



# Interpretability Methodologies for Machine Learning in Medical Imaging

Mauricio Reyes, PhD.

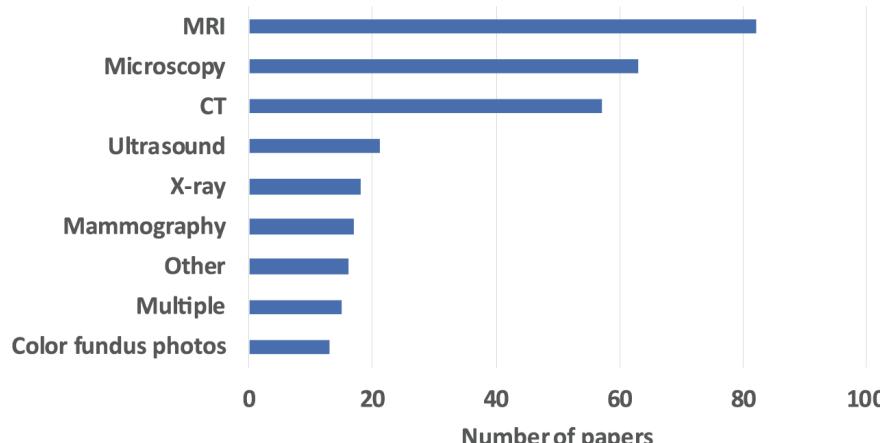
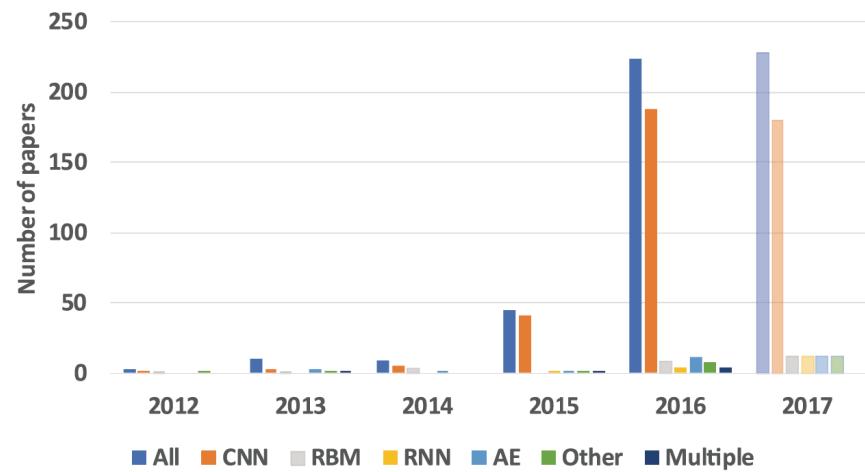
Healthcare Imaging A.I.

University of Bern/ Insel Data Science Center

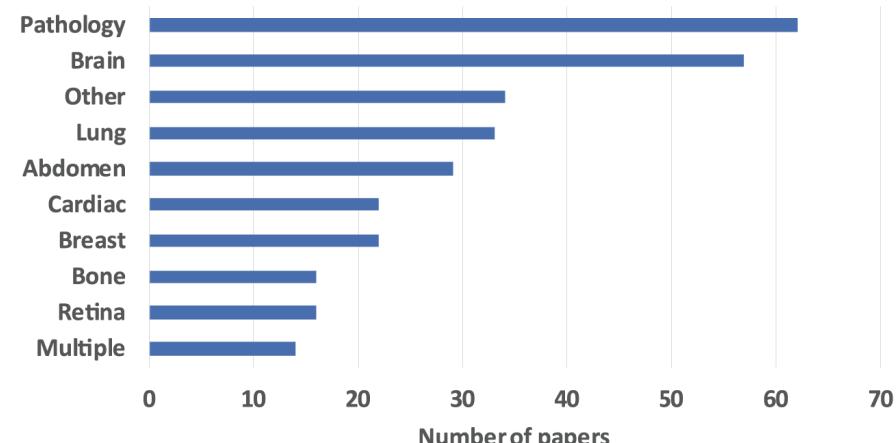
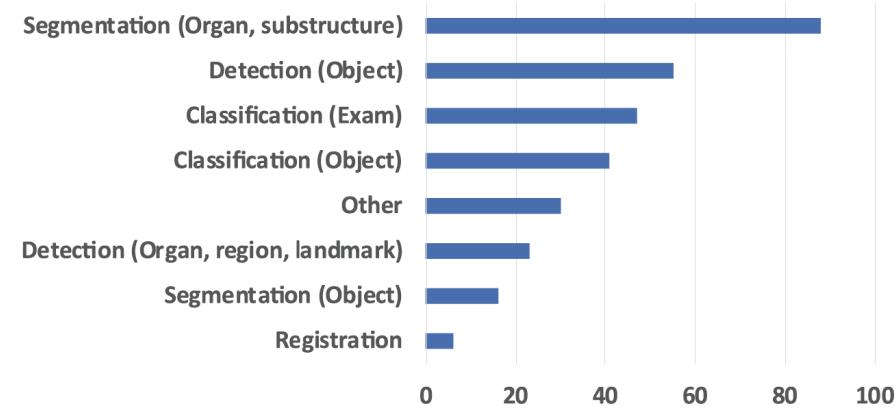
# Table of contents

- PART I
  - Definitions: What is Interpretability
  - Why do we need it (for Medical Imaging)
  - Taxonomy
  - Details on selected methods
- PART II
  - Evaluating Interpretability
  - Radiologists opinion
  - Challenges for the future
  - Concluding words
  - Bibliography and resources
  - Quiz -> winning price
- Afternoon agenda
  - Hands-on experiments using INNVESTigate, and others such as LIME
  - Real-world computer vision and medical datasets

# DL in Medical Imaging



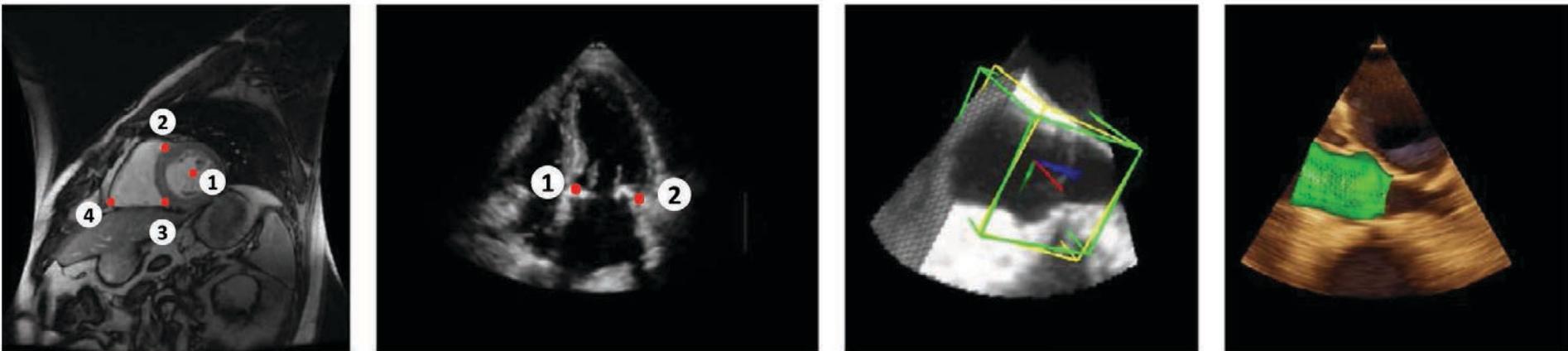
mauricio | reyes



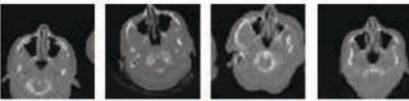
Source: Litjens et al. 2017

# DL in Medical Imaging

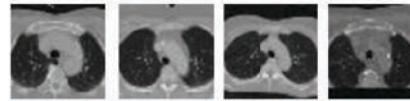
Medical Image parsing



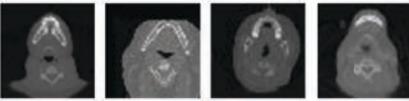
1: nose



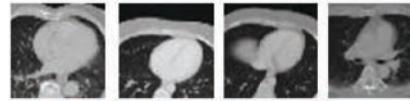
7: aorta arch



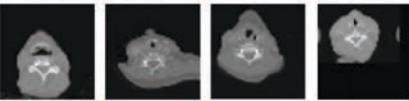
2: chin/teeth



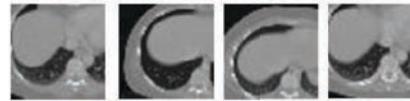
8: cardiac



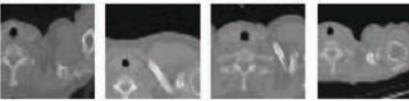
3: neck



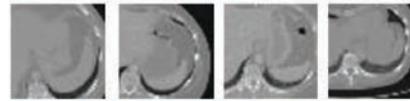
9: liver upper



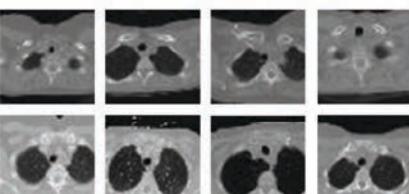
4: shoulder



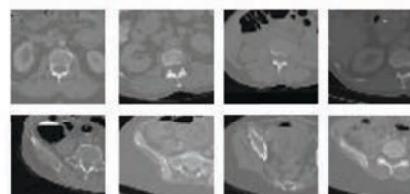
10: liver middle



5: clavicle /lung apex



11: abdomen /kidney

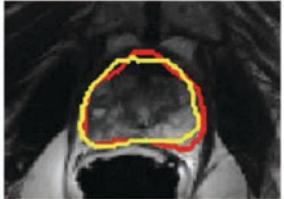


6: sternal

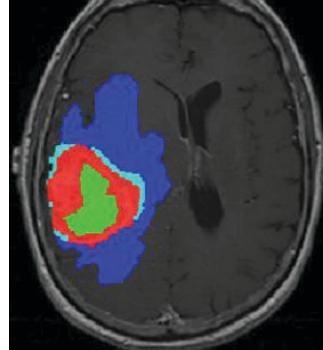
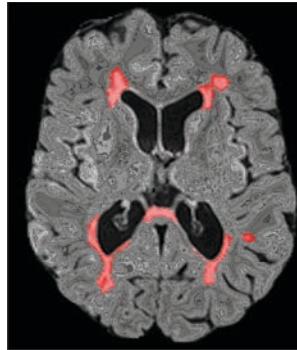
Source: Zhou et al. 2017

# DL in Medical Imaging: Versatility

Prostate



Medical Image Segmentation

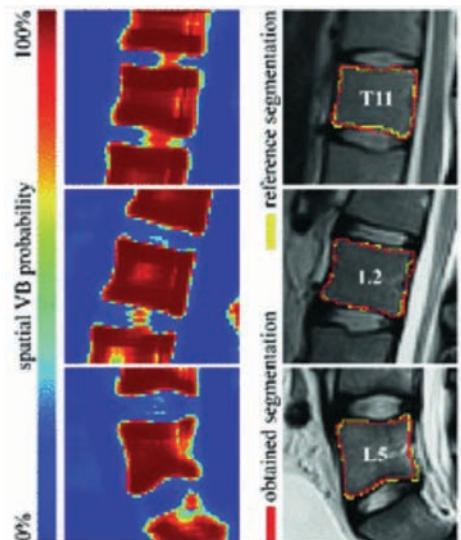


M.S

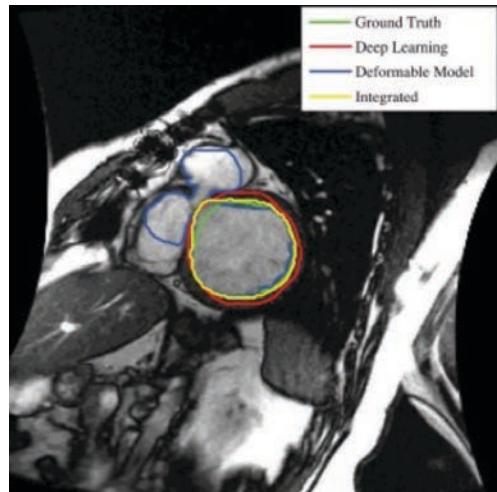
Oncology

Stroke

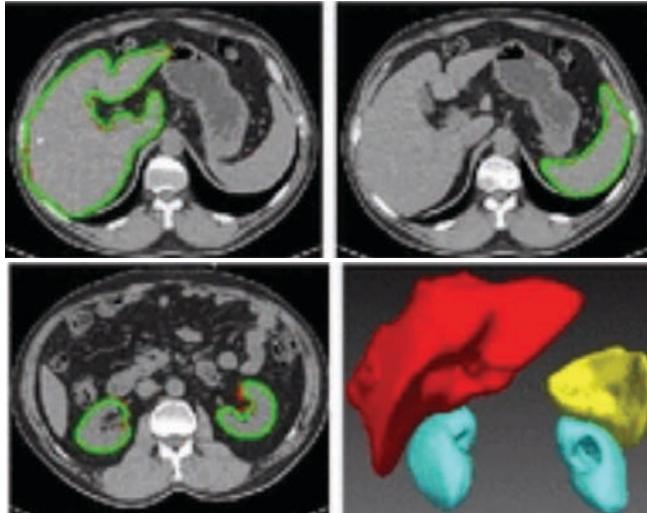
Musculoskeletal



Cardiac



Abdominal

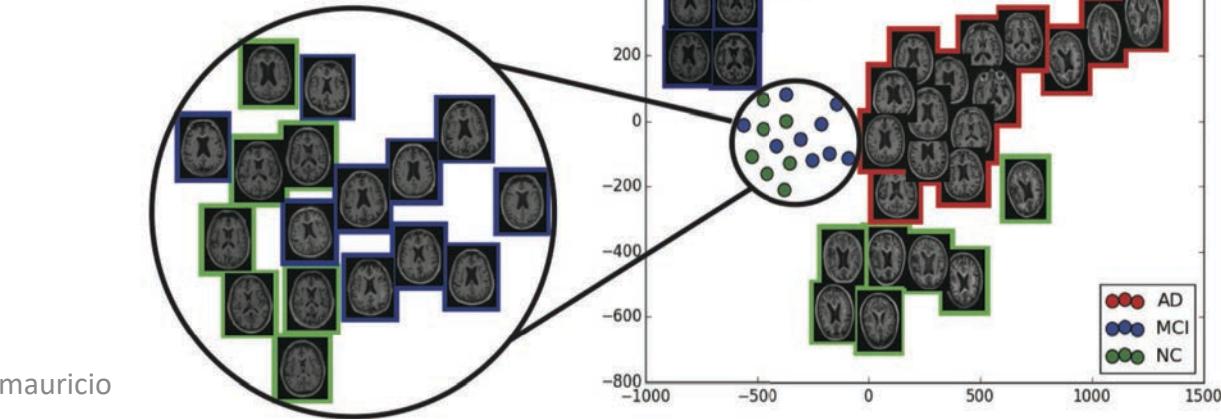


# DL in Medical Imaging

## Medical Image Classification



Chest image classification

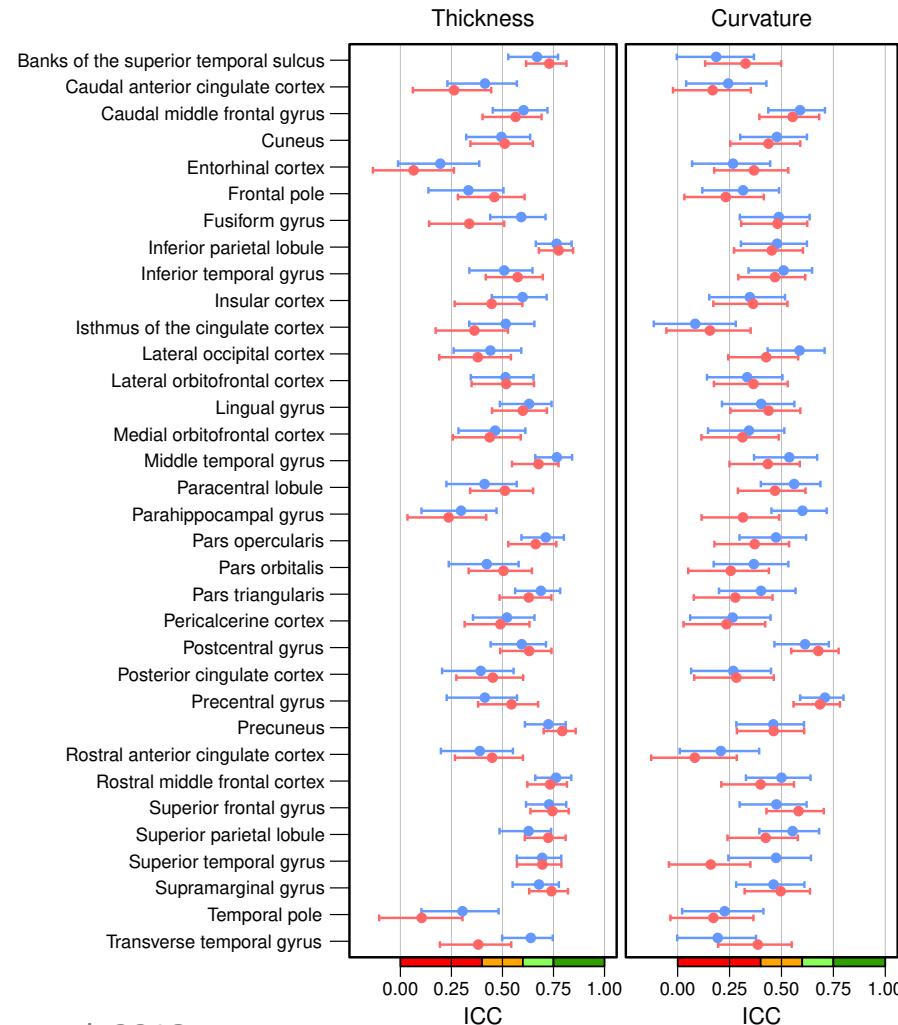
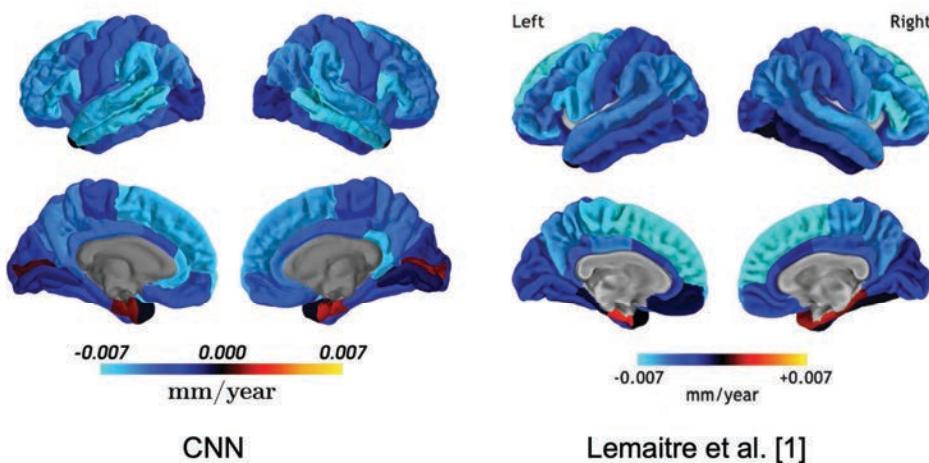
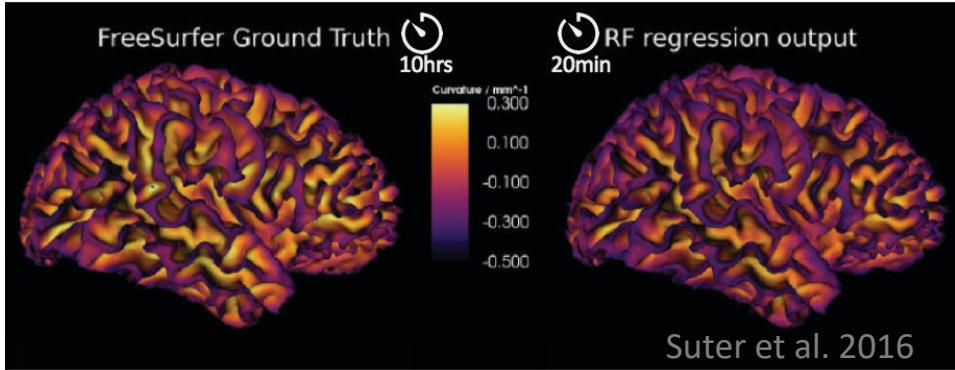


Alzheimer detection

Source: Zhou et al. 2017

# DL in Medical Imaging

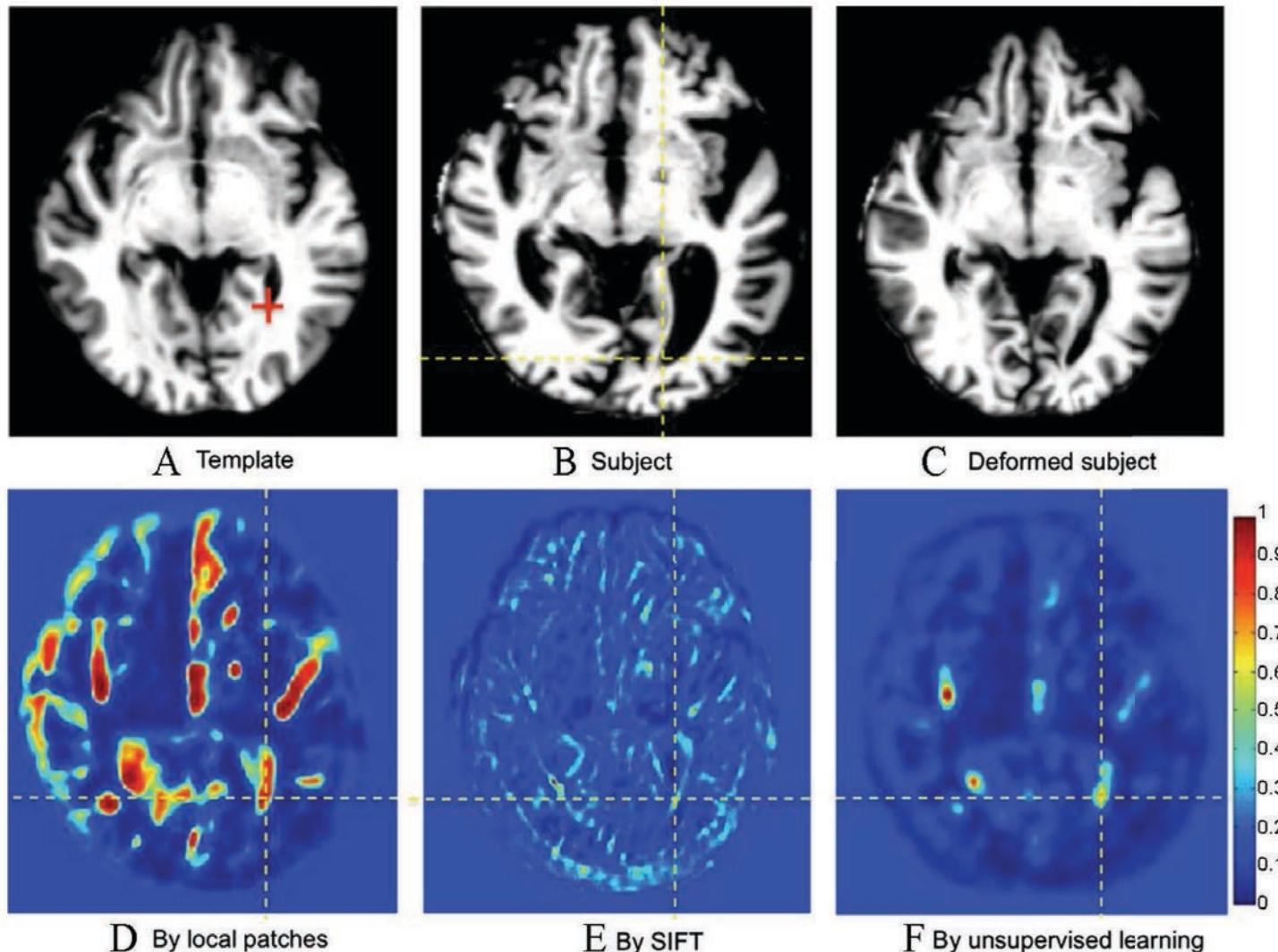
## Medical Image Quantification



Rebsamen et al. 2018

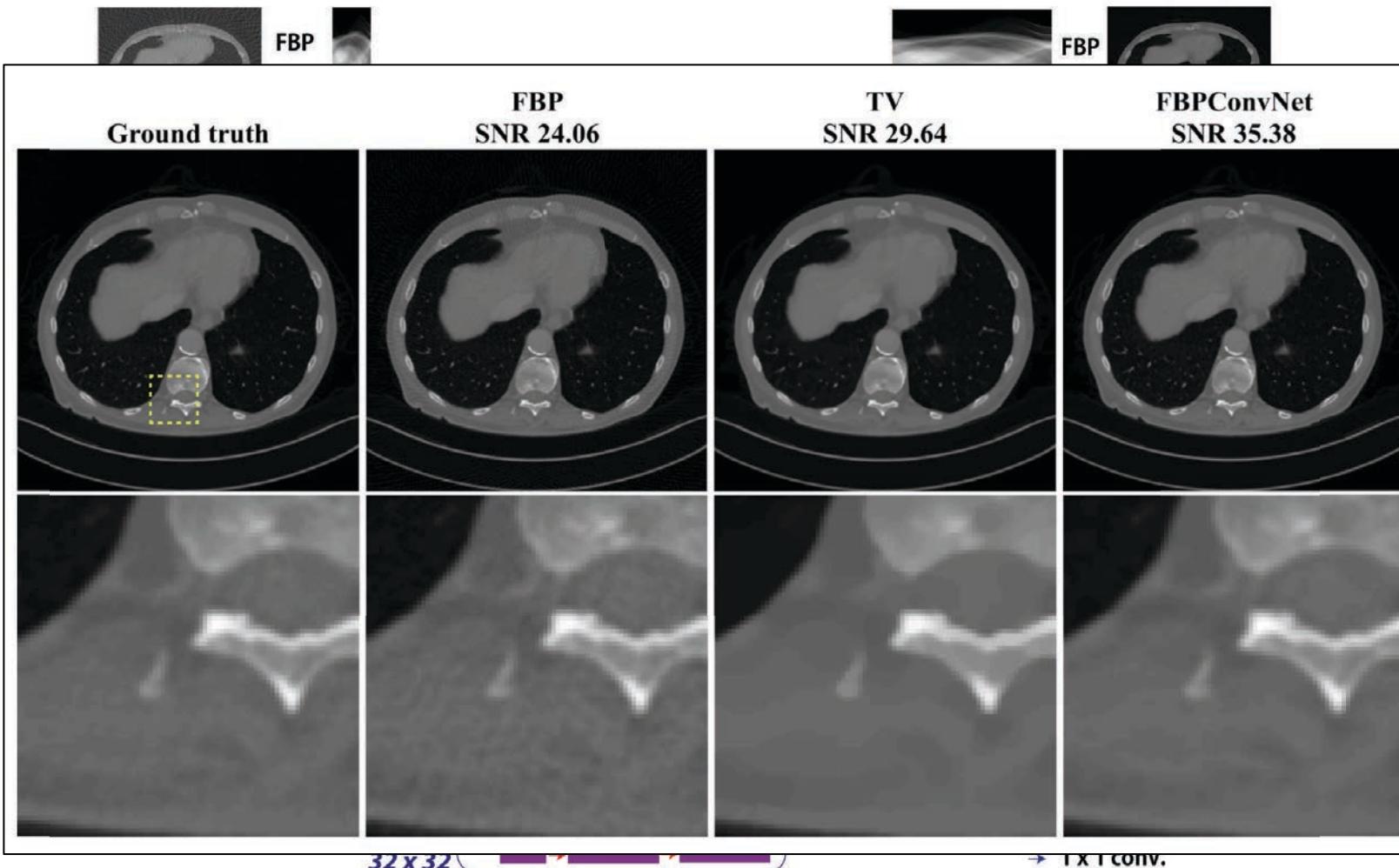
# DL in Medical Imaging

## Medical Image Registration



# DL in Medical Imaging

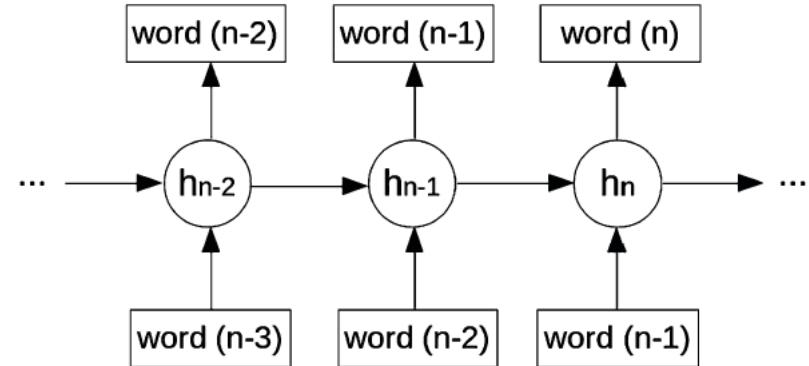
## Medical Image Reconstruction



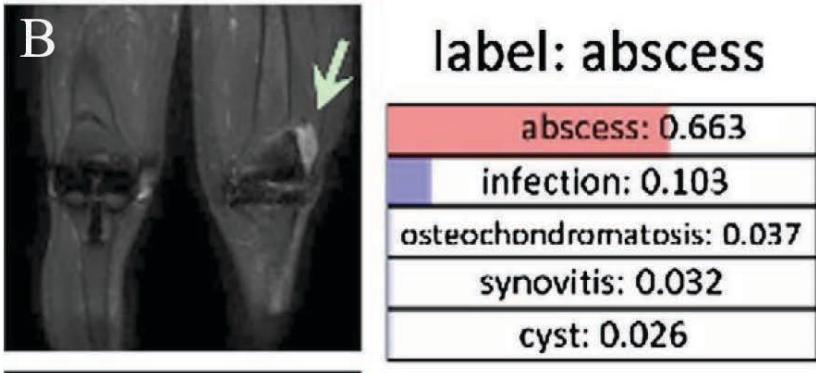
# DL in Medical Imaging

## Automated Image Interpretation

"heart"		"brain"		"liver"	
lungs	0.526600	t1	0.615066	spleen	0.759884
mediastinum	0.517008	mri	0.595027	gallbladder	0.648075
consolidating	0.486605	sagittal	0.580841	hepatomegaly	0.642022
pa	0.449816	flair	0.565445	gallstones	0.611837
chest	0.433362	t2	0.555053	pancreas	0.608356
infiltrates	0.428404	axial	0.554040	gallstone	0.606063
hyperinflated	0.413326	spgr	0.520954	steatosis	0.601081
cardiomegaly	0.410785	weighted	0.502047	dome	0.594812
hyperlucent	0.400836	technique	0.487768	portal	0.570008
pectus	0.396142	astrocytoma	0.480527	ascites	0.551869
great	0.395712	gbm	0.476956	hepatosplenomegaly	0.540501
ectatic	0.394560	gradient	0.476593	hepatic	0.537453
shifted	0.389205	oligodendrogloma	0.465892	cirrhosis	0.530389
ray	0.389091	postcontrast	0.463686	fatty	0.522134



Word neural embeddings

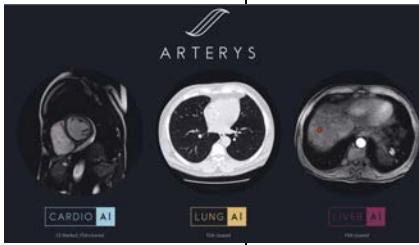


... for example series 701 image 12 and series 401 image 27 with **findings** suggesting minimally enhancing rim laterally for example series 1101 image 21 may ... the **findings** suggest a fluid collection with ... the location suggests possibility of a **synovial** collection **synovial** thickening as the appearance is nonspecific correlation with clinical findings is recommended regarding the possibility of an **infection abscess**

Feb. 2018

## Arterys Receives First FDA Clearance for Broad Oncology Imaging Suite with Deep Learning

FDA clearance covers all solid tumors. Initial launch will include Liver AI and Lung AI oncology software to empower clinicians to quickly measure and track lesions and nodules in MRI and CT scans



## As FDA signals wider AI approval, hospitals have a role to play

By Mike Miliard | May 31, 2018 | 03:27 PM



With more machine learning tools expected to get the go-ahead soon, health systems should be partnering with vendors to supply data for better algorithms.

April. 2018

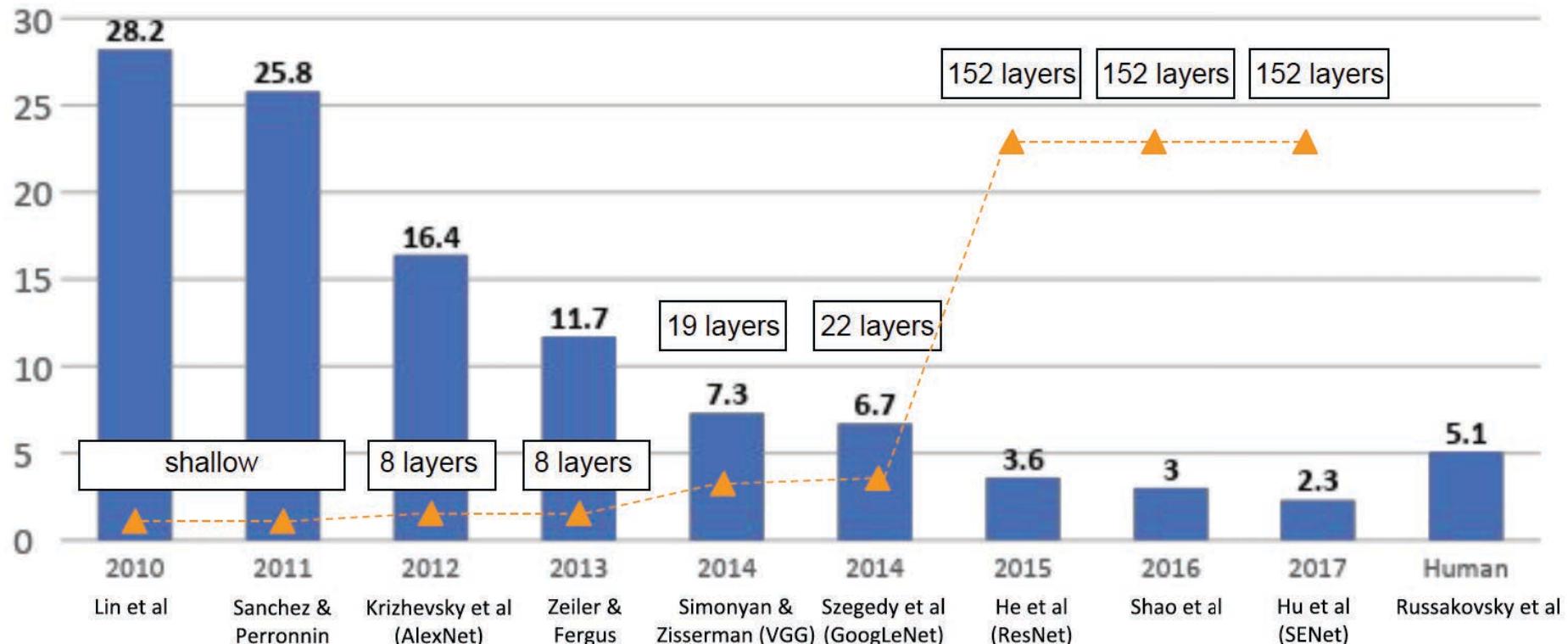
## FDA Approves First A.I. Device To Detect Diabetic Retinopathy



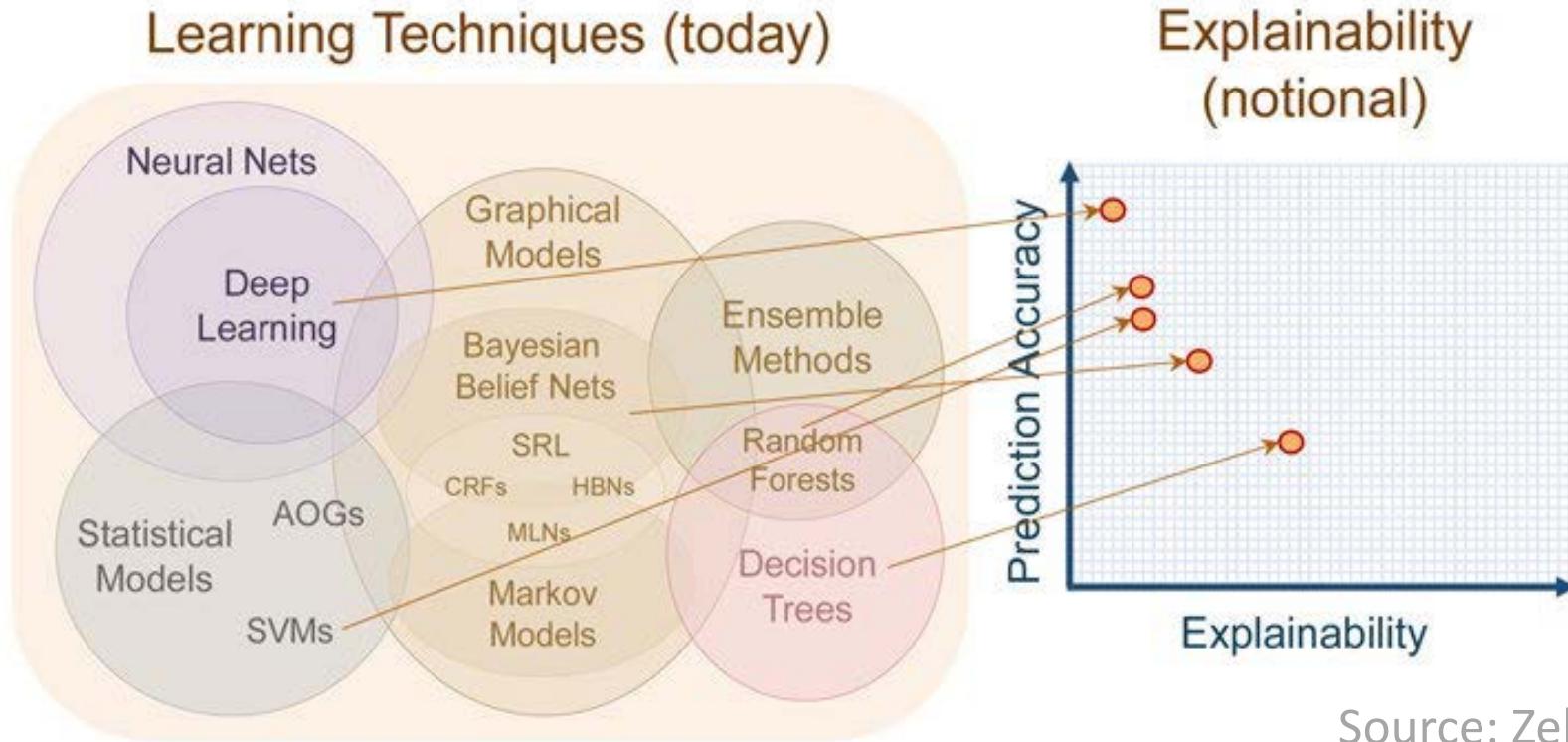
*“A.I. holds enormous promise for the future of medicine, and we’re actively developing a new regulatory framework to promote innovation in this space and support the use of AI-based technologies”.* Scott Gottlieb, FDA commissioner

# Going deeper

error rate



# Explainable A.I



Source: Zelros AI

# Definitions

- What is Interpretability?

An interpretable machine learning algorithm is described as one where  
**the link between the features used by the machine learning and the prediction itself can be understood by a human**

# Another definition

- Produce explanations without sacrificing accuracy
  - Simpler is easier to understand
  - But oversimplified is typically from an accuracy point of view, not interesting

# Explainability and Interpretability

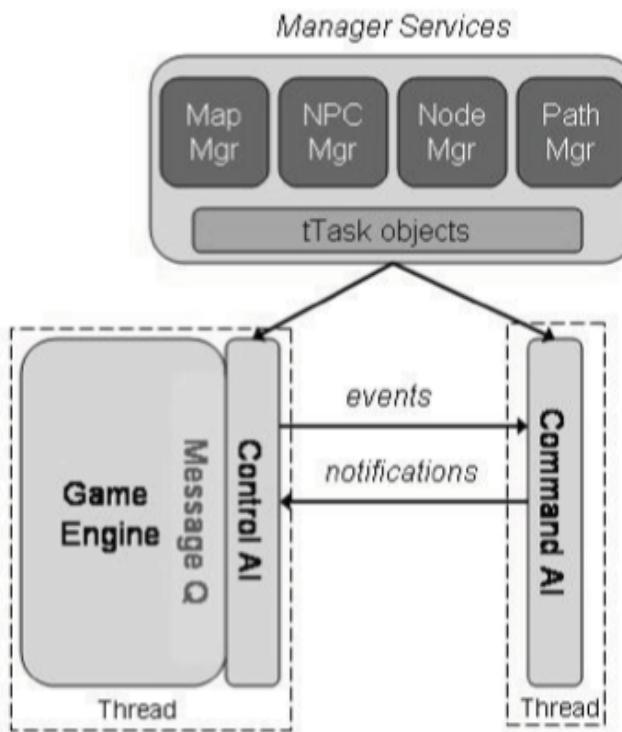
- Used interchangeably
- Explainability → “What’s the process behind” (e.g. Apple falling from a tree: gravity)
- Interpretability → “understanding/predicting causal/effect phenomena” (what happens if I cut the apple from the tree: it will fall)

# Why do we need Interpretability?

- Accountability
- Trust
- Quality Control
- Quality Assurance
- Ethical aspects
- Data exploration

# Early uses of Explainable AI (XAI)

- Van Lent, M., Fisher, W., & Mancuso, M. (2004). An explainable artificial intelligence system for small-unit tactical behavior. In *Proceedings of the National Conference on Artificial Intelligence* (pp. 900–907).



Simulator/Game “Full Spectrum Command”

# Early uses of Explainable AI (XAI)



## Recorded events:

- Weapon fire
- Unit generation/update
- Task generation/Update
- Friendly Soldier Killed in Action (KIA)
- Friendly Soldier Wounded in Action (WIA)
- Enemy Soldier Killed in Action
- Enemy Soldier Wounded in Action
- Civilian Killed in Action
- Civilian Wounded in Action
- Friendly Unit First Contact with the Enemy
- Platoon Task Started
- Platoon Task Completed

## XAI Questions:

- What is the platoon's mission?
- What is the platoon's mission status?
- How is the platoon task organized?
- How many soldiers are in the platoon?
- What is the platoon's ammo status?

# Why do we need Interpretability?

- Accountability
  - System Liability

## **European Union regulations on algorithmic decision-making and a "right to explanation"**

Bryce Goodman, Seth Flaxman

(Submitted on 28 Jun 2016 ([v1](#)), last revised 31 Aug 2016 (this version, v3))

We summarize the potential impact that the European Union's new General Data Protection Regulation will have on the routine use of machine learning algorithms. Slated to take effect as law across the EU in 2018, it will restrict automated individual decision-making (that is, algorithms that make decisions based on user-level predictors) which "significantly affect" users. The law will also effectively create a "right to explanation," whereby a user can ask for an explanation of an algorithmic decision that was made about them. We argue that while this law will pose large challenges for industry, it highlights opportunities for computer scientists to take the lead in designing algorithms and evaluation frameworks which avoid discrimination and enable explanation.

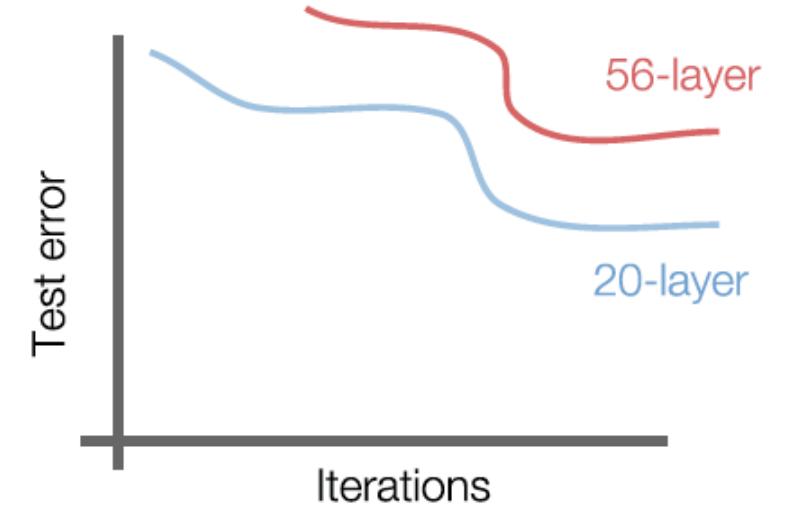
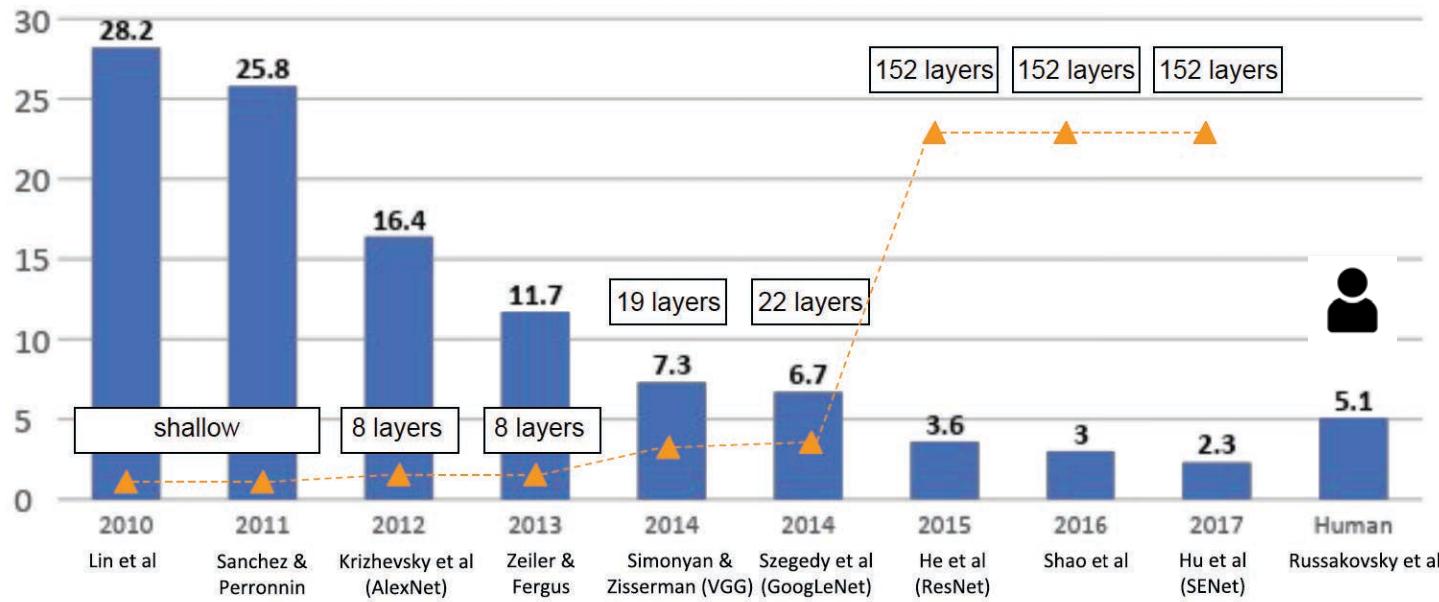
Comments: presented at 2016 ICML Workshop on Human Interpretability in Machine Learning (WHI 2016), New York, NY

# Why do we need Interpretability?

- Quality Assurance: Thorough evaluation of a model's performance
- Ensuring robustness and knowledge of breaking points of an algorithm

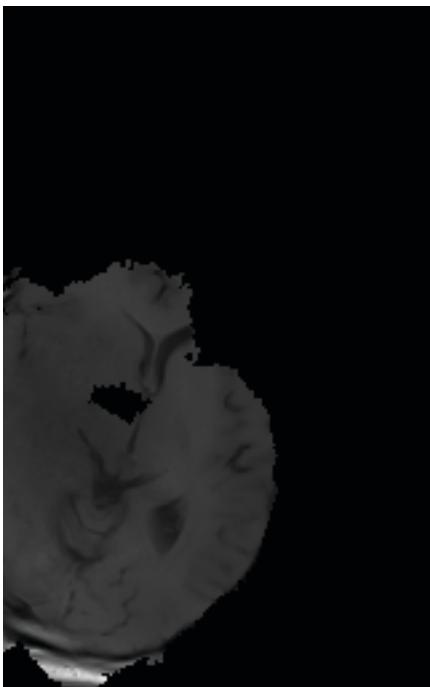
# Interpretability is needed to leverage Quality Control (QC) of A.I. systems

**Solution featuring “high degrees of freedom”**

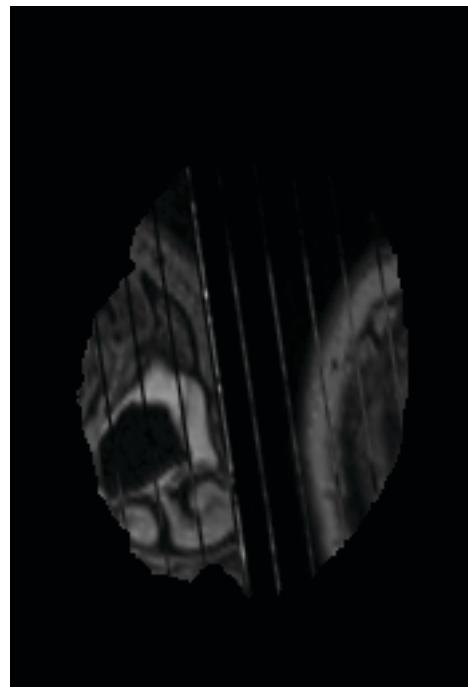


# Why do we need Interpretability?

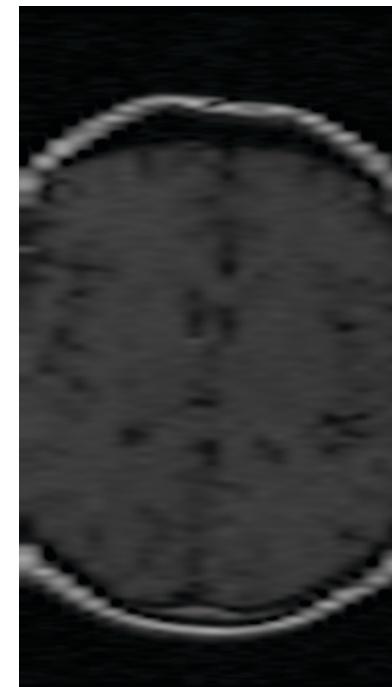
- Quality Control



flawed orientation



flawed orientation



low resolution



A.I. technology is as good as  
the training data  
characterizing the task

# Example: Automated MS Segmentation – Multi-Center Analysis



OPEN

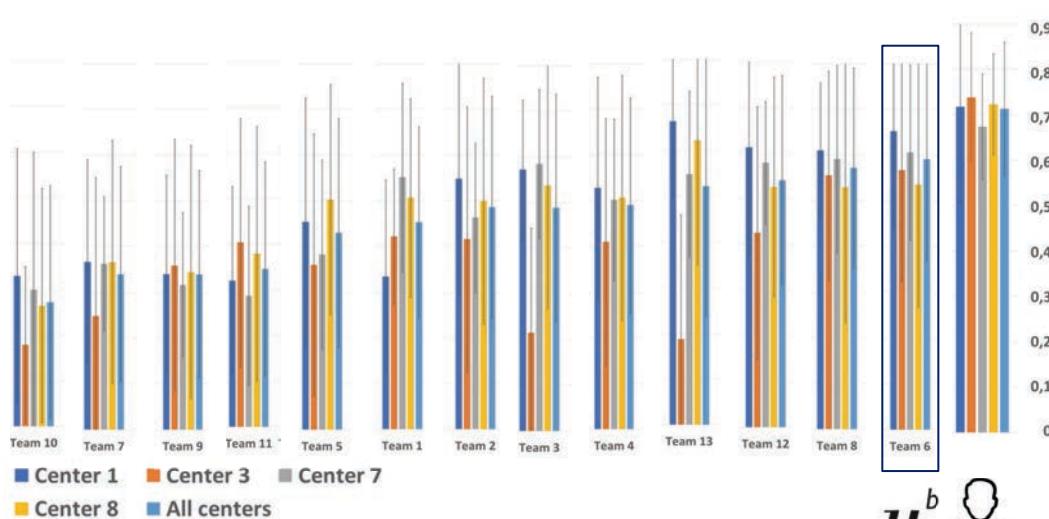
## Objective Evaluation of Multiple Sclerosis Lesion Segmentation using a Data Management and Processing Infrastructure

Received: 20 April 2018  
Accepted: 6 August 2018  
Published online: 12 September 2018

Olivier Commowick<sup>2</sup>, Audrey Istance<sup>2</sup>, Michaël Kain<sup>1</sup>, Baptiste Laurent<sup>3</sup>, Florent Leray<sup>1</sup>, Mathieu Simon<sup>1</sup>, Sorina Camarasu Pop<sup>1,4</sup>, Pascal Girard<sup>4</sup>, Roxana Améï<sup>2</sup>, Jean-Christophe Ferré<sup>5,1</sup>, Anne Kerbrat<sup>6,1</sup>, Thomas Toudias<sup>8</sup>, Frédéric Cervenansky<sup>9</sup>, Tristan Glatard<sup>10</sup>, Jérémie Beaumont<sup>1</sup>, Senan Doyle<sup>1</sup>, Florence Forbes<sup>1,10</sup>, Jesse Knight<sup>11</sup>, April Khademi<sup>12</sup>, Amirreza Mahbod<sup>13</sup>, Chunliang Wang<sup>13</sup>, Richard McKinley<sup>14</sup>, Franca Wagner<sup>15</sup>, John Muschelli<sup>15</sup>, Elizabeth Sweeney<sup>15</sup>, Eloy Roua<sup>16</sup>, Xavier Lladó<sup>16</sup>, Michel M. Santos<sup>17</sup>, Wellington P. Santos<sup>18</sup>, Abel G. Silva-Filho<sup>17</sup>, Xavier Tomas-Fernandez<sup>19</sup>, Hélène Urien<sup>20</sup>, Isabelle Bloch<sup>20</sup>, Sergi Valverde<sup>16</sup>, Mariano Cabezas<sup>16</sup>, Francisco Javier Vera-Olmos<sup>21</sup>, Norberto Malpica<sup>21</sup>, Charles Guttmann<sup>22</sup>, Sandra Vukusic<sup>2</sup>, Gilles Edan<sup>6,1</sup>, Michel Dojat<sup>23</sup>, Martin Styner<sup>14</sup>, Simon K. Warfield<sup>15</sup>, François Cotten<sup>13</sup> & Christian Barillot<sup>1</sup>



SIEMENS



Scanner	Modality	Matrix	Slices	Voxel resolution (mm)
GE Discovery 3T	Sagittal 3D FLAIR	512 × 512	224	0.47 × 0.47 × 0.9
	Sagittal 3D T1	512 × 512	248	0.47 × 0.47 × 0.6
	Axial 2D DP-T2	512 × 512	From 28 to 44	0.43 × 0.43 × 3 Gap: 0.5
Philips Ingenia 3T	Sagittal 3D FLAIR	336 × 336	261	0.74 × 0.74 × 0.7
	Sagittal 3D T1	336 × 336	200	0.74 × 0.74 × 0.85
	Axial 2D PD-T2	512 × 512	46	0.45 × 0.45 × 3
Siemens Aera 1.5T	Sagittal 3D FLAIR	256 × 224	128	1.03 × 1.03 × 1.25
	Sagittal 3D T1	256 × 256	176	1.08 × 1.08 × 0.9
	Axial 2D PD-T2	320 × 320	25	0.72 × 0.72 × 4 Gap: 1.2
Siemens Verio 3T	Sagittal 3D FLAIR	512 × 512	144	0.5 × 0.5 × 1.1
	Sagittal 3D T1	256 × 256	176	1 × 1 × 1
	Axial 2D PD-T2	240 × 320	44	0.69 × 0.69 × 3

Multi-vendor, multi-center

- Center 3 (orange) → Unknown to models, lowest performance



# Why do we need Interpretability?

- Trust
  - Essential in fields such as medicine where technology can play a crucial role
  - In radiology, AI and the potential of restructuring the radiologist's workflow



This CVPR paper is the Open Access version, provided by the Computer Vision Foundation.  
Except for this watermark, it is identical to the version available on IEEE Xplore.

## DeepFool: a simple and accurate method to fool deep neural networks

Seyed-Mohsen Moosavi-Dezfooli, Alhussein Fawzi, Pascal Frossard  
École Polytechnique Fédérale de Lausanne  
`{seyed.moosavi, alhussein.fawzi, pascal.frossard}` at epfl.ch

Published as a conference paper at ICLR 2019

## IMAGENET-TRAINED CNNs ARE BIASED TOWARDS TEXTURE; INCREASING SHAPE BIAS IMPROVES ACCURACY AND ROBUSTNESS

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Full Citation: Nguyen A, Yosinski J, Clune J. Deep Neural Networks are Easily Fooled: High Confidence Predictions for Unrecognizable Images. In Computer Vision and Pattern Recognition (CVPR '15), IEEE, 2015.

## Deep Neural Networks are Easily Fooled: High Confidence Predictions for Unrecognizable Images

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RESEARCH ARTICLE

## Variable generalization performance of a deep learning model to detect pneumonia in chest radiographs: A cross-sectional study

John R. Zech Marcus A. Badgeley Manway Liu, Anthony B. Costa, Joseph J. Titano, Eric Karl Oermann

Published: November 6, 2018 • <https://doi.org/10.1371/journal.pmed.1002683>



## Explaining DL decisions via attention maps



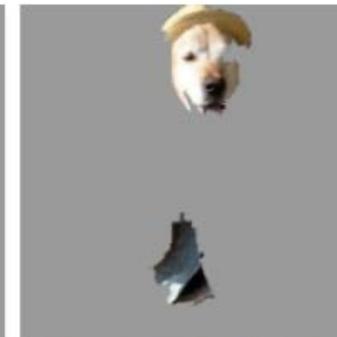
(a) Original Image



(b) Explaining *Electric guitar*



(c) Explaining *Acoustic guitar*



(d) Explaining *Labrador*

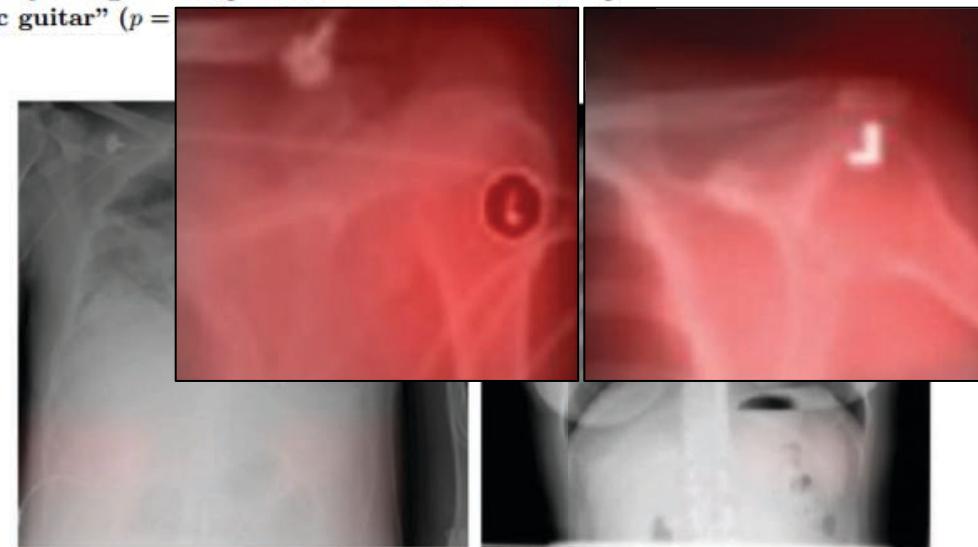
**Figure 4:** Explaining an image classification prediction made by Google's Inception neural network. The top 3 classes predicted are "Electric Guitar" ( $p = 0.32$ ), "Acoustic guitar" ( $p =$



(a) Husky classified as wolf



(b) Explanation



DL learned to detect clinical site!

# IMAGENET-TRAINED CNNS ARE BIASED TOWARDS TEXTURE; INCREASING SHAPE BIAS IMPROVES ACCURACY AND ROBUSTNESS

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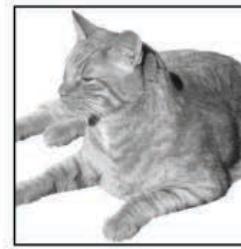
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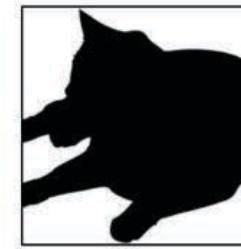
**Wieland Brendel**  
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[wieland.brendel@bethgelab.org](mailto:wieland.brendel@bethgelab.org)



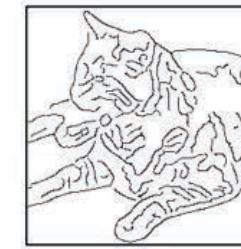
original



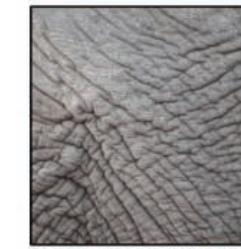
greyscale



silhouette



edges



texture

# IMAGENET-TRAINED CNNS ARE BIASED TOWARDS TEXTURE; INCREASING SHAPE BIAS IMPROVES ACCURACY AND ROBUSTNESS

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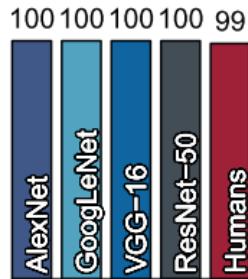
**Patricia Rubisch**  
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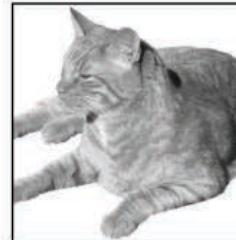
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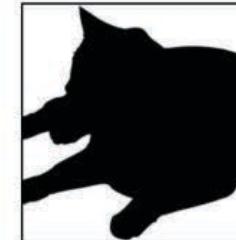
**Wieland Brendel**  
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[wieland.brendel@bethgelab.org](mailto:wieland.brendel@bethgelab.org)



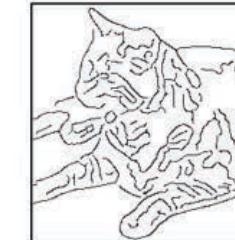
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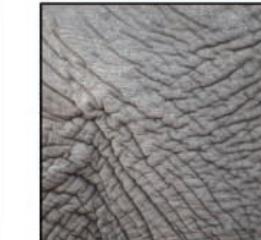
greyscale



silhouette



edges



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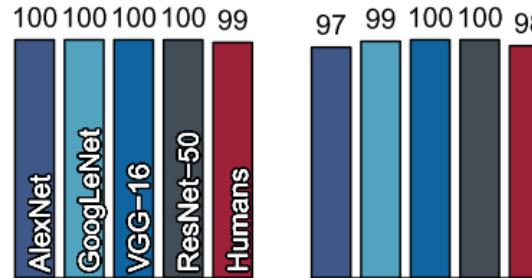
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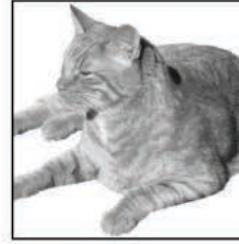
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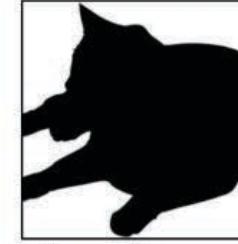
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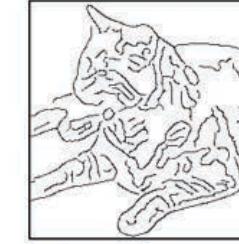
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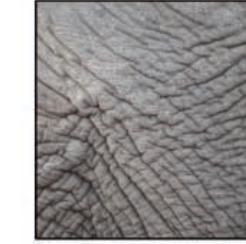
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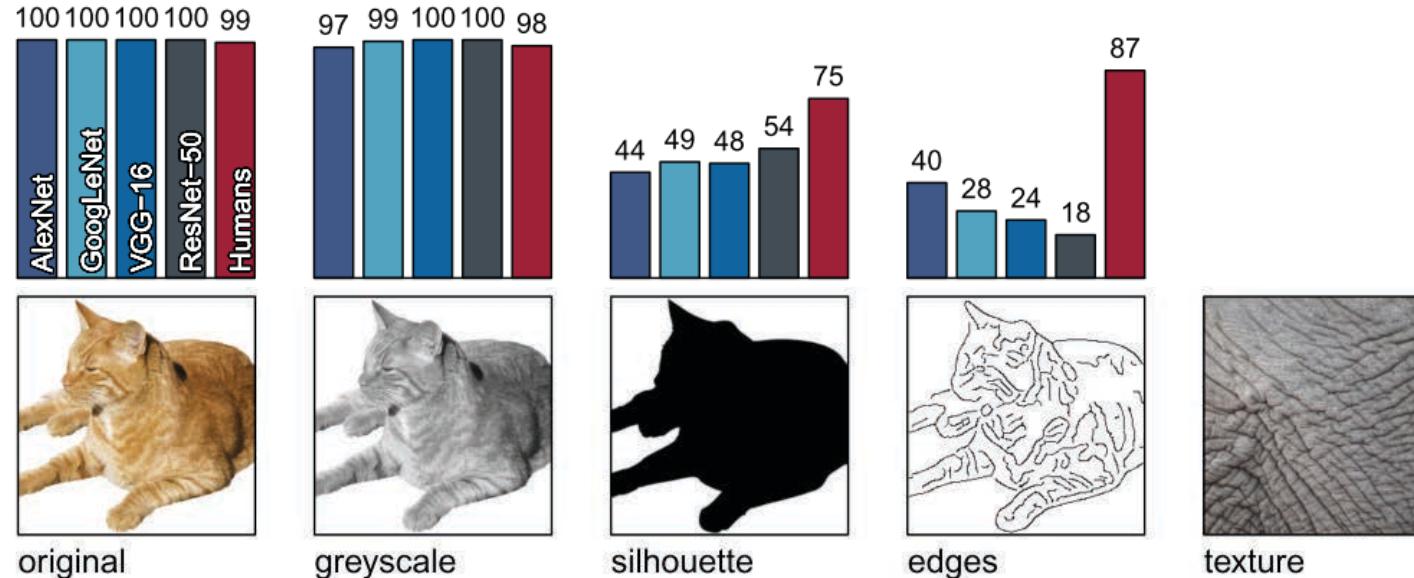
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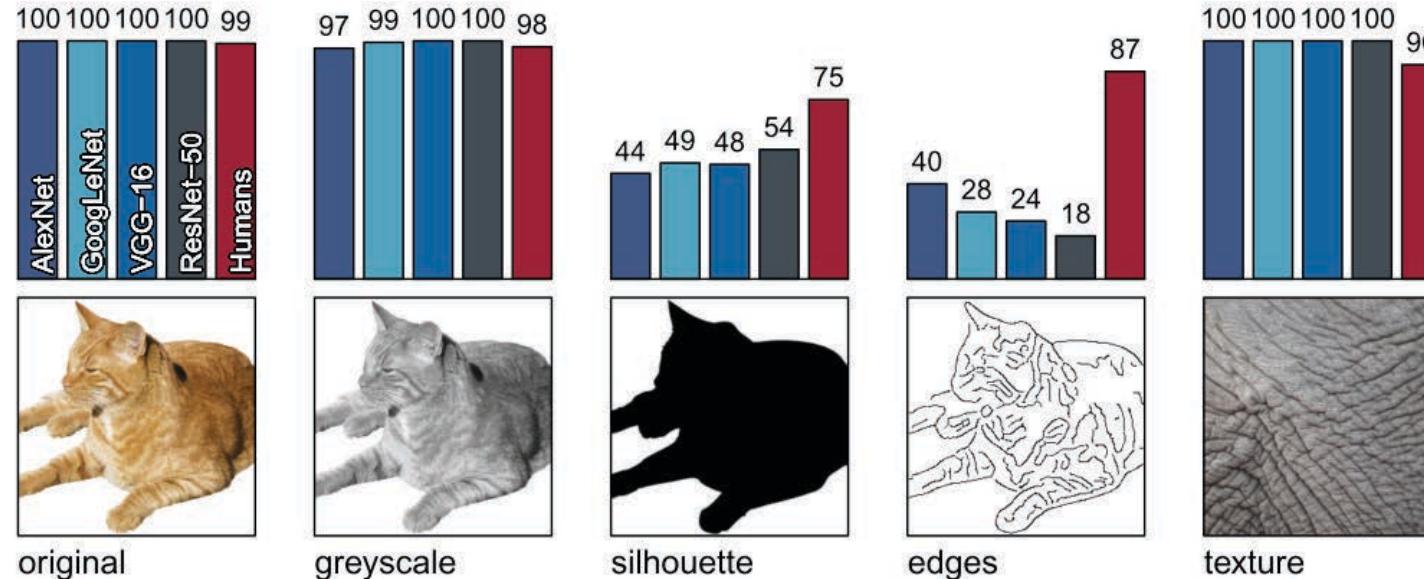
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# Ethics of AI in Radiology: European and North American Multisociety Statement

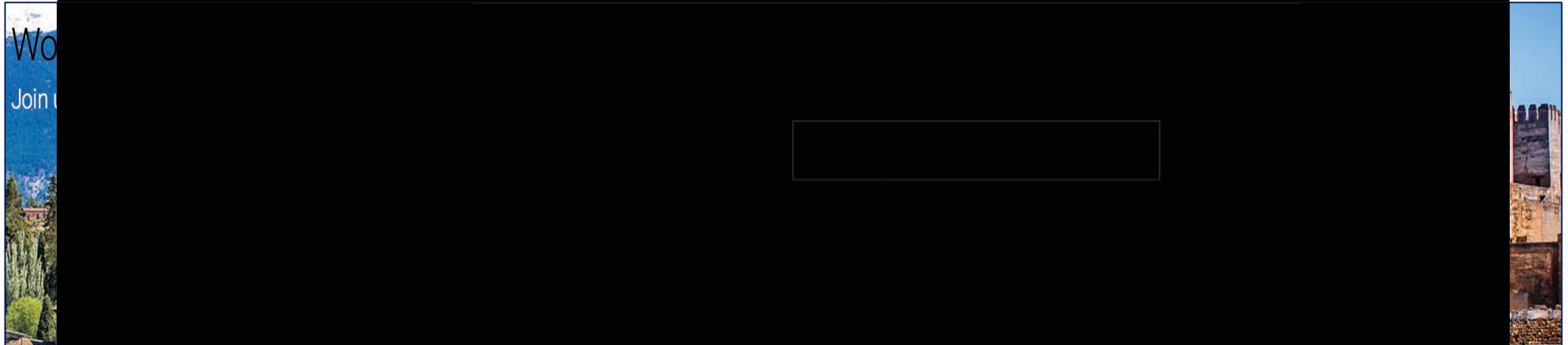
## *Transparency, interpretability, and explainability*

*Transparency, interpretability, and explainability are **necessary to build patient and provider trust**. When a radiologist makes a mistake, we want to know why, in part because we want to know whether the mistake is excusable. We want to know whether the mistake reflects malintent or negligence, or occurred due to other factors.*

*Similarly, if an algorithm fails or contributes to an adverse clinical event or malpractice, radiologists need to be able to understand **why** it produced the result that it did, and **how** it reached a decision.*



# Enhancing Interpretability of machine learning



# Taxonomy

- **Black-boxes** operating methods: No need to have “access” to the internal of models. Also referred to as model-agnostic.
- **White-boxes:** These are methods that require access to the internals of the models. Gradient-based models are one example of white box interpretability models.
- **By output:**
  - Visualization, or saliency maps: Provide pixel-wise values reflecting their importance to the performance of the model being interpreted
  - Concepts: summary statement or keyword.
  - Feature importance: explain models by expressing importance of features E.g. high weights of a model.

# Let's check some of these approaches

Christoph Molnar @ChristophMolnar · May 17

Explanation algorithms for neural network predictions are like yogurts in a supermarket. Choice overload.

LRP  
LIME  
Integrated Gradients  
deconvnet  
Occlusion  
DeepShap  
DeepLift  
Deep Taylor Decomposition  
Gradient\* Input  
Grad-CAM  
Guided Backpropagation  
Saliency Map  
...



# Partial Dependence Plot (PDP) – Friedman et al. 2001

- shows the marginal effect that one or two features have on the predicted outcome of a machine learning model
- PDP can show whether the relationship between the target and a feature is linear, monotonous or more complex.

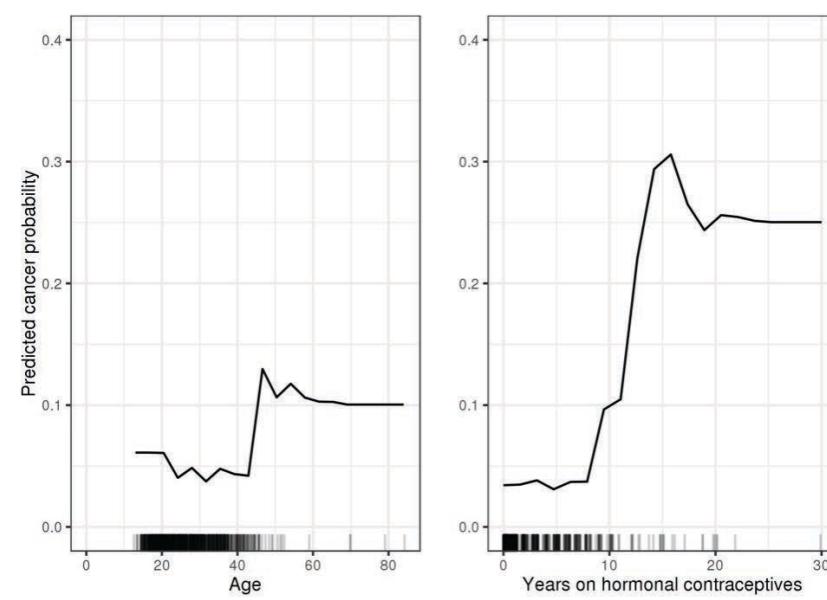
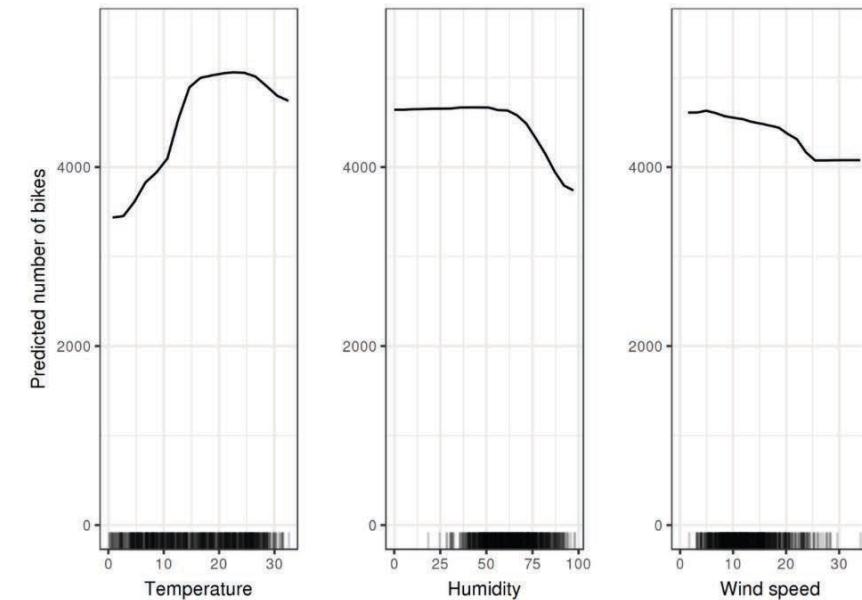
$$\hat{f}_{x_S}(x_S) = E_{x_C} \left[ \hat{f}(x_S, x_C) \right] = \int \hat{f}(x_S, x_C) d\mathbb{P}(x_C) = \hat{f}_{x_S}(x_S) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_S, x_C^{(i)})$$

Feature being explained – variable      Marginalized over other features – Actual values

- Global method: The method considers all instances and gives a statement about the global relationship of a feature with the predicted outcome.

# Partial Dependence Plot (PDP) – Friedman et al. 2001

Example: bike rental – Relation to temperature, humidity, windspeed

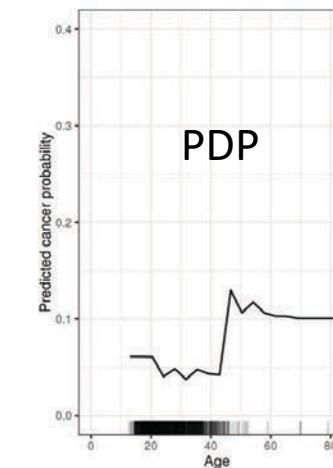
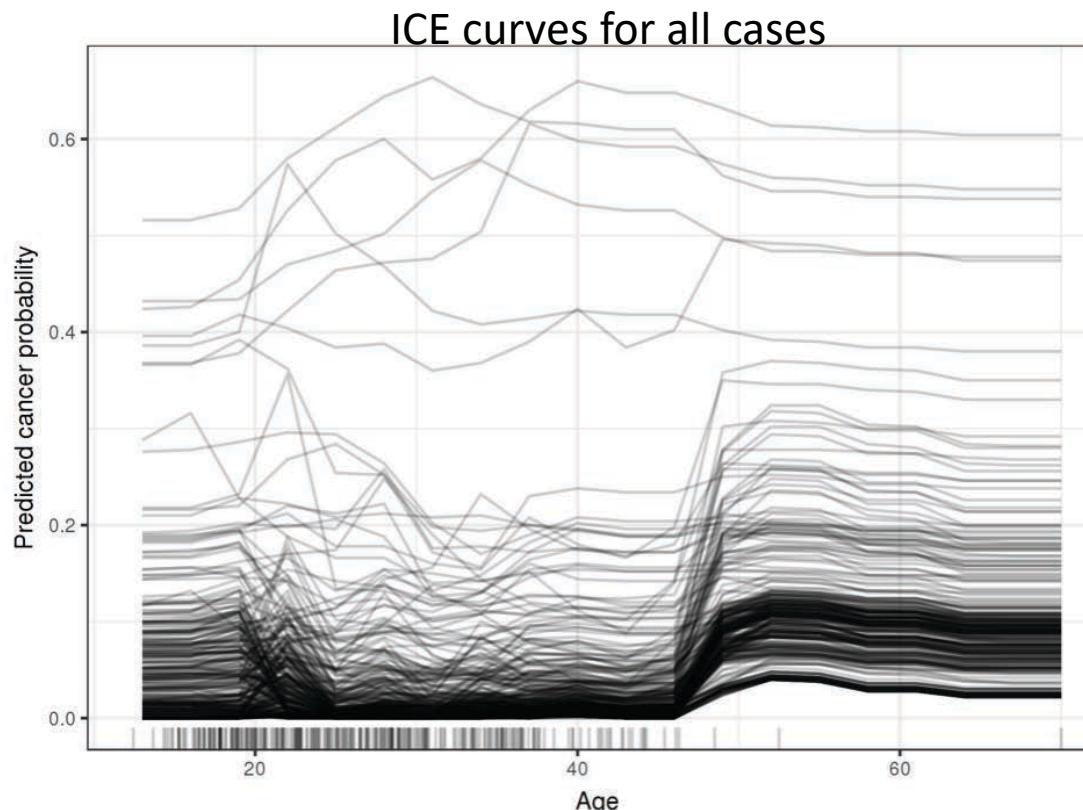


## Pros/Cons of PDP:

- Simple
- Easy to implement
- Does not account for correlated features
- More than 3 features is hard to visualize
- Doesn't show feature distribution
- Effects might cancel out

# Individual Conditional Expectation (ICE)

- ICE shows how the instance's prediction changes when a feature changes. One feature at a time
- PDP is the average of ICE over all features



$$\hat{f}_{x_S}(x_S) = \left\{ \hat{f}(x_S, x_C) \right\}_{i=1..N}$$

Actual values for other features

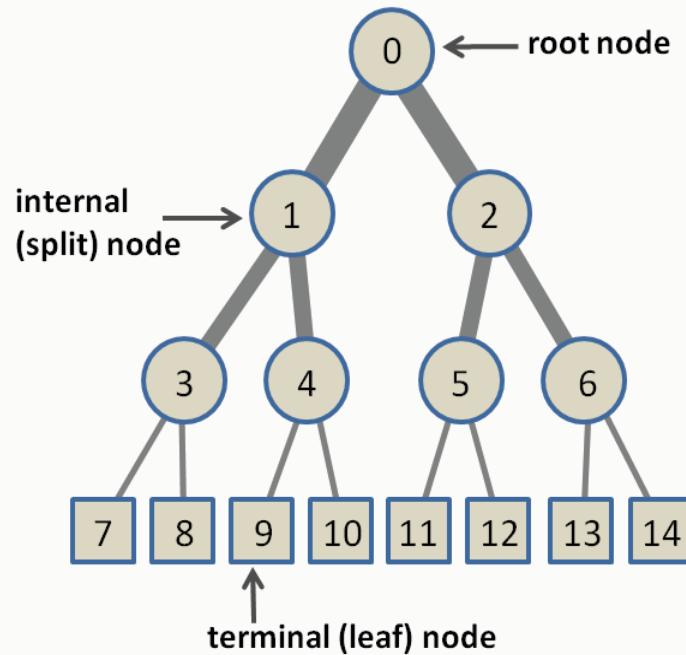
Variable - e.g. grid search

i<sup>th</sup> case

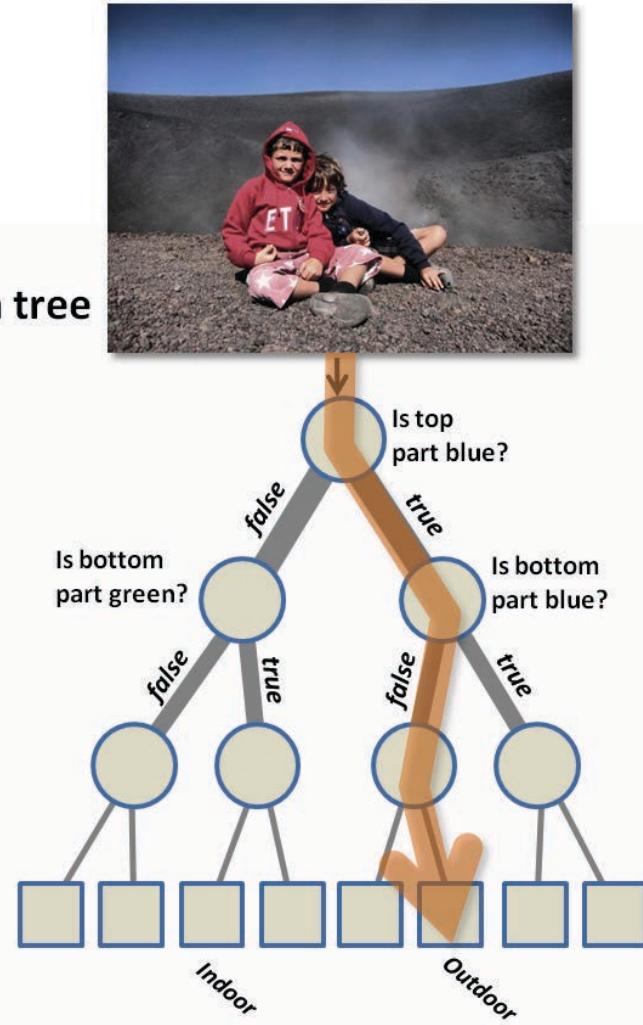
# Decision trees

## General Concept

A general tree structure

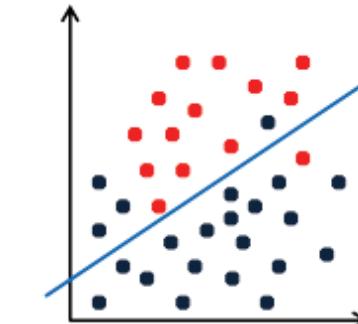
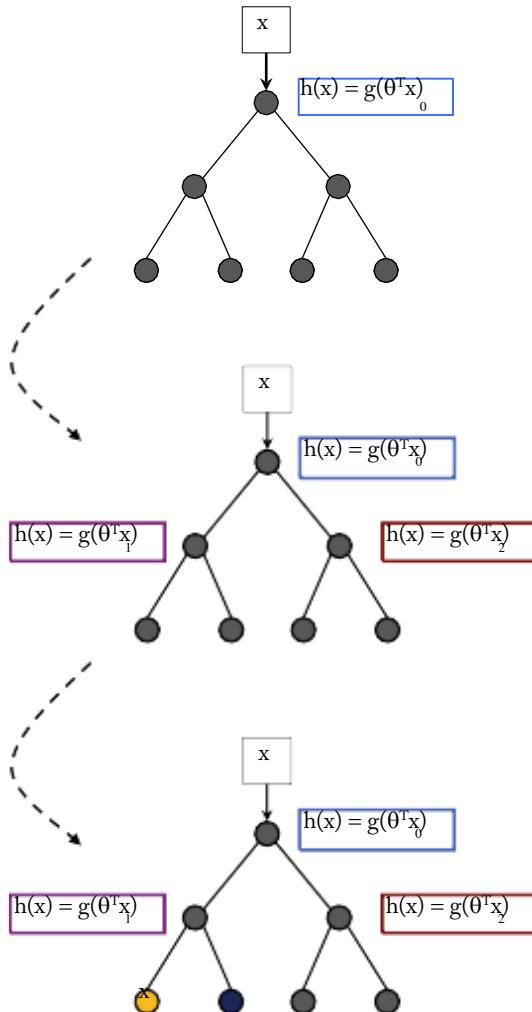


A decision tree



# Transitioning from linear to non-linear classifier

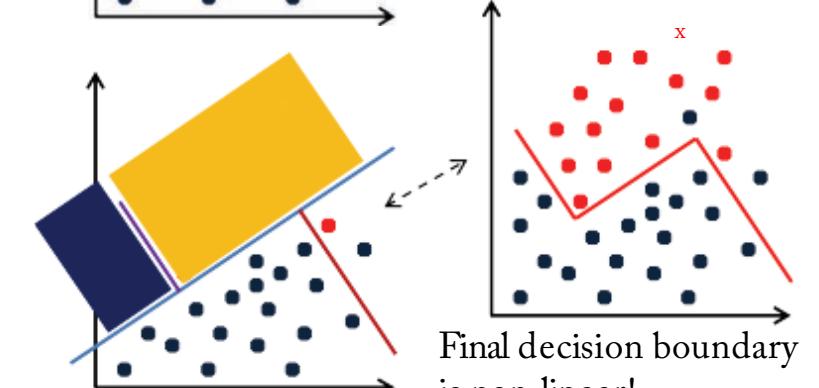
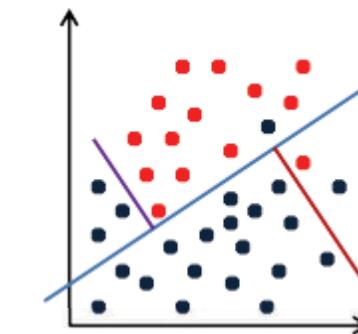
- \*Small\* trees structure are interpretable
- Good for visualization
- Capture interactions among features
- However, subject to depth (D): number of terminal nodes is  $2^D$



Idea: Combination of simple classifiers to more complex ones

$$h(x) = g(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}}$$

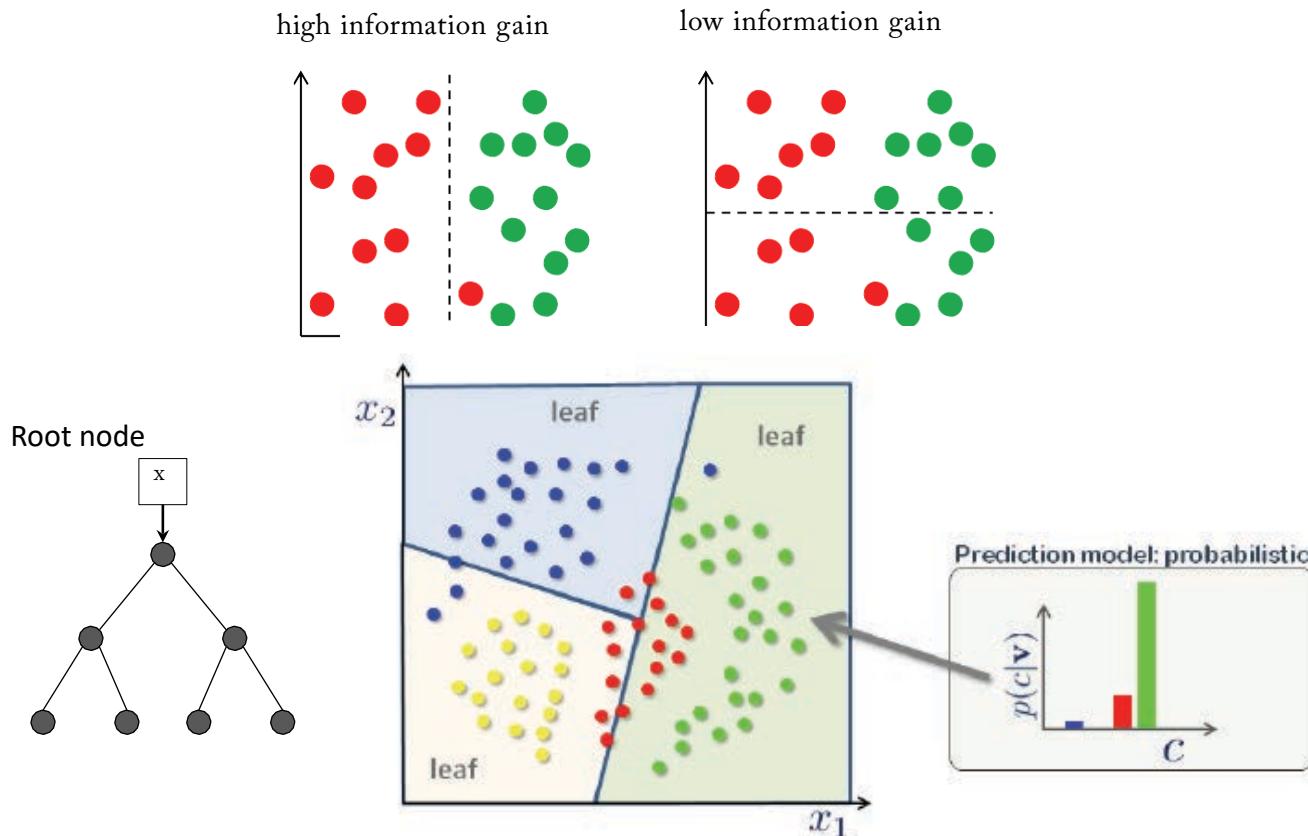
$$\begin{aligned} p(y = \text{'red'} | x) &= h(x) \\ p(y = \text{'blue'} | x) &= 1 - h(x) \end{aligned}$$



Final decision boundary  
is non-linear!

# Interpretation of Decision Trees

- A model can be interpreted by analyzing the feature importance
- A feature is important when it maximally reduces impurity of split data
- Tree structure describes feature importance (e.g. root node features are most important)



## Information Gain - IG

$$IG = H(S) - \sum_{i \in \{L, R\}} \frac{|S^i|}{|S|} H(S^i)$$

## Entropy

$$H(S) = \sum_{y \in \mathcal{Y}} p(y) \log p(y).$$

## Alternative, Gini Index

$$GI = 1 - \sum p(y)$$

- IG favors smaller but varied partitions; GI favors larger partitions

# Linking note to DL methods

Decision Forests, Convolutional Networks and the Models in-Between  
Microsoft Research Technical Report 2015-58

## Deep Neural Decision Forests

Yani Ioannou<sup>1</sup> Duncan Robertson<sup>2</sup> Darko Zikic<sup>2</sup> Peter Kontschieder<sup>2</sup>

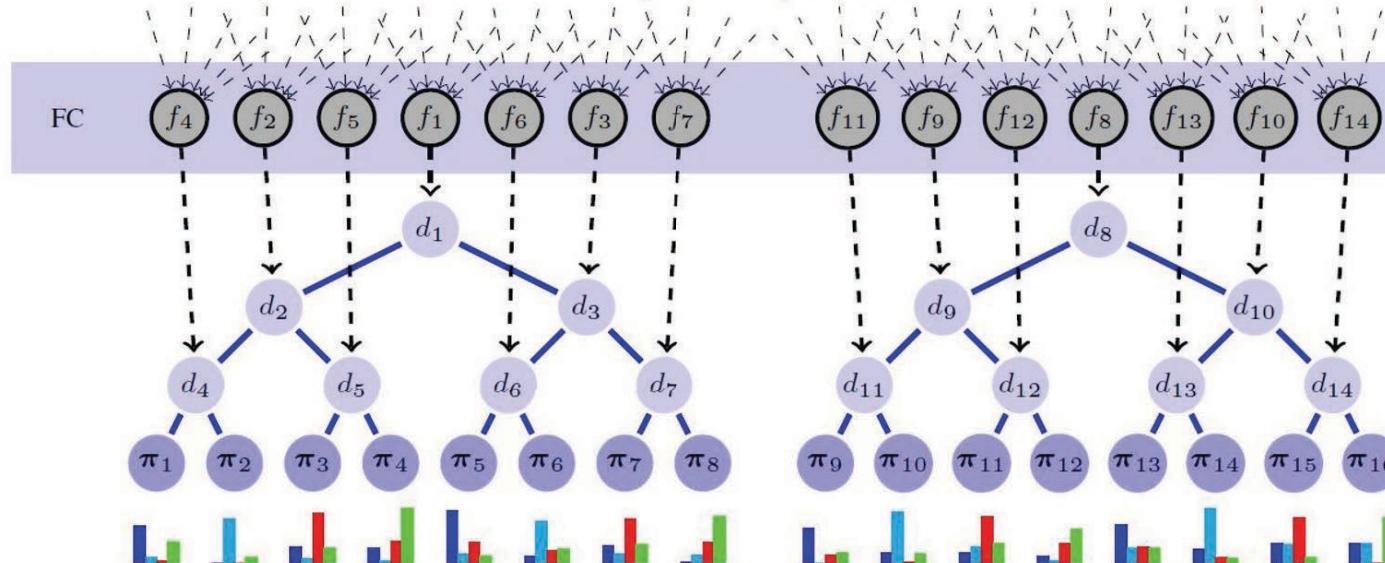
Jamie Shotton<sup>2</sup> Matthew Brown<sup>3</sup> Antonio Criminisi<sup>2</sup>

<sup>1</sup>University of Cambridge, <sup>2</sup>Microsoft Research, <sup>3</sup>University of Bath

Peter Kontschieder<sup>1</sup> Madalina Fiterau<sup>\*2</sup> Antonio Criminisi<sup>1</sup> Samuel Ro

Microsoft Research<sup>1</sup> Carnegie Mellon University<sup>2</sup> Fondazione Bruno Kessler<sup>3</sup>  
Cambridge, UK Pittsburgh, PA Trento, Italy

Deep CNN with parameters  $\Theta$



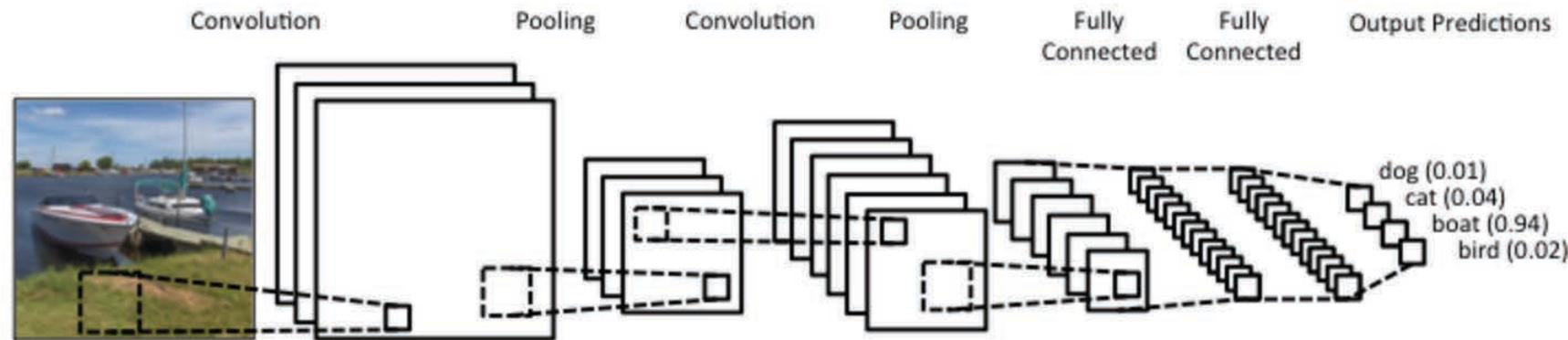


# Interpretable DL

# Convolutional Neural Networks

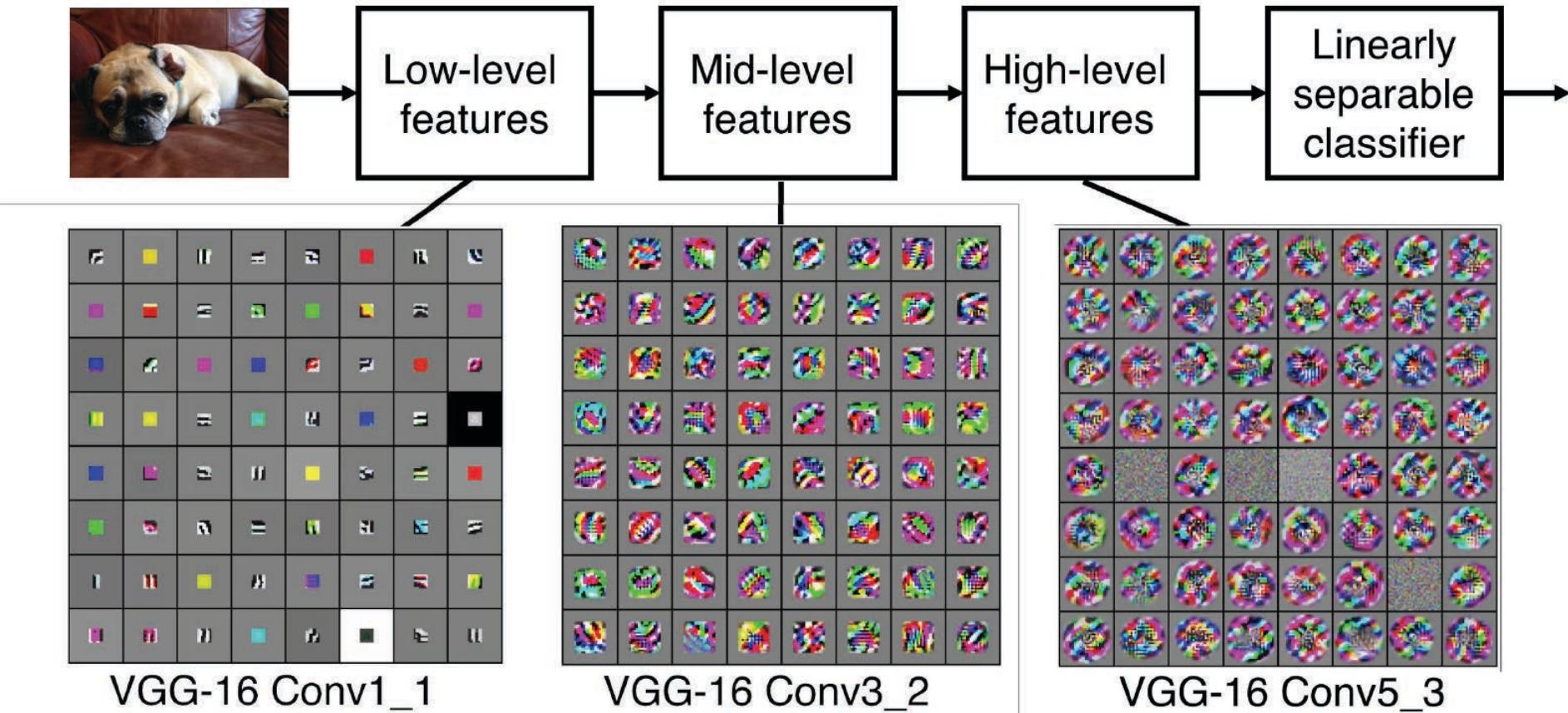
Typical structure:

- Convolution layers
- Pooling or subsampling layers
- Fully connected layers

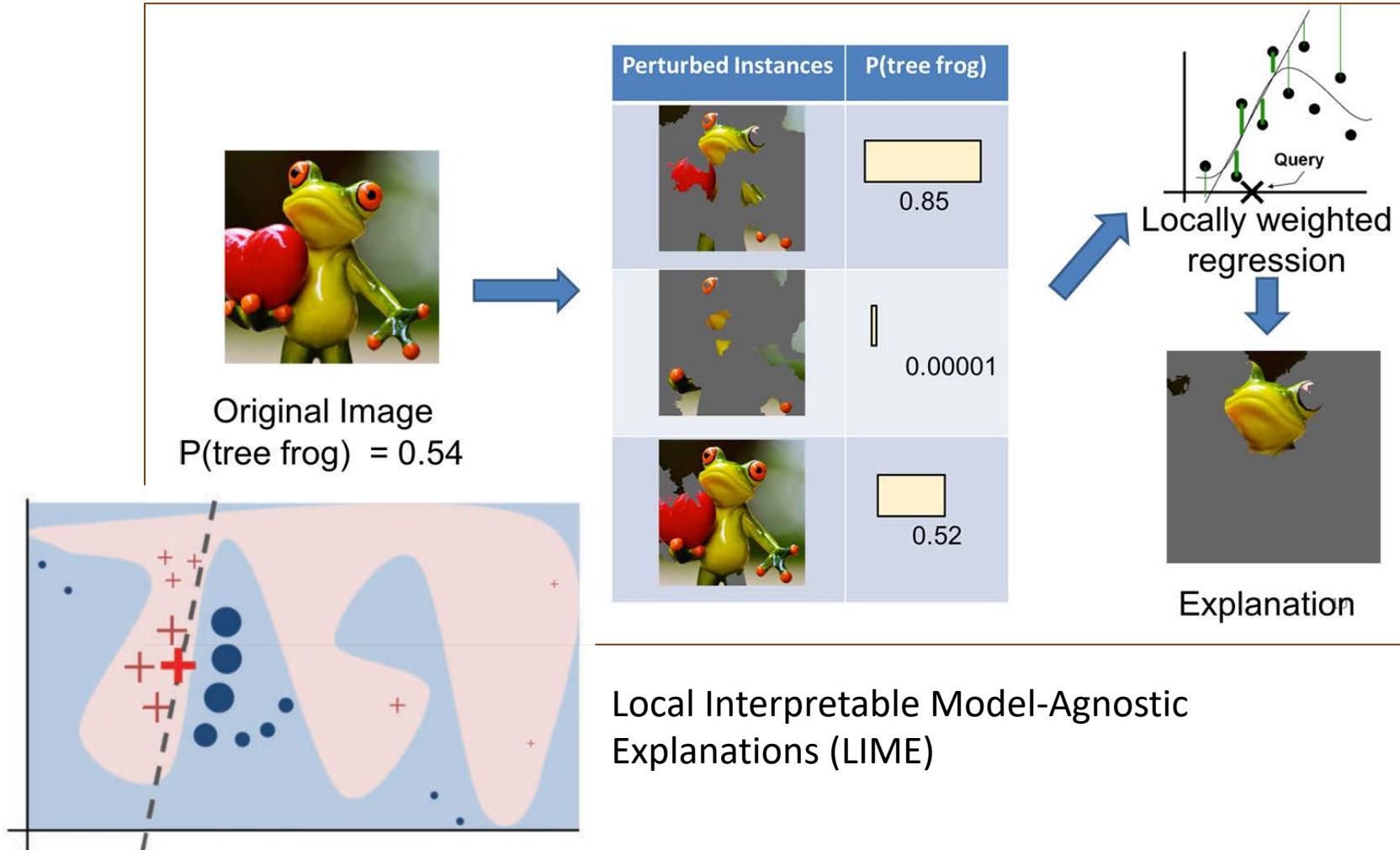


# Convolutional Neural Networks

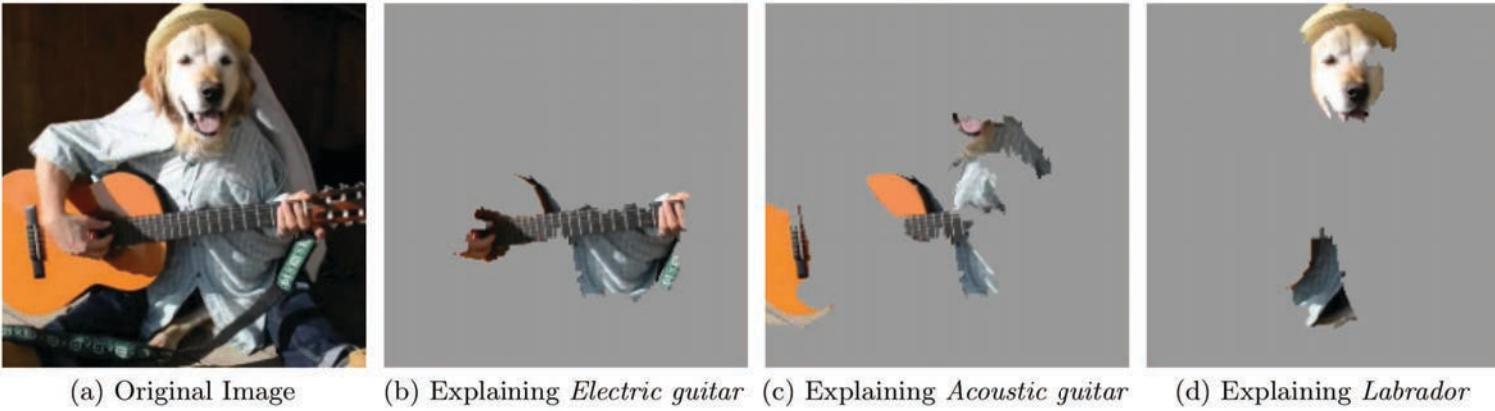
## Preview



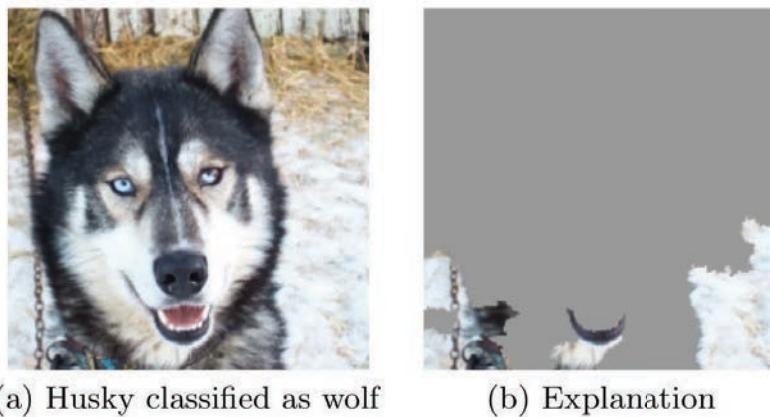
# “Why Should I Trust You?” Explaining the Predictions of Any Classifier: Local Interpretable Model-agnostic Explanations (LIME) – Ribeiro et al . 2017



# “Why Should I Trust You?” Explaining the Predictions of Any Classifier: Local Interpretable Model-agnostic Explanations (LIME) – Ribeiro et al . 2017



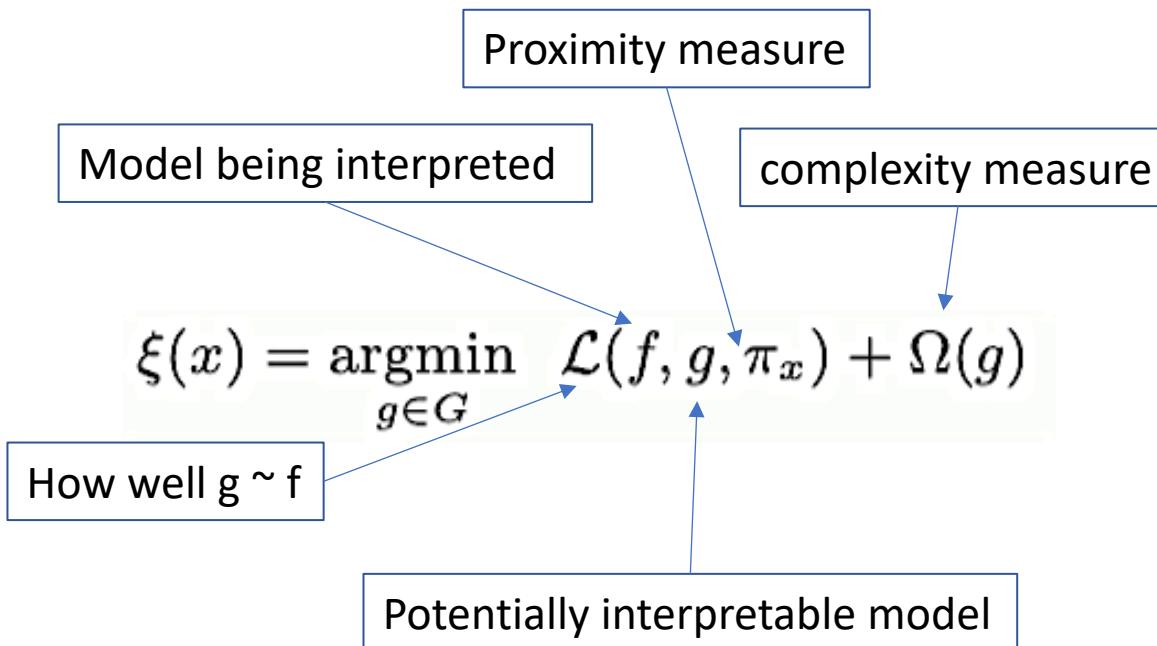
**Figure 4:** Explaining an image classification prediction made by Google’s Inception neural network. The top 3 classes predicted are “Electric Guitar” ( $p = 0.32$ ), “Acoustic guitar” ( $p = 0.24$ ) and “Labrador” ( $p = 0.21$ )



**Figure 11:** Raw data and explanation of a bad model’s prediction in the “Husky vs Wolf” task.

# “Why Should I Trust You?” Explaining the Predictions of Any Classifier: Local Interpretable Model-agnostic Explanations (LIME) – Ribeiro et al . 2017

## Local Interpretable Model-Agnostic Explanations (LIME)



---

### Algorithm 1 Sparse Linear Explanations using LIME

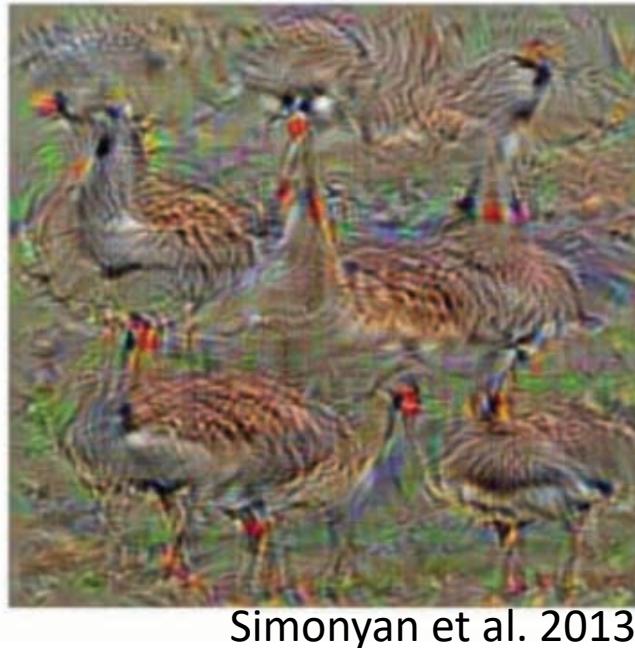
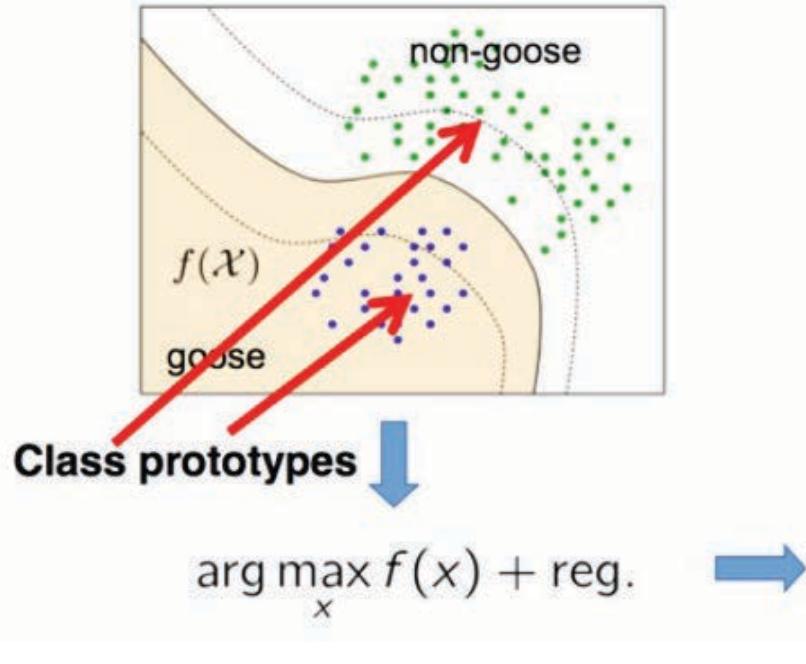
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**Require:** Classifier  $f$ , Number of samples  $N$   
**Require:** Instance  $x$ , and its interpretable version  $x'$   
**Require:** Similarity kernel  $\pi_x$ , Length of explanation  $K$

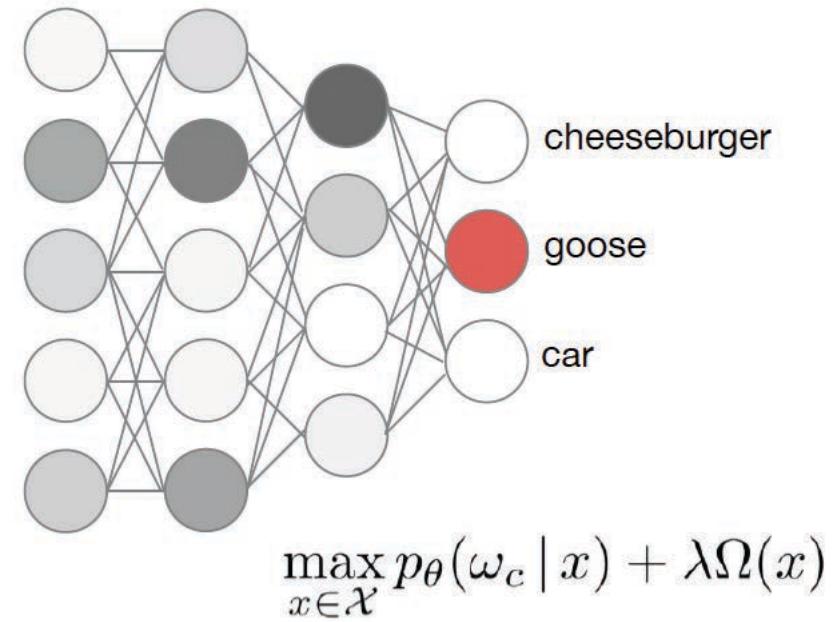
```
 $\mathcal{Z} \leftarrow \{\}$ 
for  $i \in \{1, 2, 3, \dots, N\}$  do
     $z'_i \leftarrow \text{sample\_around}(x')$ 
     $\mathcal{Z} \leftarrow \mathcal{Z} \cup \langle z'_i, f(z_i), \pi_x(z_i) \rangle$ 
end for
 $w \leftarrow \text{K-Lasso}(\mathcal{Z}, K)$   $\triangleright$  with  $z'_i$  as features,  $f(z)$  as target
return  $w$ 
```

---

# Explaining by finding prototype class members



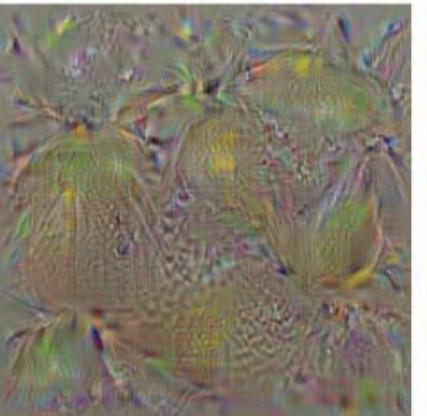
- Global explanation technique
- Find pattern maximizing class activation
- Not-necessarily a real image



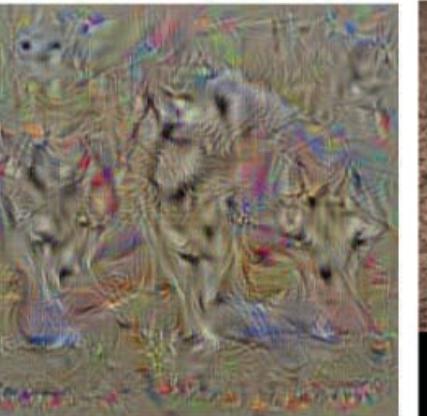
Simonyan et al. 2013. Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps



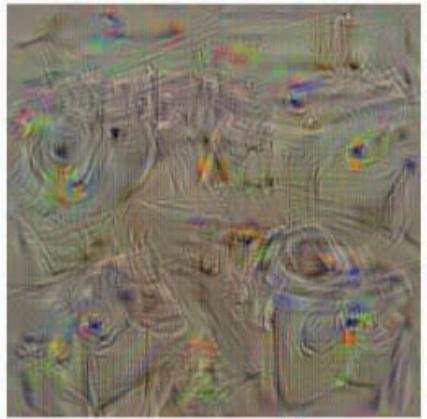
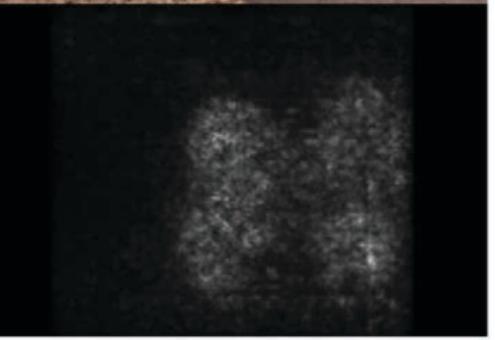
bell pepper



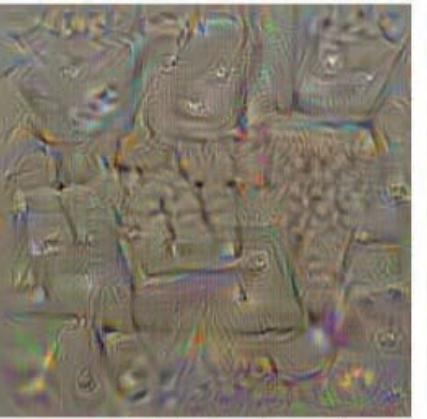
lemon



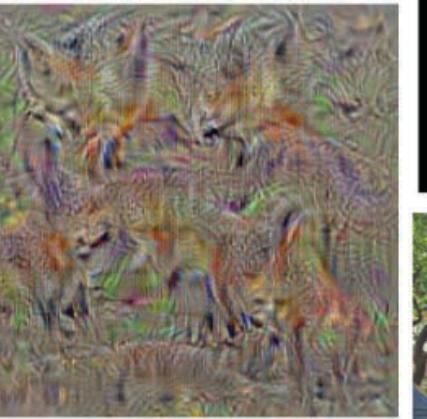
husky



washing machine



computer keyboard



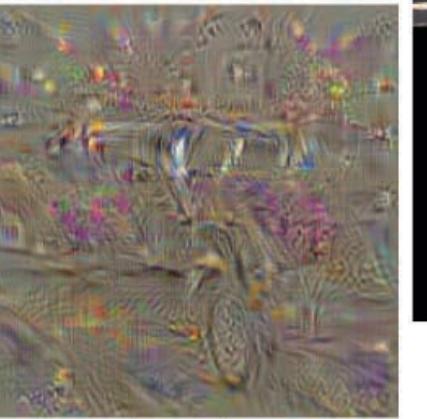
kit fox



goose



ostrich



limousine

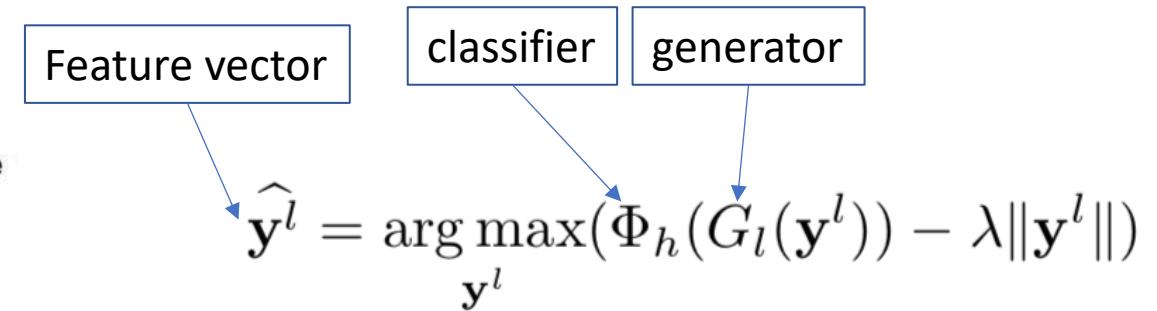
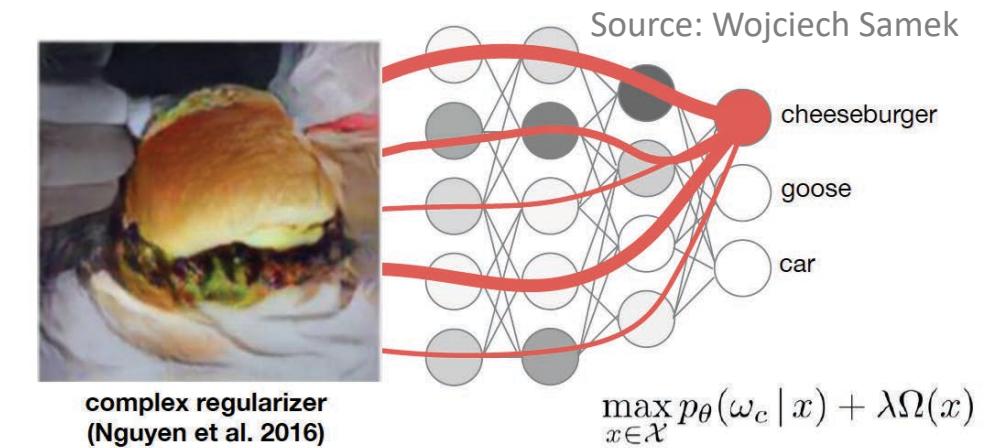
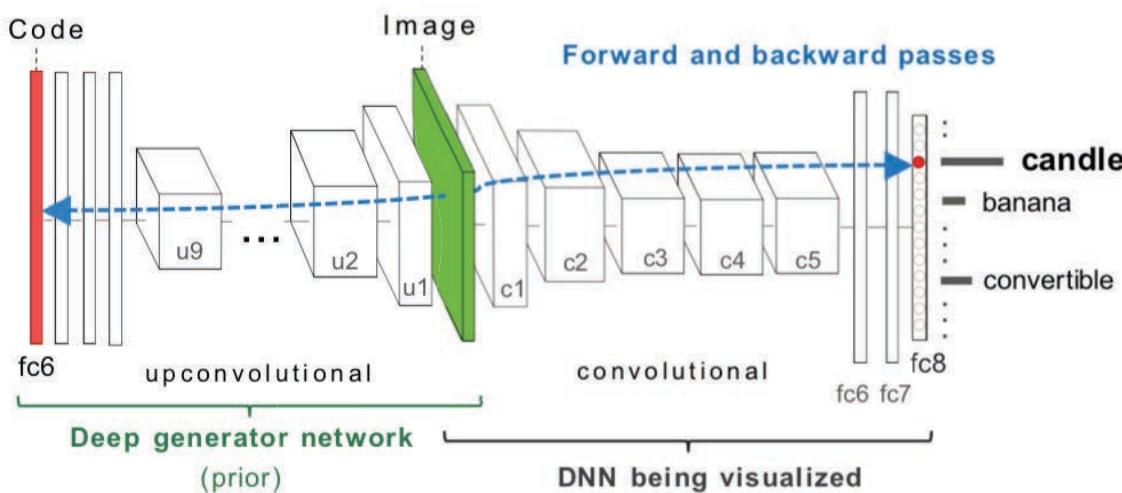
Simonyan et al. 2013. Deep Inside Convolutional Networks:  
Visualising Image Classification Models and Saliency Maps

# Synthesizing the preferred inputs for neurons in neural networks via deep generator networks

- Nguyen et al. 2016

## Regularization via generative adversarials

- 1.- Forwards pass of gradients
- 2- Detect maximum activation
- 3.- Backward pass of “FC6” into encoder



- Prior generator and DNN can be trained separately

# Synthesizing the preferred inputs for neurons in neural networks via deep generator networks

- Nguyen et al. 2016

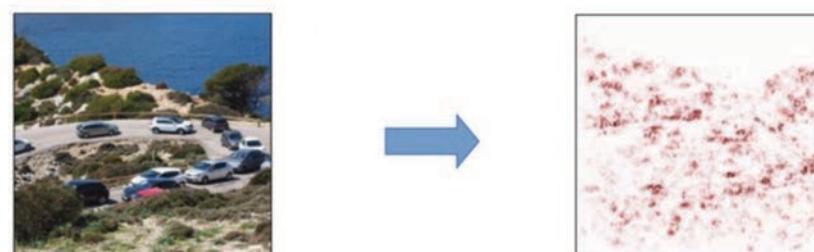


# Gradient-based methods

- Idea: magnitude of gradient reflects importance (attribution) of input to output scores

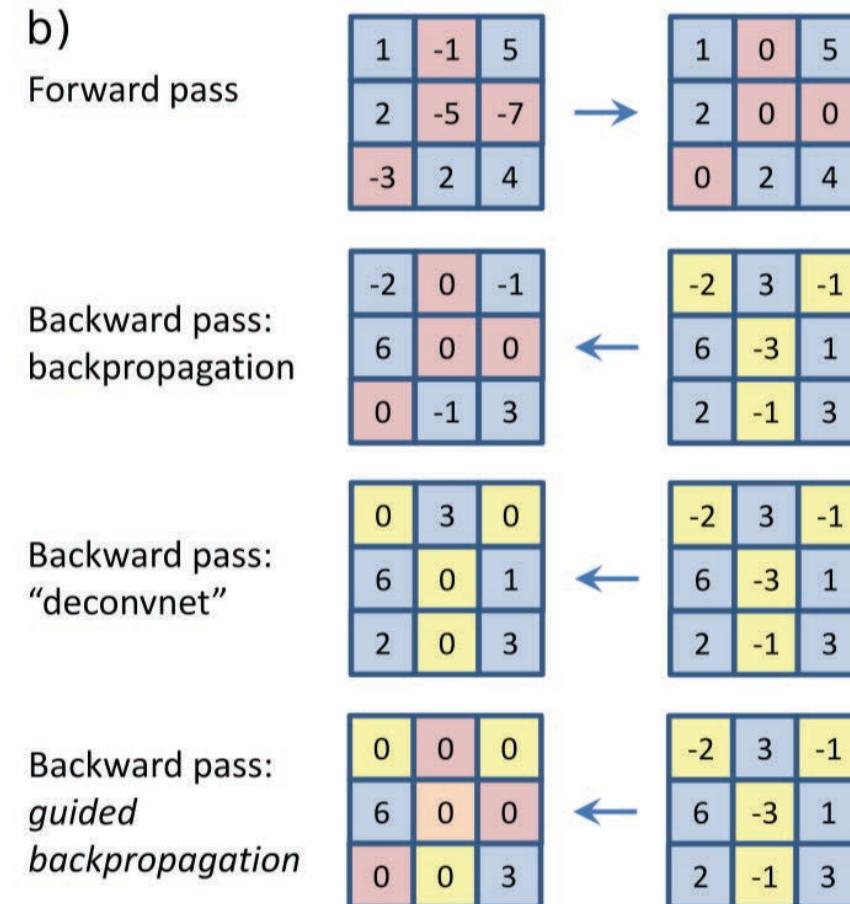
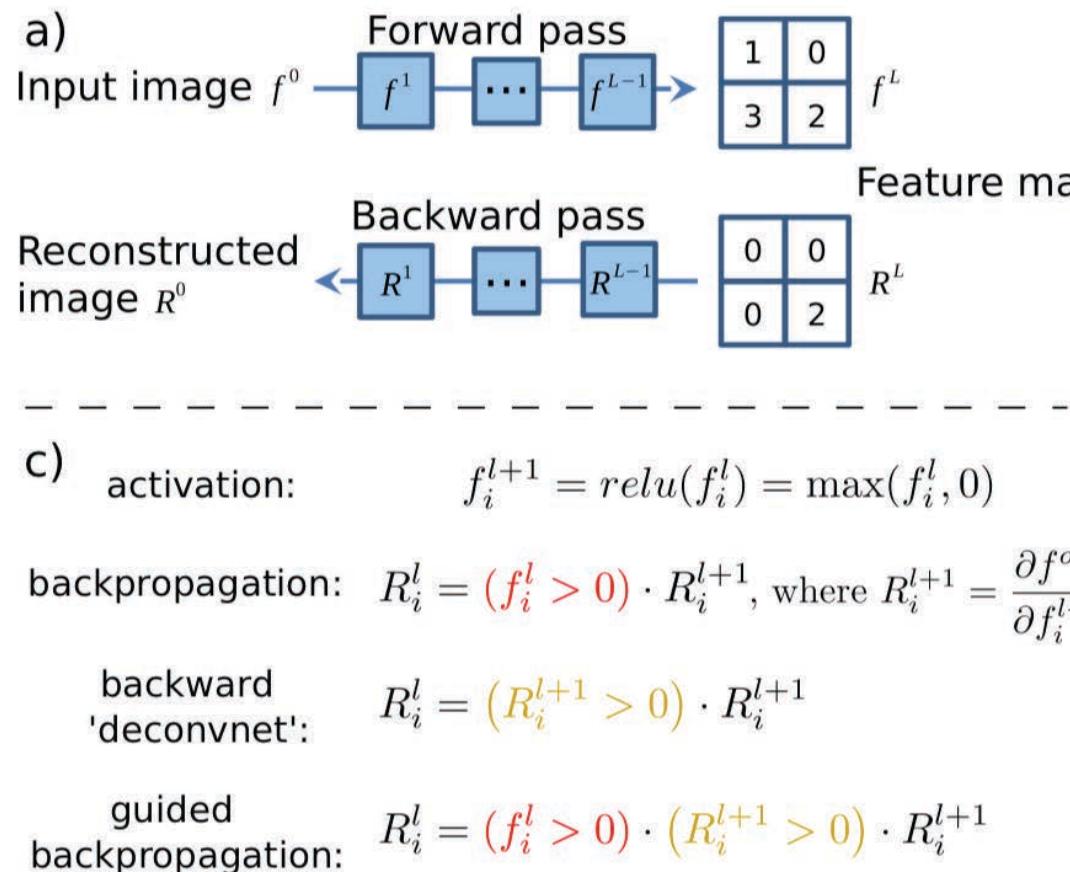
$$R = \sum \left( \frac{\delta S}{\delta x_i} \right)^2$$

Variations:



- Input \* Gradient  $x * \frac{\delta f}{\delta x_i}$  → Addresses gradient saturation and reduces diffusivity – Shrikumar et al. 2016
- Deconvnet: inverts direction of applying activation; zero outs negative activations – Zeiler et al. 2014
- Guided-backpropagation: deconvnet + filters out negative forward activations - Springenberg et al. 2015
- Integrated gradients: sums over scaled versions of input; addresses gradient saturation – Sundararajan et al. 2017
- Grad-CAM: includes a neuron importance weight (detailed later) - Selvaraju et al. 2017

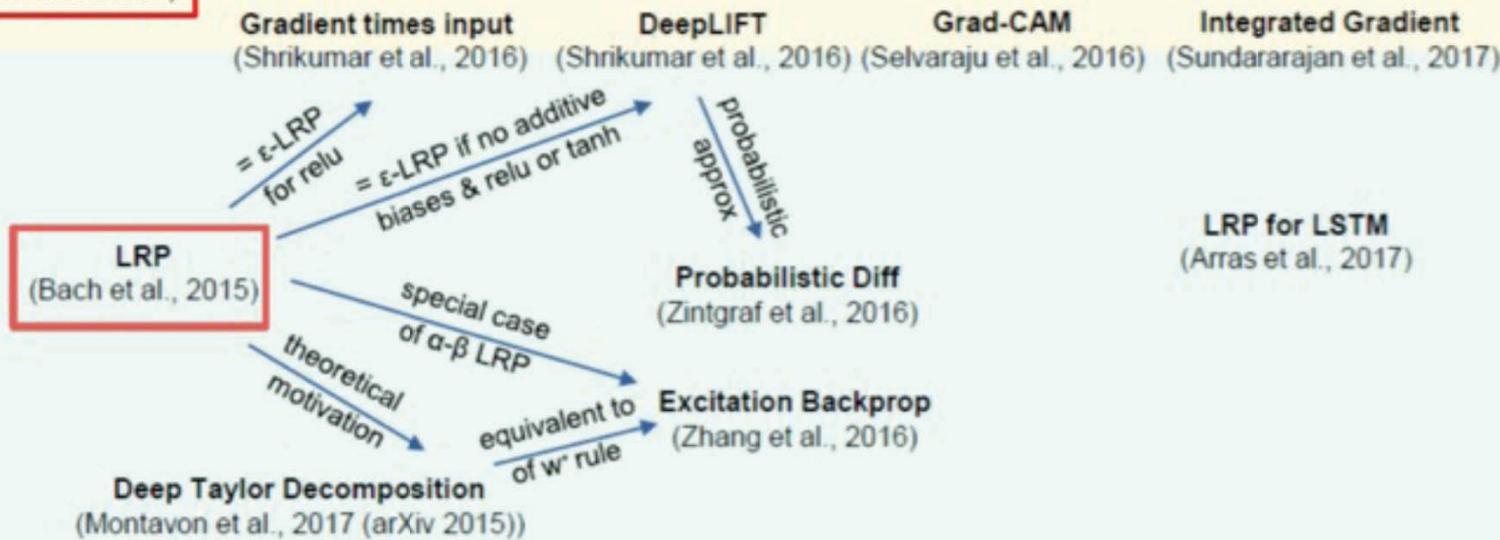
# Differences between backprop, deconvnet and guided-backpropagation





Gradient vs. Decomposition  
 (Montavon et al., 2018)

## Decomposition



## Optimization

LIME  
 (Ribeiro et al., 2016)

Meaningful Perturbations  
 (Fong & Vedaldi 2017)

PatternLRP  
 (Kindermans et al., 2017)

## Deconvolution

Deconvolution  
 (Zeiler & Fergus 2014)

Guided Backprop  
 (Springenberg et al. 2015)

## Understanding the Model

Feature visualization  
 (Erhan et al. 2009)

Deep Visualization  
 (Yosinski et al., 2015)

Inverting CNNs  
 (Dosovitskiy & Brox, 2015)

Synthesis of preferred inputs  
 (Nguyen et al. 2016)

Inverting CNNs  
 (Mahendran & Vedaldi, 2015)

RNN cell state analysis  
 (Karpathy et al., 2015)

Network Dissection  
 (Zhou et al. 2017)

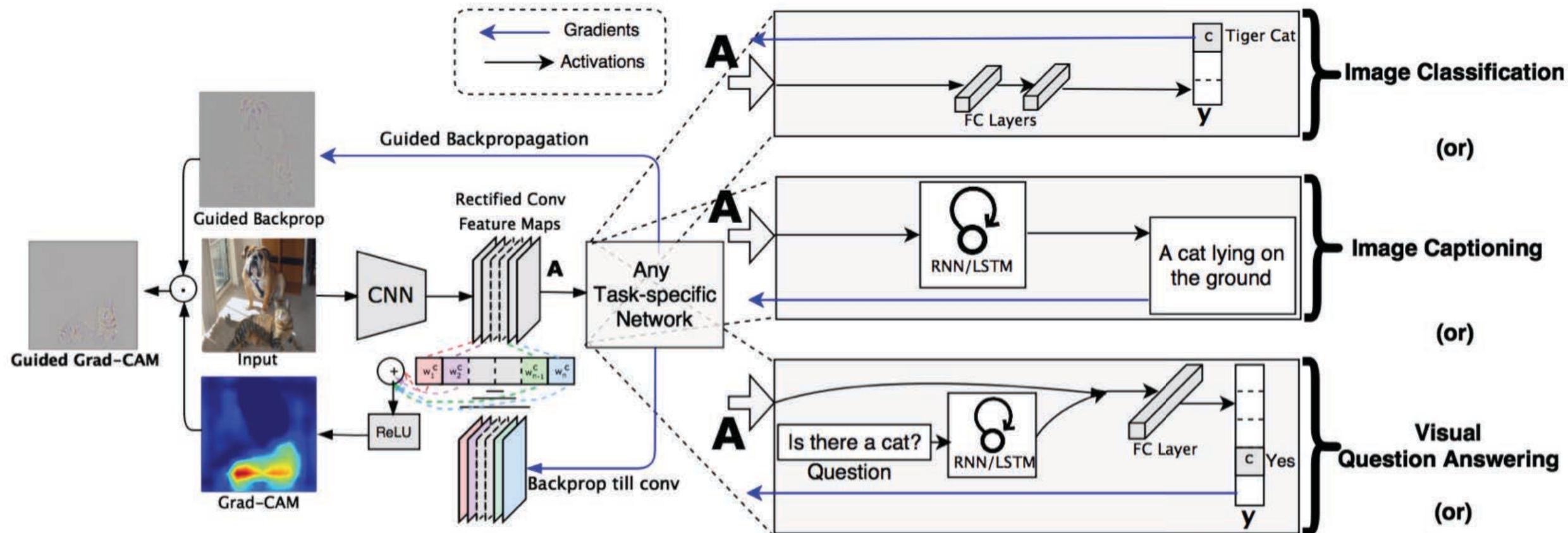
# Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization - Selvaraju et al. 2017

- Generalization of CAM: Zhou et al. Learning Deep Features for Discriminative Localization. In *CVPR*, 2016.
  - Applicable to any CNN-based (CAM requires conv feature maps → global average pooling → softmax layer)
- Motivation – Good visualization is class-specific and detailed



# Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization - Selvaraju et al. 2017

**Guided-Grad-CAM:** Uses Grad-CAM ask mask for Guided Backprop

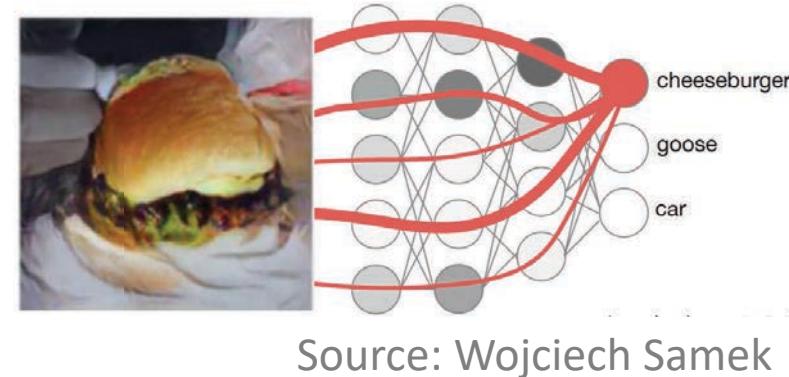


# Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization - Selvaraju et al. 2017

Single forward and (partial) backward pass

**Neuron importance weights**  $\alpha_k^c = \underbrace{\frac{1}{Z} \sum_i \sum_j}_{\text{global average pooling}} \underbrace{\frac{\partial y^c}{\partial A_{ij}^k}}_{\text{gradients via backprop}}$

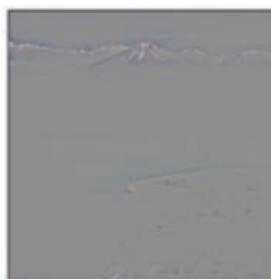
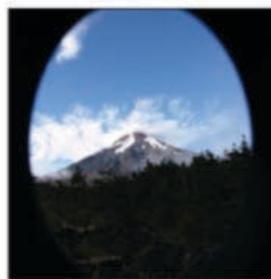
$A^k$ : kth feature map  
 $y^c$ : score for class c (before softmax)



$$L_{\text{Grad-CAM}}^c = \text{ReLU} \left( \underbrace{\sum_k \alpha_k^c A^k}_{\text{linear combination}} \right)$$

# Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization - Selvaraju et al. 2017

Failure analysis: Cases where VGG failed and corresponding visualizations



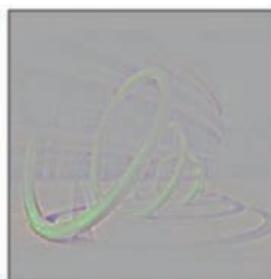
Ground truth: volcano



Ground truth: volcano



Ground truth: beaker



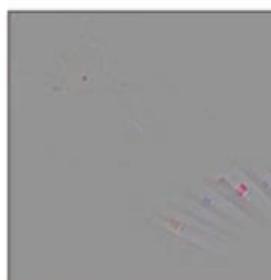
Ground truth: coil



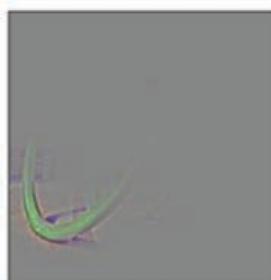
Predicted: sandbar



Predicted: car mirror



Predicted: syringe



Predicted: vine snake

# Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization - Selvaraju et al. 2017

## Human studies

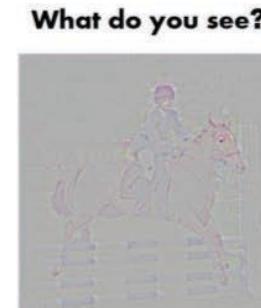
“Which of the two object categories is depicted in the image?”

- N=43, amazon mechanical turk
- Humans recognized correct class in 61.23% vs 44.44% guided backprop

“Which model is more trustable?”

VGG vs. AlexNet

*“Remarkably, we find that human subjects are able to identify the more accurate classifier (VGG over AlexNet) despite viewing identical predictions from the two, simply from the different explanations generated from the two.”*



Your options:  
 Horse  
 Person

**Both robots predicted: Person**  
Robot A based its decision on      Robot B based its decision on

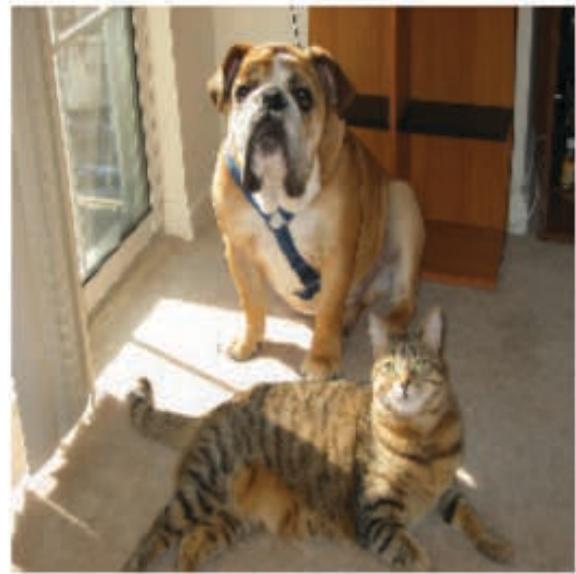


**Which robot is more reasonable?**

- Robot A seems clearly more reasonable than robot B
- Robot A seems slightly more reasonable than robot B
- Both robots seem equally reasonable
- Robot B seems slightly more reasonable than robot A
- Robot B seems clearly more reasonable than robot A

# Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization - Selvaraju et al. 2017

Robustness to adversarial examples: Examples where VGG got “fooled”



Boxer: 0.40 Tiger Cat: 0.18

(a) Original image



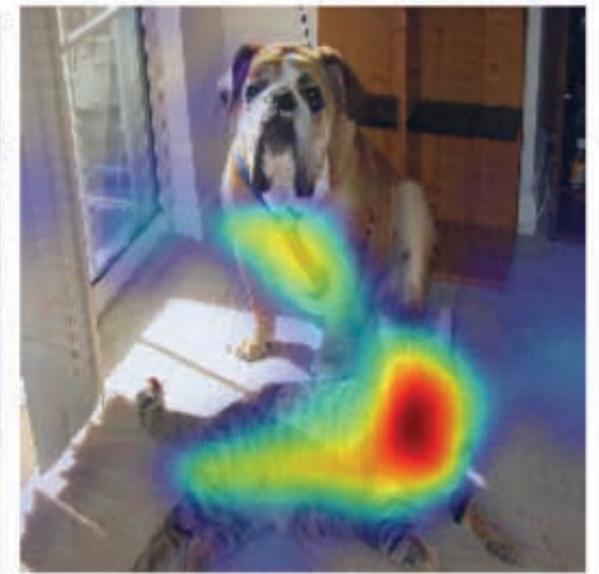
Airliner: 0.9999

(b) Adversarial image



Boxer: 1.1e-20

(c) Grad-CAM “Dog”

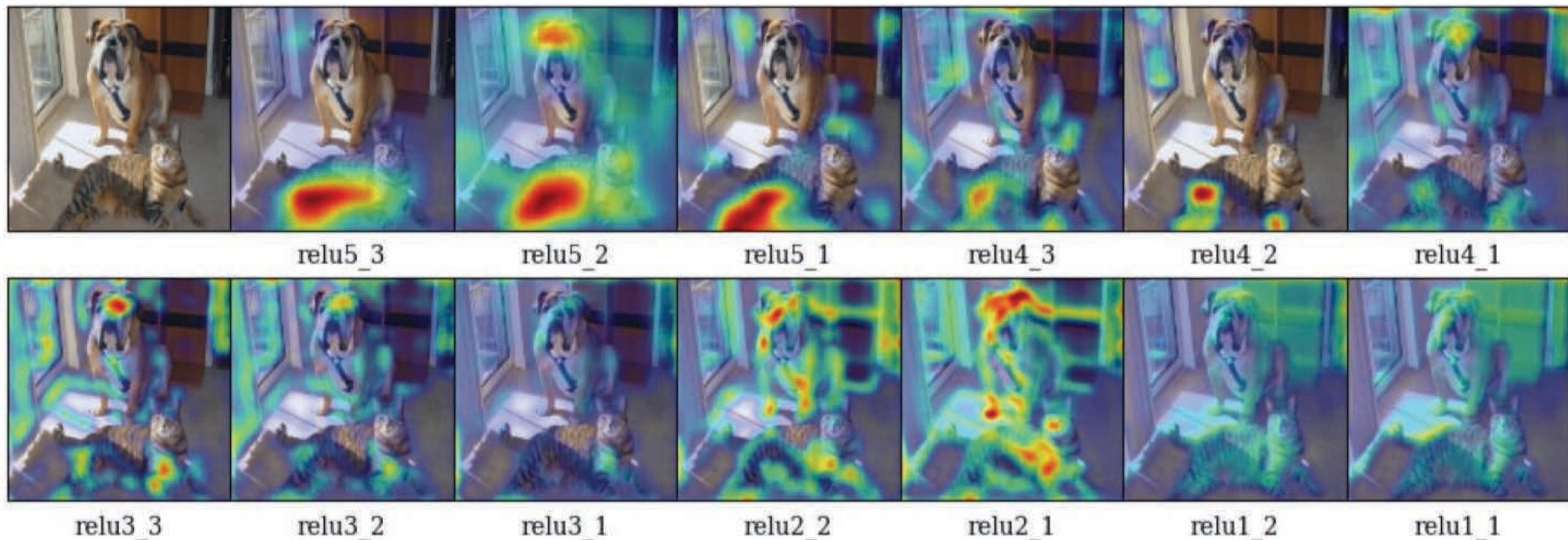


Tiger Cat: 6.5e-17

(d) Grad-CAM “Cat”

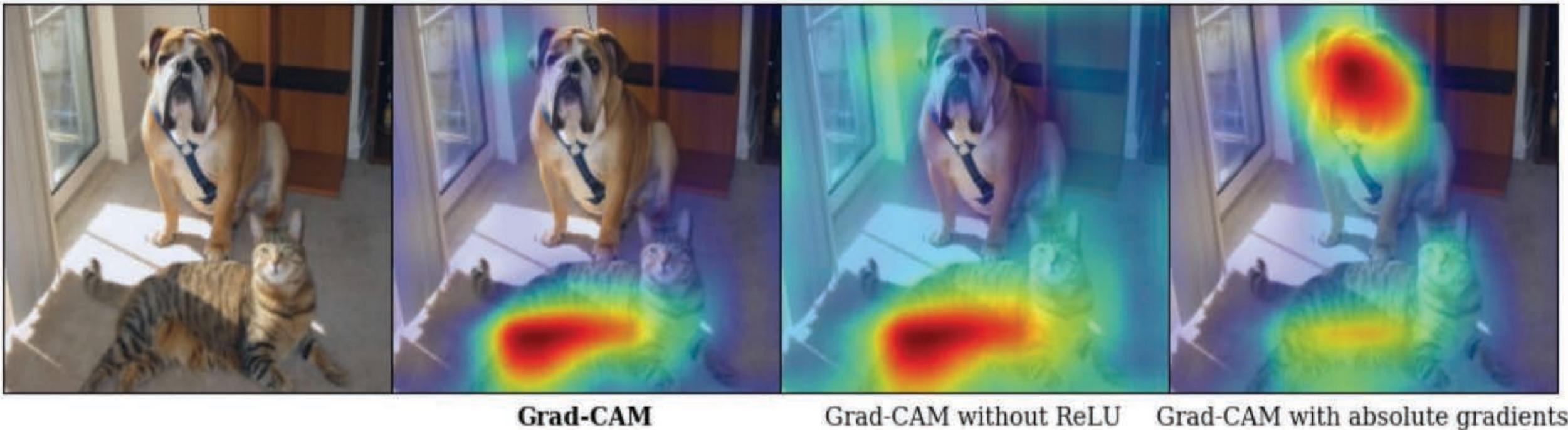
# Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization - Selvaraju et al. 2017

## Layer-wise analysis



# Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization - Selvaraju et al. 2017

## Ablation study



# Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization - Selvaraju et al. 2017

Effect of global average pooling vs. global max pooling



**Grad-CAM**

Grad-CAM with  
Global Max Pooled gradients

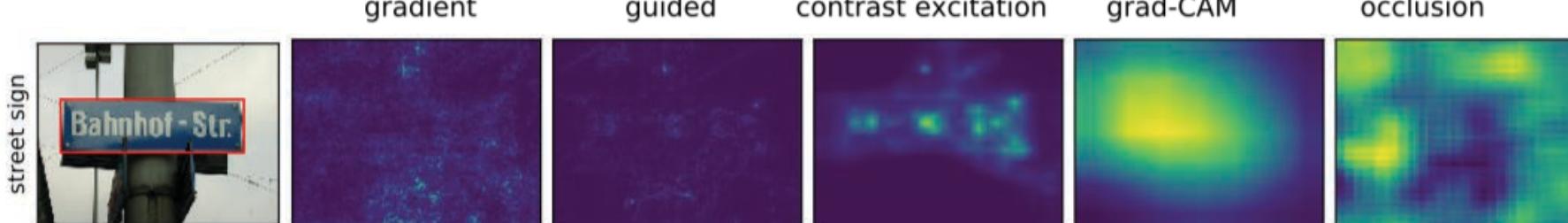
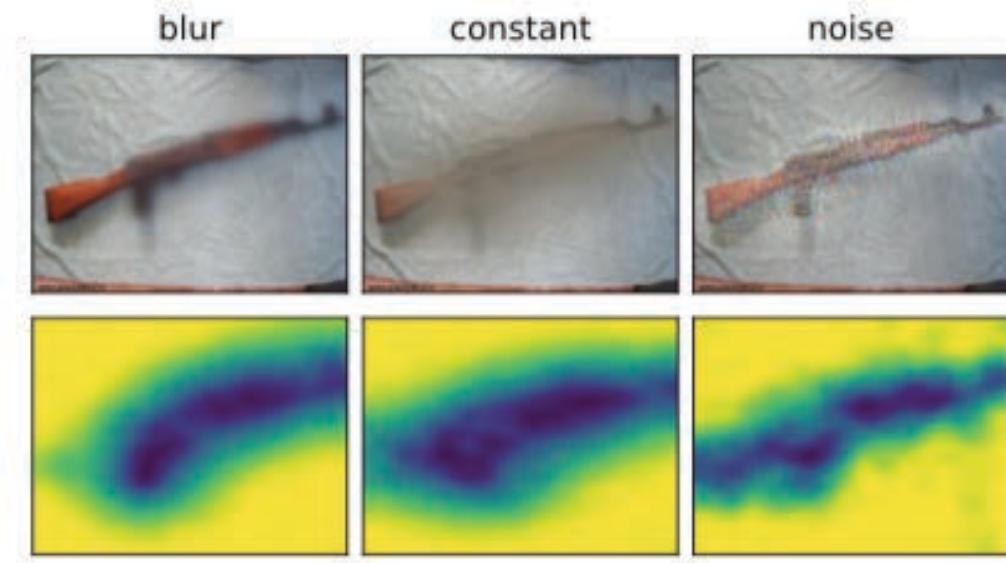
# Interpretable Explanations of Black Boxes by Meaningful Perturbation - Fong et al. 2018

**Motivation:** Saliency (gradient-based) approaches are not specific enough

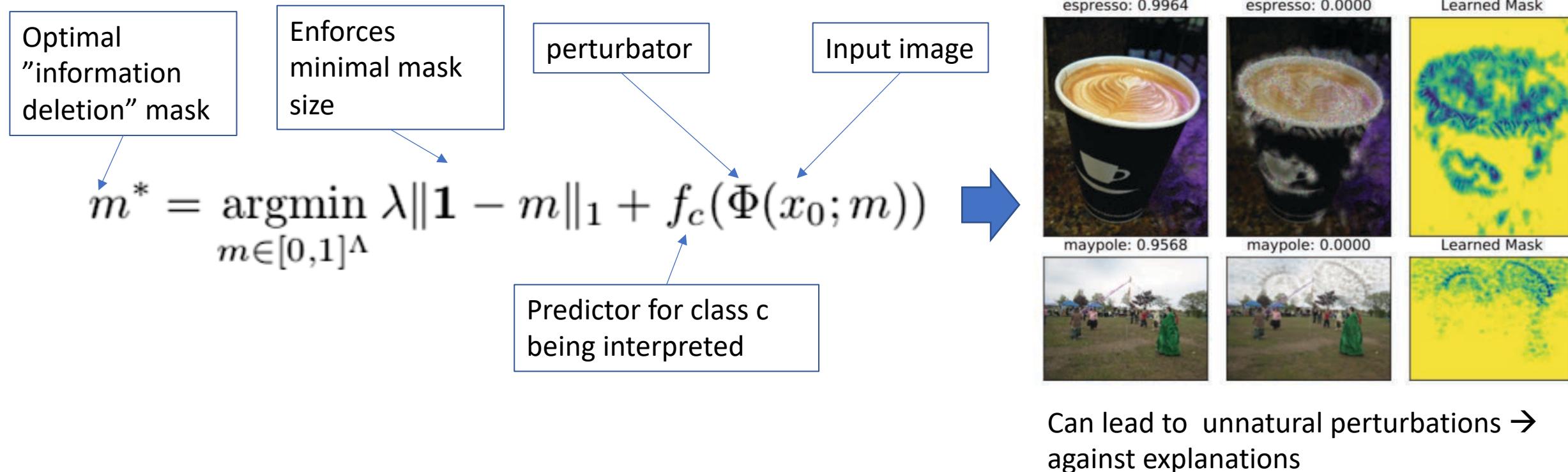
**Key idea:** select the right perturbation\* to study the effect on the prediction function  $f(x)$

Meaning of an explanation depends on the meaning of the changes applied to the input  $x$

\*Perturbation  $\longleftrightarrow$  type of information deletion



# Interpretable Explanations of Black Boxes by Meaningful Perturbation - Fong et al. 2018

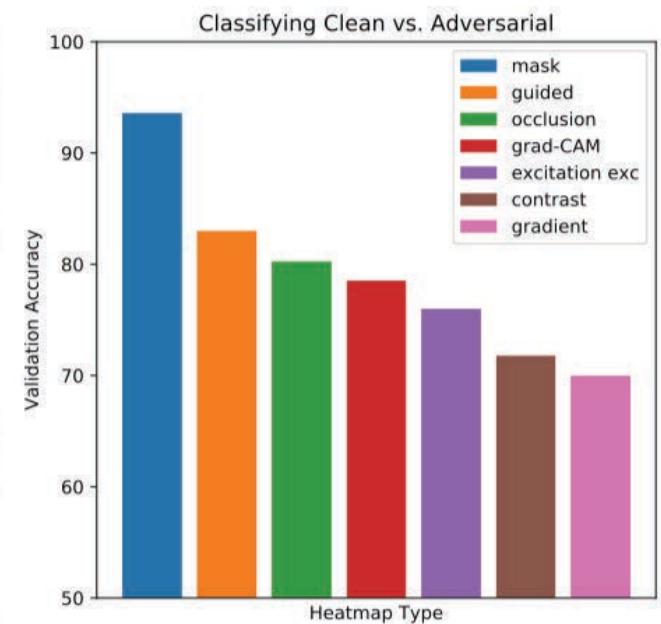
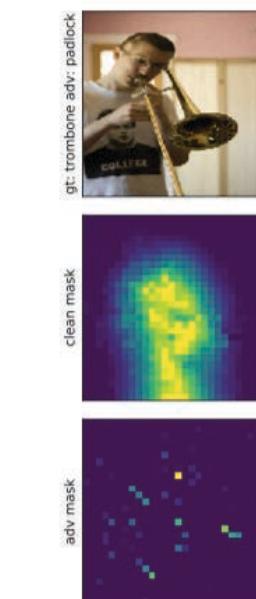


# Interpretable Explanations of Black Boxes by Meaningful Perturbation - Fong et al. 2018

$$\min_{m \in [0,1]^\Lambda} \lambda_1 \|\mathbf{1} - m\|_1 + \lambda_2 \sum_{u \in \Lambda} \|\nabla m(u)\|_\beta^\beta + \mathbb{E}_\tau [f_c(\Phi(x_0(\cdot - \tau), m))]$$

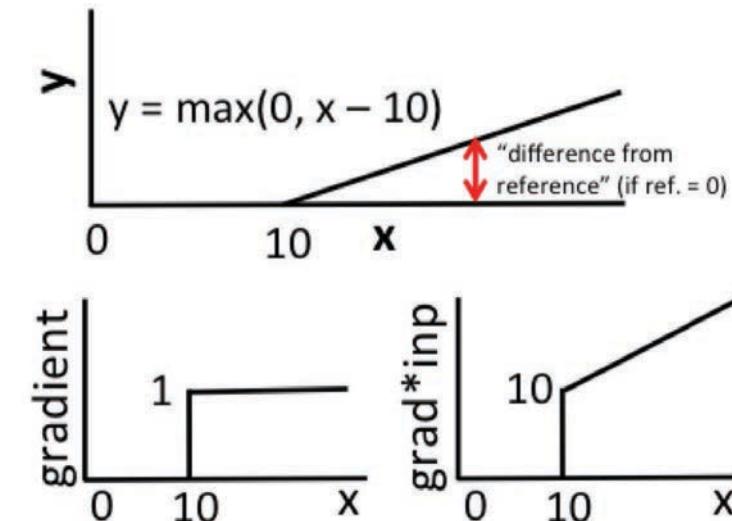
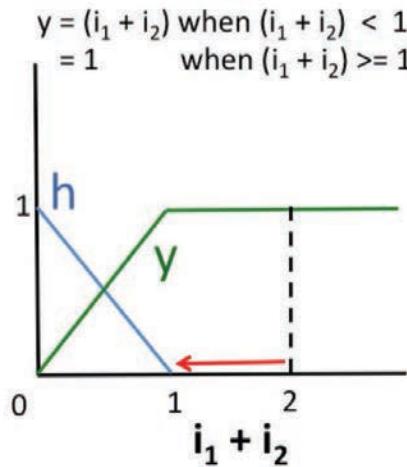
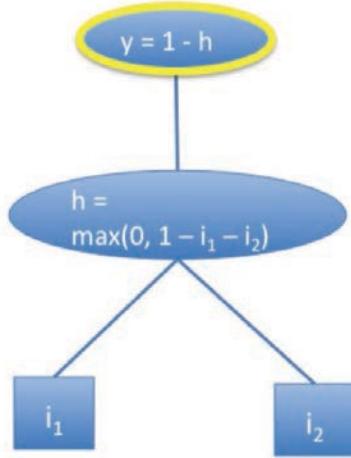
Expectation

Add variability to the mask (via jitter)



# DeepLift - Learning Important Features Through Propagating Activation Differences – Shrikumar et al. 2017

- Also part of the “gradient backpropagation” family of methods
- Motivation: zero gradients not necessarily mean no attribution; consider positive and negative attributions
- Idea: measure importance by assessing difference to a “reference”



# DeepLift - Learning Important Features Through Propagating Activation Differences – Shrikumar et al. 2017

- “reference”? → default or neutral state ?(e.g. black image)

$$\sum_{i=1}^n C_{\Delta x_i \Delta t} = \Delta t$$

Difference between neuron output and its reference value

Contribution measure: difference to delta\_t attributed to differences in input x

Positive and negative contributions

$$\Delta x_i = \Delta x_i^+ + \Delta x_i^-$$
$$C_{\Delta x_i \Delta t} = C_{\Delta x_i^+ \Delta t} + C_{\Delta x_i^- \Delta t}$$

Dense and conv. layers

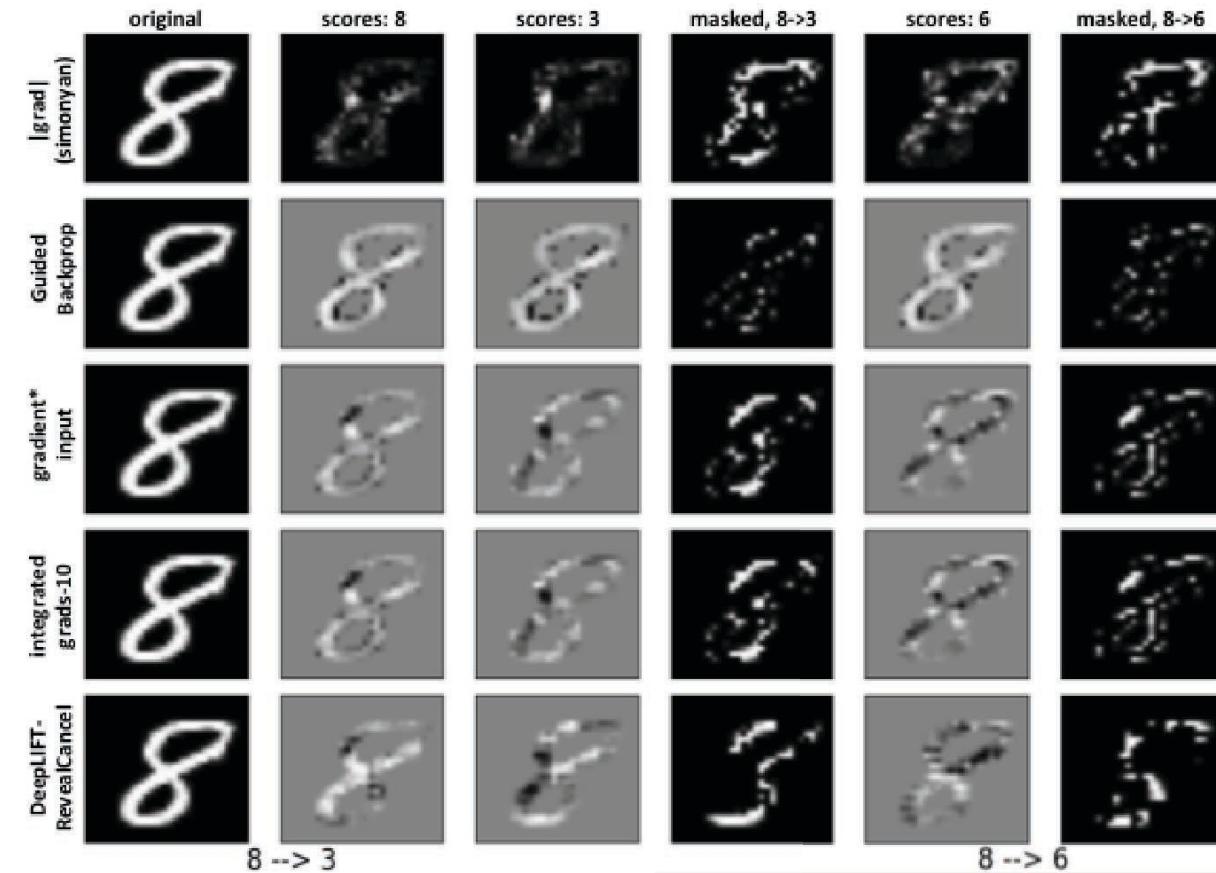
$$C_{\Delta x_i^+ \Delta y^+} = 1\{w_i \Delta x_i > 0\} w_i \Delta x_i^+$$
$$C_{\Delta x_i^- \Delta y^+} = 1\{w_i \Delta x_i > 0\} w_i \Delta x_i^-$$
$$C_{\Delta x_i^+ \Delta y^-} = 1\{w_i \Delta x_i < 0\} w_i \Delta x_i^+$$
$$C_{\Delta x_i^- \Delta y^-} = 1\{w_i \Delta x_i < 0\} w_i \Delta x_i^-$$

Non-linear (e.g. ReLU)

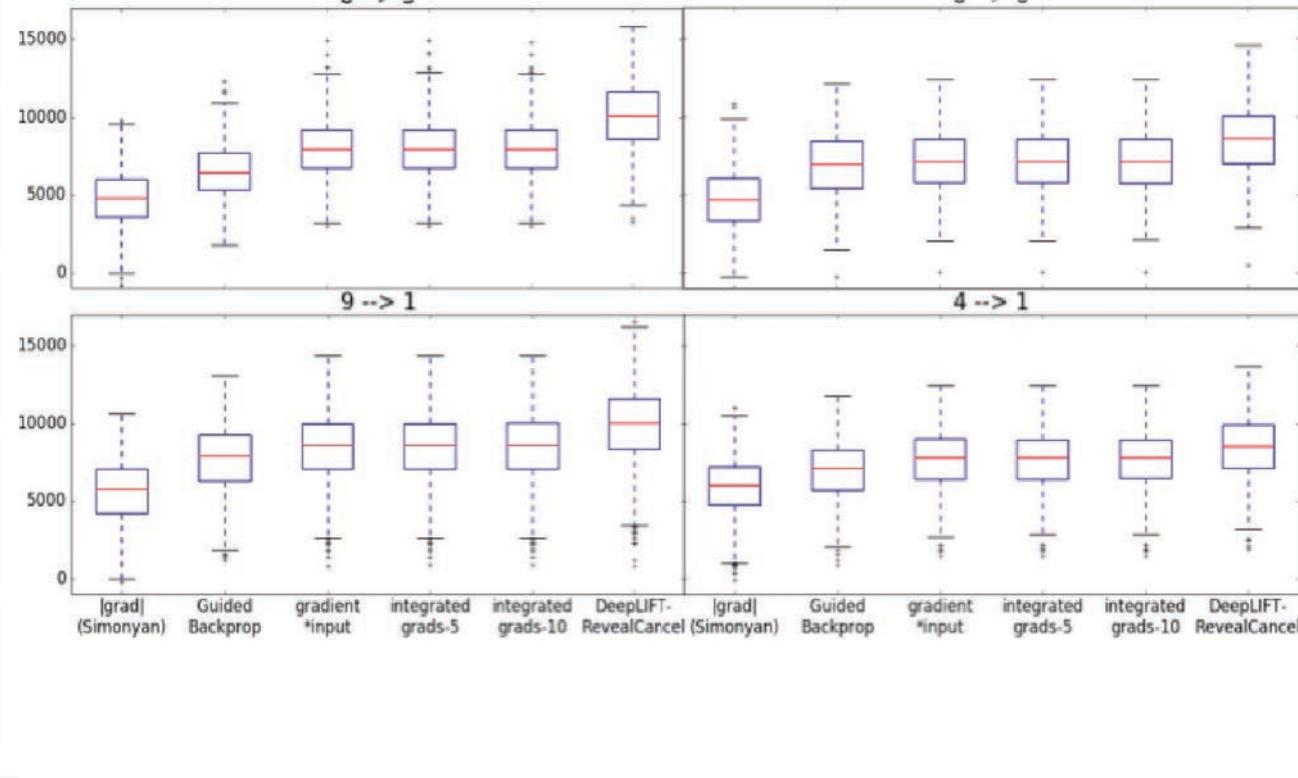
$$C_{\Delta x \Delta y} = \Delta y \quad \text{Approximates gradient}$$

# DeepLift - Learning Important Features Through Propagating Activation Differences – Shrikumar et al. 2017

Evaluation on MNIST: maximizing transition between digits



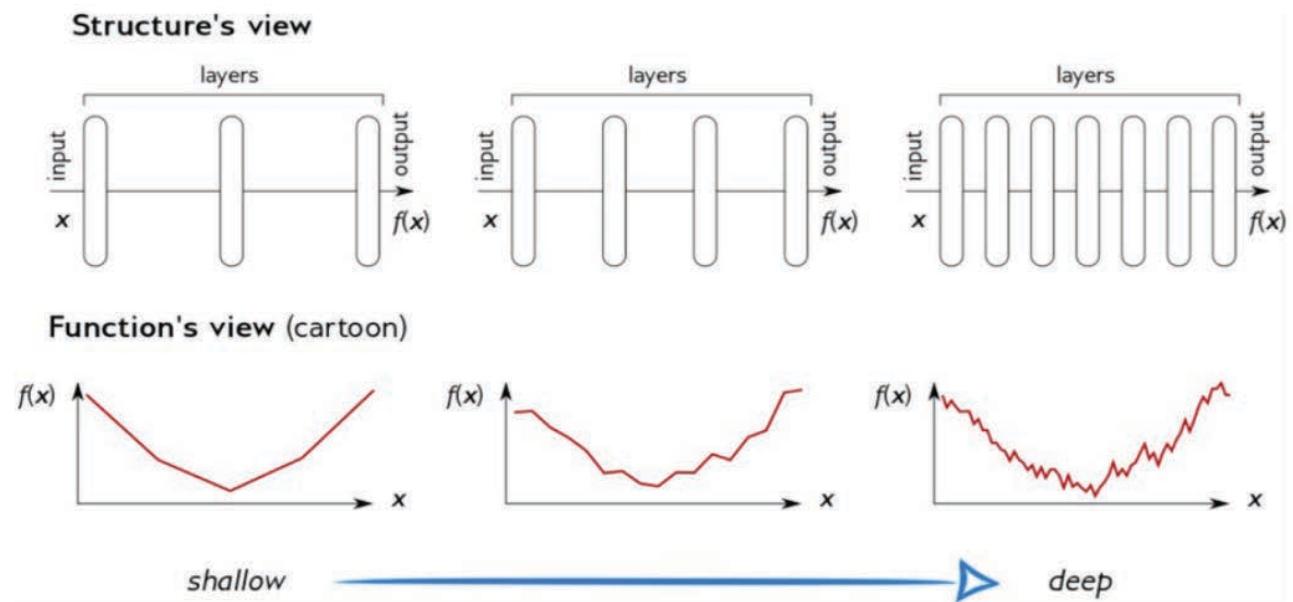
log-odds scores of target vs. original class after the mask is applied



# Layer-wise Relevance Propagation (LRP) -

Bach et al., PLOS ONE, 2015

- Motivation: Gradient methods suffering from shattered gradient problem → depth affects reliability of computed input gradients
- Sensitivity explains changes to the prediction function, not the function's value itself.

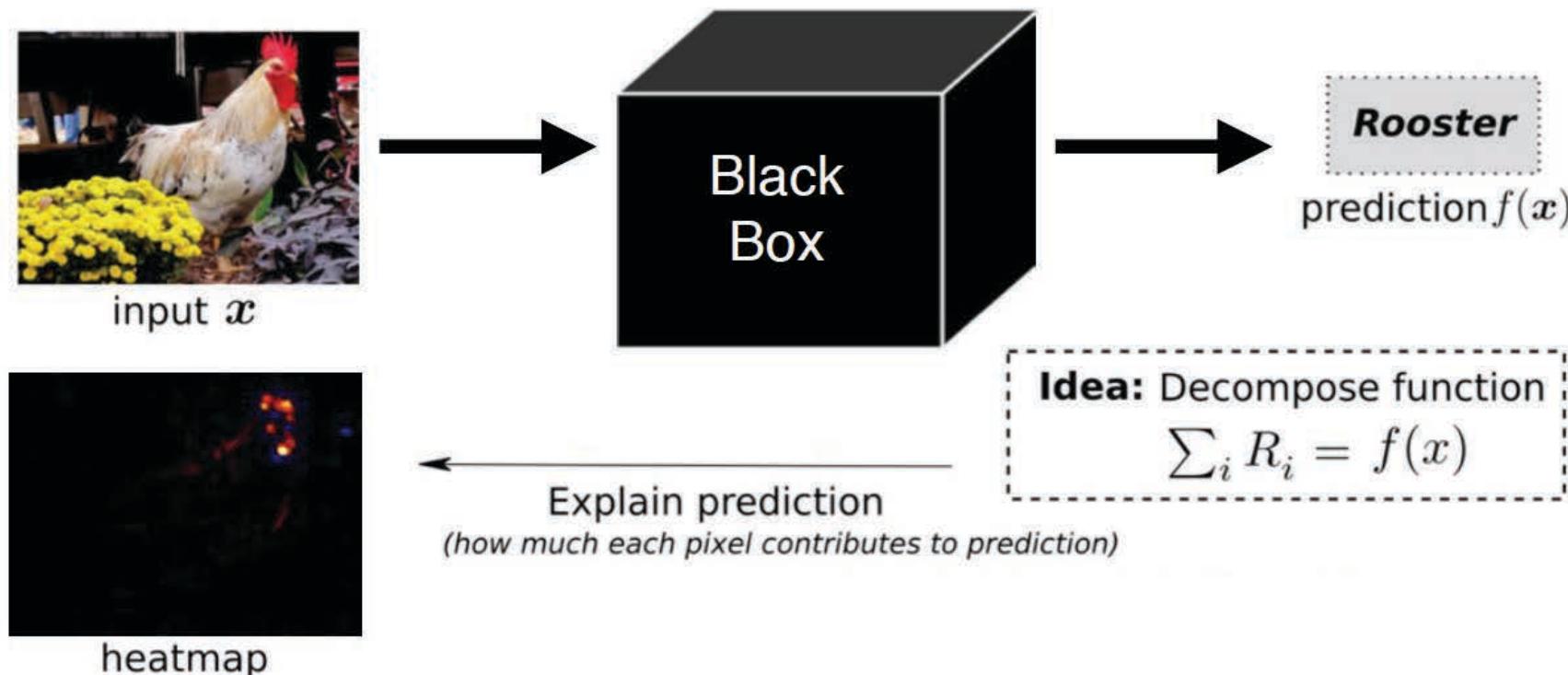


Source: Wojciech Samek

# Layer-wise Relevance Propagation (LRP) -

Bach et al., PLOS ONE, 2015

**Idea:** Decompose prediction function  $f(x)$  as a sum of layer-wise relevance values

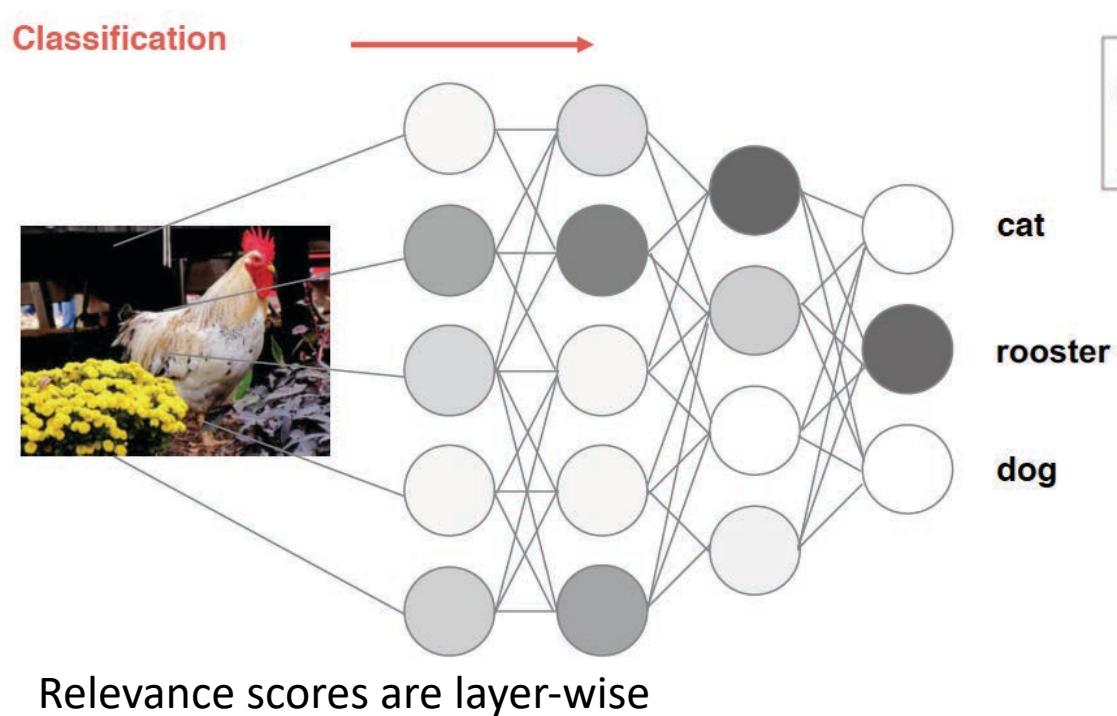


Source: Wojciech Samek

# Layer-wise Relevance Propagation (LRP) -

Bach et al., PLOS ONE, 2015

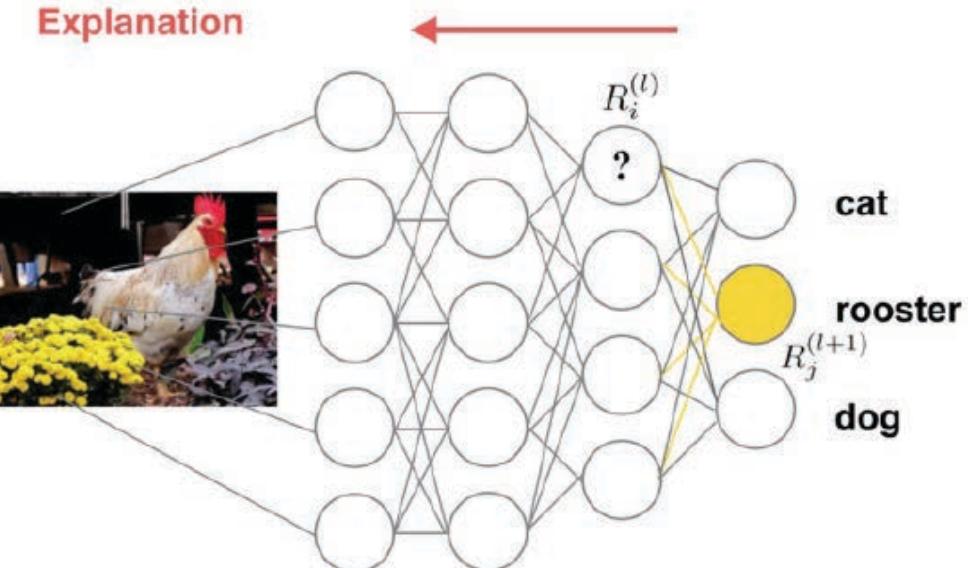
**Idea:** Decompose prediction function  $f(x)$  as a sum of layer-wise relevance values



$$f(x) = \dots = \sum_{d \in l+1} R_d^{(l+1)} = \sum_{d \in l} R_d^{(l)} = \dots = \sum_d R_d^{(1)}$$

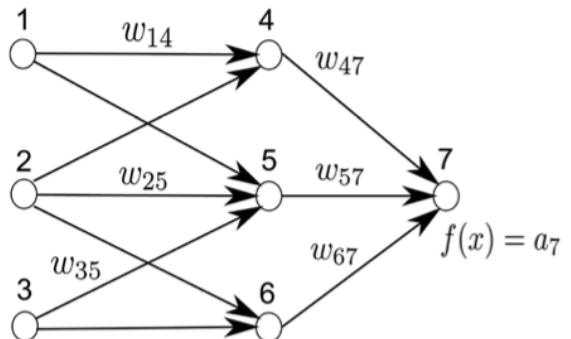
Initialization

$$R_j^{(l+1)} = f(x)$$

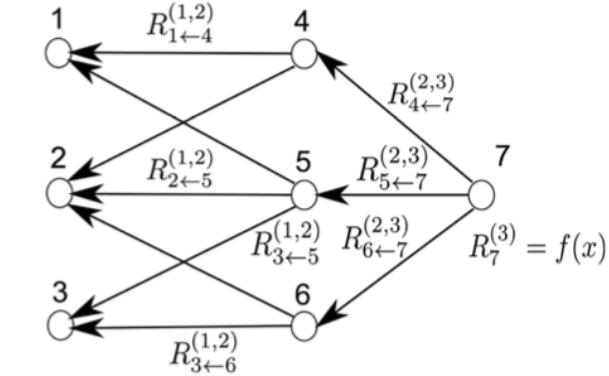


# Layer-wise Relevance Propagation (LRP) -

Bach et al., PLOS ONE, 2015



Testing



Relevance propagation

Conditions

$$R_7^{(3)} = R_{4 \leftarrow 7}^{(2,3)} + R_{5 \leftarrow 7}^{(2,3)} + R_{6 \leftarrow 7}^{(2,3)}$$

$$R_4^{(2)} = R_{1 \leftarrow 4}^{(1,2)} + R_{2 \leftarrow 4}^{(1,2)}$$

$$R_5^{(2)} = R_{1 \leftarrow 5}^{(1,2)} + R_{2 \leftarrow 5}^{(1,2)} + R_{3 \leftarrow 5}^{(1,2)}$$

$$R_6^{(2)} = R_{2 \leftarrow 6}^{(1,2)} + R_{3 \leftarrow 6}^{(1,2)}$$

As a function of activations “a” and neuron weights “w”. Example:

$$R_4^{(2)} = R_4^{(2)} \frac{a_1 w_{14}}{\sum_{i=1,2} a_i w_{i4}} + R_4^{(2)} \frac{a_2 w_{24}}{\sum_{i=1,2} a_i w_{i4}}$$

General formulation

$$R_{i \leftarrow k}^{(l,l+1)} = R_k^{(l+1)} \frac{a_i w_{ik}}{\sum_h a_h w_{hk}}$$

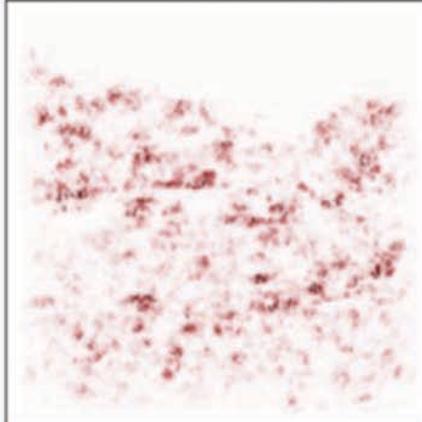
# Layer-wise Relevance Propagation (LRP) -

Bach et al., PLOS ONE, 2015

Image



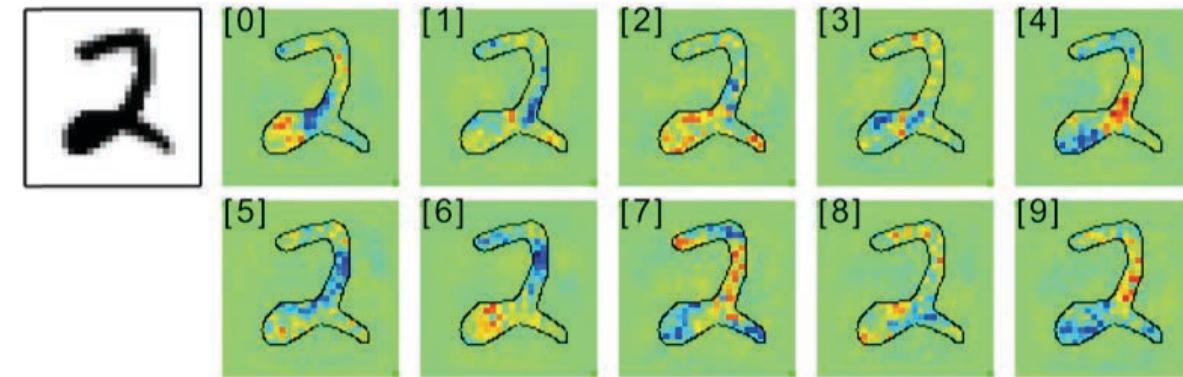
Sensitivity Analysis



LRP / Deep Taylor



Interpreting MNIST predictions

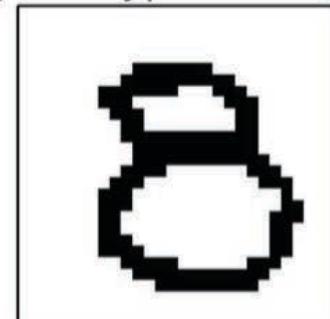


Explains what influences prediction "cars".

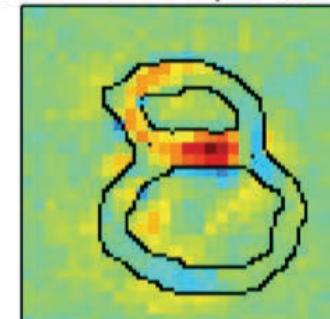
Explains prediction "cars" as is.

original image

$y=1.0$   $yp=23.93$  [8]

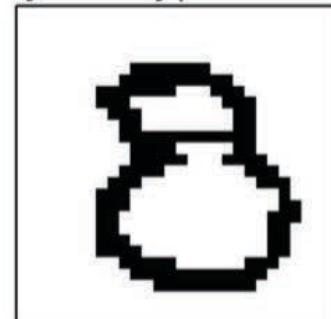


heatmap [8]



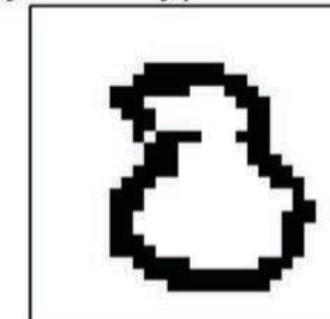
1% flipped

$y=1.0$   $yp=12.33$



2% flipped

$y=0.67$   $yp=8.36$  [0]



# Sanity Checks for Saliency Maps

Julius Adebayo\*, Justin Gilmer<sup>#</sup>, Michael Muelly<sup>#</sup>, Ian Goodfellow<sup>#</sup>, Moritz Hardt<sup>#†</sup>, Been Kim<sup>#</sup>

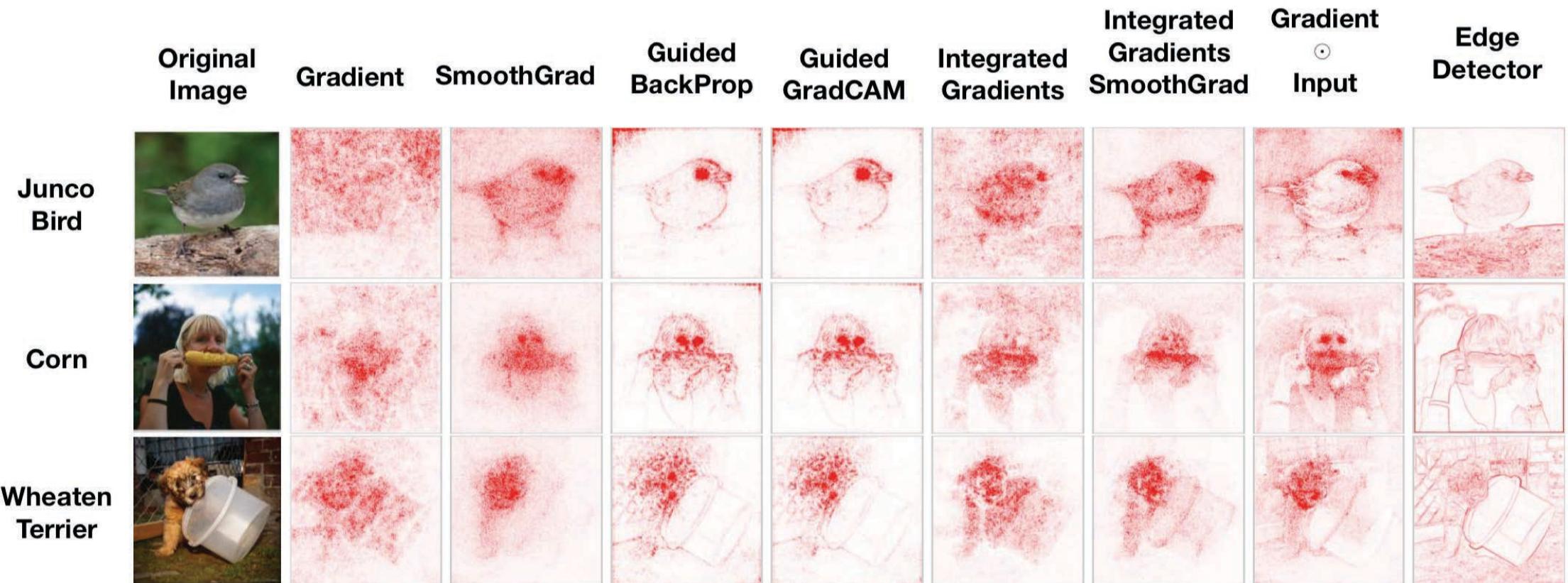
juliusad@mit.edu, {gilmer, muelly, goodfellow, mrtz, beenkim}@google.com

<sup>#</sup>Google Brain

<sup>†</sup>University of California Berkeley

**Motivation:** Objective Evaluation of Interpretability Methods

**Observation:** Some methods are independent of the model and data processing.



# Sanity Checks for Saliency Maps

Julius Adebayo\*, Justin Gilmer<sup>#</sup>, Michael Muelly<sup>#</sup>, Ian Goodfellow<sup>#</sup>, Moritz Hardt<sup>#†</sup>, Been Kim<sup>#</sup>

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<sup>#</sup>Google Brain

<sup>†</sup>University of California Berkeley

Observation: Some methods are independent of the model and data generating process

- The **model parameter randomization test**: perturbations to model parameters
- The **data randomization test** : perturbations to labels

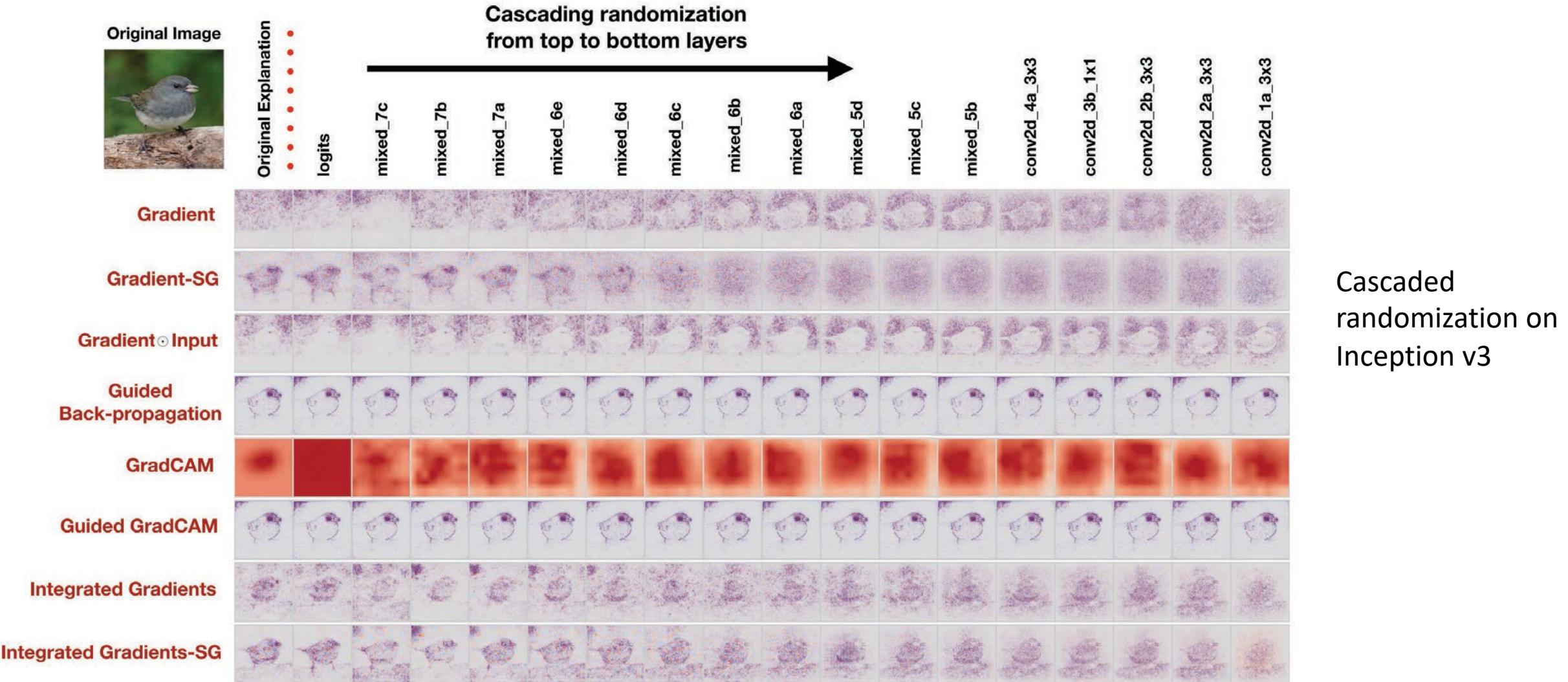
Other quantitative ways include:

- “Fragility”: find adversarial examples that most affect the saliency maps
- As surrogate for image classification, i.e. thresholded saliency maps used as localization ROI

Assessing similarity among maps

- Structural similarity maps – SSIM
- Spearman rank correlation
- Pearson correlation of the histogram of gradients (HOGs)

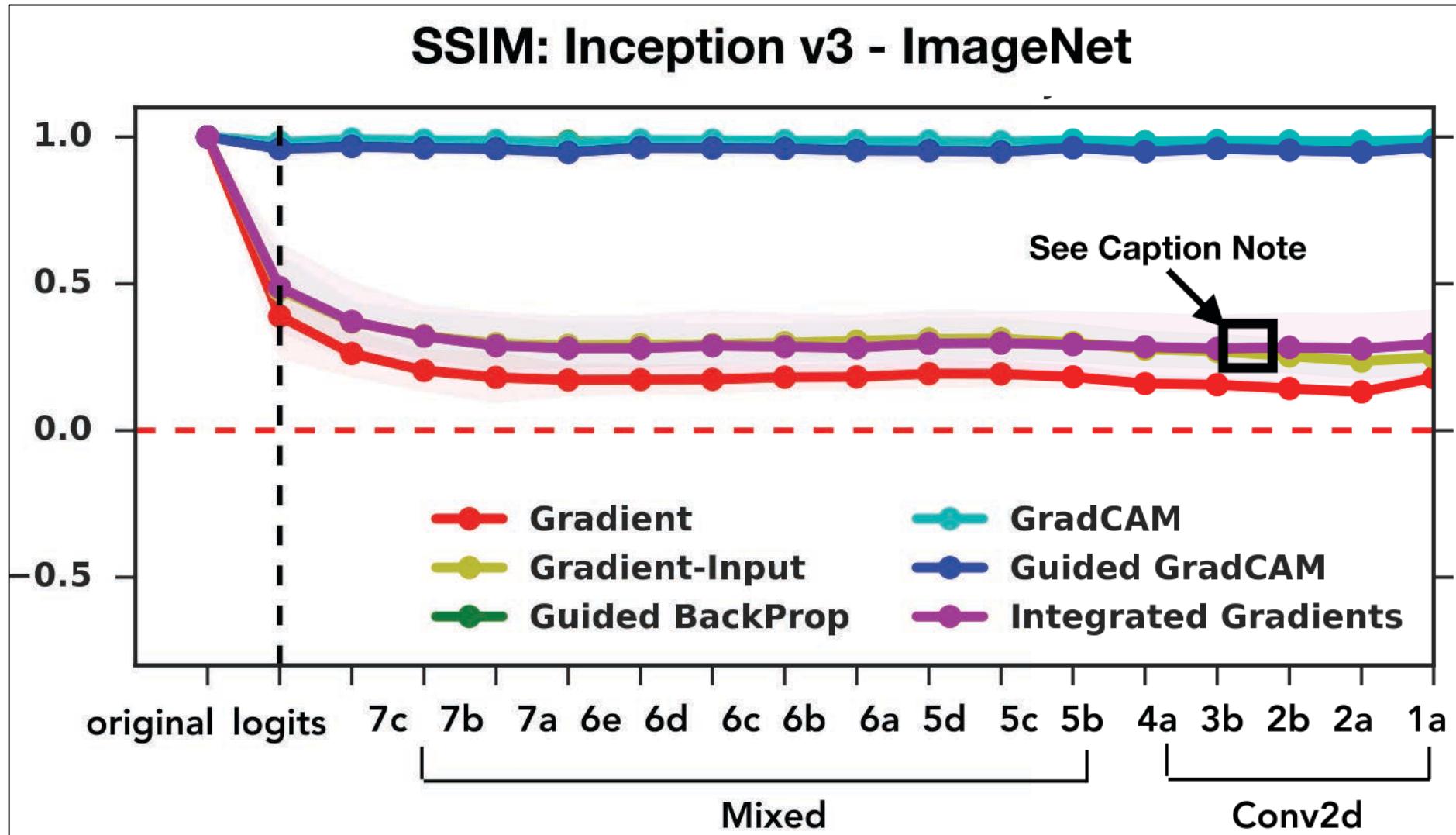
# Sanity Checks for Saliency Maps



Findings:

Gradients & GradCAM passed the sanity checks, while Guided BackProp & Guided GradCAM fail

# Sanity Checks for Saliency Maps

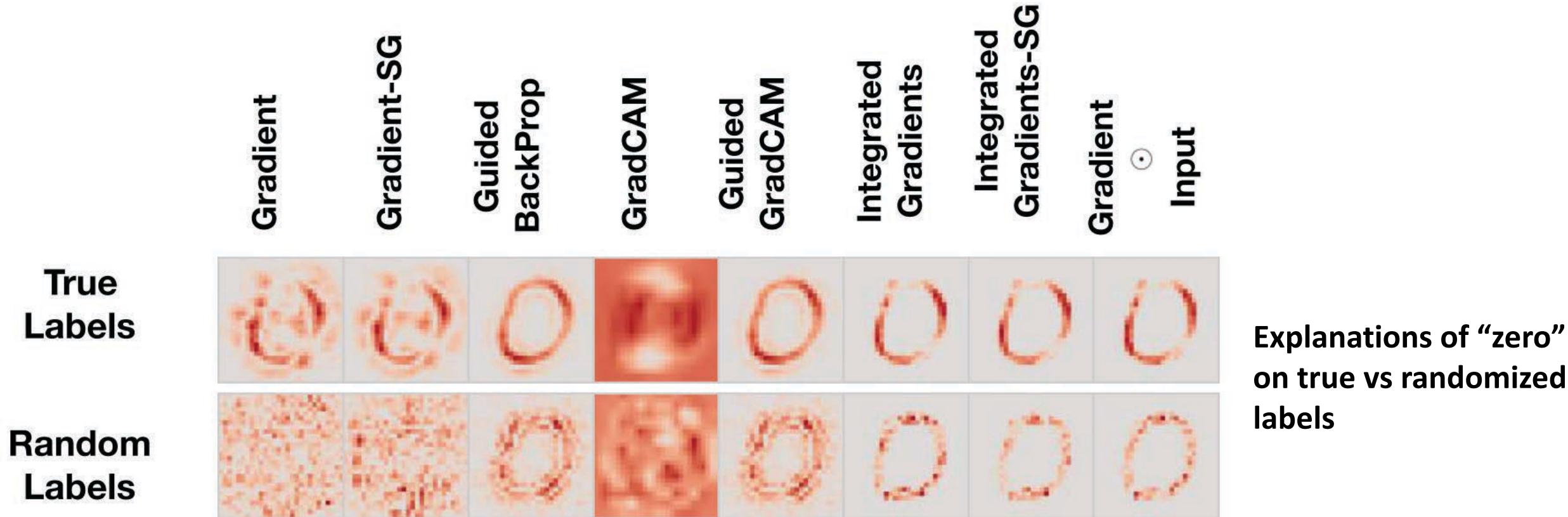


Cascaded  
randomization on  
Inception v3 –  
SSIM across layers

See Caption Note

# Sanity Checks for Saliency Maps

## Absolute-Value Visualization



Findings:

Gradients & GradCAM passed the sanity checks, while Guided BackProp & Guided GradCAM fail

# Sanity Checks for Saliency Maps

Julius Adebayo\*, Justin Gilmer<sup>#</sup>, Michael Muelly<sup>#</sup>, Ian Goodfellow<sup>#</sup>, Moritz Hardt<sup>#†</sup>, Been Kim<sup>#</sup>

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<sup>#</sup>Google Brain

<sup>†</sup>University of California Berkeley

Other findings/confirmation from previous works:

- LRP and DeepLIFT are equivalent to (input \* gradient) for ReLU network w/o positive biases.
- Explanations of methods of the type “input \* gradient” are heavily based on input structure → edge detector effect
- Explanations that do not depend on model parameters or training data might still depend on the model architecture, and thus provide some useful information about the prior incorporated in the model architecture.

See more benchmarking here:

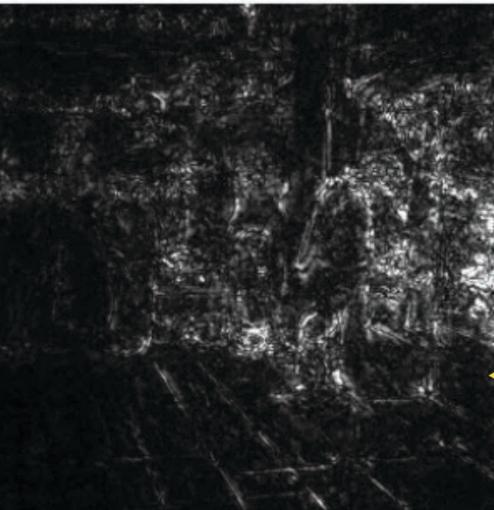
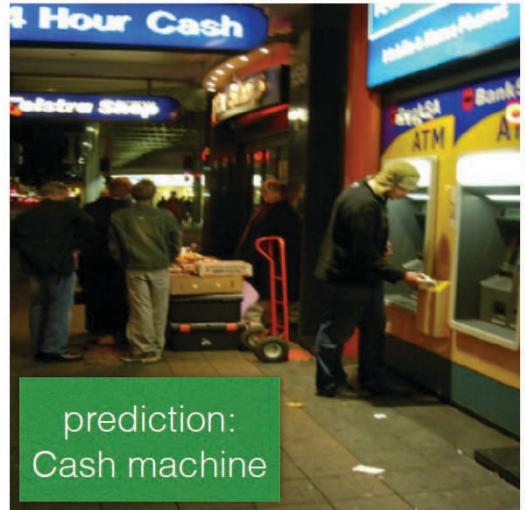
- DeepLIFT often approximates Integrated gradients (IG)
- DeepLIFT != IG and fail to produce meaningful results when applied to RNNs with multiplicative interactions (e.g. LSTM)

Published as a conference paper at ICLR 2018					
Method	Attribution $R_i^c(x)$				
	ReLU	Tanh	Sigmoid	Softplus	
TOWARDS GRADIENT FOR DEEP	$x_i \cdot \frac{\partial S_c(x)}{\partial x_i}$				
Marco Ancona Department of Co ETH Zurich, Swit marco.ancona@inf.	$(x_i - \bar{x}_i) \cdot \int_{\alpha=0}^1 \frac{\partial S_c(\tilde{x})}{\partial (\tilde{x}_i)} \Big _{\tilde{x}=\bar{x}+\alpha(x-\bar{x})} d\alpha$				
<u>ε-LRP</u>	$x_i \cdot \frac{\partial^g S_c(x)}{\partial x_i}, \quad g = \frac{f(z)}{z}$				
DeepLIFT	$(x_i - \bar{x}_i) \cdot \frac{\partial^g S_c(x)}{\partial x_i}, \quad g = \frac{f(z) - f(\bar{z})}{z - \bar{z}}$				
Occlusion-1	$S_c(x) - S_c(x_{[x_i=0]})$				

# Wrap-up saliency methods

- Many approaches have been proposed!
- Visual evaluation alone can be misleading
- Recent findings on deficiencies and similarities of gradient-based approaches
- (Recall) all these methods require access to the model architecture
- Assessment of methods is an active field of research
- Seemingly lack of integration of expert-knowledge (e.g. more methodological way of defining “reference” points for interpretability)

# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017



Were there more pixels on the cash machine than on the person?

Did the 'human' concept matter?  
Did the 'glasses' or 'paper' matter?

Which concept mattered more?

Is this true for all other cash machine predictions?

Wouldn't it be great if we can **quantitatively** measure how important any of these **user-chosen concepts** are?

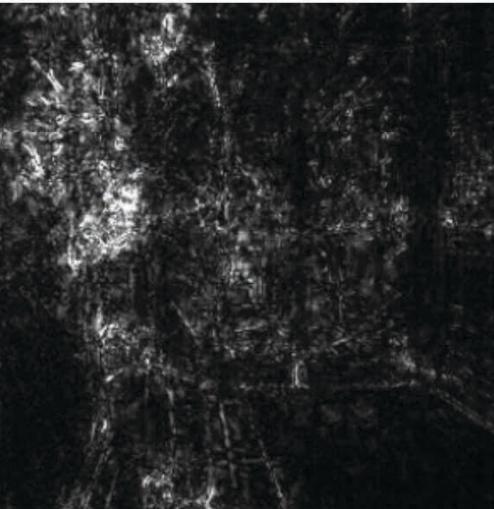
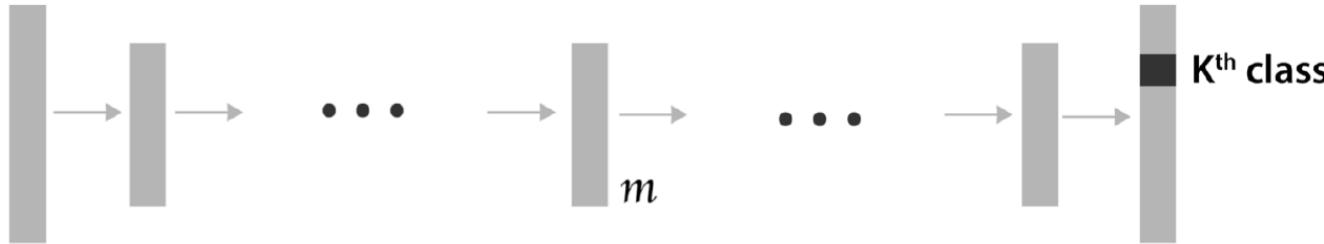


Image source: Kim Been

## Testing with Concept Activation Vectors – TCAV – Kim et al. 2017



**Quantitative** explanation: how much a concept (e.g., gender, race) was important for a prediction in a trained model.

...even if the concept was not part of the training.

# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017

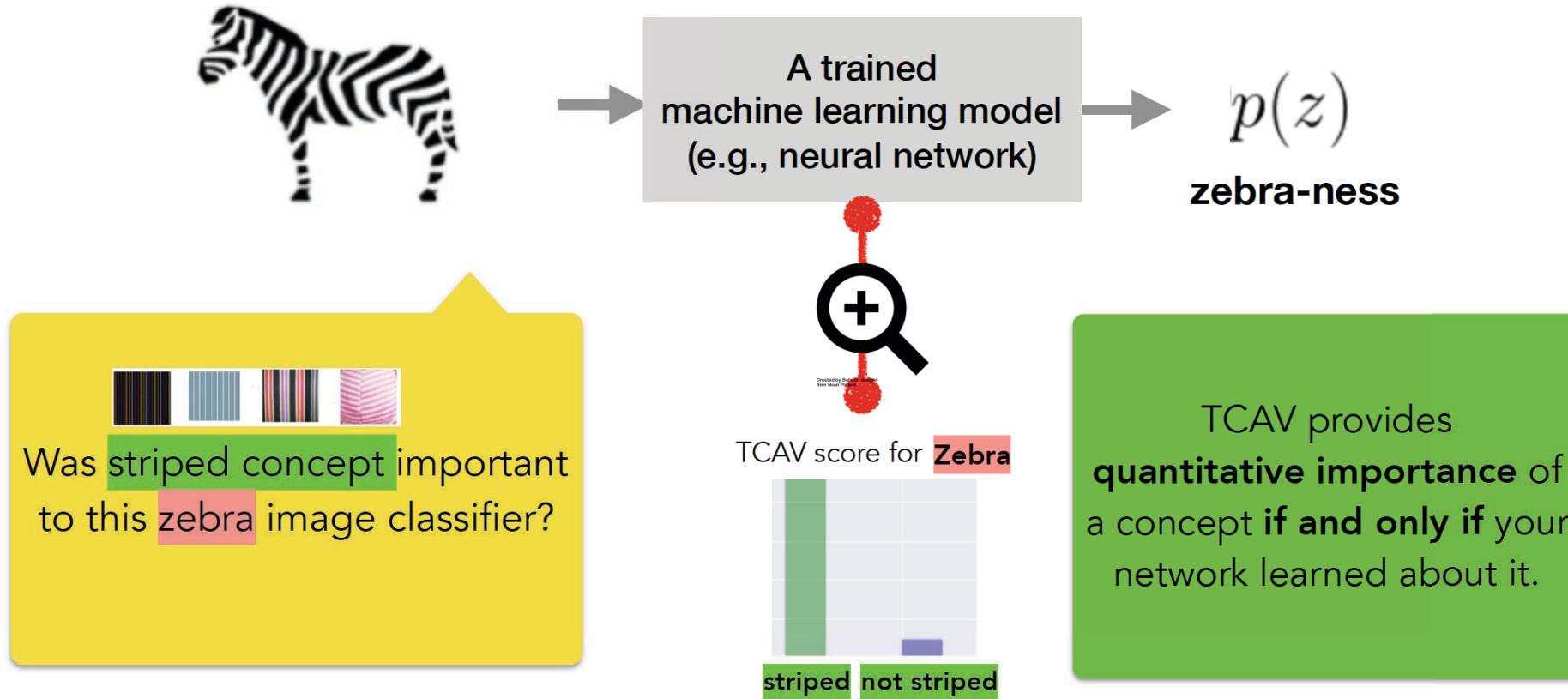


Image source: Kim Been

# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017

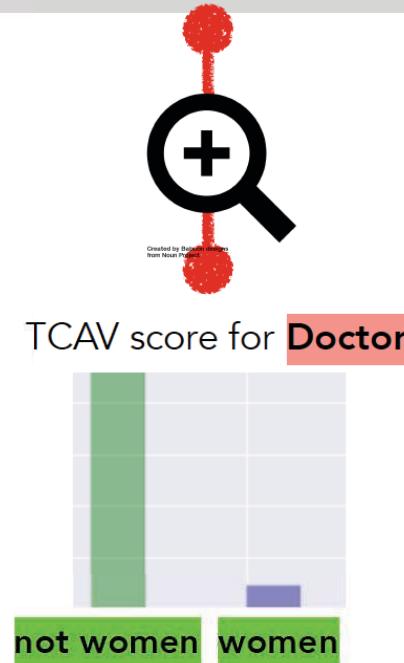


A trained  
machine learning model  
(e.g., neural network)

$$p(z)$$

**Doctor-ness**

Was gender concept important  
to this doctor image classifier?



TCAV provides  
**quantitative importance** of  
a concept **if and only if** your  
network learned about it.

# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017

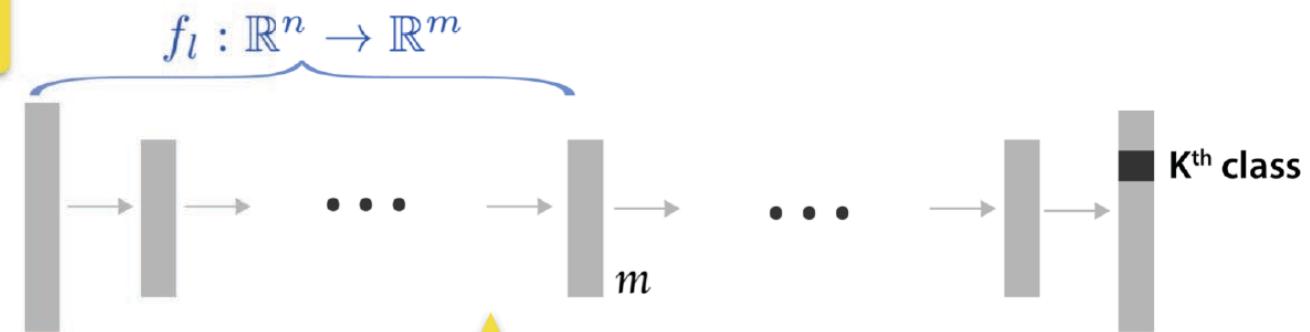
## Inputs:

a



Examples of  
concepts

Random  
images



A trained network under investigation  
and  
Internal tensors

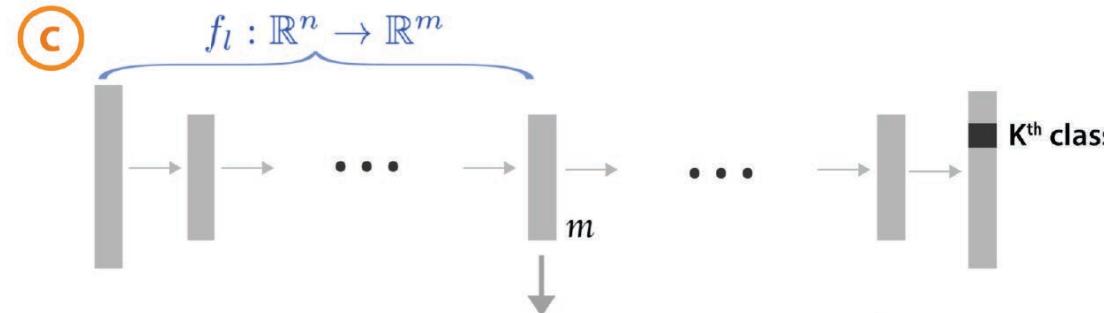
# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017

## Inputs:

a



c

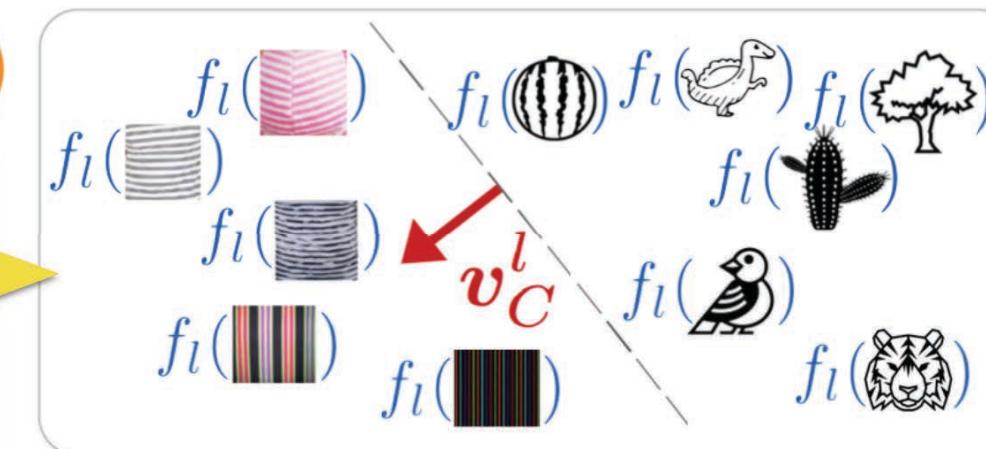


d

Train a linear classifier to separate activations.

CAV ( $v_C^l$ ) is the vector **orthogonal** to the decision boundary.

[Smilkov '17, Bolukbasi '16, Schmidt '15]

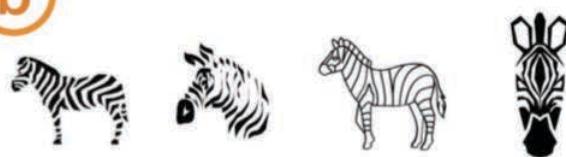


# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017

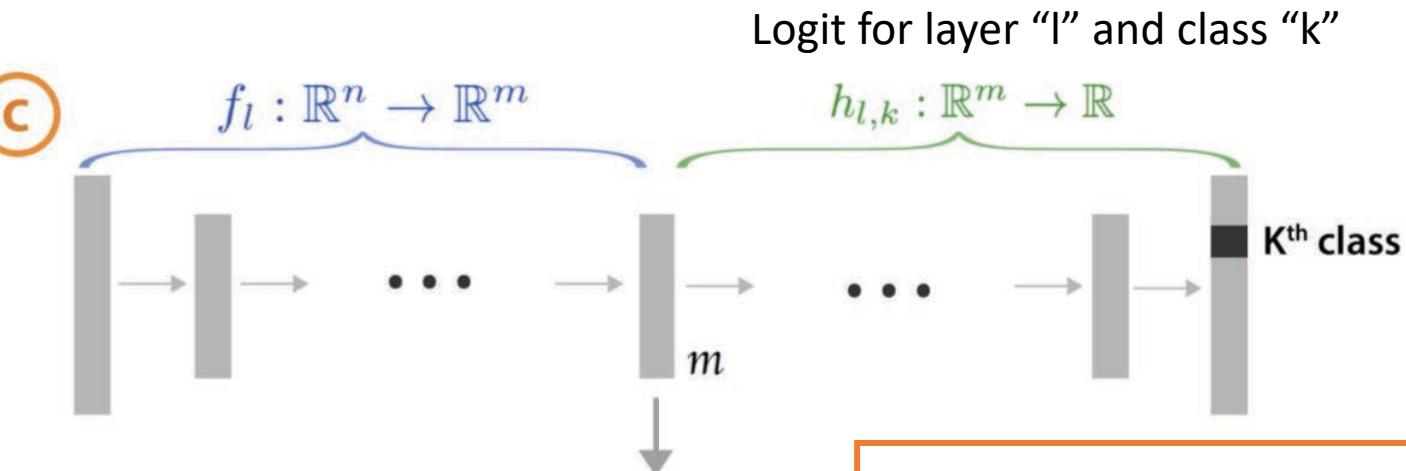
a



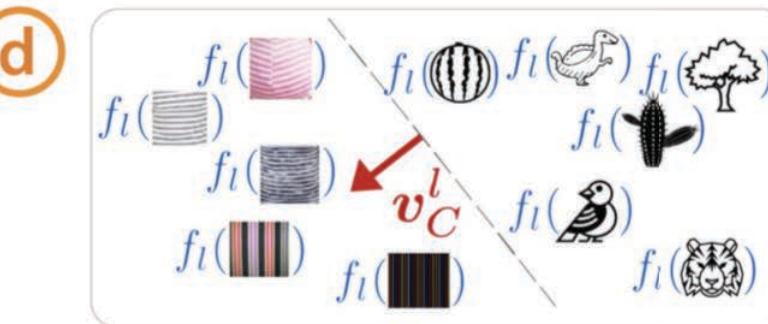
b



c



d



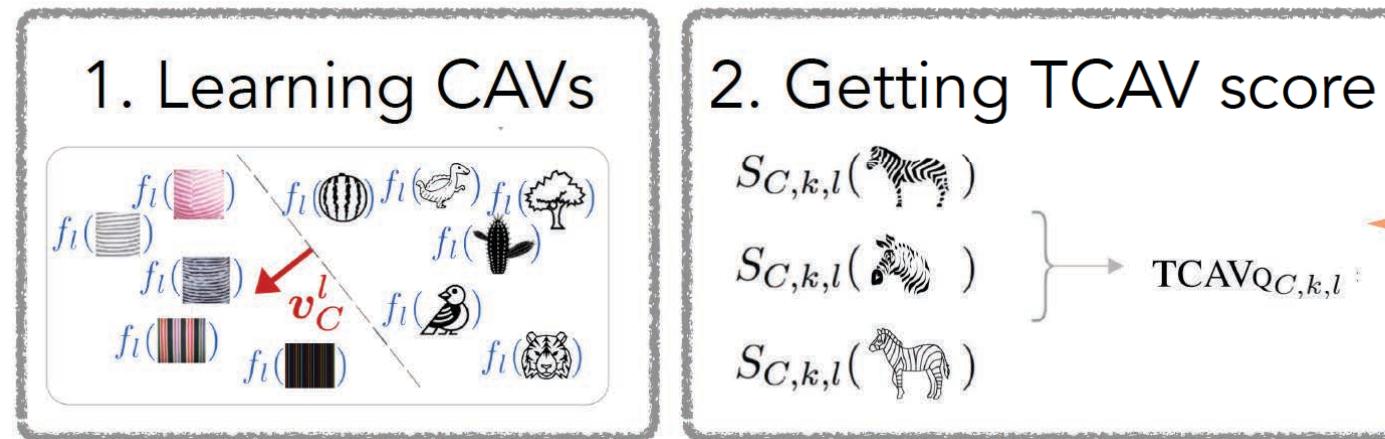
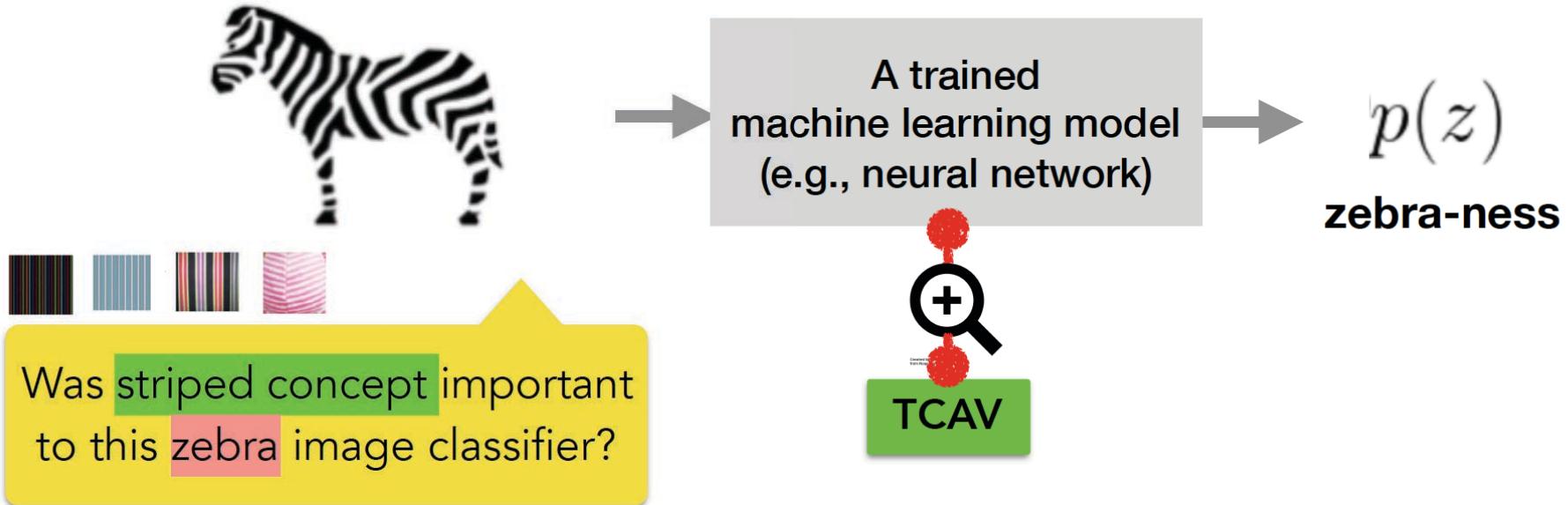
e

Conceptual sensitivity of class "k" to concept "C"

$$S_{C,k,l}( \text{zebra} )$$

$$= \nabla h_{l,k}(f_l(\text{zebra})) \cdot v_C^l$$

# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017

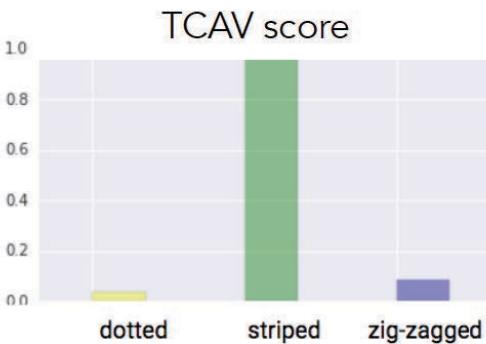
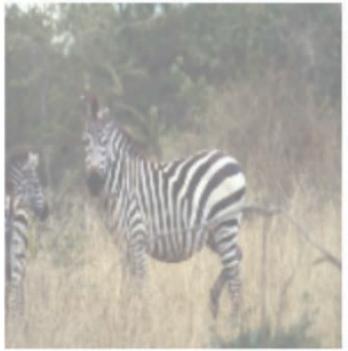


2. How are the CAVs useful to get explanations?

Image source: Kim Been

# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017

## TCAV



$$\begin{aligned} \text{zebra-ness} &\rightarrow \frac{\partial p(z)}{\partial \mathbf{v}_C^l} = S_{C,k,l}(x) \\ \text{striped CAV} &\rightarrow \frac{\partial \mathbf{v}_C^l}{\partial \mathbf{v}_C^l} = S_{C,k,l}(x) \end{aligned}$$

### Directional derivative with CAV

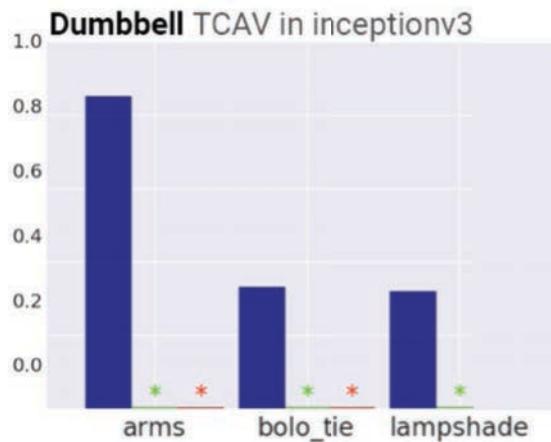
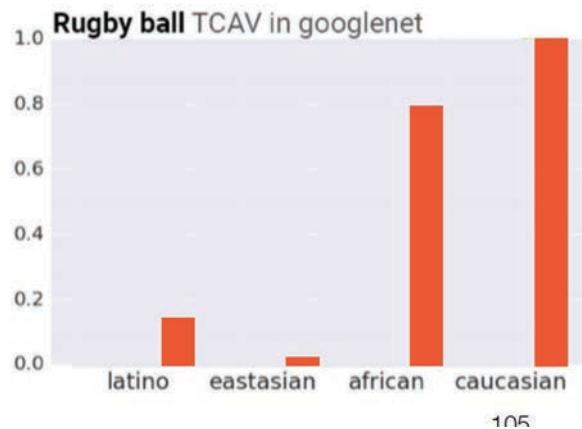
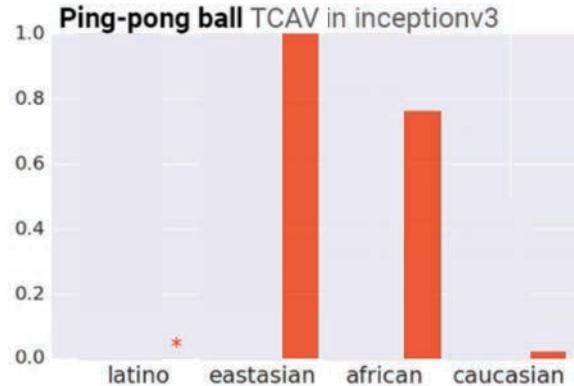
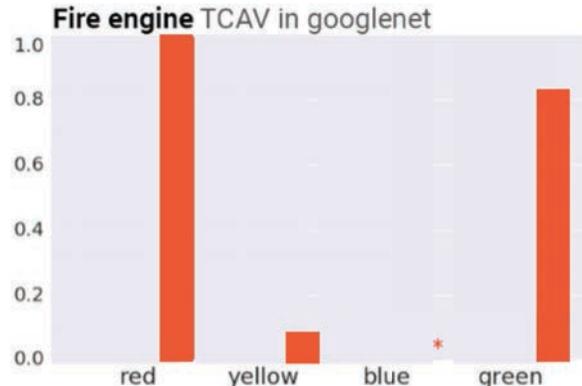
$$\left. \begin{array}{l} S_{C,k,l}(\text{zebra}) \\ S_{C,k,l}(\text{striped}) \\ S_{C,k,l}(\text{zig-zagged}) \\ S_{C,k,l}(\text{solid}) \end{array} \right\}$$

$$\text{TCAV}_{Q_{C,k,l}} = \frac{|\{x \in X_k : S_{C,k,l}(x) > 0\}|}{|X_k|}$$

fraction of  $k$ -class inputs whose  $l$ -layer activation vector was positively influenced by concept  $C$

# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017

## TCAV in Two widely used image prediction models



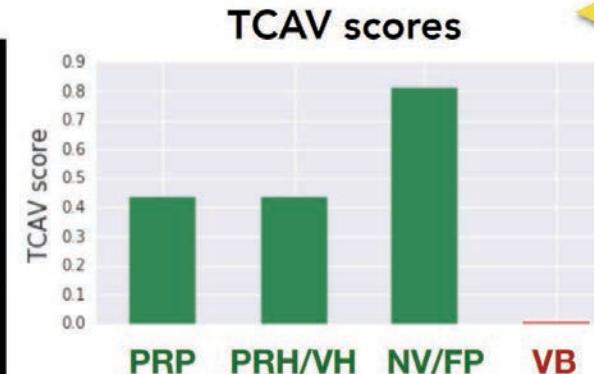
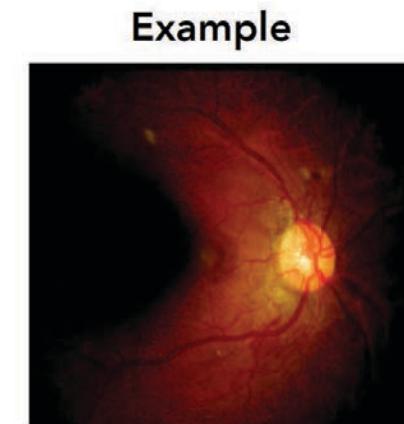
TCAV facilitates spotting of biases in the datasets

# Testing with Concept Activation Vectors – TCAV – Kim et al. 2017

## Example application to Diabetic Retinopathy (DR)

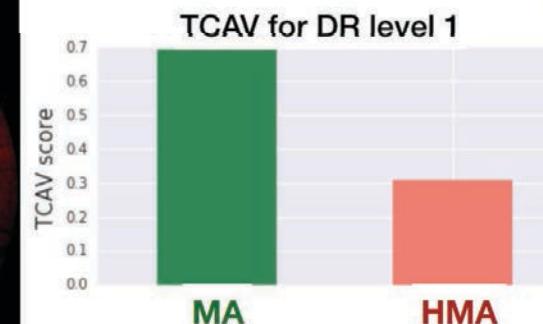
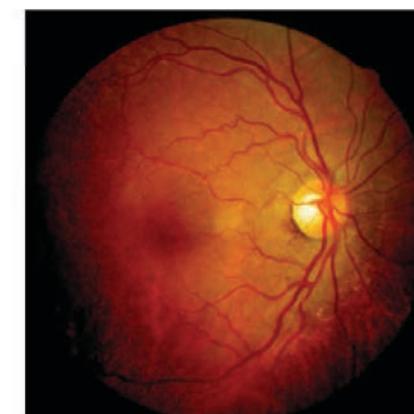
Prediction class      Prediction accuracy

DR level 4      High



TCAV shows the model is **consistent** with doctor's knowledge when model is **accurate**

DR level 1      Med



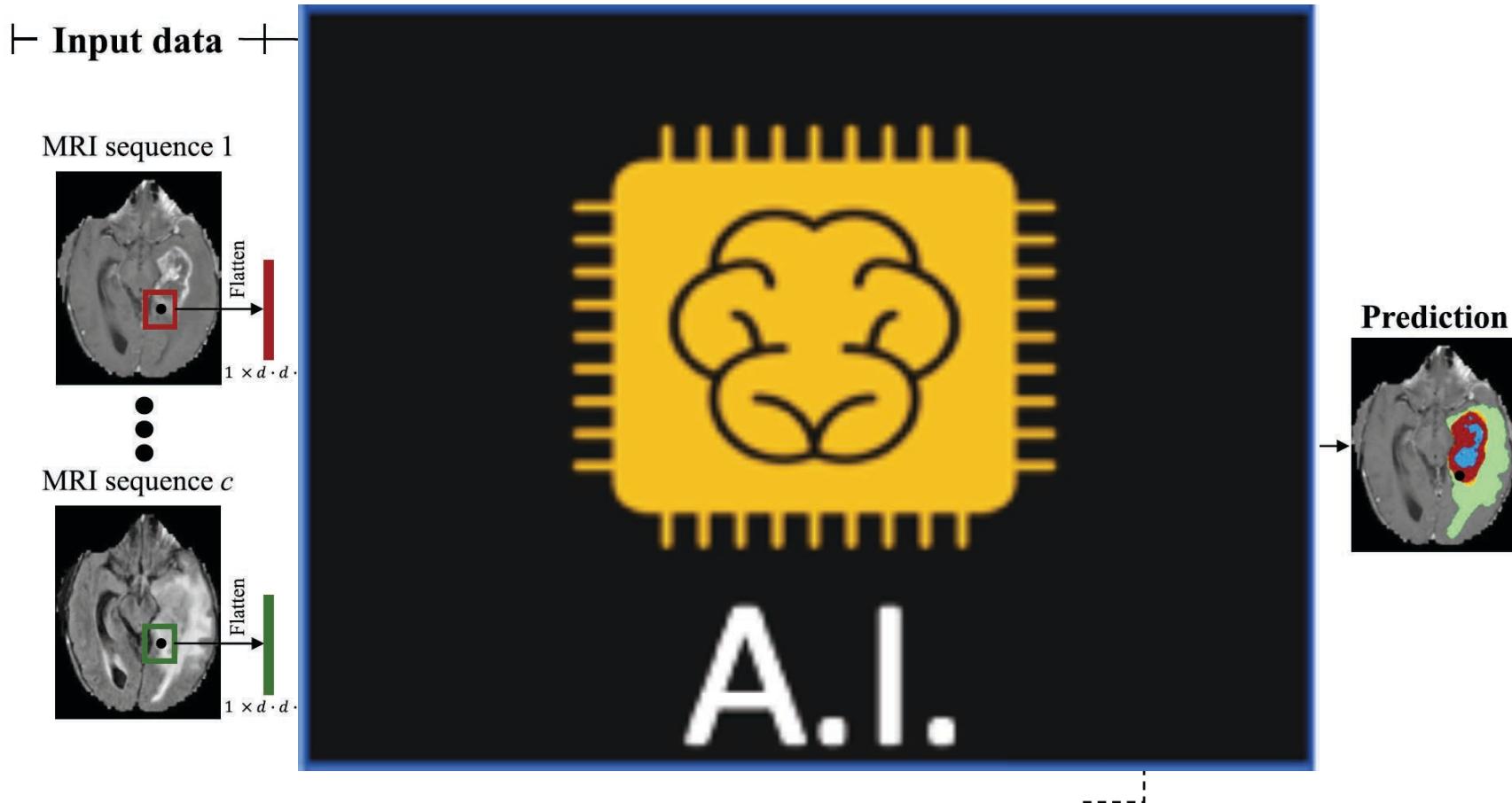
TCAV shows the model is **inconsistent** with doctor's knowledge for classes when model is less accurate

Green: domain expert's label on concepts belong to the level  
Red: domain expert's label on concepts does not belong to the level

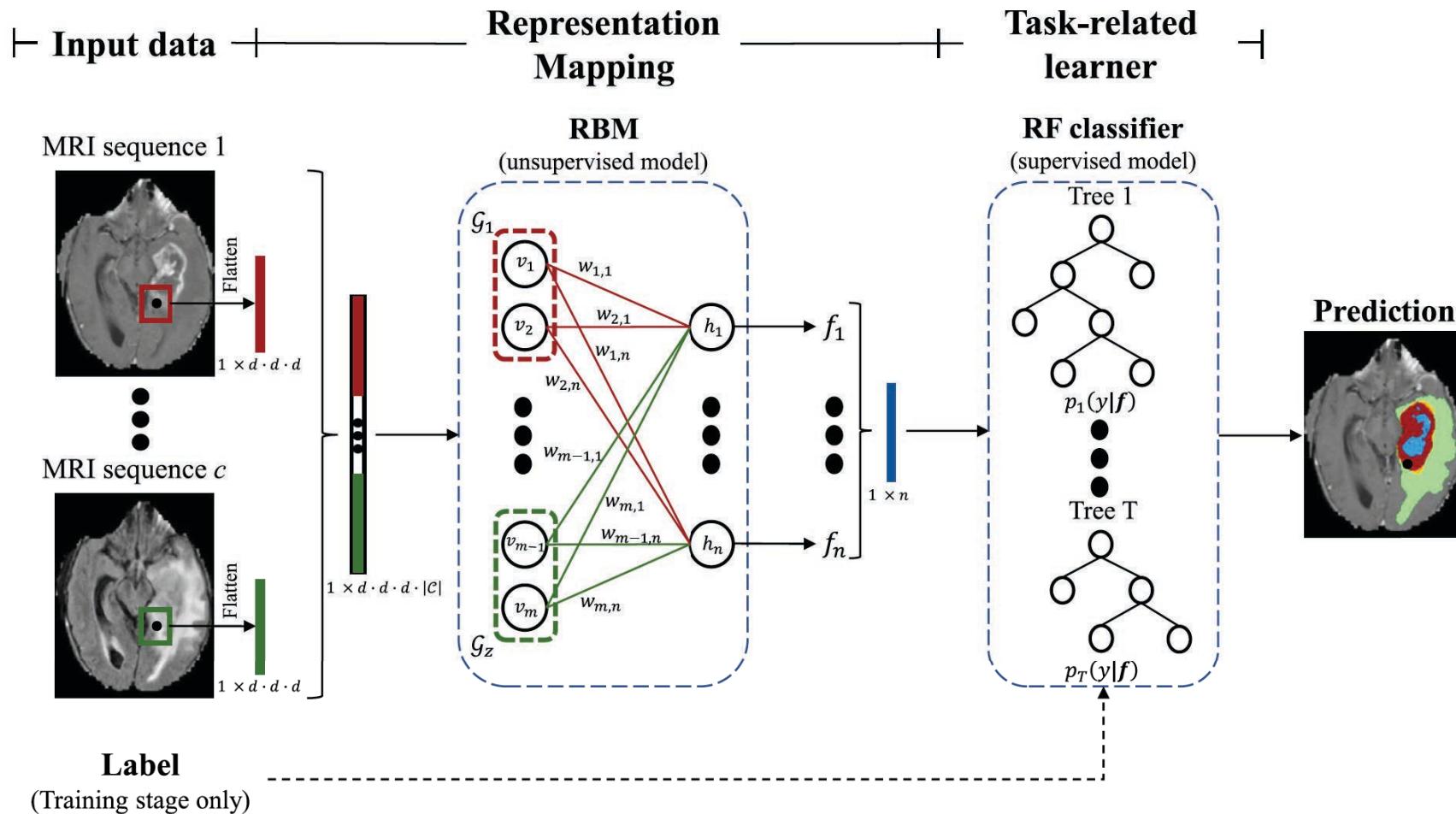
Image source: Kim Been

# Enhancing Interpretability of Learned Features in Multisequence-MRI

Example task:  
Automated brain tumor  
segmentation from  
multisequence MRI



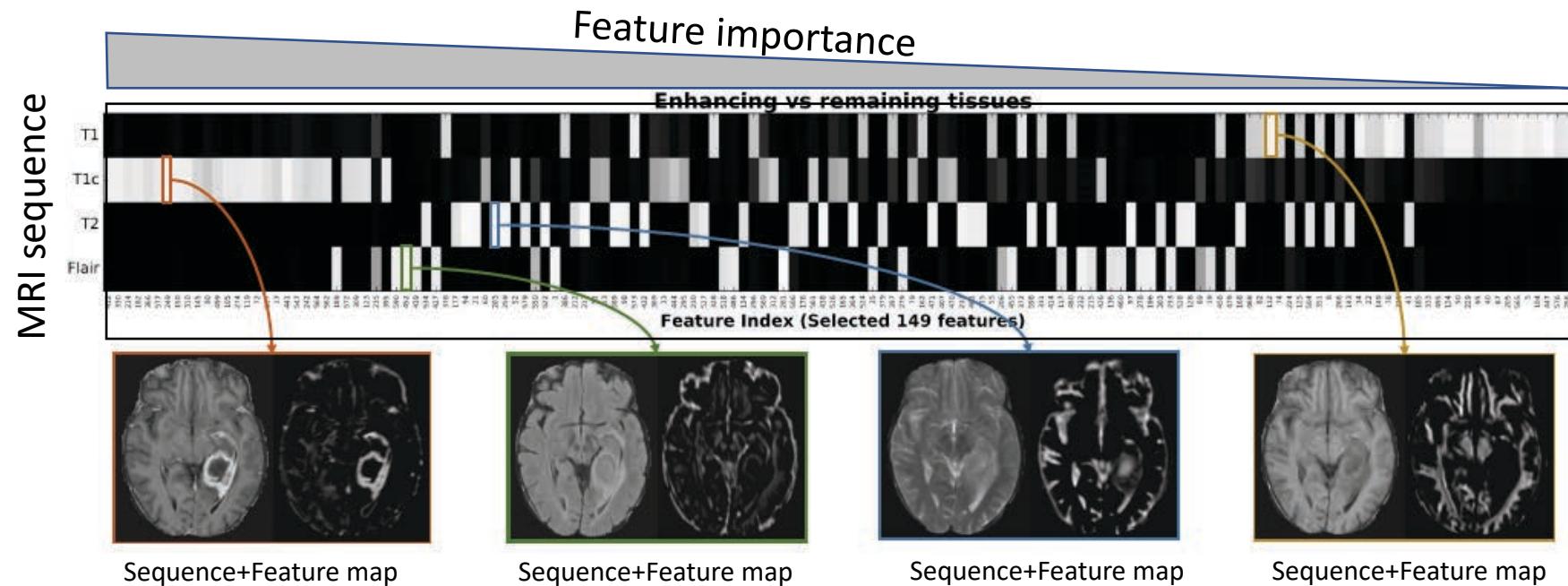
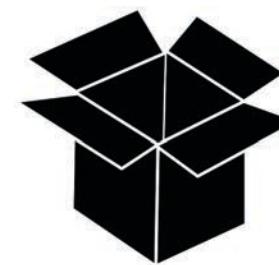
# Enhancing Interpretability of Learned Features in Multisequence-MRI



Pereira et al. 2018

# Enhancing interpretability of machine learning algorithms

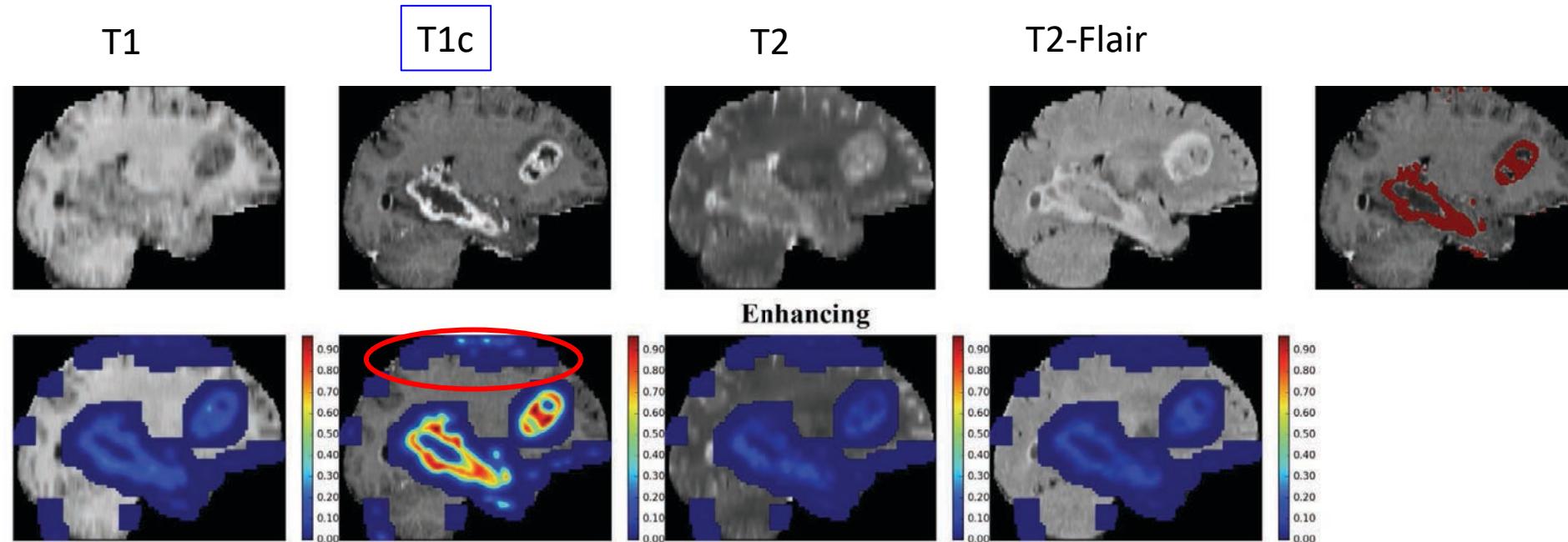
- *How is the machine using the information?*
- *Which sequence is more important?*
- *If it fails, why does it fail?*
- *Quality Certification*



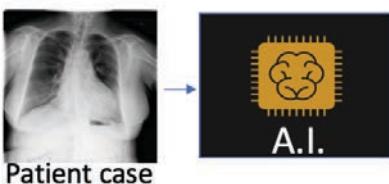
# Enhancing interpretability of machine learning algorithms

*Which Sequence is used most for the task of tumor-enhancing segmentation?*

- *T1c (agrees with clinical practice)*
- *Method also detects bias from pre-processing*

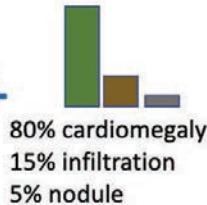


# Combining interpretability approaches



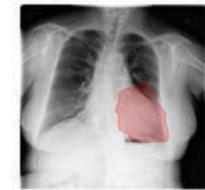
+ output probabilities

1 "cardiomegaly"



+ output probabilities  
+ visual saliency

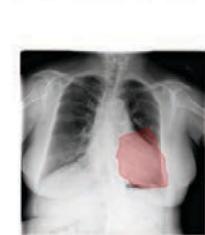
2 "cardiomegaly" +



Areas of attention

+ output probabilities  
+ visual saliency  
+ explain by example

3 "cardiomegaly" + +



Areas of attention

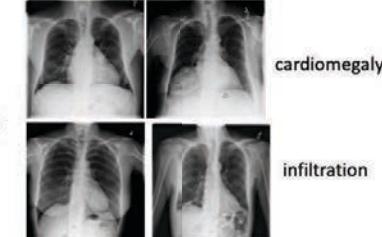
+ output probabilities  
+ visual saliency  
+ explain by example  
+ semantic explanation

4 "cardiomegaly" + +



Areas of attention

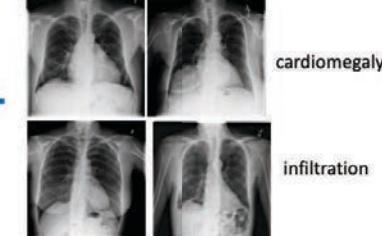
Matched real cases



cardiomegaly

infiltration

Matched real cases



cardiomegaly

infiltration

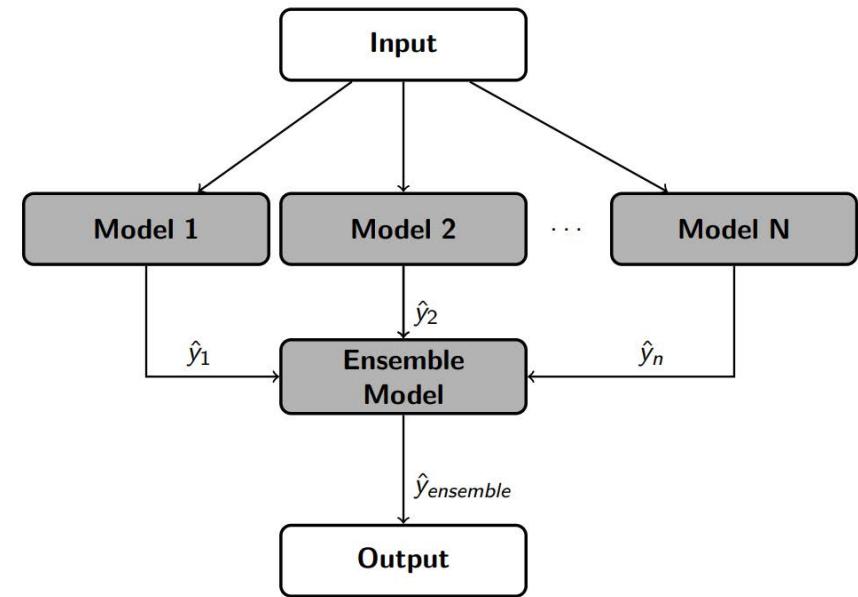
+ "Enlargement  
heart region"

# How to produce complementary explanations using an Ensemble Model – Silva et al. 2019 (IJCNN)

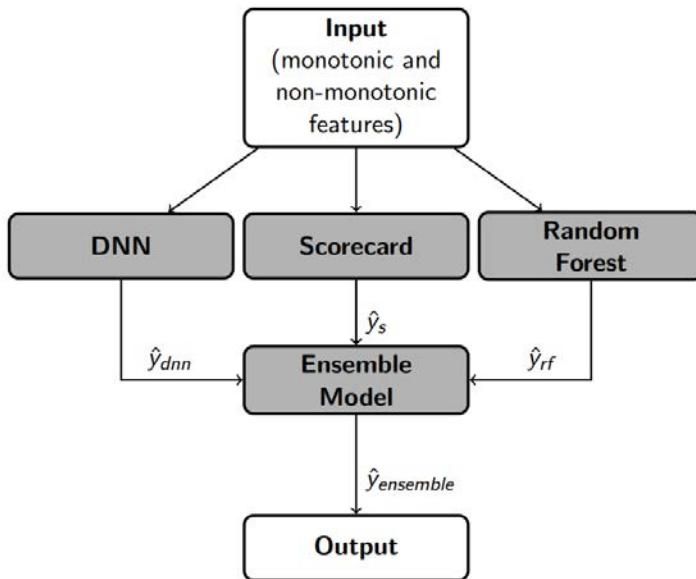
- Motivation – Generating explanations is not easy: model complexity + variability in application domains and target users. Most adequate type of explanation may vary with the example under evaluation.

- Ensemble Model:
  - Different models inside a global one
  - Improvement in quality + diversity of explanations

$$E_{global}(x) = \operatorname{argmax}_{E_n(x)} \operatorname{corr}(E_n(x))$$



# How to produce complementary explanations using an Ensemble Model – Silva et al. 2019 (IJCNN)



**Input image**  
**(Prediction: {Common, Atypical})**



Similar case

Why?: Both images have light and dark brown color and atypical presence of dots/globules.



Opponent case

Why?: It doesn't have light brown color or atypical dots/globules. It has blue whitish veil and pigmented network.

**Random Forest:** Lack of regression, presence brown color and lack of white color.

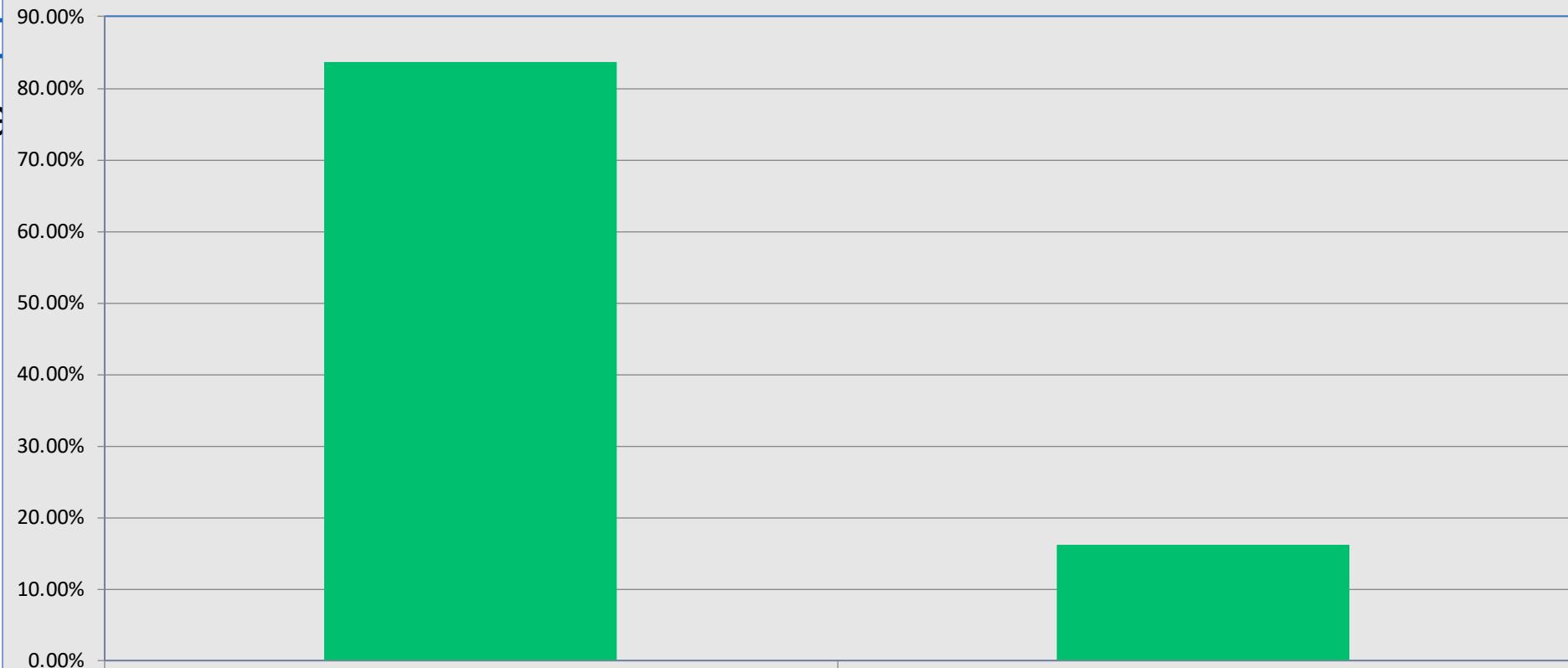
**Scorecard:** Presence of brown color, lack of atypical dots and asymmetry.

# How do experts perceive interpretable A.I. new

Do you think interpretability/explainability methods  
for A.I. systems are a must for the future of radiology  
and A.I.?

- [ht](#)

Please

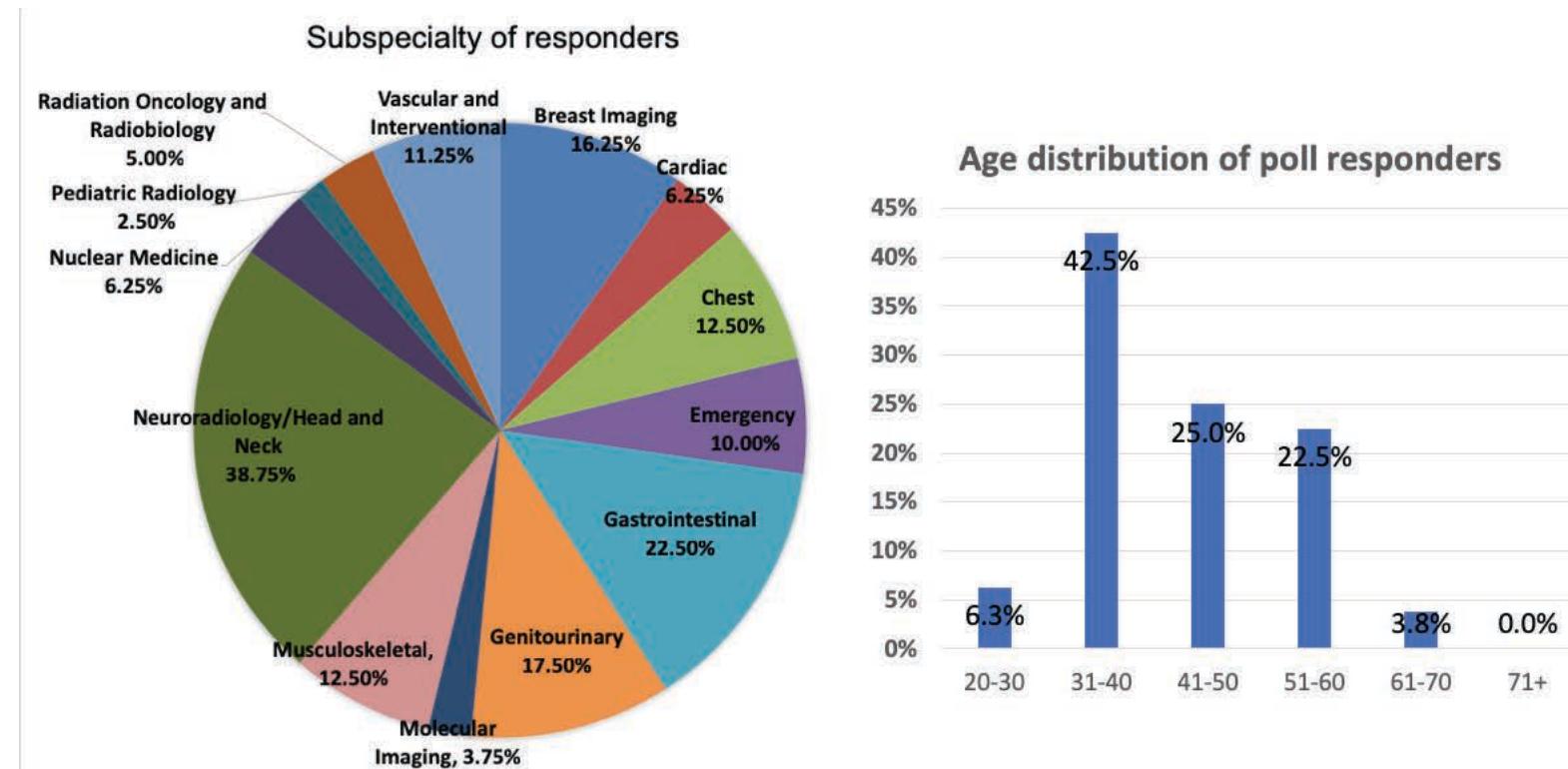


Yes, absolutely, I want to have security about  
their answers

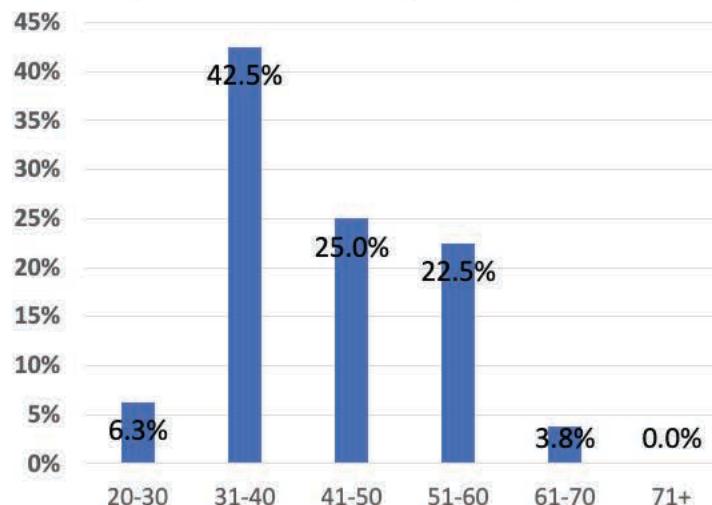
No, as long as they do their job I'm O.K without  
having means to interpret/explain A.I. results

# How do experts perceive interpretable A.I. – needed?

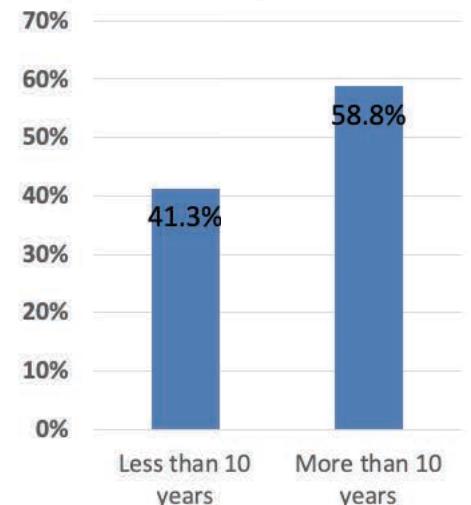
80 responders  
Online survey



**Age distribution of poll responders**

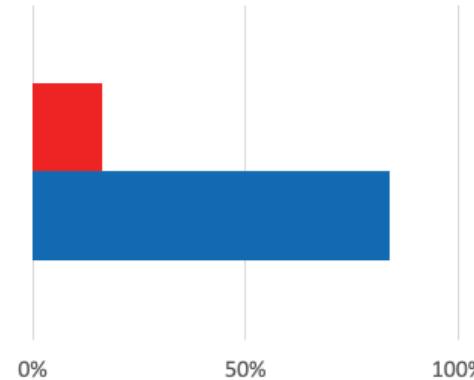


**Years of experience**



# How do experts perceive interpretable A.I. – needed?

■ No, as long as they do their job I'm O.K without having means to interpret/explain A.I. results



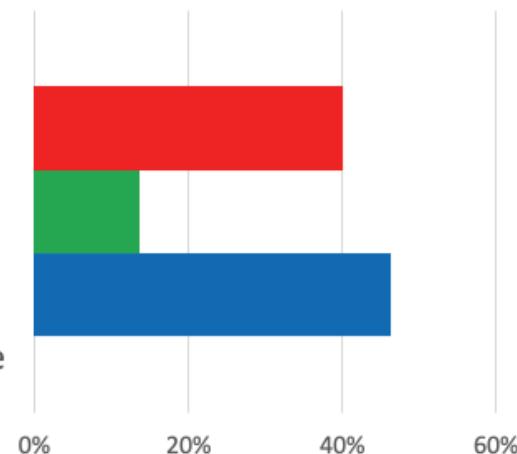
■ Yes, absolutely, I want to have security about their answers

**Do you think interpretability/explainability methods for A.I. systems are a must for the future of radiology and A.I.?**

■ It does not matter as long as it is understandable and not time consuming

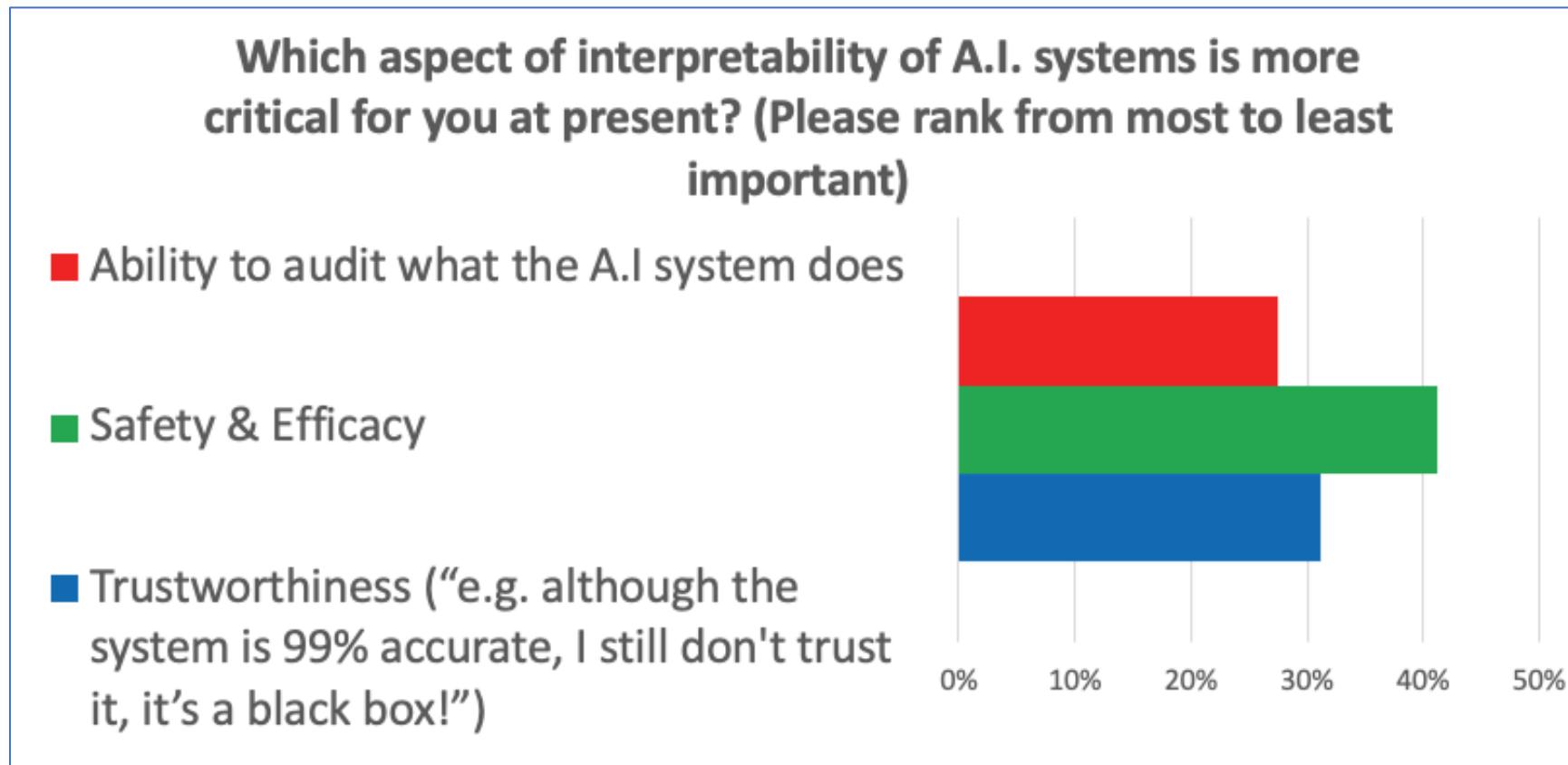
■ Statement (e.g. “lesion detected due to hyper-intensity, increased contrast levels, volume and shape irregularity”)

■ Visual cues, such as highlighted areas on an image that the A.I. system uses for decision-making



**What kind of information would you prefer from interpretability methods? (Please rank from most to least important)**

# How do experts perceive interpretable A.I. – needed?



*"Primum non nocere – First, to do no harm"*

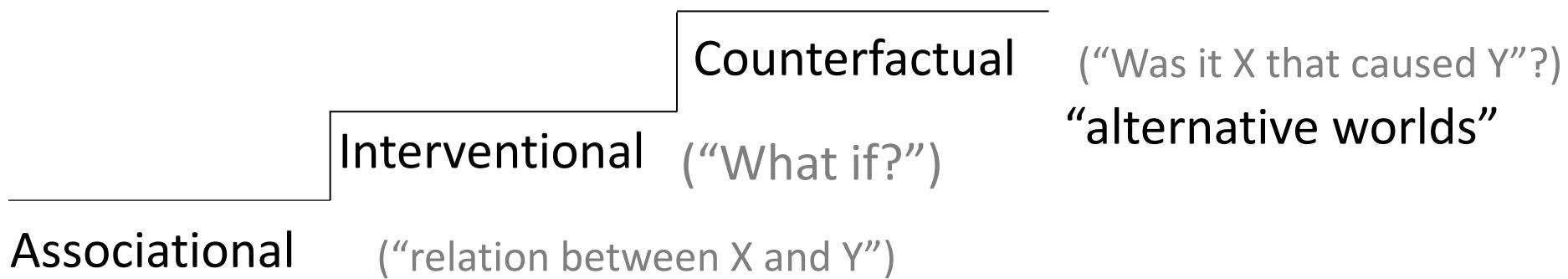
# Improved Interpretability: Deep Learning meets Causal Inference

## CONTRIBUTED ARTICLES

### The Seven Tools of Causal Inference, with Reflections on Machine Learning

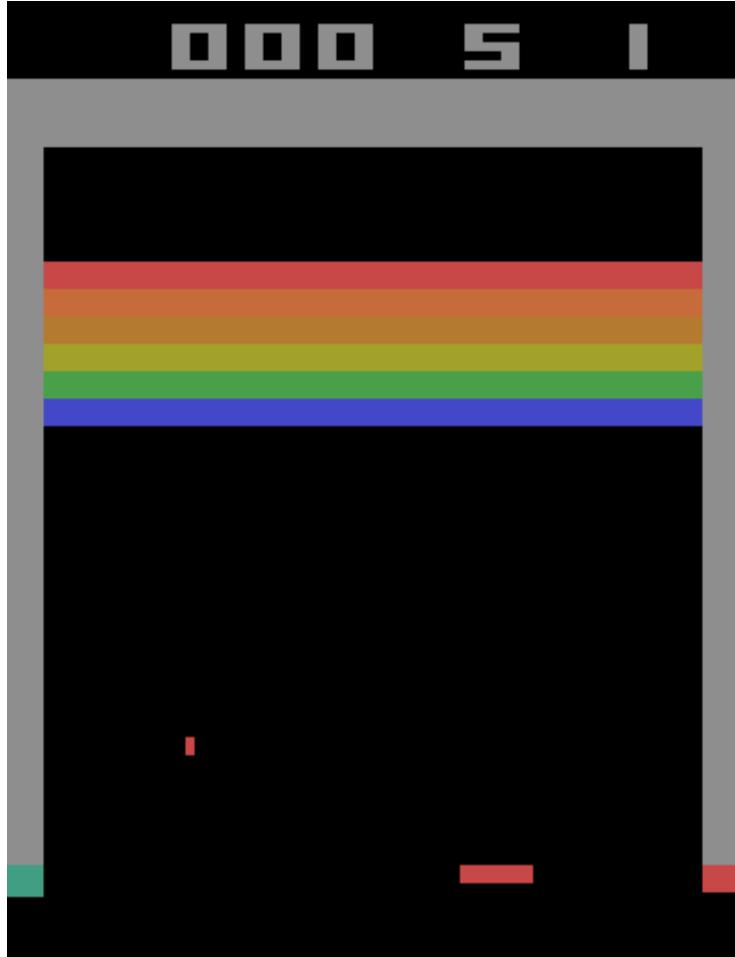
By Judea Pearl

Communications of the ACM, March 2019, Vol. 62 No. 3, Pages 54-60  
10.1145/3241036



Counterfactual calls for “alternative worlds”  $\longleftrightarrow$  A.I

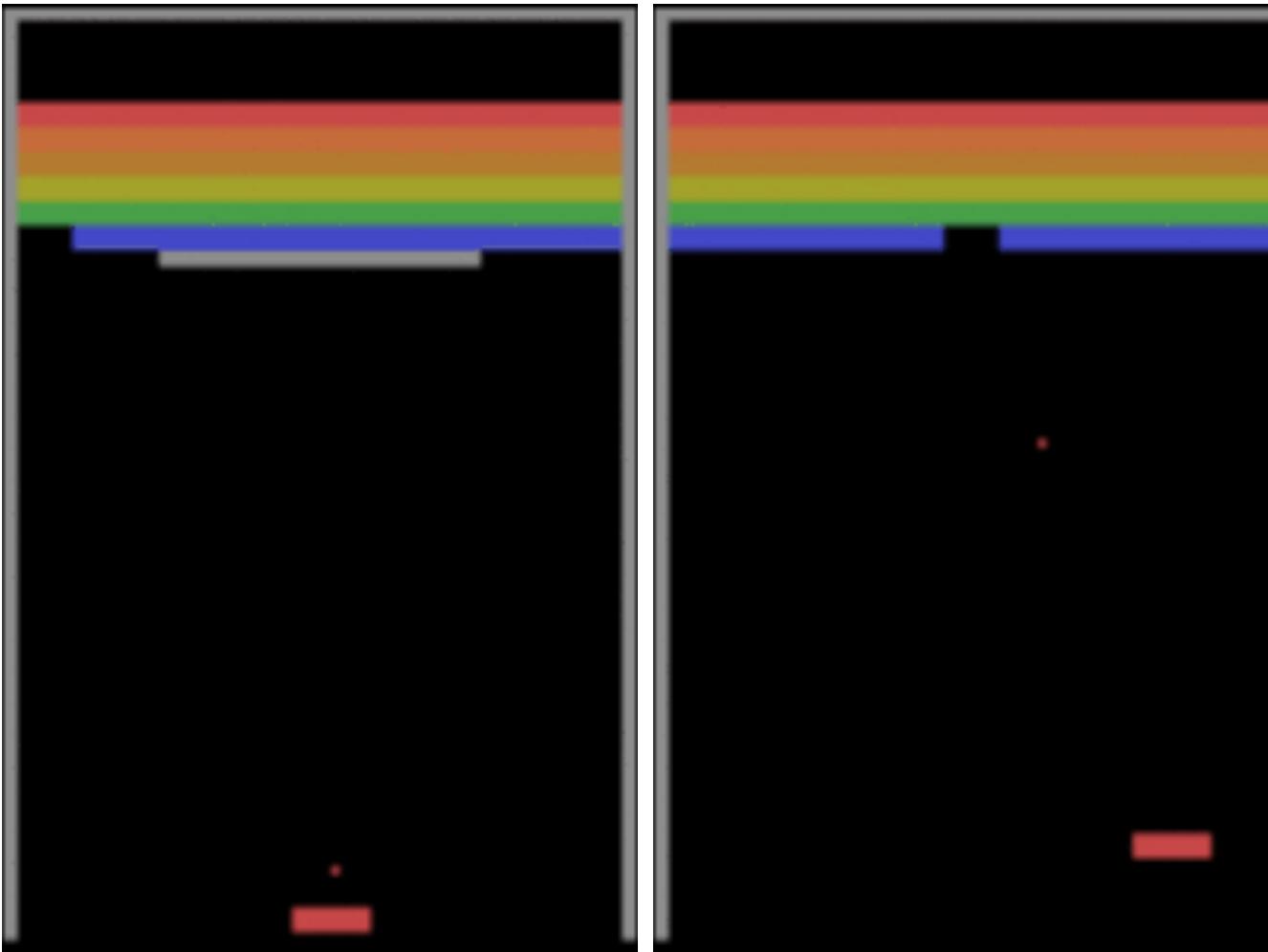
# Improved Interpretability: Deep Learning meets Causal Inference



2014 - DeepMind teaches  
itself to play breakout

..but can the A.I. system adapt  
to small changes?

# Improved Interpretability: Deep Learning meets Causal Inference



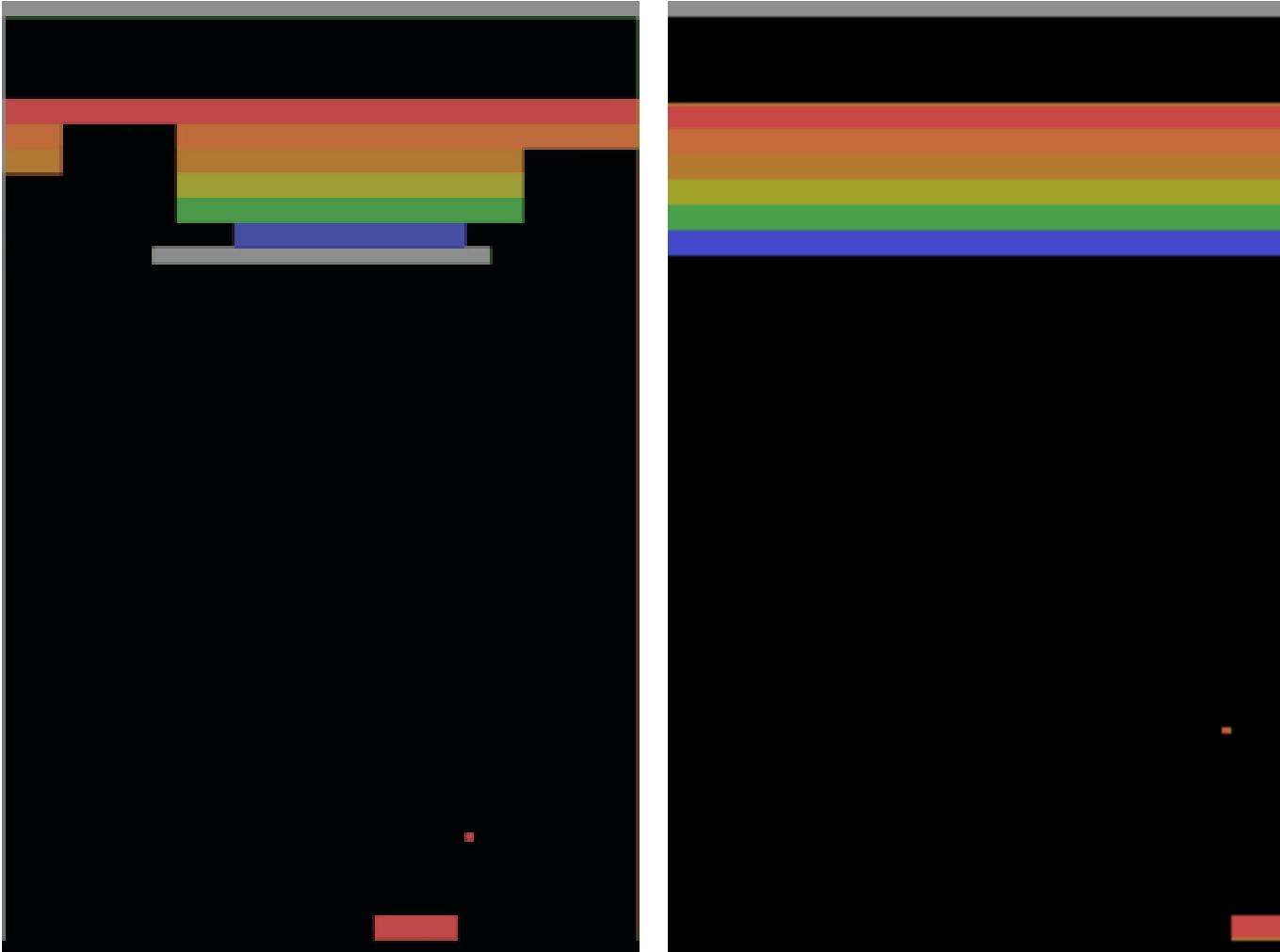
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**Schema Networks: Zero-shot Transfer with a Generative Causal Model of Intuitive Physics**

---

Ken Kansky Tom Silver David A. Mély Mohamed Eldawy Miguel Lázaro-Gredilla Xinghua Lou  
Nimrod Dorfman Szymon Sidor Scott Phoenix Dileep George

# Improved Interpretability: Deep Learning meets Causal Inference



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## Schema Networks: Zero-shot Transfer with a Generative Causal Model of Intuitive Physics

---

Ken Kansky Tom Silver David A. Mély Mohamed Eldawy Miguel Lázaro-Gredilla Xinghua Lou  
Nimrod Dorfman Szymon Sidor Scott Phoenix Dileep George

- Better modeling of cause-effect
- Better generalization through a conceptual representation
- Causal-Effect can leverage **better explanations** of systems

# Let's wrap-up



- Interpretability of ML systems is not a new topic, but propelled by new findings from the DL community and efforts to safely translate this technology to (medical) applications. Complexity and Prevalence.
- The goal of interpretability is \*NOT\* to understand every part but to have enough information for the task at hand.
- Interpretability can leverage: auditability, trust, adoptability, understanding of system's inner workings.
- Lot of work in visualization techniques; active area of research
- Benchmarking of interpretability methods is still an unexplored area.
- Likely a task-dependent combination of approaches will ultimately succeed.  
*Tradeoff succinct-yet-rich explanation*

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# Resources

- iMIMIC websites
  - 2018 edition, check material section  
<https://imimic.bitbucket.io/resources.html>
  - 2019 edition (talks and accepted contributions to be posted)  
<http://imimic-workshop.com>
- Awesome book from Christoph Molnar:  
<https://christophm.github.io/interpretable-ml-book/>
- INNvestigate - <https://github.com/albermax/investigate/>

# Hands-on session

- Use of INNvestigate on two datasets
- Apply methods seen during morning session

# VISUM Summer School

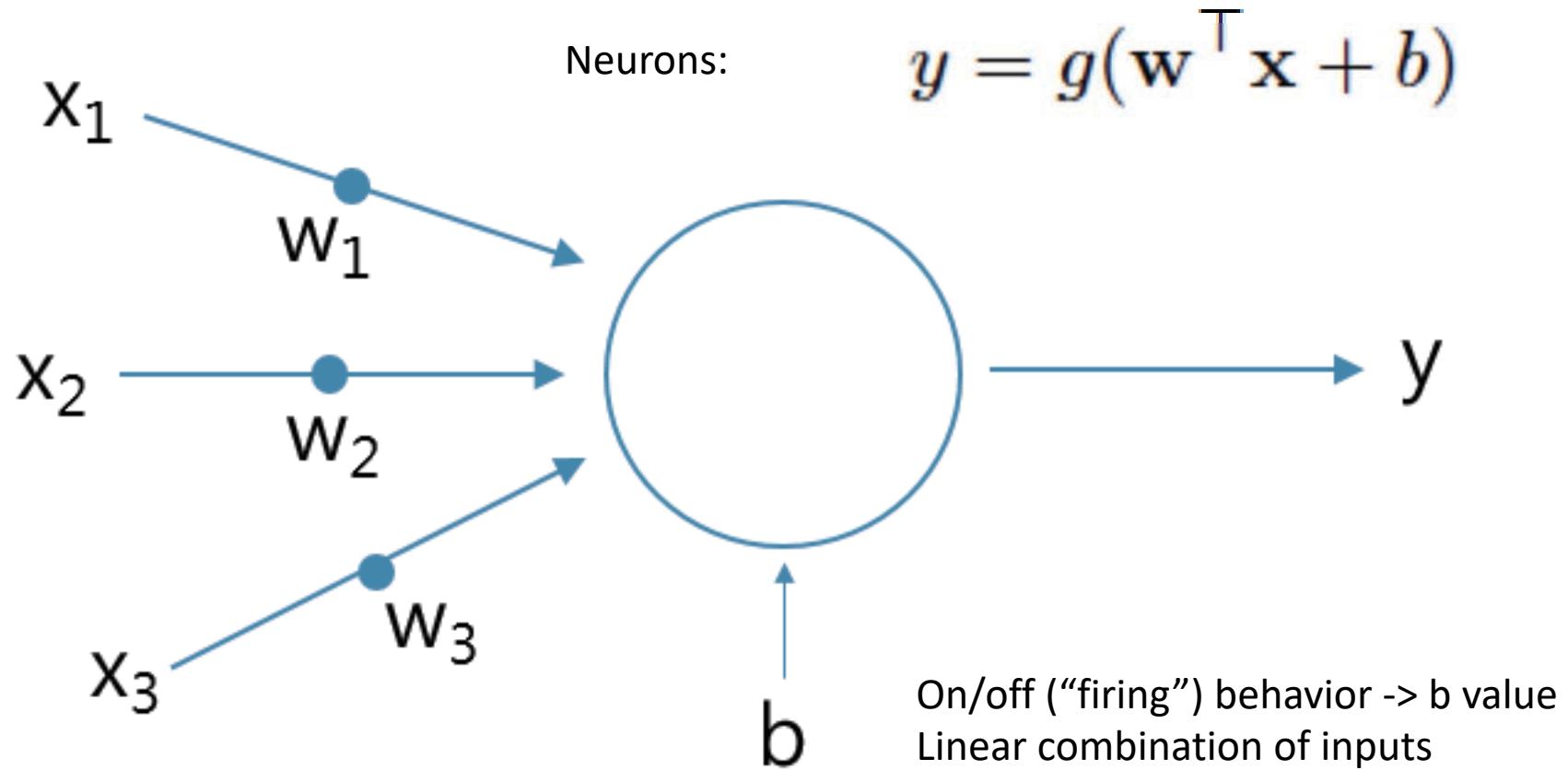


VISion Understanding and Machine intelligence

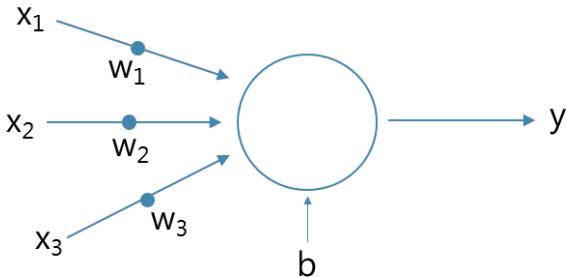


..and a short quiz now

# From neuron to neural nets

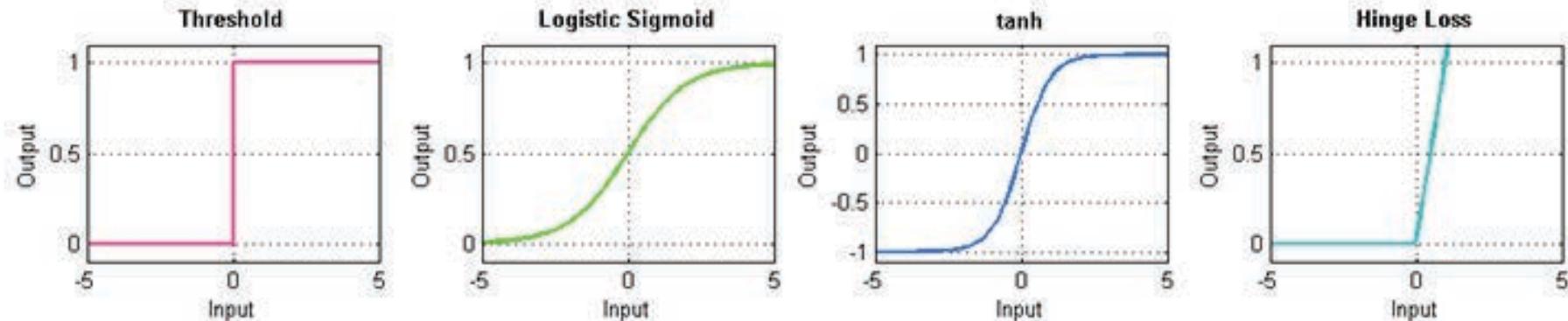


# Neural Nets: Activation functions

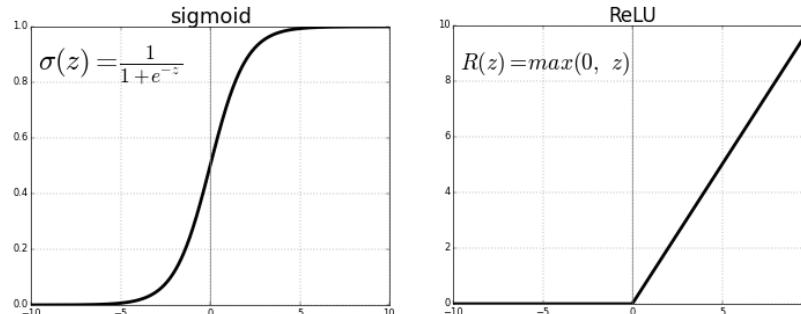


$$y = g(\mathbf{w}^\top \mathbf{x} + b)$$

Activation Function “g”

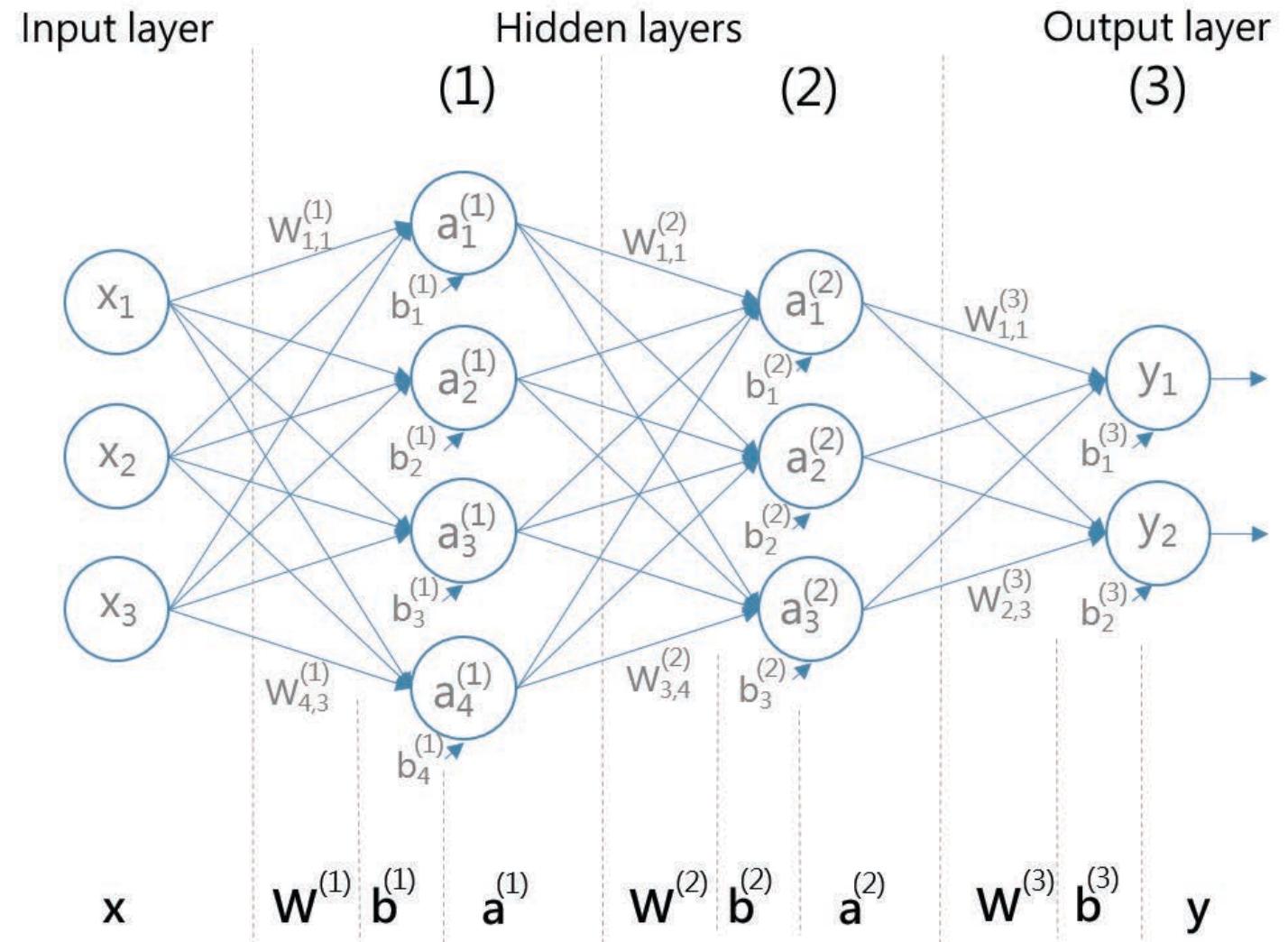


Most used: sigmoid and ReLU



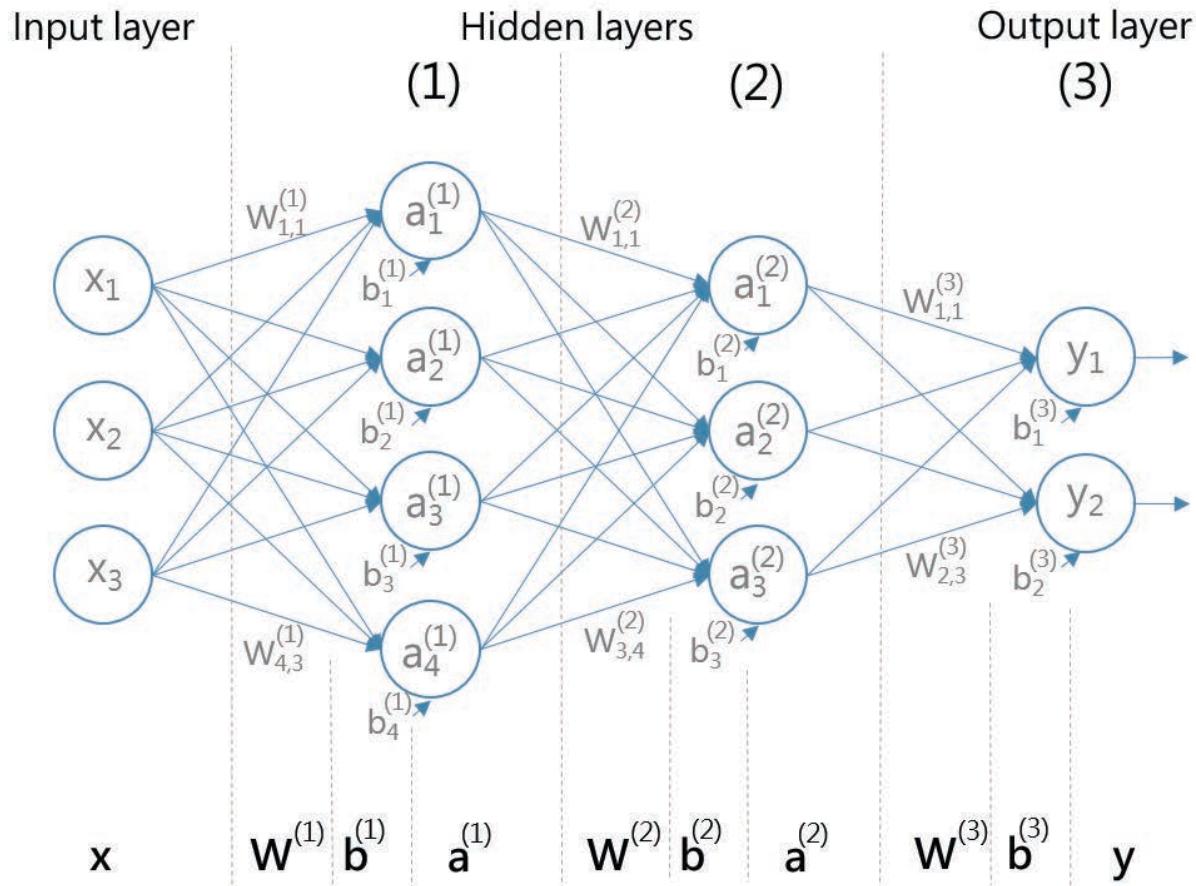
(We'll talk later about issues with sigmoid)

# Neural Nets: Layers



# Neural Nets: Math behind layers

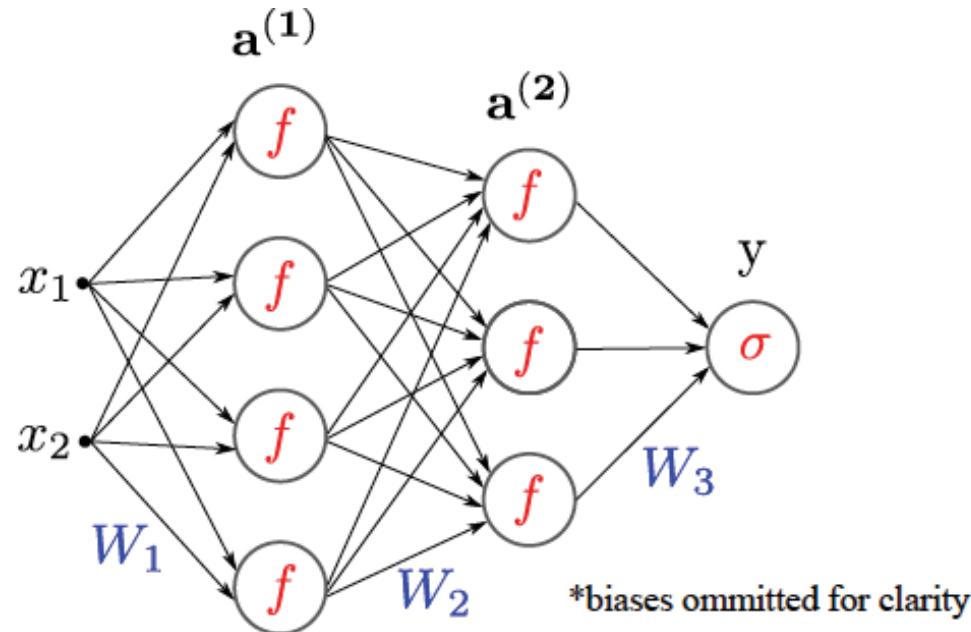
$$\mathbf{a}^{(1)} = g^{(1)} \left( \mathbf{W}^{(1)} \mathbf{x} + \mathbf{b}^{(1)} \right) \quad \mathbf{a}^{(l)} = g^{(l)} \left( \mathbf{W}^{(l)} \mathbf{a}^{(l-1)} + \mathbf{b}^{(l)} \right)$$



# Multilayer Perceptron (MLP)

## Characteristics and Training a MLP

- Adjust weights to minimize error -> supervised
- Backpropagation -> backward propagation of errors
- Gradient Descent
- Fully connected: output of a neuron connects to all downstream neurons



# Training is an optimization process

- Gradient descent

Numerical gradient: slow :, approximate :, easy to write :) Analytic gradient: fast :, exact :, error-prone :)

In practice: Derive analytic gradient, check your implementation with numerical gradient

(Kingma & Ba 2015)

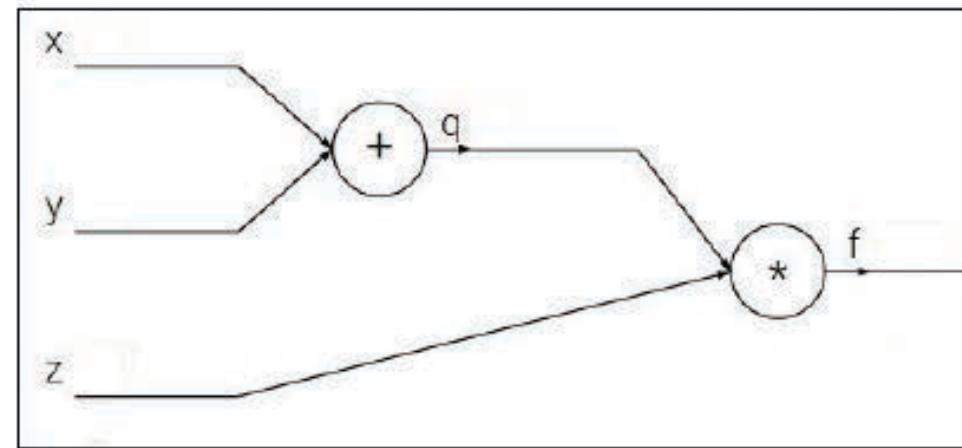
- Adam optimization is the most popular to date

# Simple example Backpropagation

credits: Fei-Fei CS231

Backpropagation: a simple example

$$f(x, y, z) = (x + y)z$$



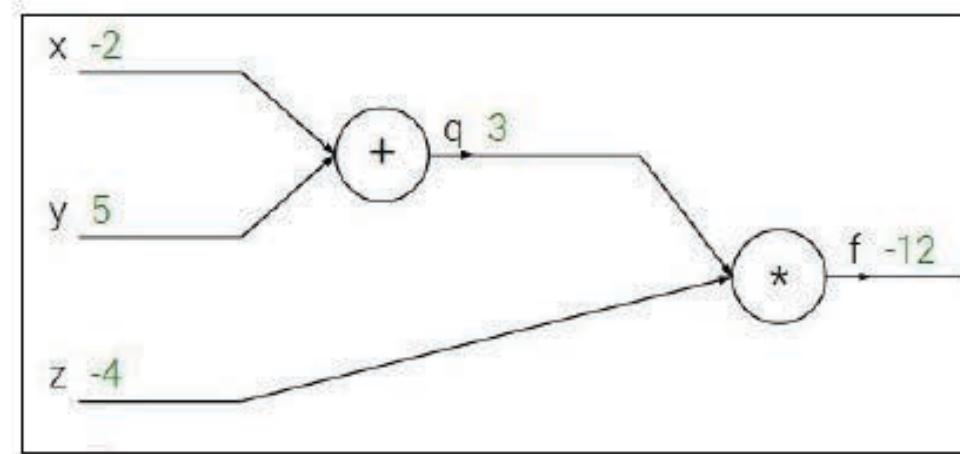
# Simple example Backpropagation

credits: Fei-Fei CS231

Backpropagation: a simple example

$$f(x, y, z) = (x + y)z$$

e.g.  $x = -2$ ,  $y = 5$ ,  $z = -4$



# Simple example Backpropagation

credits: Fei-Fei CS231

Backpropagation: a simple example

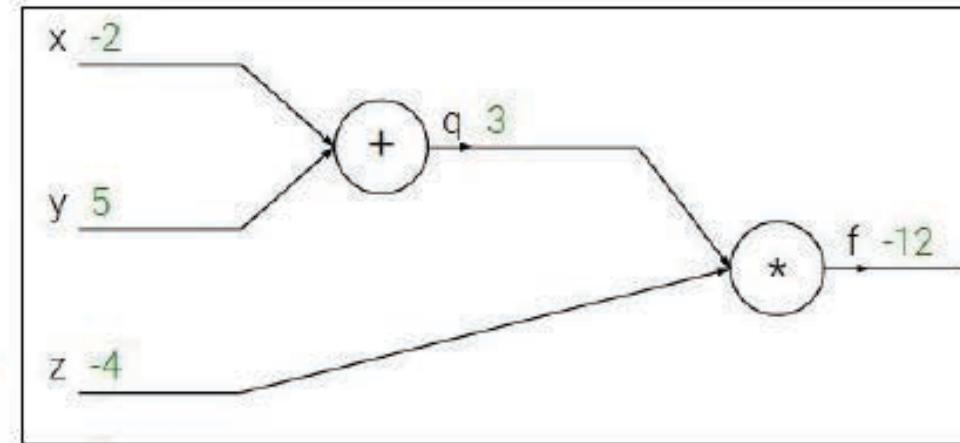
$$f(x, y, z) = (x + y)z$$

e.g.  $x = -2, y = 5, z = -4$

$$q = x + y \quad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



# Simple example Backpropagation

credits: Fei-Fei CS231

Backpropagation: a simple example

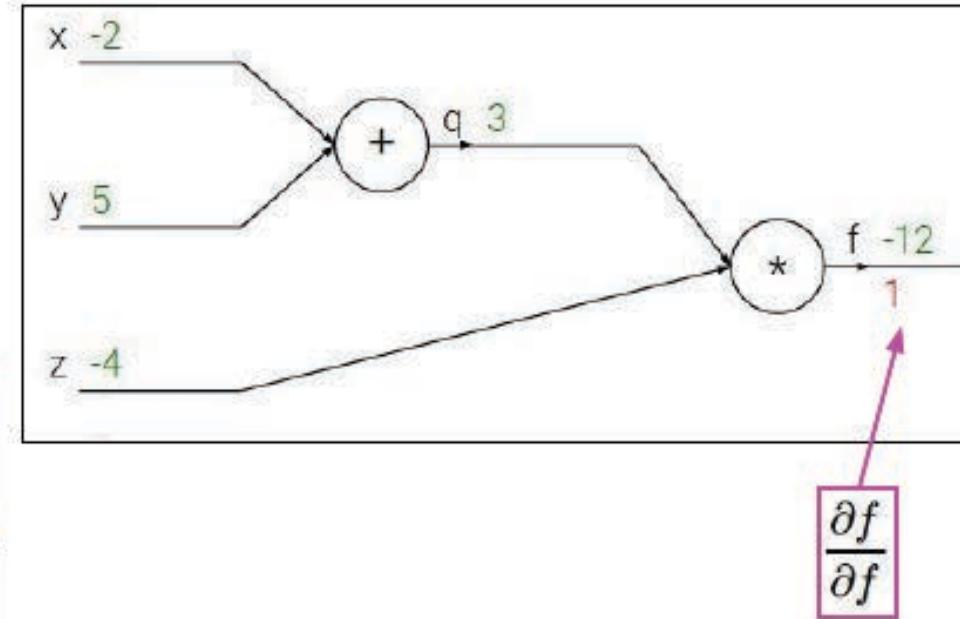
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# Simple example Backpropagation

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Backpropagation: a simple example

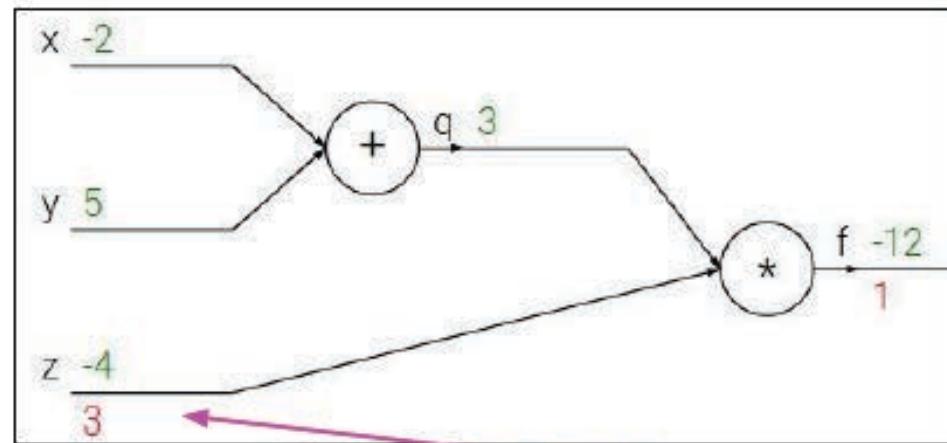
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Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial z}$$

# Simple example Backpropagation

credits: Fei-Fei CS231

Backpropagation: a simple example

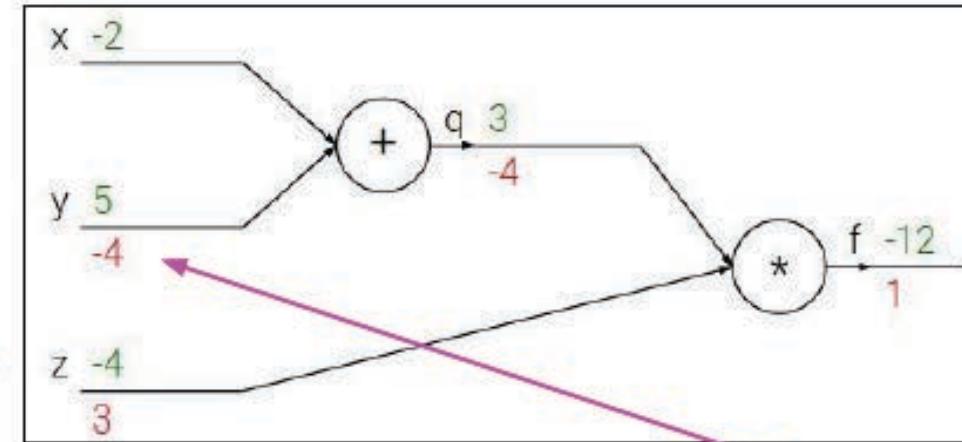
$$f(x, y, z) = (x + y)z$$

e.g.  $x = -2$ ,  $y = 5$ ,  $z = -4$

$$q = x + y \quad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Chain rule:

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial y}$$

Upstream  
gradient      Local  
gradient

$$\frac{\partial f}{\partial y}$$

# Simple example Backpropagation

credits: Fei-Fei CS231

