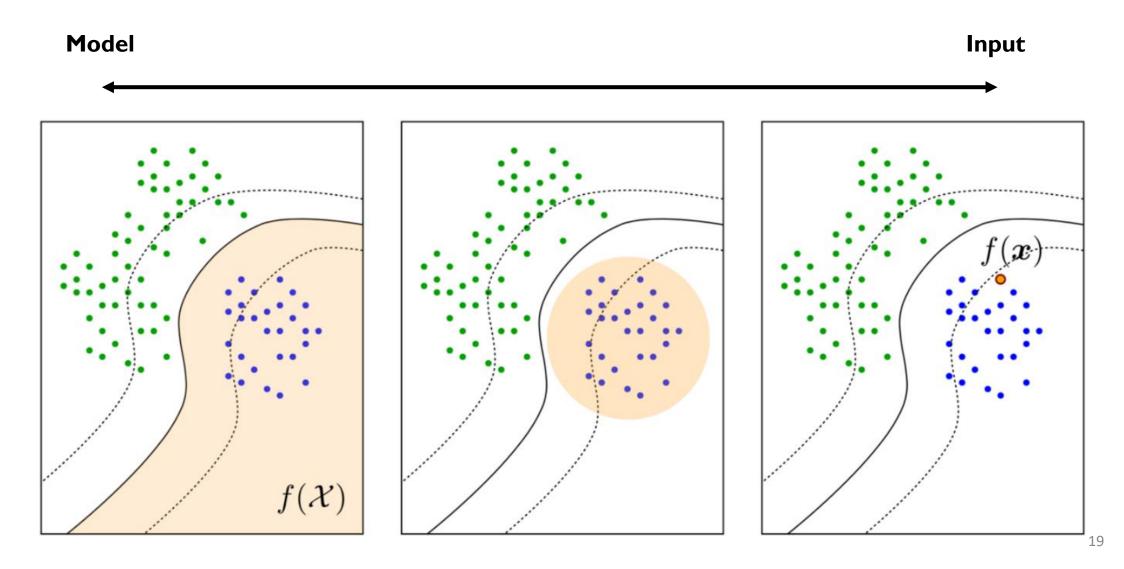
What pattern / image maximally activates a particular neuron?



dumbbell

Explain why input x has been classified as f(x).





### Part I Summary

#### I. What is interpretability in Deep Learning?

- Converting implicit information in DNN to (human) interpretable information

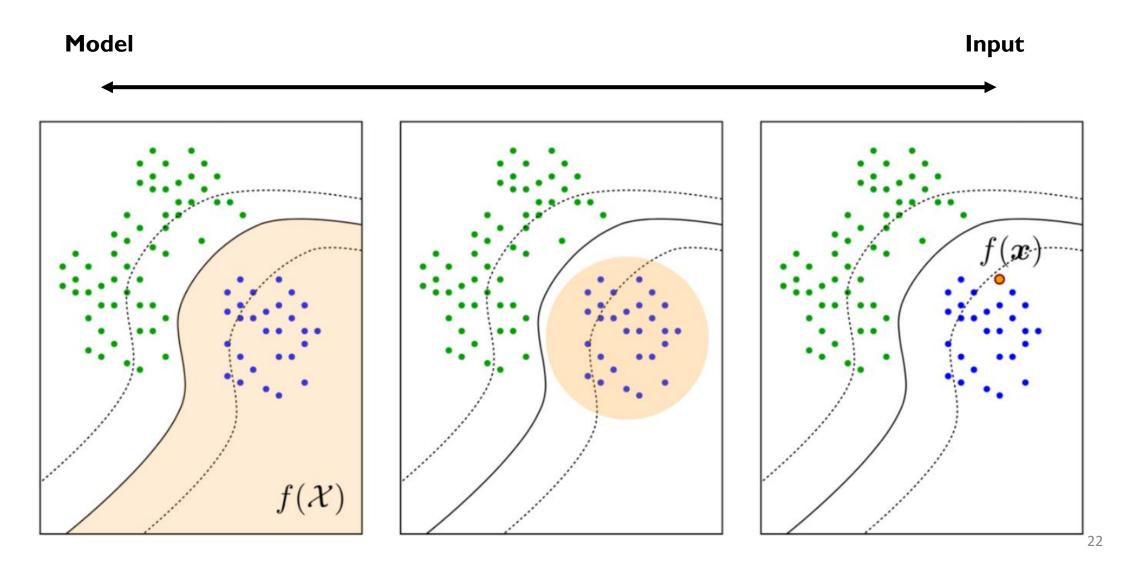
#### 2. Why do we need interpretability in Deep Learning?

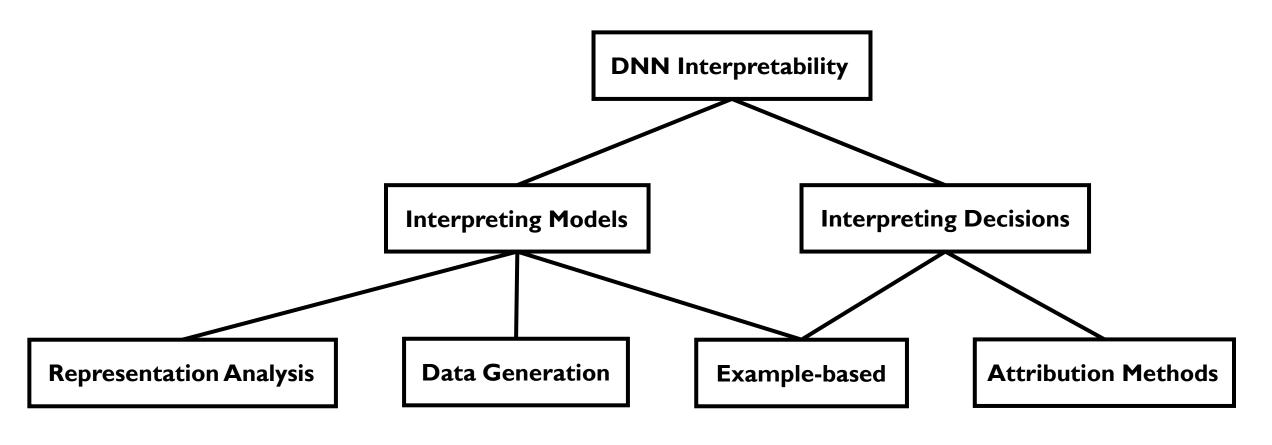
- Verify model works as intended
- Debug classifier
- Make discoveries
- Right to explanation

#### 3. Types of Interpretability in ML

- Ante-hoc Interpretability: choose an interpretable model and train it
- Post-hoc Interpretability: choose a complex model and develop a special technique to interpret it
- Post-hoc interpretability techniques can be classified by degree of "locality"

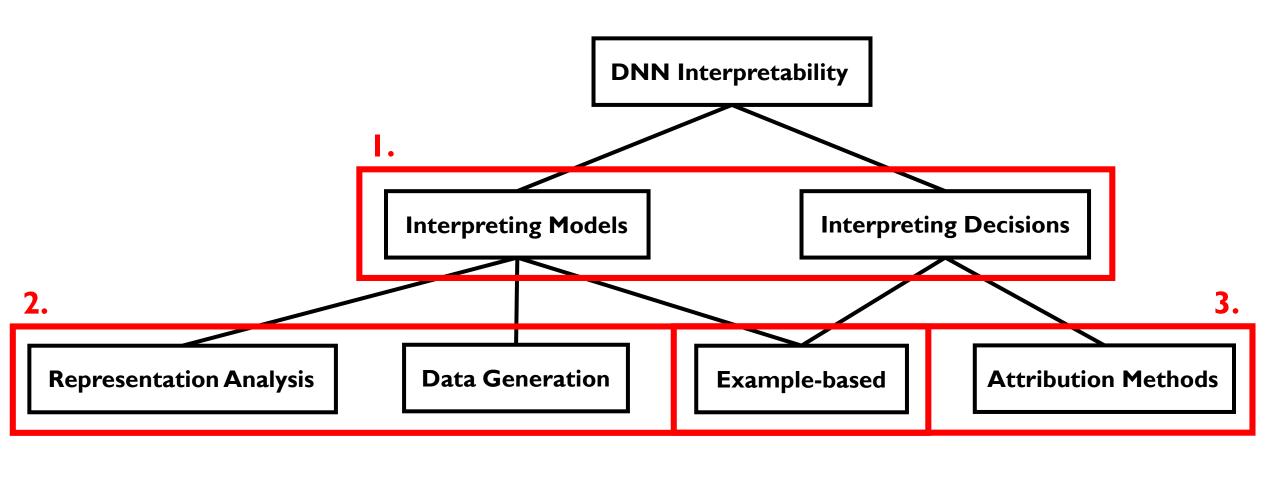
### Part 2 – Interpreting Deep Neural Networks

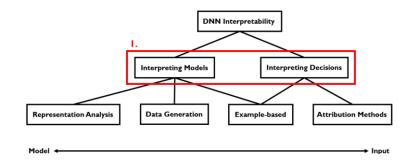




Model ← Input

Model





### **Interpreting Models**

(Macroscopic)

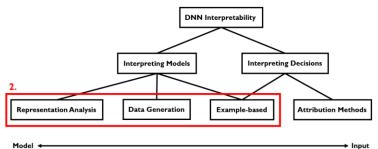
- "Summarize" DNN with a simpler model (e.g. decision tree)
- Find prototypical example of a category
- Find pattern maximizing activation of a neuron

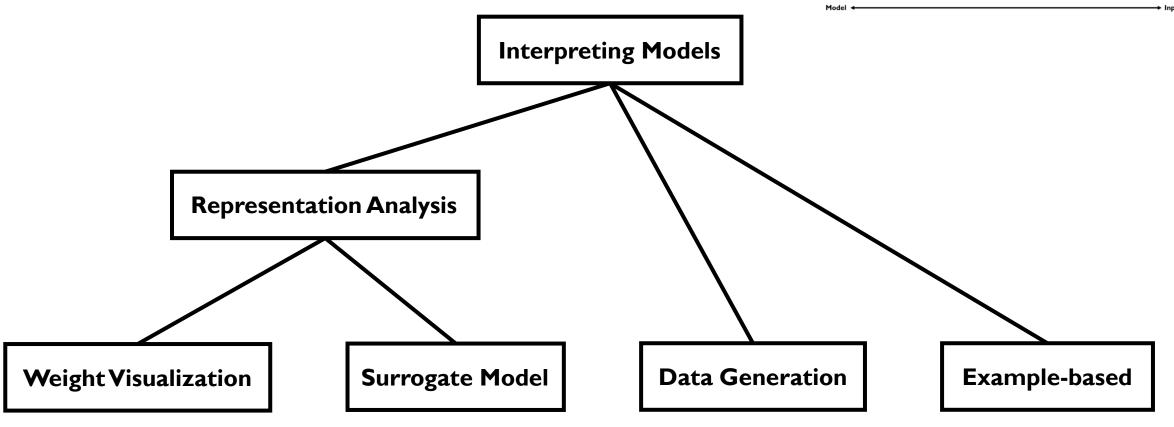
Better understand internal representations

### Interpreting Decisions (Microscopic)

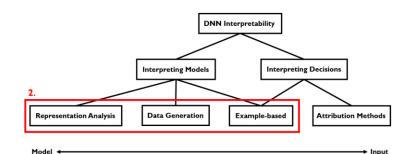
- Why did DNN make this decision
- Verify that model behaves as expected
- Find evidence for decision

Important for practical applications





Model ← Input



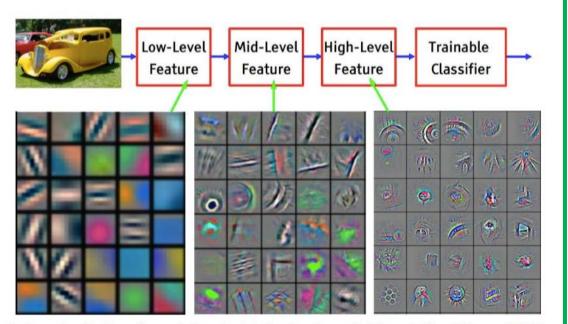
Weight Visualization

**Surrogate Model** 

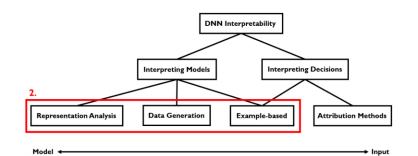
**Data Generation** 

**Example-based** 

- Filter visualization in Convolutional Neural Networks
- Can understand what kind of features CNN has learned
- Still too many filters!



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

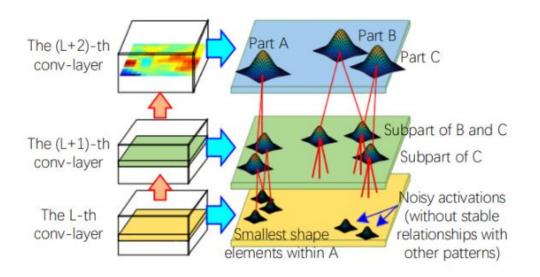


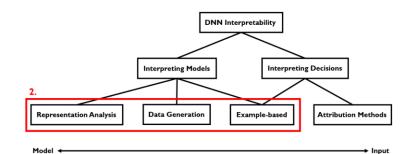
Weight Visualization

**Surrogate Model** 

**Data Generation** 

- "Summarize" DNN with a simpler model
- E.g. Decision trees, graphs or linear models





Weight Visualization

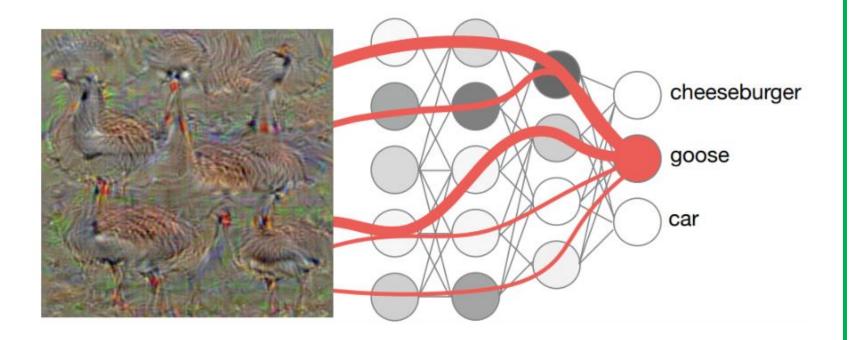
**Surrogate Model** 

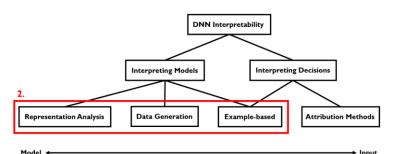
**Data Generation** 

**Example-based** 

#### **Activation Maximization**

- Find pattern maximizing activation of a neuron



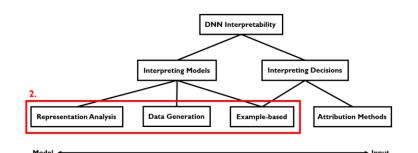


Weight Visualization

Surrogate Model

**Data Generation** 

$$\max_{x \in \mathcal{X}} p_{\theta}(\omega_c \,|\, x) + \lambda \Omega(x)$$

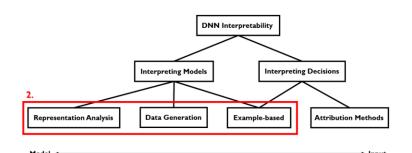


Weight Visualization

**Surrogate Model** 

**Data Generation** 

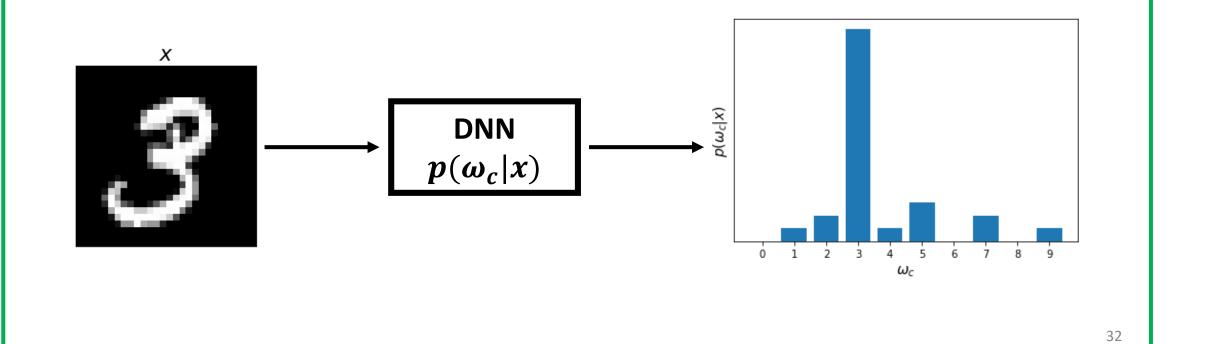
$$\max_{x \in \mathcal{X}} p_{\theta}(\omega_c \,|\, x) + \lambda \Omega(x)$$
Class Probability Regularization Term

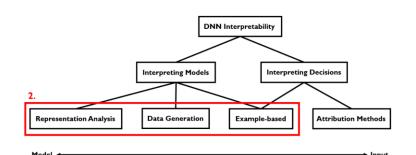


Weight Visualization

**Surrogate Model** 

**Data Generation** 

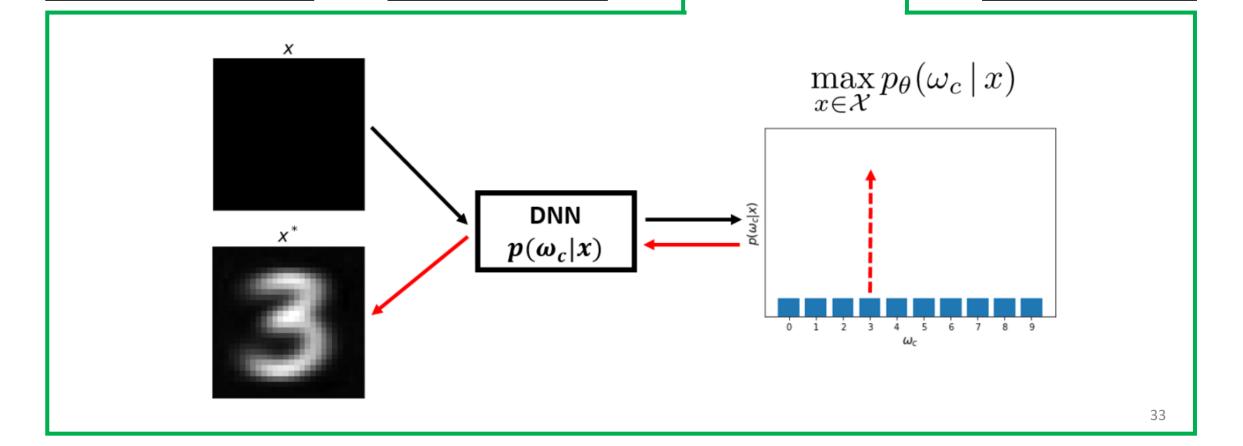


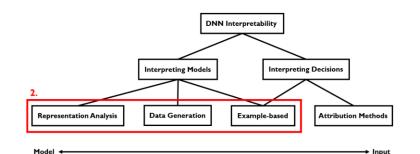


Weight Visualization

**Surrogate Model** 

**Data Generation** 

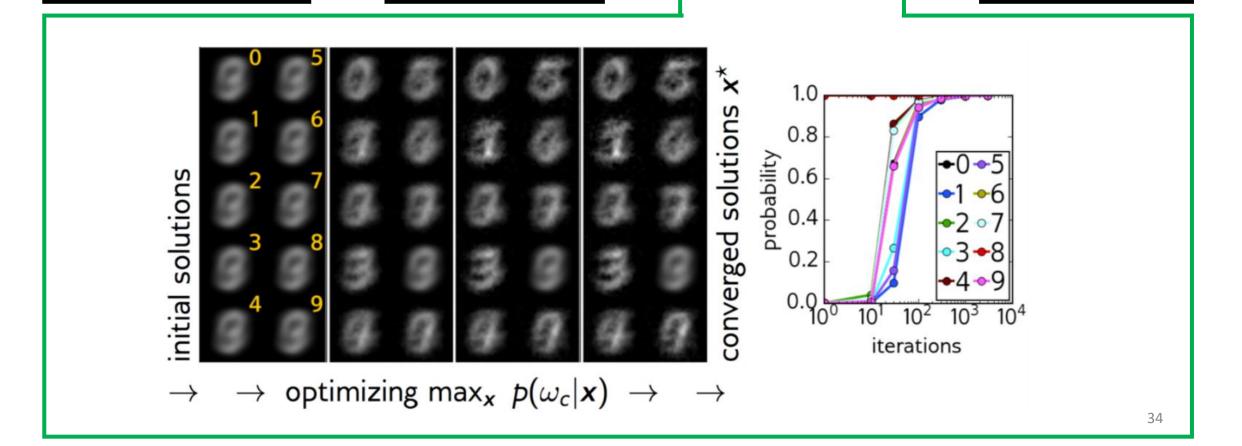


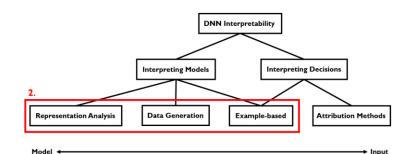


Weight Visualization

**Surrogate Model** 

**Data Generation** 





Weight Visualization

**Surrogate Model** 

**Data Generation** 

**Example-based** 

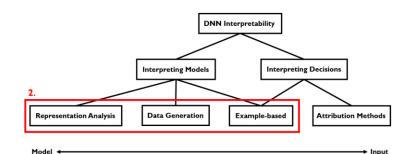
goose



ostrich



Images from **Simonyan et al**. **2013** "Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps"



Weight Visualization

**Surrogate Model** 

**Data Generation** 

**Example-based** 

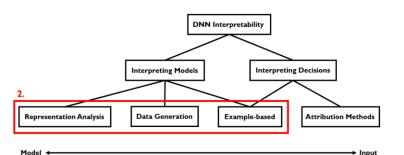
#### Advantages

- AM builds typical patterns for given classes (e.g. beaks, legs)
- Unrelated background objects are not present in the image

#### Disadvantages

- Does not resemble class-related patterns
- Lowers the quality of the interpretation for given classes

Redefine optimization problem!



Weight Visualization

**Surrogate Model** 

**Data Generation** 

**Example-based** 

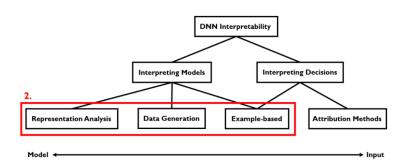
- Does not resemble class-related patterns
- Lowers the quality of the interpretation for given classes

Redefine optimization problem!

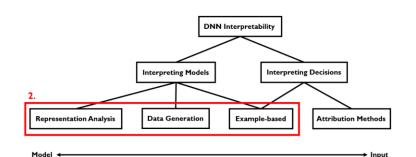
Force the generated data  $x^*$  to match the data more closely

Find the input pattern that maximizes class probability

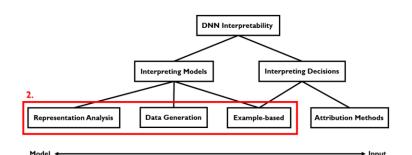
Find the most likely input pattern for a given class



**Surrogate Model** Weight Visualization **Example-based Data Generation** Find the input pattern that Find the most likely input maximizes class probability pattern for a given class



**Surrogate Model** Weight Visualization **Data Generation Example-based**  $\max_{x \in \mathcal{X}} p_{\theta}(\omega_c \mid x) + \lambda \Omega(x)$ 



Weight Visualization

**Surrogate Model** 

**Data Generation** 

**Example-based** 

Find the input pattern that maximizes class probability

Find the most likely input pattern for a given class

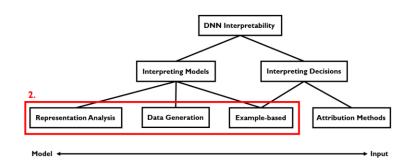
Activation Maximization with Expert

$$p(\mathbf{x}|\omega_c) \propto p(\omega_c|\mathbf{x}) \cdot p(\mathbf{x})$$
original

Activation Maximization in Code Space

$$\max_{\mathbf{z}\in\mathcal{Z}} p(\omega_c|\underbrace{g(\mathbf{z})}_{\mathbf{x}}) + \lambda \|\mathbf{z}\|^2 \qquad \mathbf{x}^* = g(\mathbf{z}^*)$$

These two techniques require an unsupervised model of the data, either a density model p(x) or a generator g(z)



Weight Visualization

**Surrogate Model** 

**Data Generation** 

**Example-based** 

simple AM (initialized to mean)



simple AM (init. to class means)



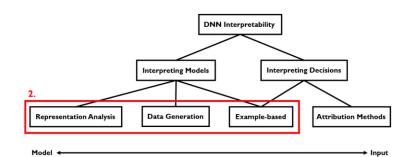
AM-density (init. to class means)



AM-gen (init. to class means)



**Observation:** Connecting to the data leads to sharper visualizations.



Weight Visualization

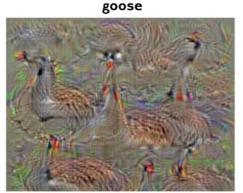
**Surrogate Model** 

**Data Generation** 

**Example-based** 

#### **Activation Maximization**

#### ----



ostrich



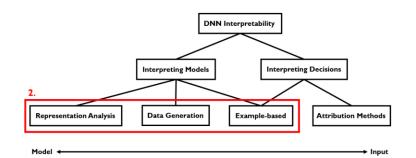
Images from **Simonyan et al. 2013** "Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps"

#### Activation Maximization in Code Space

Images from **Nguyen et al. 2016**. "Synthesizing the preferred inputs for neurons in neural networks via deep generator networks"



**Observation:** Connecting to the data leads to sharper visualizations.



Weight Visualization

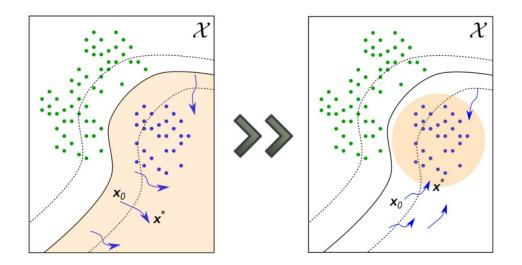
**Surrogate Model** 

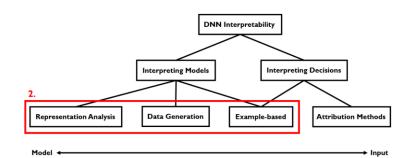
**Data Generation** 

**Example-based** 

#### Summary

- DNNs can be interpreted by finding input patterns that maximize a certain output quantity.
- Connecting to the data improves the interpretability of the visualization.





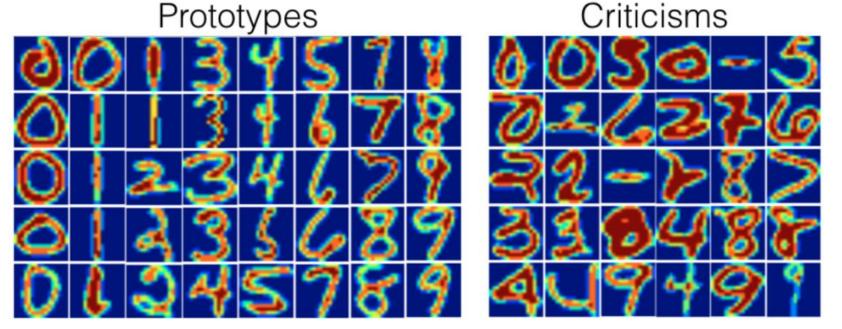
Weight Visualization

**Surrogate Model** 

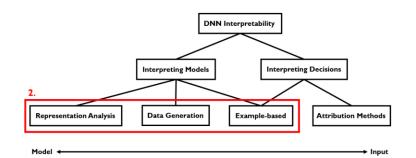
**Data Generation** 

**Example-based** 

- Find image instances that represent / do not represent the image class



"Examples are not Enough, Learn to Criticize! Criticism for Interpretability", https://people.csail.mit.edu/beenkim/papers/KIM2016NIPS MMD.pdf



Weight Visualization

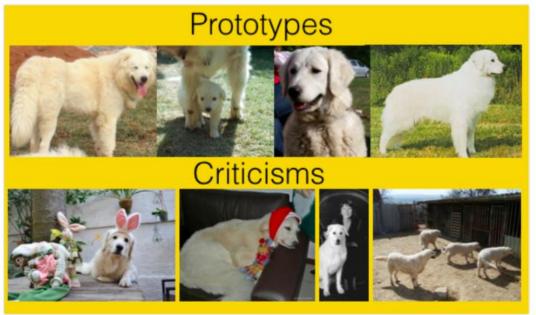
**Surrogate Model** 

**Data Generation** 

**Example-based** 

- Find image instances that represent / do not represent the image class





"Examples are not Enough, Learn to Criticize! Criticism for Interpretability", https://people.csail.mit.edu/beenkim/papers/KIM2016NIPS\_MMD.pdf

#### Limitation of Model Interpretations

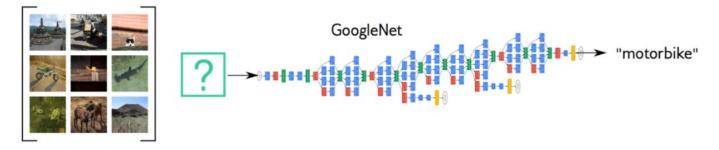
Question: What would be the best image to interpret the class "motorcycle"?



- Summarizing a concept or a category like "motorcycle" into a single image is difficult.
- A good interpretation would grow as large as the diversity of the concept to interpret.

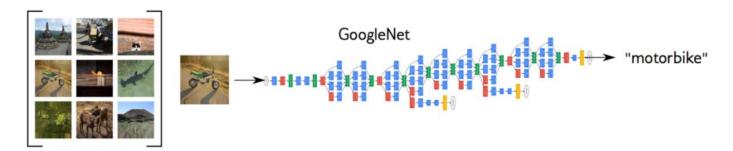
#### Limitation of Model Interpretations

#### Finding a prototype:

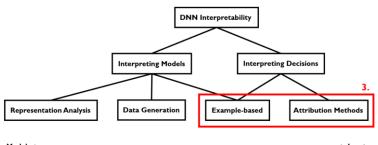


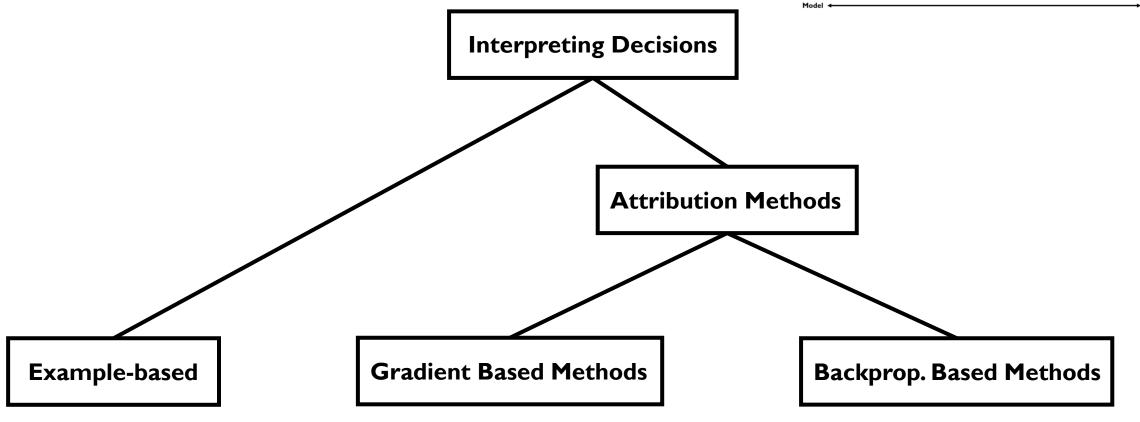
Question: How does a "motorbike" typically look like?

#### **Decision explanation:**

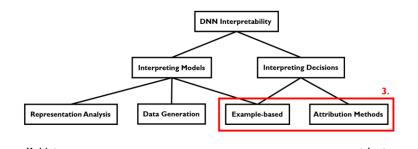


Question: Why is this example classified as a motorbike?





Model ← Input



**Example-based** 

**Attribution Methods** 

**Gradient Based** 

Backprop. Based

- Which training instance influenced the decision most?
- Still does not specifically highlight which features were important.

'Sunflower': 59.2% conf.

Original



Influence: 0.09



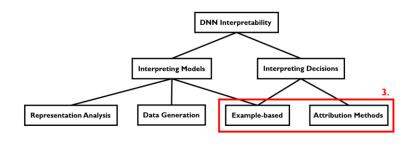
Influence: 0.14



Influence: 0.42



<sup>&</sup>quot;Understanding Black-box Predictions via Influence Functions", https://arxiv.org/pdf/1703.04730.pdf "Interpretation of Neural Networks is Fragile", https://arxiv.org/pdf/1710.10547.pdf



**Example-based** 

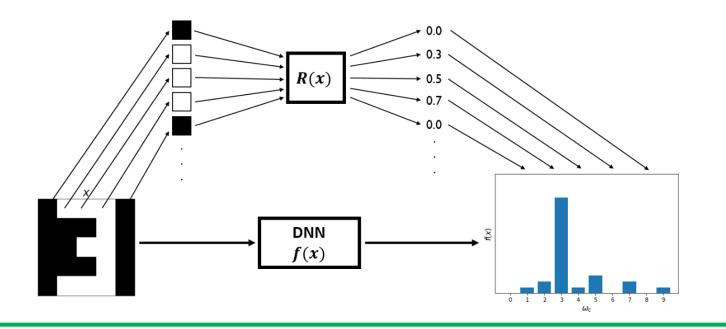
**Attribution Methods** 

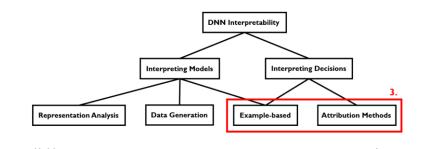
**Gradient Based** 

Backprop. Based

50

Given an image  $x \in \mathbb{R}^n$  and a decision f(x), assign to each pixel  $x_1, x_2, ..., x_n$  attribution values  $R_1(x), R_2(x), ..., R_n(x)$ .





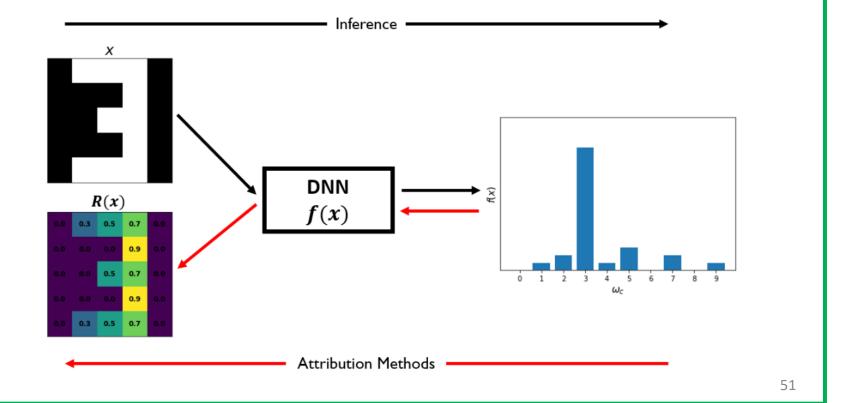
**Example-based** 

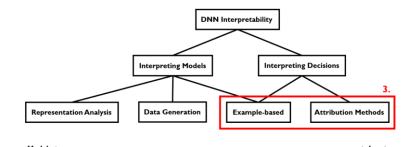
**Attribution Methods** 

**Gradient Based** 

Backprop. Based

Usually visualized as heatmaps





**Example-based** 

**Attribution Methods** 

**Gradient Based** 

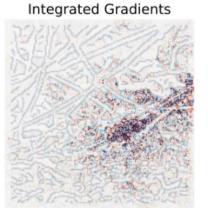
Backprop. Based

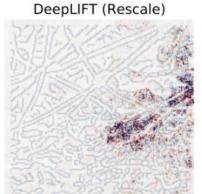
Usually visualized as heatmaps

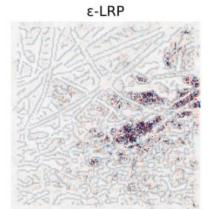
Original (label: "garter snake")

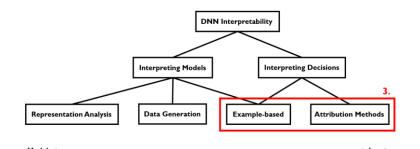


Grad \* Input









**Example-based** 

**Attribution Methods** 

**Gradient Based** 

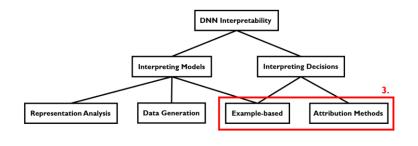
Backprop. Based

#### The Baseline Attribution Method Saliency Map

- Gradient of the decision f(x) with respect to the input image x:

$$Saliency(\mathbf{x}) \coloneqq \nabla_{\mathbf{x}} f(\mathbf{x}) = \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}$$

- Can be calculated through backpropagation.



**Example-based** 

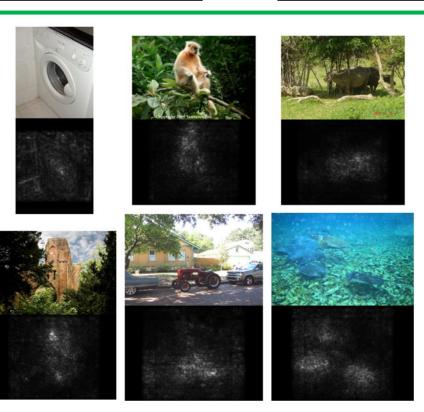
**Attribution Methods** 

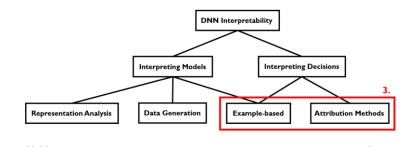
**Gradient Based** 

Backprop. Based

#### The Baseline Attribution Method Saliency Map

- Saliency maps are very noisy!
- Only roughly correlated with the object(s) of interest.





**Example-based** 

**Attribution Methods** 

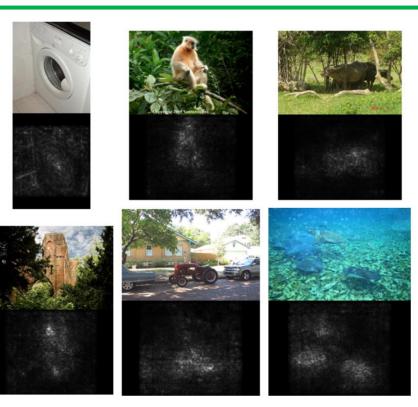
**Gradient Based** 

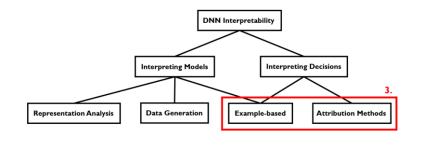
**Backprop. Based** 

#### The Baseline Attribution Method Saliency Map

- Saliency maps are very noisy!
- Only roughly correlated with the object(s) of interest.

Question: How to improve saliency maps?





**Example-based** 

**Attribution Methods** 

**Gradient Based** 

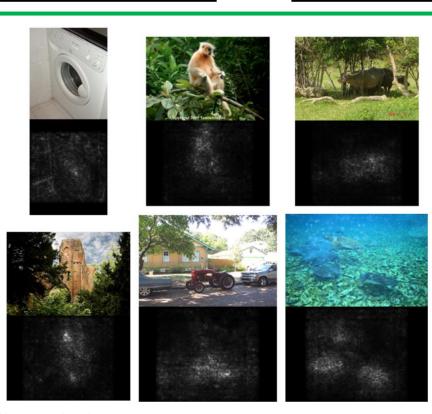
Backprop. Based

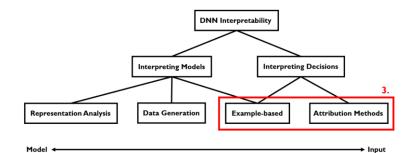
#### The Baseline Attribution Method Saliency Map

- Saliency maps are very noisy!
- Only roughly correlated with the object(s) of interest.

Question: How to improve saliency maps?

Question: Why are saliency maps noisy?





**Example-based** 

**Attribution Methods** 

**Gradient Based** 

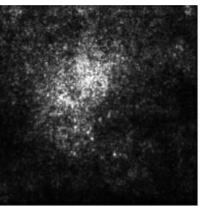
Backprop. Based

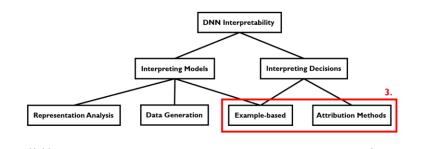
**Question:** Why are saliency maps noisy?

Hypothesis I — Saliency maps are truthful

- Certain pixels scattered randomly across the image are central to how the network is making a decision.
- Noise is important!







**Example-based** 

**Attribution Methods** 

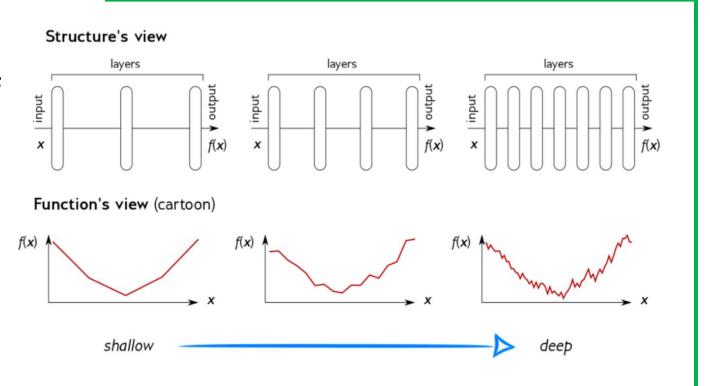
**Gradient Based** 

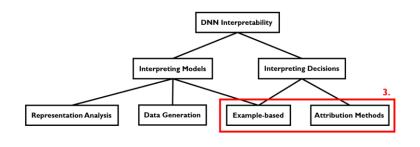
Backprop. Based

Question: Why are saliency maps noisy?

Hypothesis 2 — Gradients are discontinuous

- DNN uses piecewise-linear functions (ReLU activation, max-pooling, etc.).
- Sudden jumps in the importance score over infinitesimal changes in the input.





**Example-based** 

**Attribution Methods** 

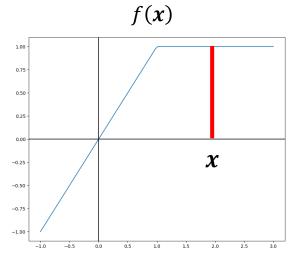
**Gradient Based** 

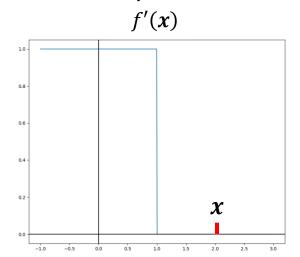
Backprop. Based

**Question:** Why are saliency maps noisy?

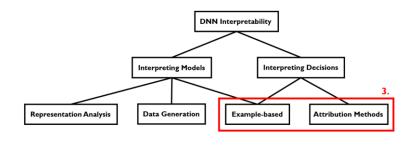
Hypothesis 3 - f(x) saturates

- A feature may have a strong effect globally, but with a small derivative locally.





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**Example-based** 

**Attribution Methods** 

**Gradient Based** 

Backprop. Based

Question: How to improve saliency maps?

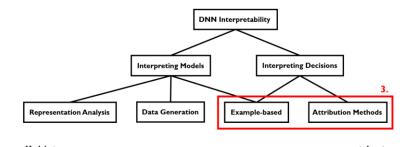
$$Saliency(\mathbf{x}) \coloneqq \nabla_{\mathbf{x}} f(\mathbf{x}) = \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}$$

**Gradient-based Methods** 

- Perturb the input x to  $x^*$  and use  $\nabla_{x^*} f(x^*)$ .
- Some methods take the average over the perturbation set  $\{x_1^*, x_2^*, ..., x_n^*\}$ .

**Backprop-based Methods** 

- Modify the backpropagation algorithm.



**Example-based** 

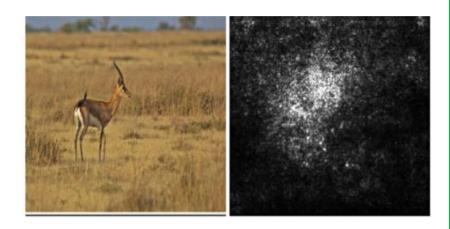
**Attribution Methods** 

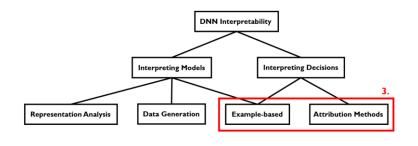
**Gradient Based** 

Backprop. Based

#### Summary

- Attribution method assigns "attribution score" to each input pixel.
- Baseline attribution method Saliency Map is noisy.
- Hypothesis I: Saliency maps are truthful.
- Hypothesis 2: Gradients are discontinuous.
- Hypothesis 3: f(x) saturates.
- Two solution approaches: Gradient based method and Backprop. based method.





**Example-based** 

**Attribution Methods** 

**Gradient Based** 

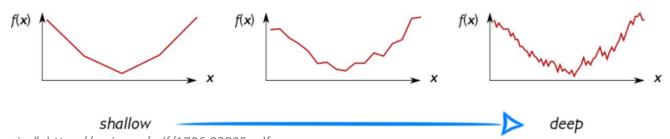
Backprop. Based

**I.SmoothGrad** Hypothesis 2 – Gradients are discontinuous

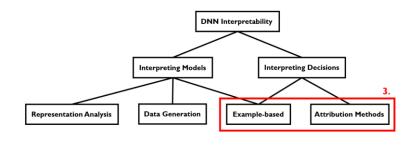
SmoothGrad(
$$\mathbf{x}$$
) :=  $\frac{1}{n} \sum_{1}^{n} \frac{\partial f(\mathbf{x}^*)}{\partial \mathbf{x}^*}$ ,  $\mathbf{x}^* = \mathbf{x} + \mathcal{N}(\mathbf{0}, \sigma^2)$ 

Gaussian smoothing

Function's view (cartoon)



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**Example-based** 

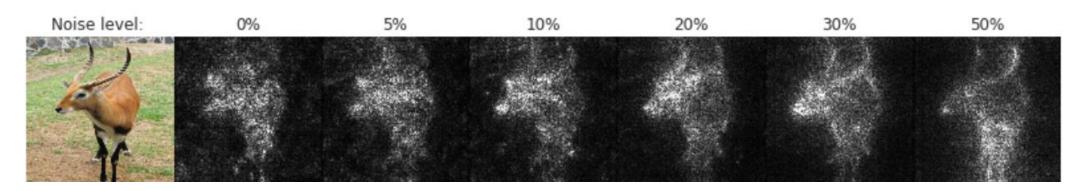
**Attribution Methods** 

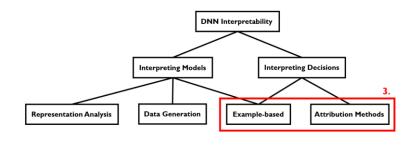
**Gradient Based** 

Backprop. Based

**I. SmoothGrad** Hypothesis 2 – Gradients are discontinuous

SmoothGrad(
$$\mathbf{x}$$
) :=  $\frac{1}{n} \sum_{1}^{n} \frac{\partial f(\mathbf{x}^*)}{\partial \mathbf{x}^*}$ ,  $\mathbf{x}^* = \mathbf{x} + \mathcal{N}(0, \sigma^2)$ 





**Example-based** 

**Attribution Methods** 

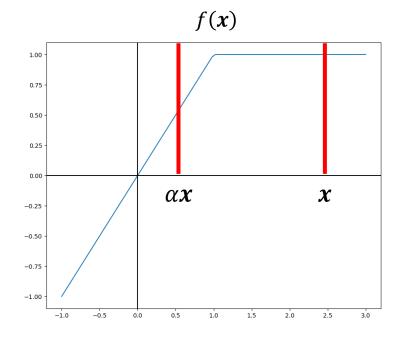
**Gradient Based** 

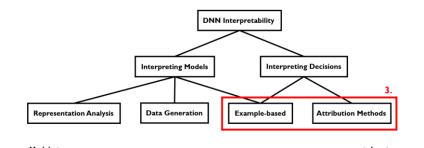
Backprop. Based

**2. Interior Gradient** Hypothesis 3 - f(x) saturates

$$IntGrad(x) := \frac{\partial f(x^*)}{\partial x^*}, \quad x^* = \alpha x, \quad 0 < \alpha \le 1$$

- Appropriate  $\alpha$  will trigger informative activation functions





**Example-based** 

**Attribution Methods** 

**Gradient Based** 

Backprop. Based

#### 2. Interior Gradient

$$IntGrad(\mathbf{x}) \coloneqq \frac{\partial f(\mathbf{x}^*)}{\partial \mathbf{x}^*},$$

$$x^* = \alpha x$$
.

$$0 < \alpha < 1$$







 $\alpha = 0.04$ 



 $\alpha = 0.06$ 



 $\alpha = 0.08$ 



$$\alpha = 0.1$$



$$\alpha = 0.2$$



$$\alpha = 0.4$$



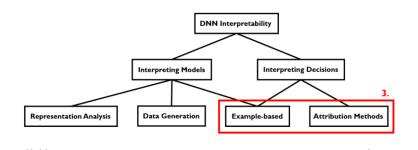
$$\alpha = 0.6$$



$$\alpha = 0.8$$



$$\alpha = 1.0$$



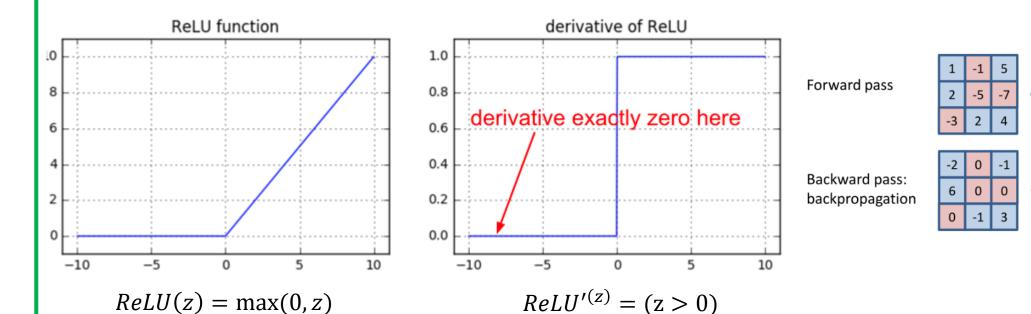
**Example-based** 

**Attribution Methods** 

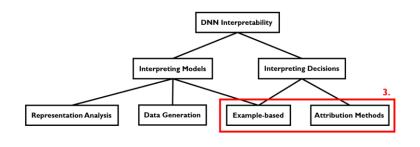
**Gradient Based** 

Backprop. Based

#### Review: Backpropagation at ReLU



"Striving for Simplicity: The All Convolutional Net", https://arxiv.org/pdf/1412.6806.pdf



**Example-based** 

**Attribution Methods** 

**Gradient Based** 

**Backprop. Based** 

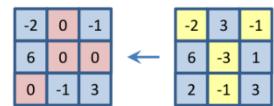
#### I. Deconvnet

- Maps feature pattern to input space (image reconstruction)
- To obtain valid feature reconstruction, pass the reconstructed signal through ReLUs
- Removing noise by removing negative gradient

Forward pass

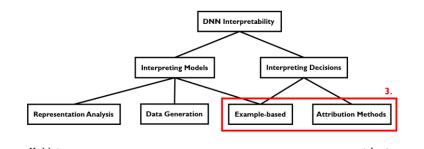
1	-1	5		1	0	5
2	-5	-7	$\rightarrow$	2	0	0
-3	2	4		0	2	4

Backward pass: backpropagation



Backward pass: "deconvnet"

0	3	0	<b>←</b>	-2	3	-1
6	0	1		6	-3	1
2	0	3		2	-1	3



**Example-based** 

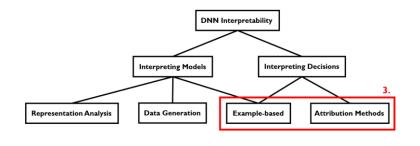
**Attribution Methods** 

**Gradient Based** 

**Backprop. Based** 

#### 2. Guided Backpropagation

- Combine Deconvnet with Backpropagation
- Removing negative gradient + consider forward activations



**Example-based** 

**Attribution Methods** 

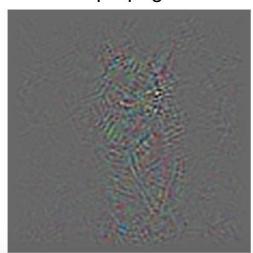
**Gradient Based** 

**Backprop. Based** 

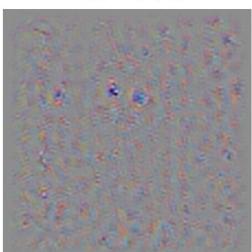
Input image



Backpropagation



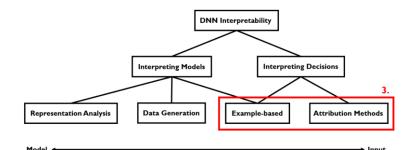
Deconvolution



**Guided Backprop** 



**Observation:** Removing more gradient leads to sharper visualizations



**Example-based** 

**Attribution Methods** 

**Gradient Based** 

Backprop. Based

#### **Other Attribution Methods**

- Gradient \* Input https://arxiv.org/pdf/1704.02685.pdf
- Integrated Gradient https://arxiv.org/pdf/1703.01365.pdf
- Layer-wise Relevance Propagation https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0130140
- Deep Taylor Decomposition https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0130140
- DeepLIFT https://arxiv.org/pdf/1704.02685.pdf
- PatternNet and PatternAttribution https://arxiv.org/pdf/1705.05598.pdf

#### Part 2 Summary

#### I. Interpreting Models vs. Interpreting Decisions

- Interpreting models: macroscopic view, better understand internal representations
- Interpreting decision: microscopic view, important for practical applications

#### 2. Interpreting Models

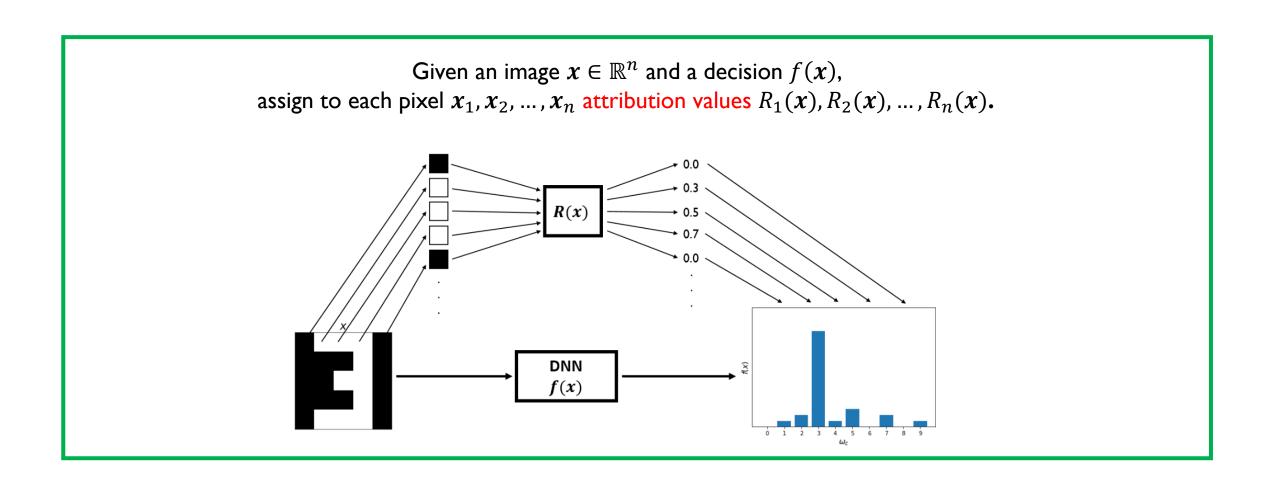
- Weight visualization
- Surrogate model
- Activation maximization
- Example-based

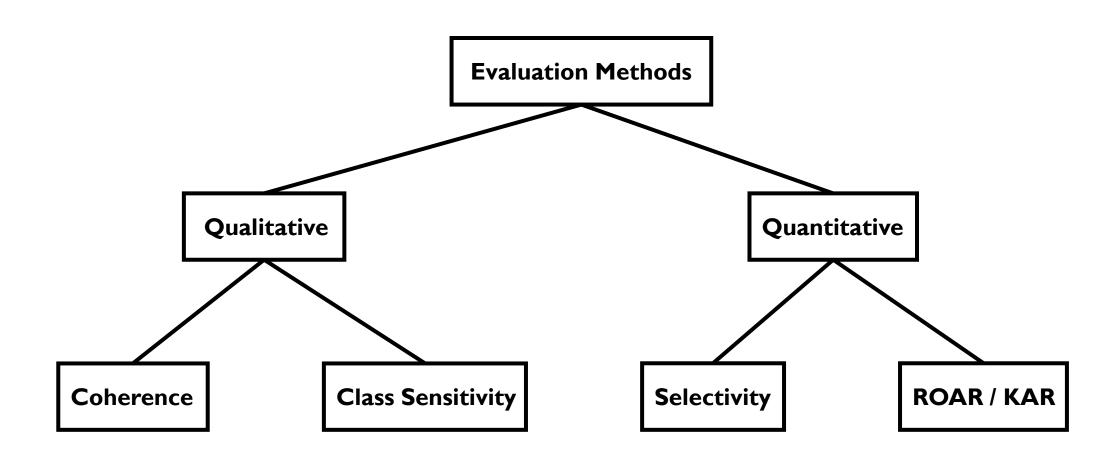
#### 3. Interpreting Decisions

- Example-based
- Attribution Methods: why are gradients noisy?
- Gradient based Attribution Methods: SmoothGrad, Interior Gradient
- Backprop. based Attribution Methods: Deconvolution, Guided Backpropagation

#### Part 3 – Evaluating Attribution Methods

### Attribution Method Review





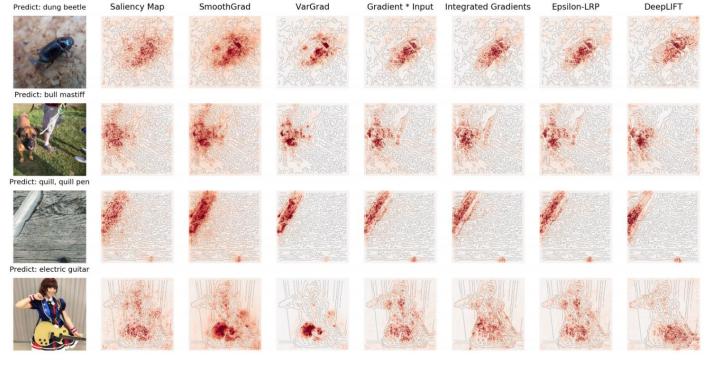
Coherence

**Class Sensitivity** 

**S**electivity

**ROAR / KAR** 

- Attributions should fall on discriminative features (e.g. the object of interest)



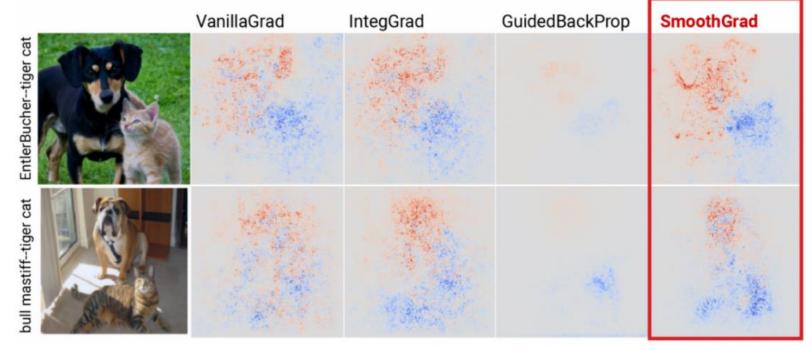
Coherence

**Class Sensitivity** 

**S**electivity

**ROAR / KAR** 

- Attributions should be sensitive to class labels



Coherence

**Class Sensitivity** 

**Selectivity** 

**ROAR / KAR** 

- Removing feature with high attribution should cause large decrease in class probability

#### **Algorithm**

Sort pixel attribution values  $R_i(x)$ 

Iterate:

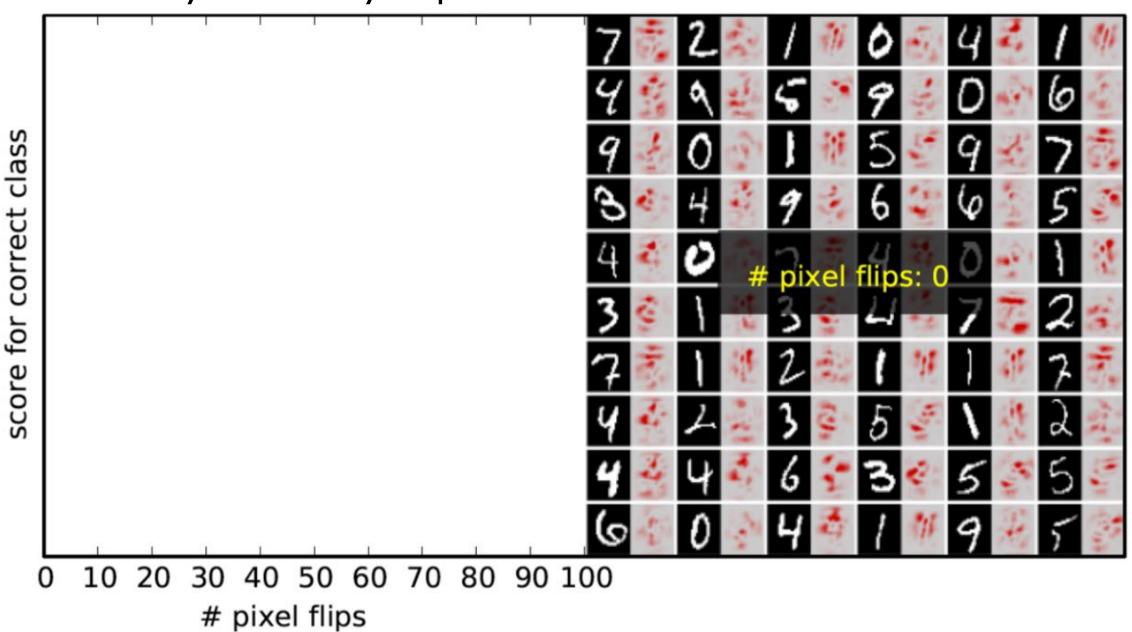
Remove pixels

Evaluate f(x)

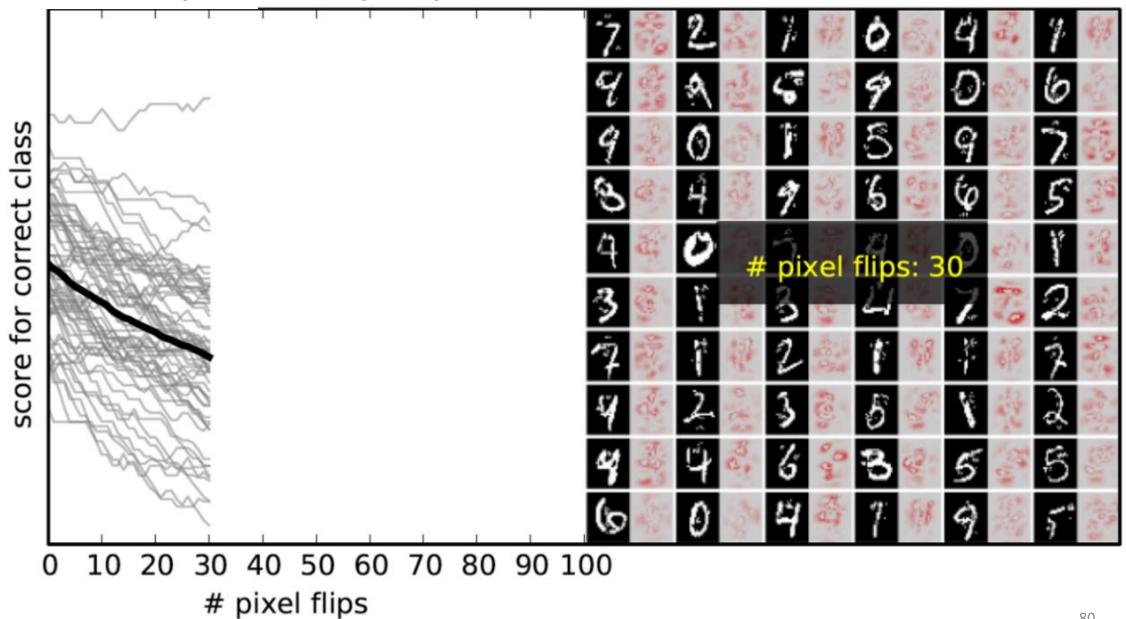
Measure decrease of f(x)

**Class Sensitivity Selectivity ROAR / KAR** Coherence comparing "pixel-flipping" procedure explanationtechniques examples heatmaps - sensitivity 2100 9 14 12 simple Taylor classification 2 i C (1) average compute current heatmap (2) remove most relevant features # features removed 78

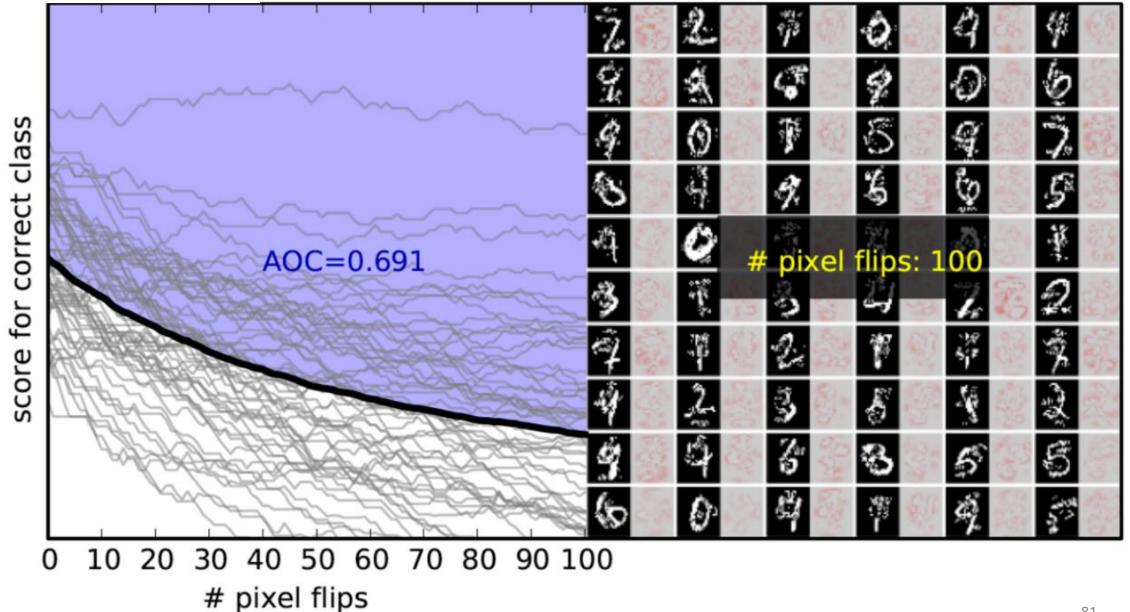
### Selectivity on Saliency Map



### Selectivity on Saliency Map



#### Selectivity on Saliency Map



Coherence

**Class Sensitivity** 

**S**electivity

**ROAR / KAR** 

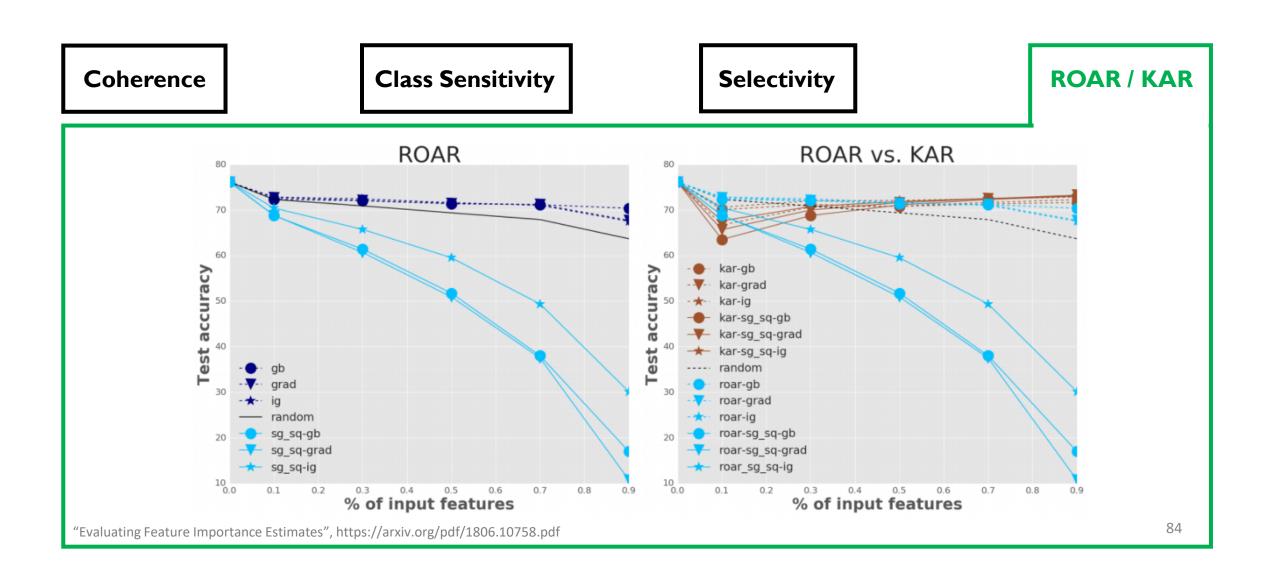
- Sensitivity may not be accurate
- Class probability may decrease because the DNN has never seen such image

#### Remove and Retrain (ROAR) / Keep and Retrain (KAR)

Measure how the performance of the classifier changes as features are removed based on the attribution method

- ROAR: replace N% of pixels estimated to be *most* important
- KAR: replace N% of pixels estimated to be *least* important
- Retrain DNN and measure change in test accuracy

**Selectivity ROAR / KAR Class Sensitivity** Coherence ROAR - RemOve And Retrain Class Class Model 2 Model 1 Prediction Prediction IwAccuracy Modification Estimate Estimator Accuracy of input of Input feature According (Attribution Method) importance Estimate 83 "Evaluating Feature Importance Estimates", https://arxiv.org/pdf/1806.10758.pdf



# Part 3 Summary

#### I. Qualitative: Coherence

- Attributions should highlight discriminative features / objects of interest

#### 2. Qualitative: Class Sensitivity

- Attributions should be sensitive to class labels

#### 3. Quantitative: Sensitivity

- Removing feature with high attribution should cause large decrease in class probability

#### 4. Quantitative: ROAR & KAR

- Problem: class probability may decrease because the DNN has never seen such image
- Solution: remove pixels, retrain and measure drop in accuracy

# Summary

#### I. Introduction to Interpretability

- Interpretability is converting implicit information in DNN to (human) interpretable information
- Ante-hoc Interpretability vs. Post-hoc Interpretability
- Post-hoc interpretability techniques can be classified by degree of "locality"

#### 2. Interpreting Deep Neural Networks

- Interpreting Models vs. Interpreting Decisions
- Interpreting Models: weight visualization, surrogate model, activation maximization, example-based
- Interpreting Decisions: example-based, attribution methods

#### 3. Evaluating Attribution Methods

- Qualitative Evaluation Methods: coherence, class sensitivity
- Quantitative Evaluation Methods: Sensitivity, ROAR & KAR

### Additional References

http://www.heatmapping.org/slides/2017\_GCPR.pdf

https://www.kth.se/social/files/58fdbdfdf276546e343765e3/Lecture8.pdf

https://ramprs.github.io/2017/01/21/Grad-CAM-Making-Off-the-Shelf-Deep-Models-Transparent-through-Visual-Explanations.html

"Methods for Interpreting and Understanding Deep Neural Networks", https://arxiv.org/pdf/1706.07979.pdf