

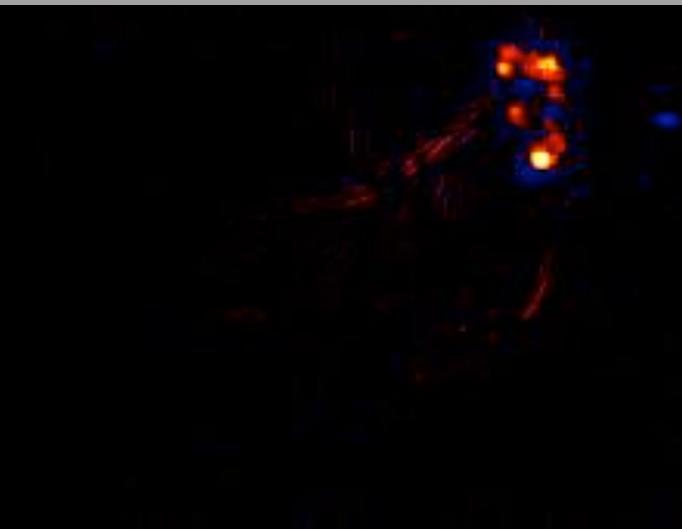


Fraunhofer

Heinrich Hertz Institute

# Interpretable & Transparent Deep Learning

Fraunhofer HHI, Machine Learning Group  
Wojciech Samek



# Record Performances with ML

## Research projects

Deep Net outperforms humans in image classification



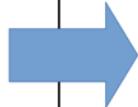
AlphaGo beats Go human champ



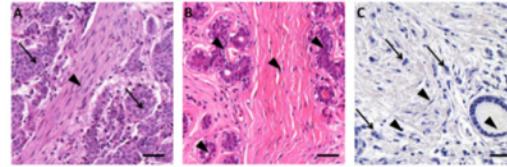
Visual Reasoning



What size is the cylinder that is left of the brown metal thing that is left of the big sphere?



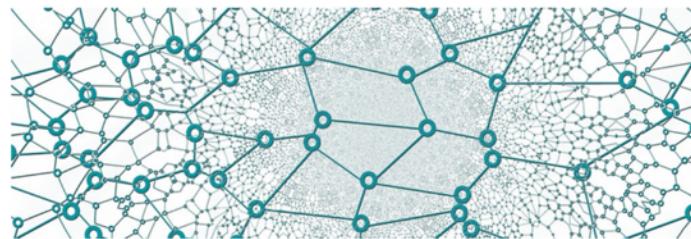
## Medical Diagnosis



## Autonomous Driving

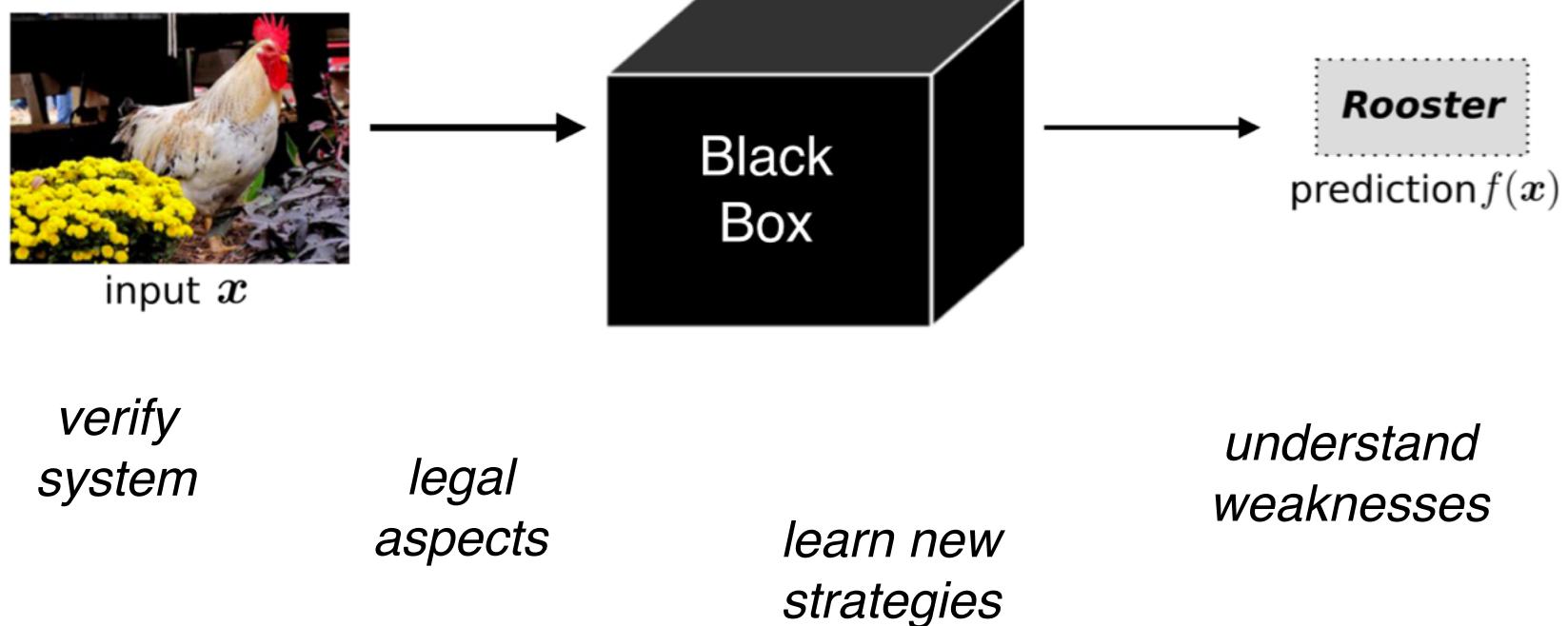


## Networks (smart grids, etc.)



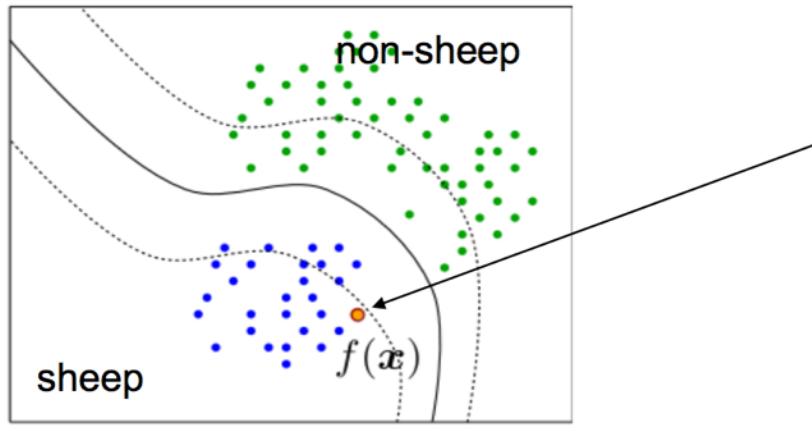
## Safety critical applications

# Need for Interpretability

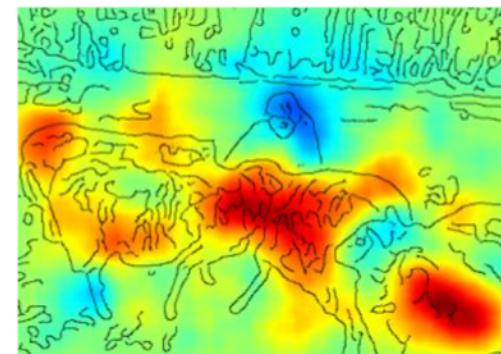


# Need for Interpretability

*“Why is a given image classified as a sheep?”*



$\text{heatmap} = LRP(x, f)$

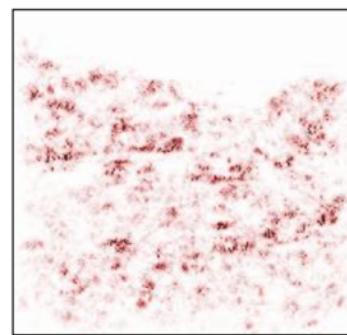


# Naive Approach: Sensitivity Analysis

## Sensitivity analysis:



$$R_i = \left( \frac{\partial f}{\partial x_i} \right)^2$$

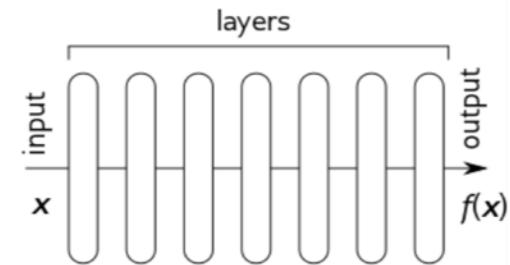
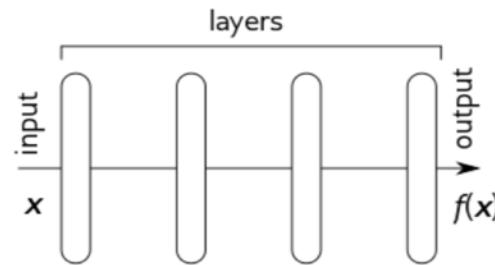
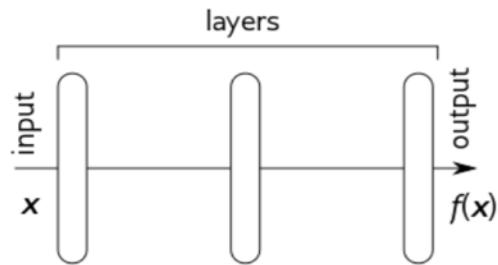


**Problem:** sensitivity analysis does not highlight cars

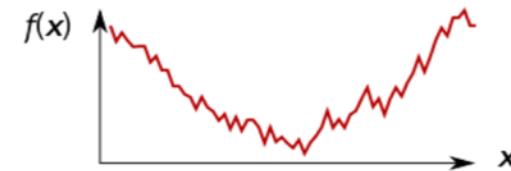
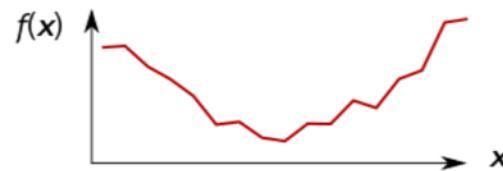
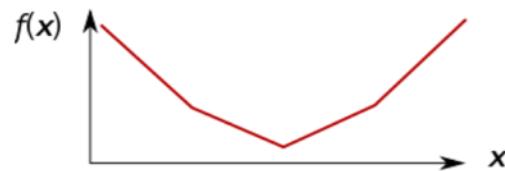
# Naive Approach: Sensitivity Analysis

Input gradient (on which sensitivity analysis is based), becomes increasingly highly varying and unreliable with neural network depth.

Structure's view



Function's view (cartoon)



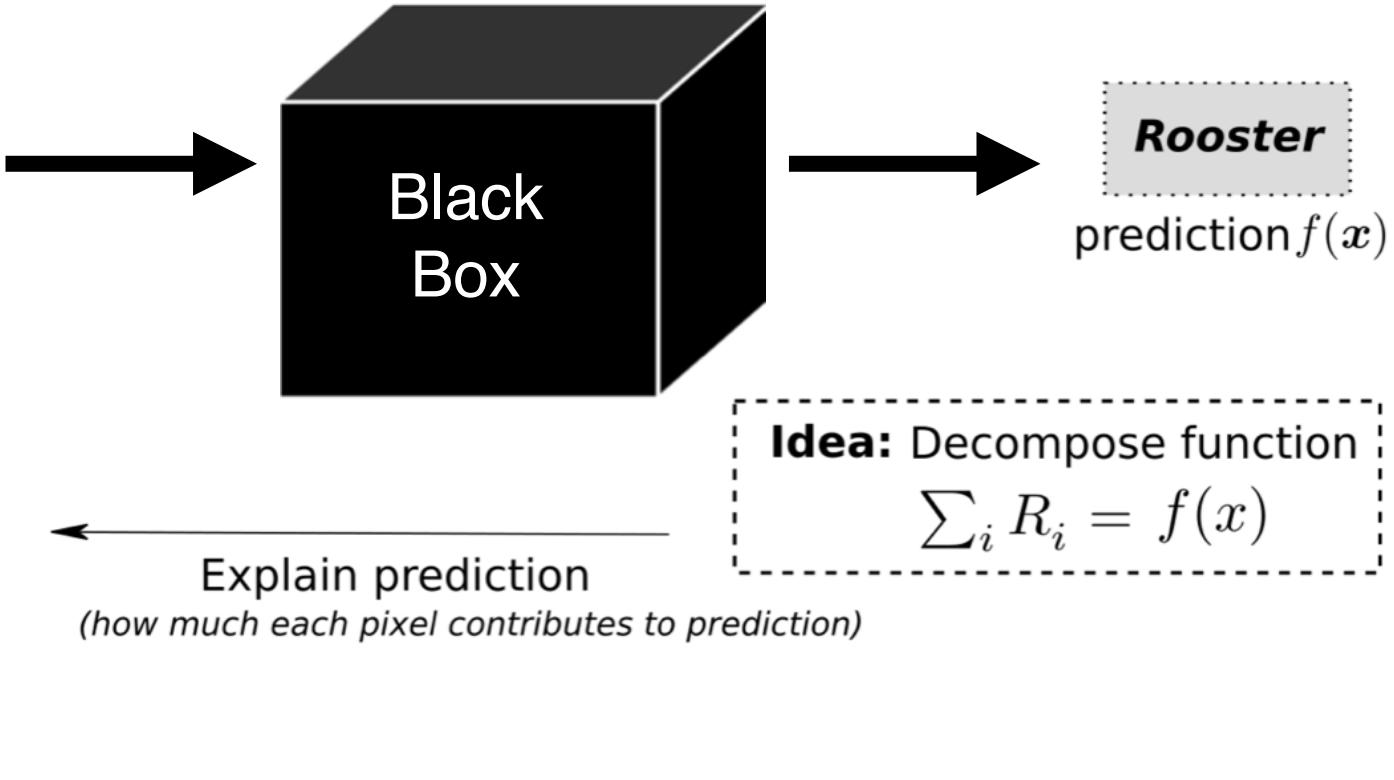
shallow

deep

# Better Approach: LRP



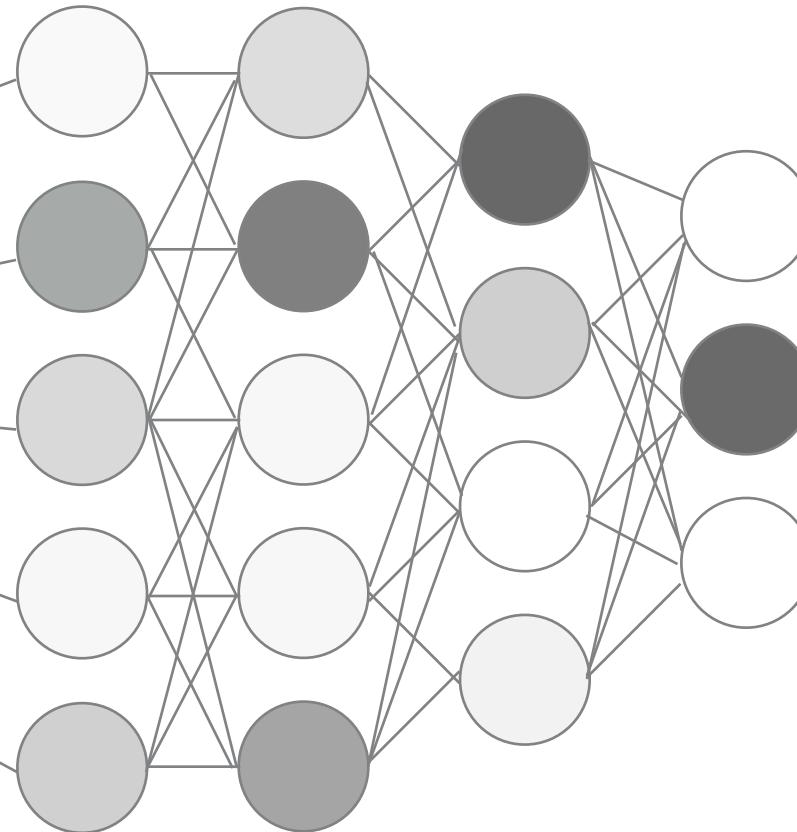
input  $x$



Layer-wise Relevance Propagation (LRP)  
(Bach et al., PLOS ONE, 2015)

# Better Approach: LRP

Classification



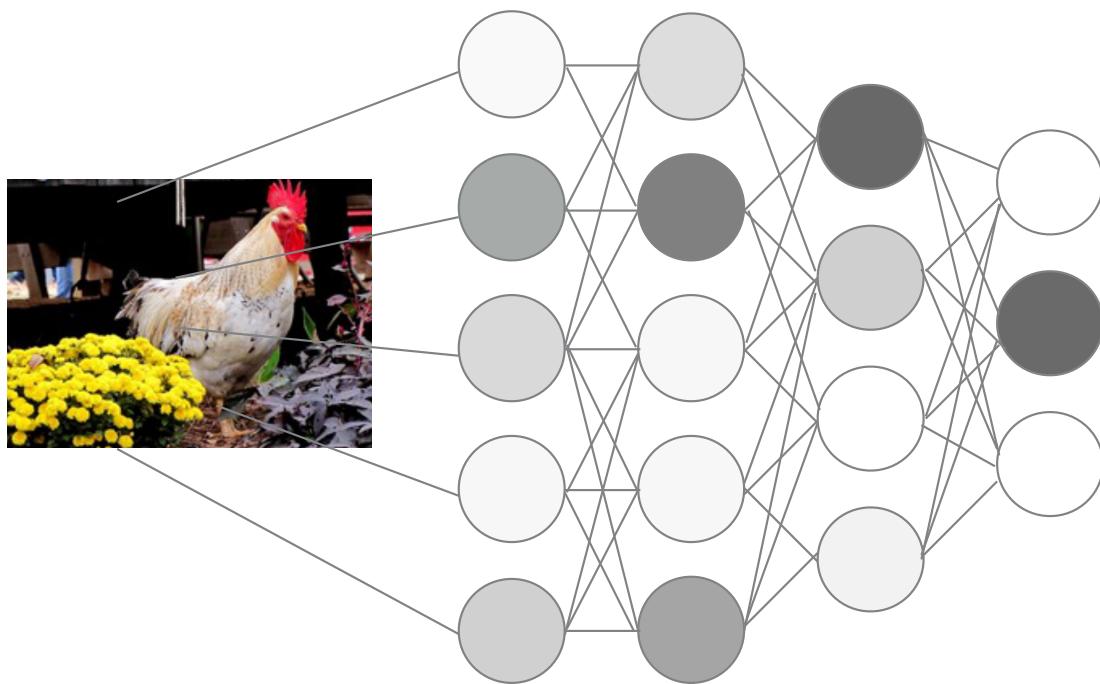
cat

rooster

dog

# Better Approach: LRP

Classification



cat

rooster

dog

Initialization

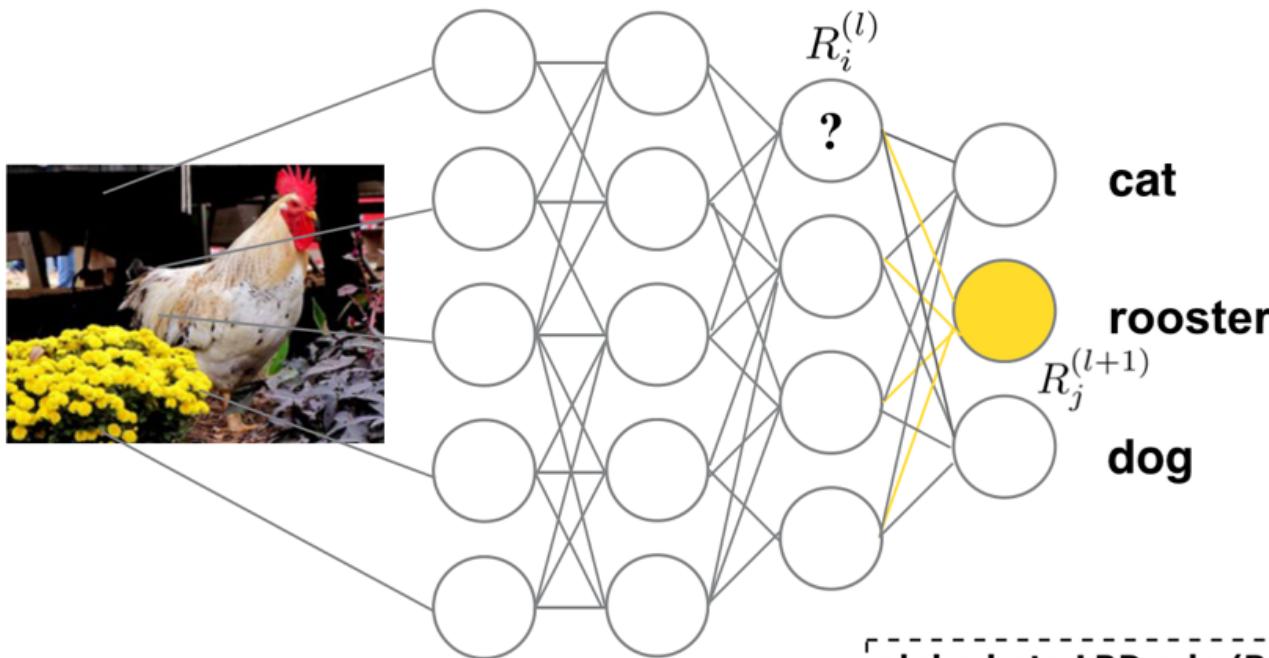
$$R_j^{(l+1)} = f(x)$$

What makes this image a “rooster image” ?

**Idea:** Redistribute the evidence for class rooster back to image space.

# Better Approach: LRP

## Explanation



**Theoretical interpretation**  
Deep Taylor Decomposition  
(Montavon et al., 2017)  
**not based on gradient !**

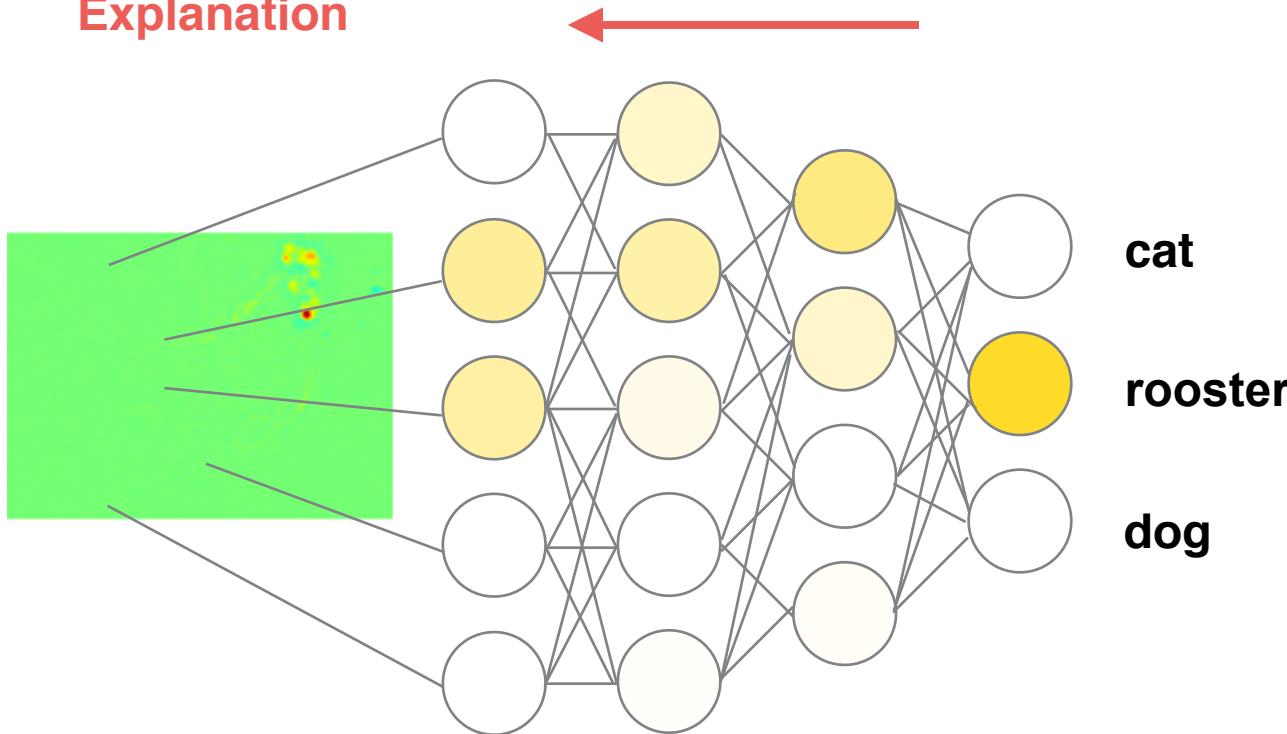
**alpha-beta LRP rule (Bach et al. 2015)**

$$R_i^{(l)} = \sum_j (\alpha \cdot \frac{(x_i \cdot w_{ij})^+}{\sum_{i'} (x_{i'} \cdot w_{i'j})^+} + \beta \cdot \frac{(x_i \cdot w_{ij})^-}{\sum_{i'} (x_{i'} \cdot w_{i'j})^-}) R_j^{(l+1)}$$

where  $\alpha + \beta = 1$

# Better Approach: LRP

Explanation

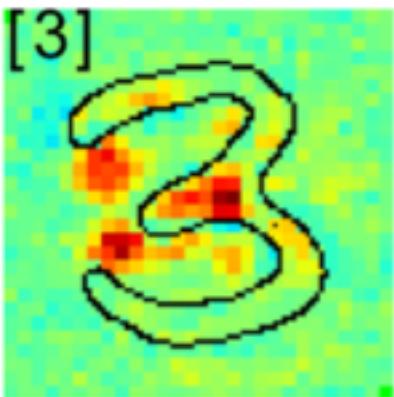


Layer-wise relevance conservation

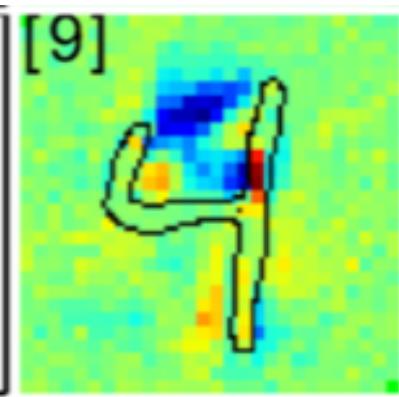
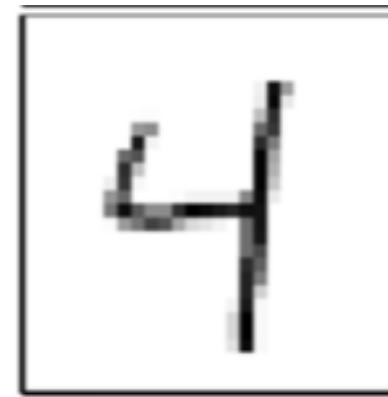
$$\sum_i R_i = \dots = \sum_i R_i^{(l)} = \sum_j R_j^{(l+1)} = \dots = f(x)$$

# Better Approach: LRP

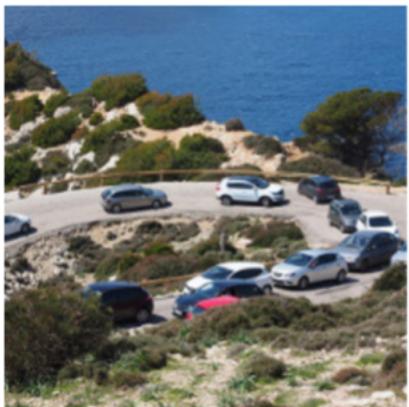
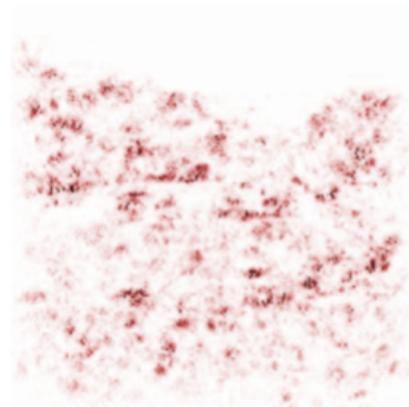
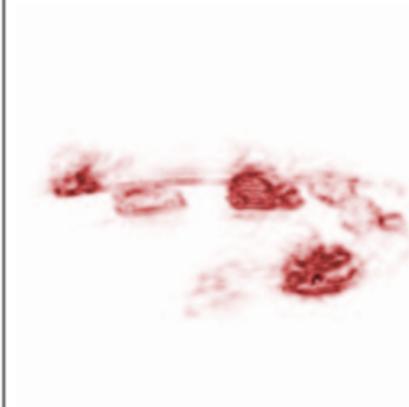
Heatmap of prediction “3”



Heatmap of prediction “9”



# Better Approach: LRP

Image	Sensitivity Analysis	LRP / Deep Taylor
		
Explains what influences prediction “cars”.		Explains prediction “cars” as is.
Slope decomposition $\sum_i R_i = \ \nabla_x f\ ^2$		Value decomposition $\sum_i R_i = f(\mathbf{x})$
		More information (Montavon et al., 2017 & 2018)

# Decomposing the Correct Quantity

slope decomposition

$$\sum_i R_i = \|\nabla_x f\|^2$$

value decomposition

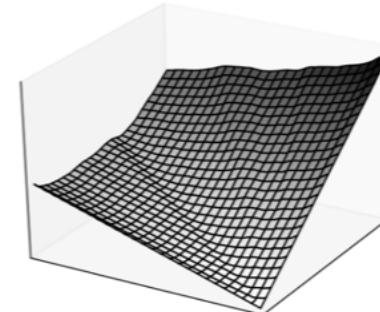
$$\sum_i R_i = f(\mathbf{x})$$

**Candidate:** Taylor decomposition

$$f(\mathbf{x}) = \underbrace{f(\tilde{\mathbf{x}})}_0 + \sum_{i=1}^d \underbrace{\frac{\partial f}{\partial x_i} \Big|_{\mathbf{x}=\tilde{\mathbf{x}}} (x_i - \tilde{x}_i)}_{R_i} + \underbrace{O(\mathbf{x}\mathbf{x}^\top)}_0$$

- Achievable for linear models and deep ReLU networks without biases, by choosing:

$$\tilde{\mathbf{x}} = \lim_{\varepsilon \rightarrow 0} \varepsilon \cdot \mathbf{x} \approx \mathbf{0}.$$

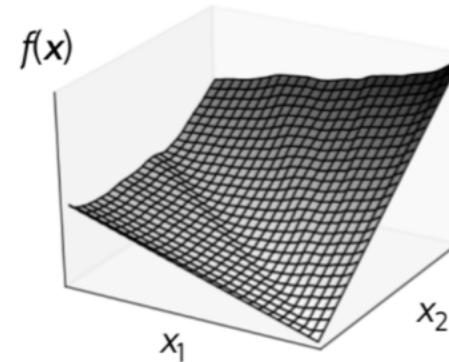


# Why Simple Taylor doesn't work?

## Two Reasons:

1

Root point is hard to find or too far → includes too much information (incl. negative evidence)



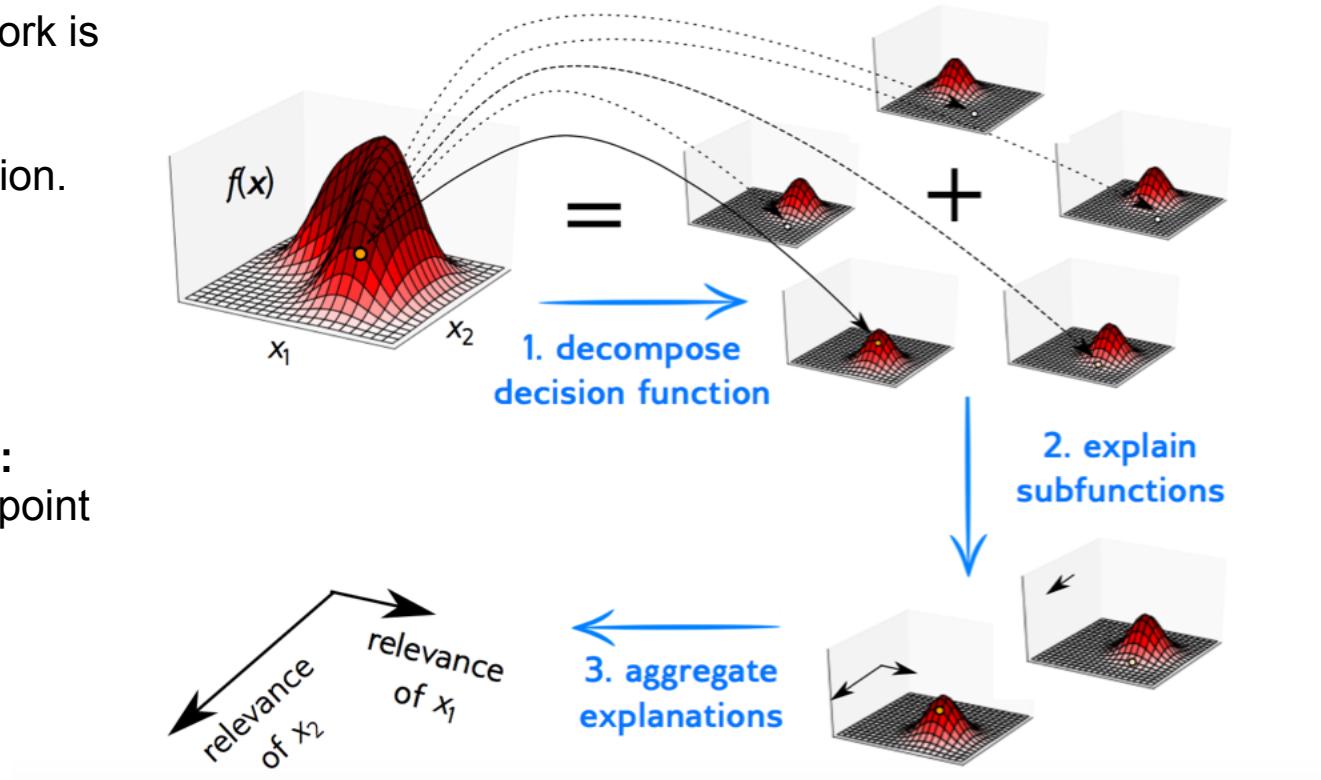
2

Gradient shattering problem → gradient of deep nets has low informative value



# Deep Taylor Decomposition

**Idea:** Since neural network is composed of simple functions, we propose a *deep* Taylor decomposition.

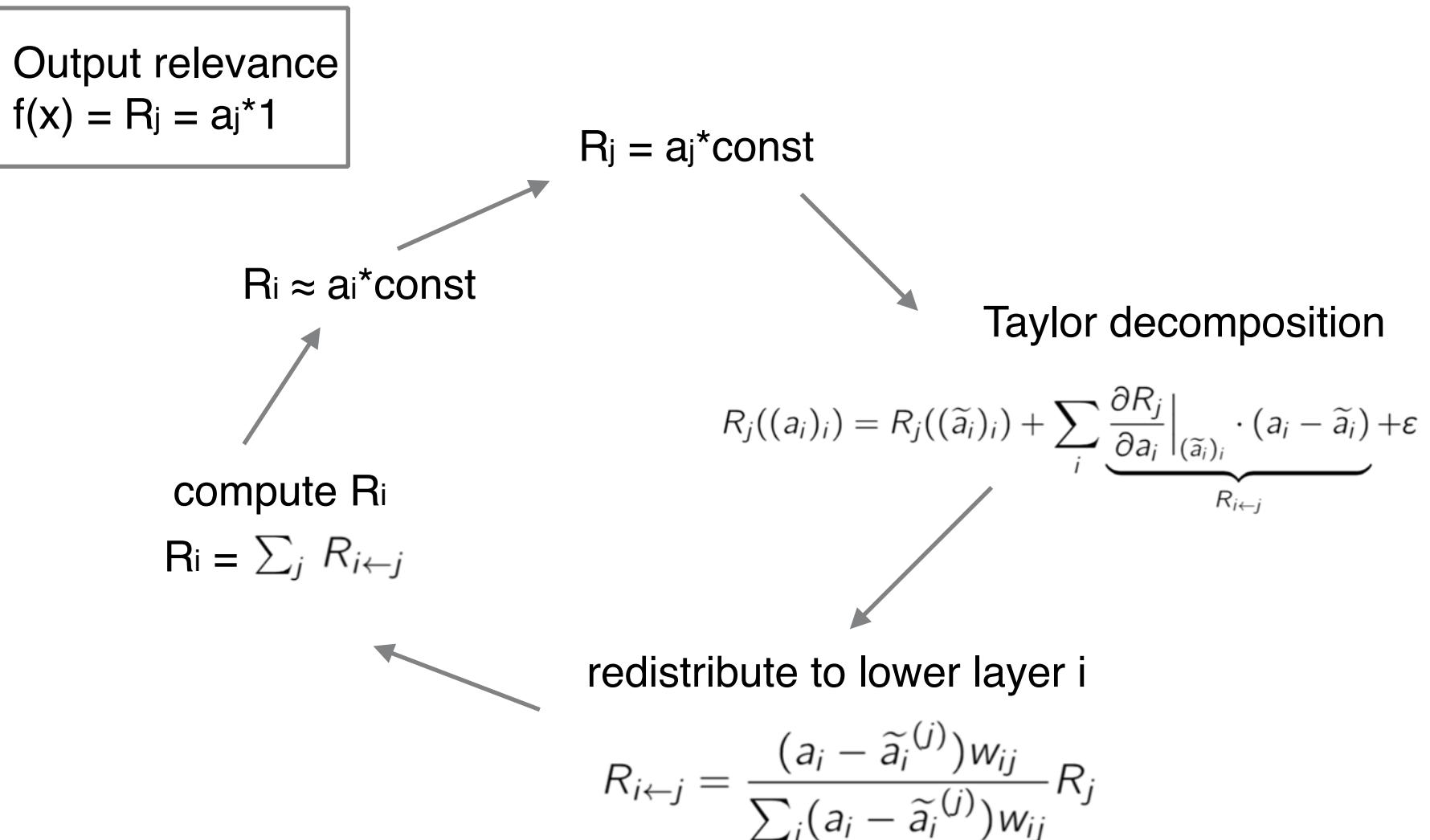


## Each explanation step:

- easy to find good root point
- no gradient shattering

(Montavon et al., 2017  
Montavon et al. 2018)

# Deep Taylor Decomposition



# Deep Taylor Decomposition

how to choose the root point  $\tilde{a}_i^{(j)}$  ?

$$R_{i \leftarrow j} = \frac{(a_i - \tilde{a}_i^{(j)}) w_{ij}}{\sum_i (a_i - \tilde{a}_i^{(j)}) w_{ij}} R_j$$

Input domain	Rule
ReLU activations ( $a_j \geq 0$ )	$R_j = \sum_k \frac{a_j w_{jk}^+}{\sum_j a_j w_{jk}^+} R_k$
Pixel intensities ( $x_i \in [l_i, h_i]$ , $l_i \leq 0 \leq h_i$ )	$R_i = \sum_j \frac{x_i w_{ij} - l_i w_{ij}^+ - h_i w_{ij}^-}{\sum_i x_i w_{ij} - l_i w_{ij}^+ - h_i w_{ij}^-} R_j$
Real values ( $x_i \in \mathbb{R}$ )	$R_i = \sum_j \frac{w_{ij}^2}{\sum_i w_{ij}^2} R_j$

# Other Explanation Methods



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

## Decomposition



# Question: Which one to choose ?

(Ribeiro et al., 2016) (Fong & Vedaldi 2017) (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)

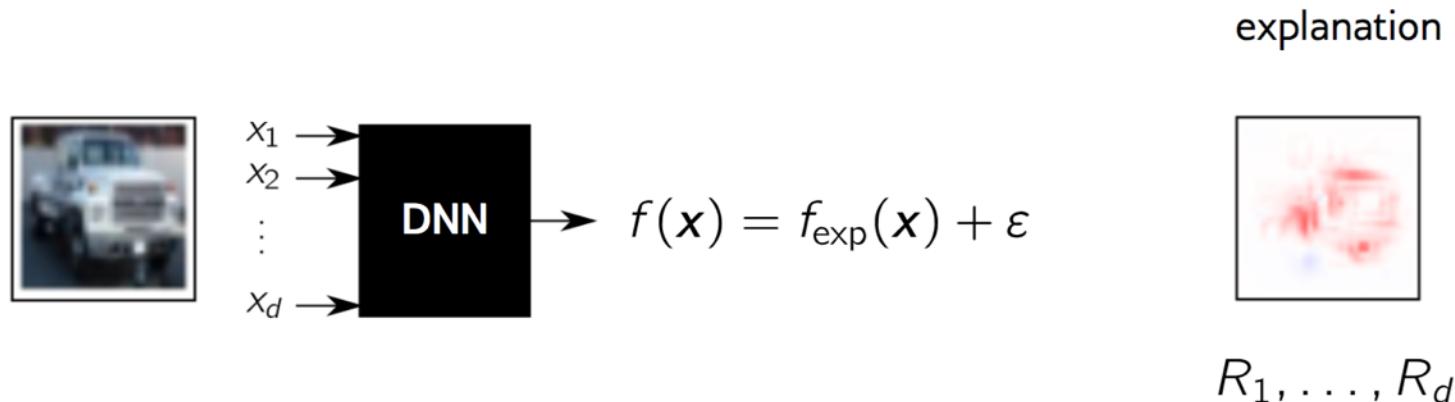
RNN cell state analysis  
(Karpathy et al., 2015)

Network Dissection  
(Zhou et al. 2017)

# Axiomatic Approach to Interpretability

## Properties 1-2: Conservation and Positivity

[Montavon'17, see also Sun'11, Landecker'13, Bach'15]



**Conservation:** Total attribution on the input features should be proportional to the amount of (explainable) evidence at the output.

$$\sum_{p=1}^d R_p = f_{\text{exp}}(\mathbf{x})$$

**Positivity:** If the neural network is certain about its prediction, input features are either relevant (positive) or irrelevant (zero).

$$\forall_{p=1}^d : R_p \geq 0$$

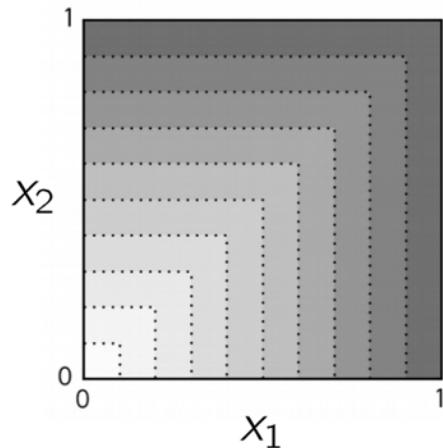
# Axiomatic Approach to Interpretability

## Property 3: Continuity [Montavon'18]

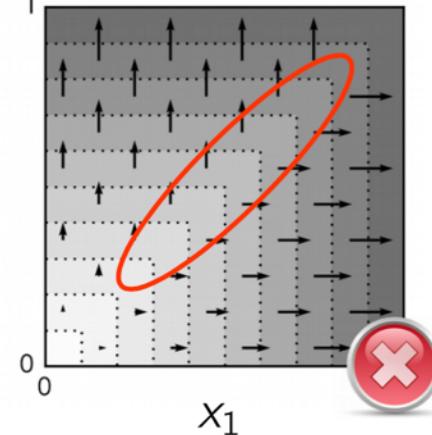
If two inputs are the almost the same, and the prediction is also almost the same, then the explanation should also be almost the same.

### Example:

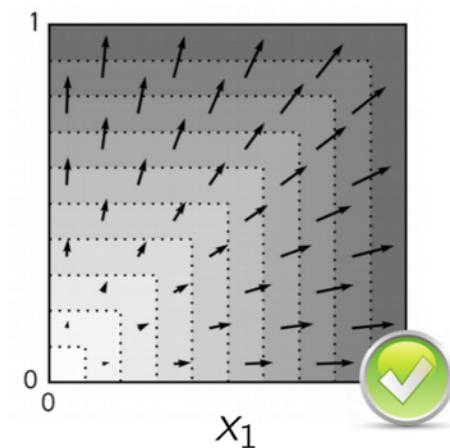
$$f(x) = \max(x_1, x_2)$$



Method 1  
discontinuity at  $x_1 = x_2$



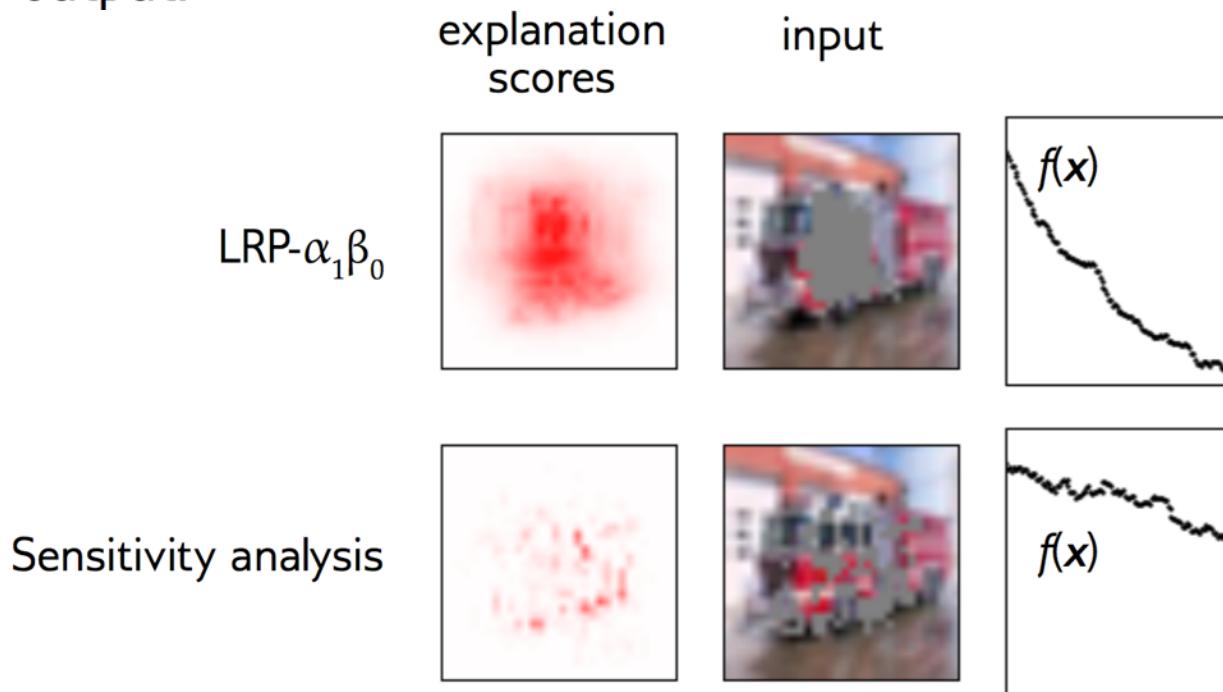
Method 2



# Axiomatic Approach to Interpretability

## Property 4: Selectivity [Bach'15, Samek'17]

Model must agree with the explanation: If input features are attributed relevance, removing them should reduce evidence at the output.



# Axiomatic Approach to Interpretability

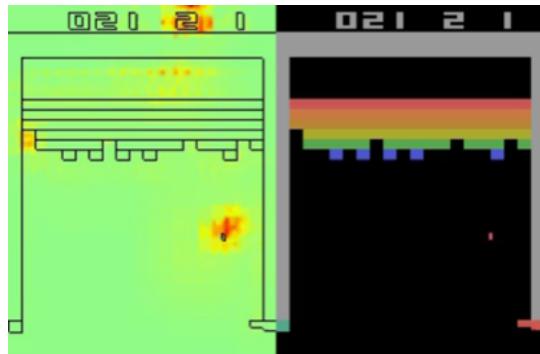
Explanation techniques	Uniform	(Gradient) <sup>2</sup>	(Guided BP) <sup>2</sup>	Gradient x Input	Guided BP x Input	LRP- $\alpha, \beta_0$	...
Properties							
1. Conservation	✓			✓	✓	✓	
2. Positivity	✓	✓	✓		✓	✓	
3. Continuity	✓		✓		✓	✓	
4. Selectivity		✓	✓	✓	✓	✓	
...							

# LRP revisited

General Images (Bach' 15, Lapuschkin'16)



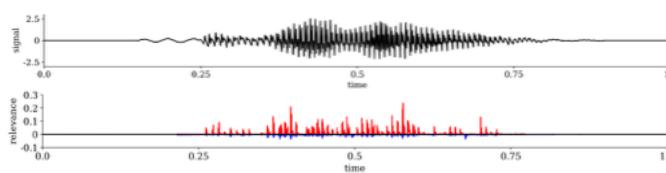
Games (Lapuschkin'19)



Faces (Lapuschkin'17)



Speech (Becker'18)



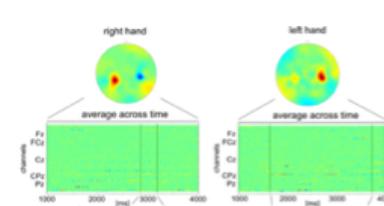
VQA (Arras'18)



Video (Anders'18)



EEG (Sturm'16)



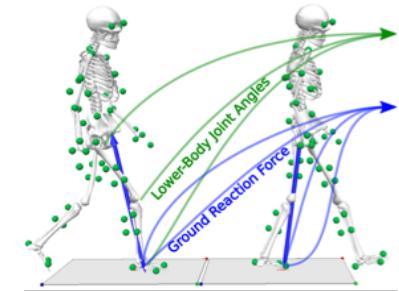
Text Analysis (Arras'16 &17)

do n't waste your money  
neither funny nor susper

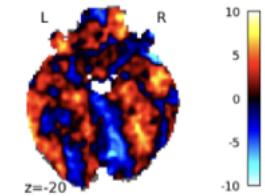
Morphing (Seibold'18)



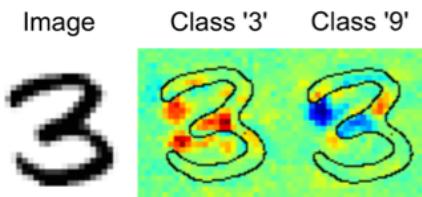
Gait Patterns (Horst'19)



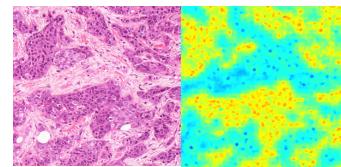
fMRI (Thomas'18)



Digits (Bach' 15)

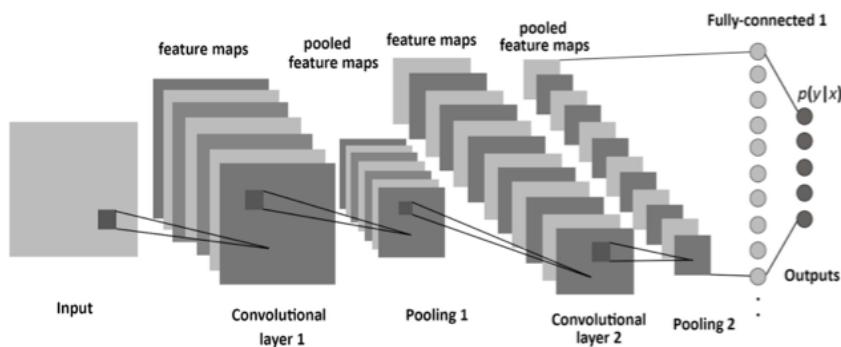


Histopathology (Binder'18)

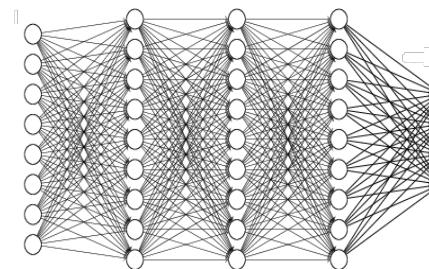


# LRP applied to different Models

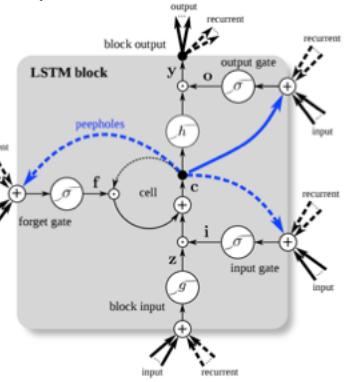
Convolutional NNs (Bach'15, Arras'17 ...)



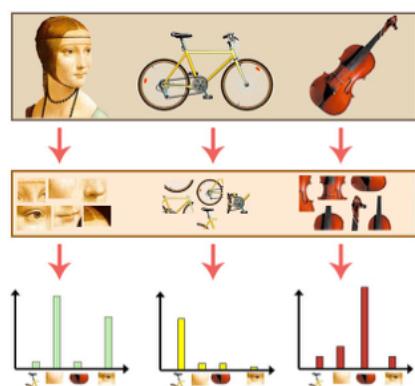
Local Renormalization Layers (Binder'16)



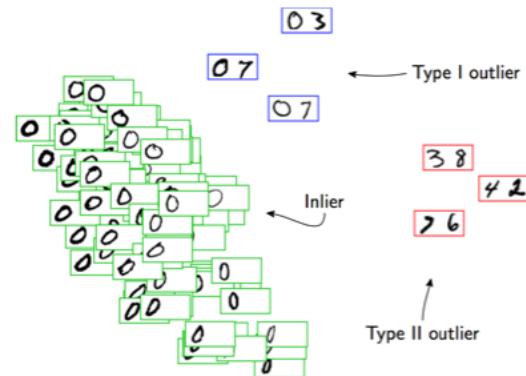
LSTM (Arras'17, Thomas'18)



Bag-of-words / Fisher Vector models  
(Bach'15, Arras'16, Lapuschkin'17, Binder'18)



One-class SVM (Kauffmann'18)



# Application: Compare Classifiers

## word2vec/CNN:

Performance: 80.19%

Strategy to solve the problem:  
identify semantically meaningful words related to the topic.

## BoW/SVM:

Performance: 80.10%

Strategy to solve the problem:  
identify statistical patterns,  
i.e., use word statistics

Yes, weightlessness does feel like falling. It may feel strange at first, but the body does adjust. The feeling is not too different from that of sky diving.

(4.1) >And what is the motion sickness  
>that some astronauts occasionally experience?  
**sci.med** It is the body's reaction to a strange environment. It appears to be induced partly to physical discomfort and part to mental distress. Some people are more prone to it than others, like some people are more prone to get sick on a roller coaster ride than others. The mental part is usually induced by a lack of clear indication of which way is up or down, ie: the Shuttle is normally oriented with its cargo bay pointed towards Earth, so the Earth (or ground) is "above" the head of the astronauts. About 50% of the astronauts experience some form of motion sickness, and NASA has done numerous tests in space to try to see how to keep the number of occurrences down.

Yes, weightlessness does feel like falling. It may feel strange at first, but the body does adjust. The feeling is not too different from that of sky diving.

(-0.6) >And what is the motion sickness  
>that some astronauts occasionally experience?  
**sci.med** It is the body's reaction to a strange environment. It appears to be induced partly to physical discomfort and part to mental distress. Some people are more prone to it than others, like some people are more prone to get sick on a roller coaster ride than others. The mental part is usually induced by a lack of clear indication of which way is up or down, ie: the Shuttle is normally oriented with its cargo bay pointed towards Earth, so the Earth (or ground) is "above" the head of the astronauts. About 50% of the astronauts experience some form of motion sickness, and NASA has done numerous tests in space to try to see how to keep the number of occurrences down.

(Arras et al. 2016 & 2017)

# Application: Compare Classifiers

Test error for various classes:

	aeroplane	bicycle	bird	boat	bottle	bus	car
Fisher	79.08%	66.44%	45.90%	70.88%	27.64%	69.67%	80.96%
DeepNet	88.08%	79.69%	80.77%	77.20%	35.48%	72.71%	86.30%
	cat	chair	cow	diningtable	dog	horse	motorbike
Fisher	59.92%	51.92%	47.60%	58.06%	42.28%	80.45%	69.34%
DeepNet	81.10%	51.04%	61.10%	64.62%	76.17%	81.60%	79.33%
	person	pottedplant	sheep	sofa	train	tvmonitor	mAP
Fisher	85.10%	28.62%	49.58%	49.31%	82.71%	54.33%	59.99%
DeepNet	92.43%	49.99%	74.04%	49.48%	87.07%	67.08%	72.12%

Image



same performance → same strategy ?

(Lapuschkin et al. 2016)

# Application: Compare Classifiers



'horse' images in PASCAL VOC 2007

C: Lothar Lenz  
[www.pferdefotoarchiv.de](http://www.pferdefotoarchiv.de)



C: Lothar Lenz  
[www.pferdefotoarchiv.de](http://www.pferdefotoarchiv.de)



C: Lothar Lenz  
[www.pferdefotoarchiv.de](http://www.pferdefotoarchiv.de)



C: Lothar Lenz  
[www.pferdefotoarchiv.de](http://www.pferdefotoarchiv.de)



C: Lothar Lenz  
[www.pferdefotoarchiv.de](http://www.pferdefotoarchiv.de)

# Application: Measure Context Use



how important  
is context ?

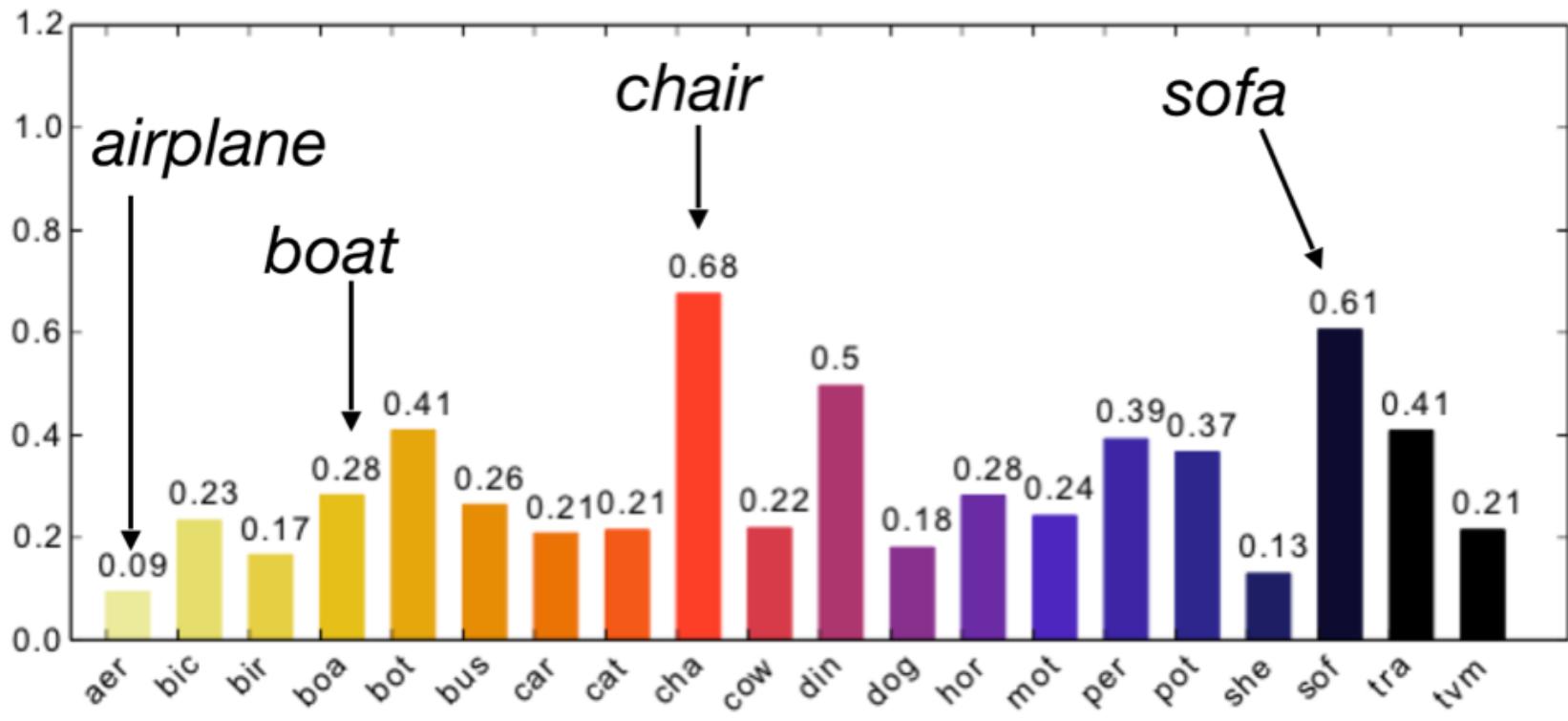
**classifier**



how important  
is context ?

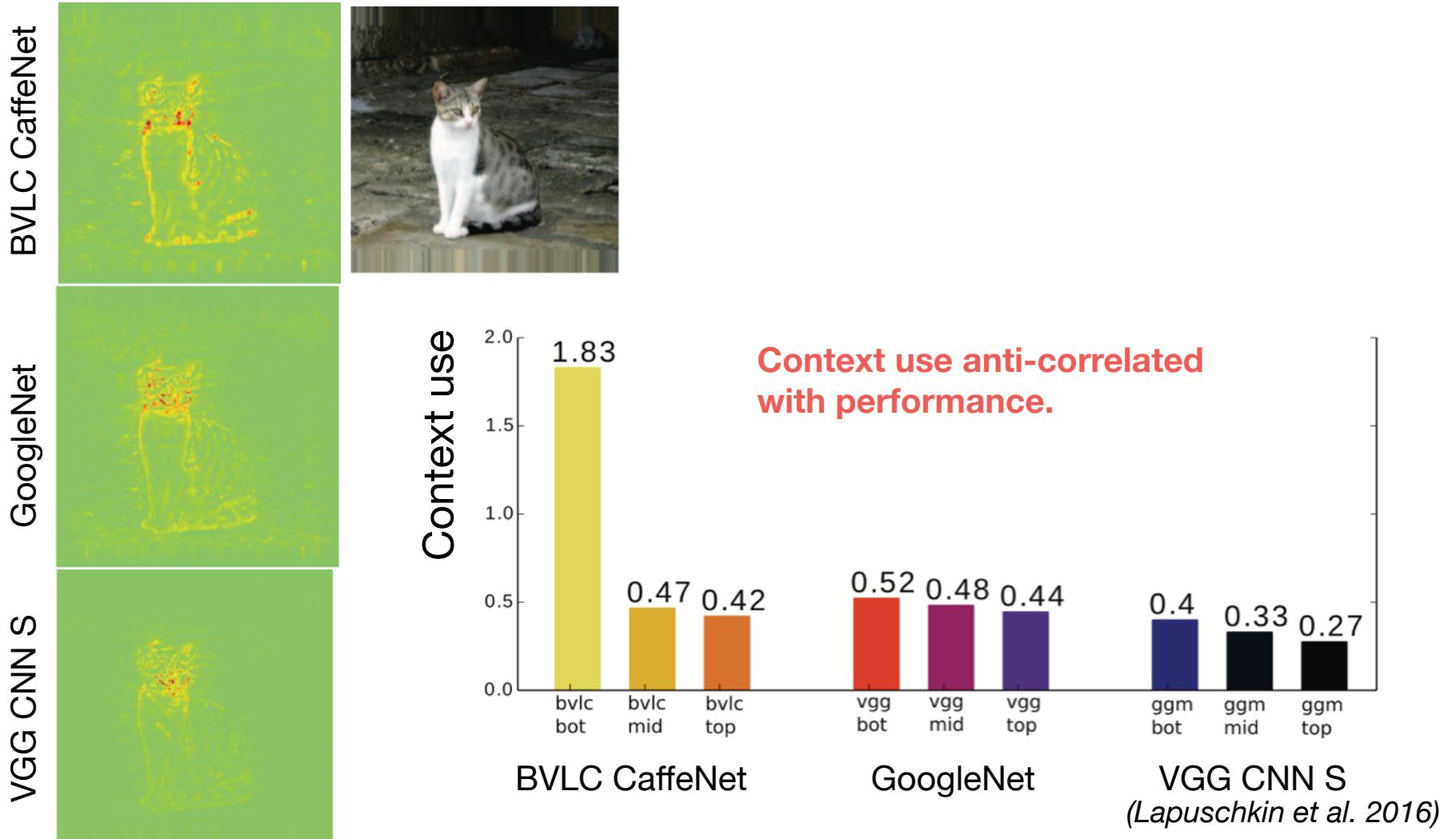
$$\text{importance of context} = \frac{\text{relevance outside bbox}}{\text{relevance inside bbox}}$$

# Application: Measure Context Use



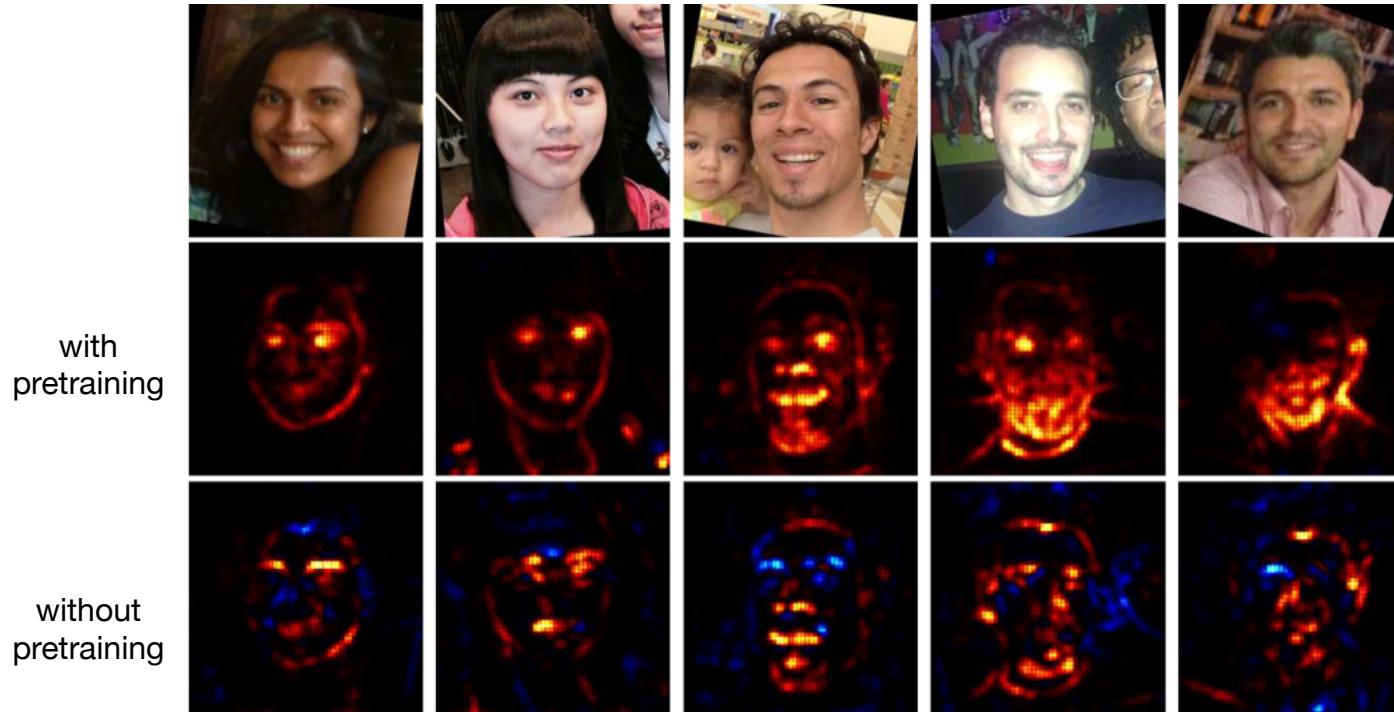
(Lapuschkin et al., 2016)

# Application: Measure Context Use



# Application: Face analysis

Gender classification

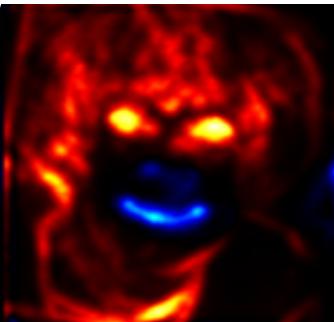
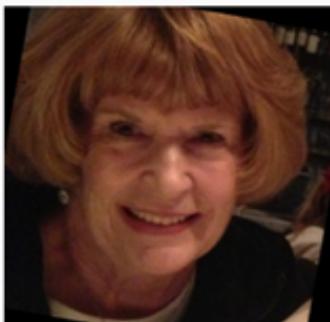


Strategy to solve the problem: Focus on chin / beard, eyes & hair,  
but without pretraining the model overfits

(Lapuschkin et al., 2017)

# Application: Face analysis

## Age classification



## Predictions

25-32 years old

Strategy to solve the problem:  
Focus on the laughing ...

60+ years old

pretraining on

ImageNet

pretraining on

IMDB-WIKI

laughing speaks against 60+  
(i.e., model learned that old  
people do not laugh)

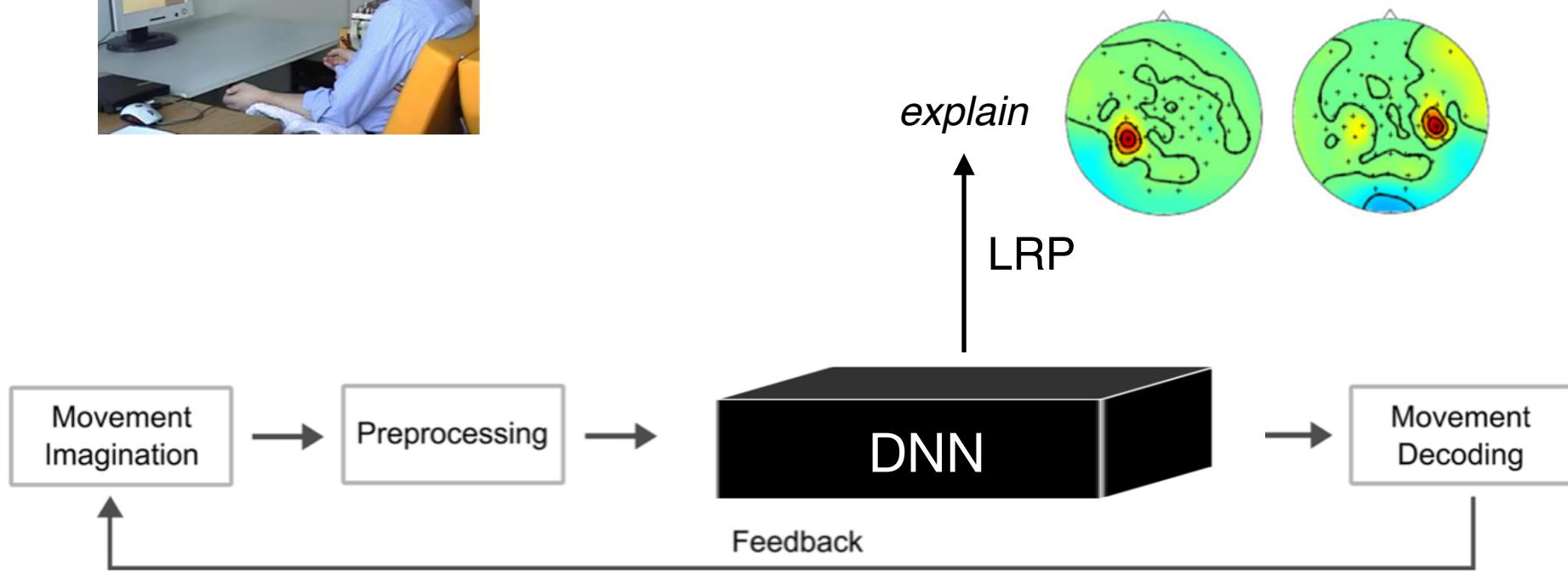
(Lapuschkin et al., 2017)

# Application: EEG Analysis

Brain-Computer  
Interfacing



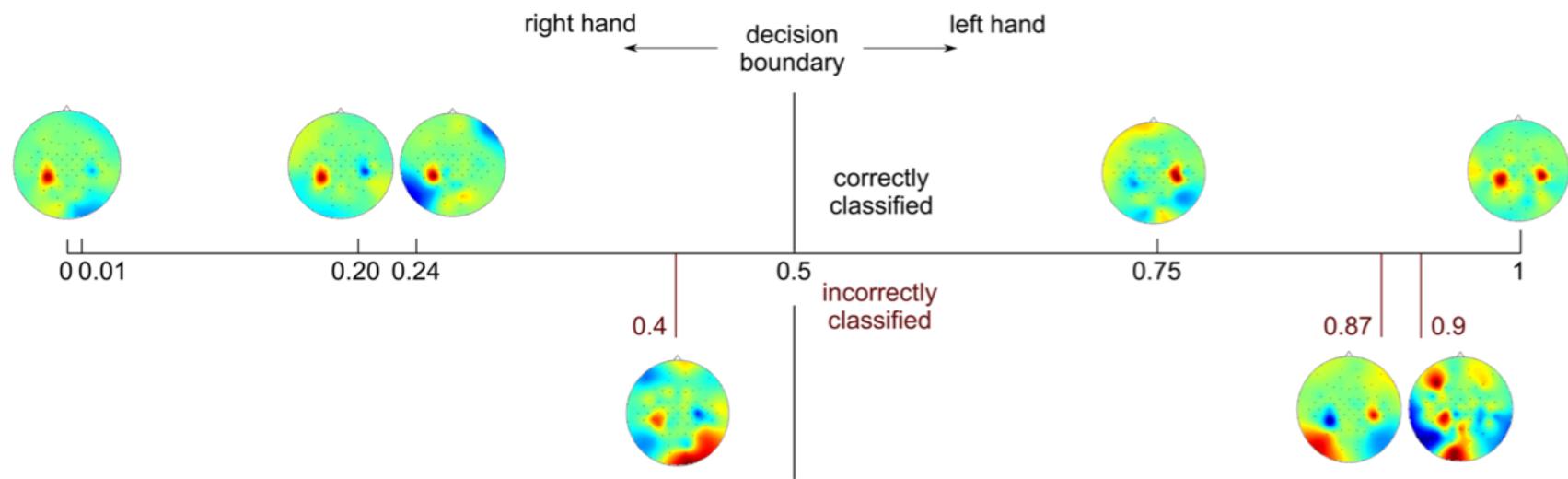
How brain works subject-dependent  
→ individual explanations



(Sturm et al. 2016)

# Application: EEG Analysis

With LRP we can analyze what made a trial being misclassified.



(Sturm et al. 2016)

# Application: Sentiment analysis

## How to handle multiplicative interactions ?

$$z_j = z_g \cdot z_s$$

$$R_g = 0 \quad R_s = R_j$$

gate neuron indirectly affect relevance distribution in forward pass

### Negative sentiment

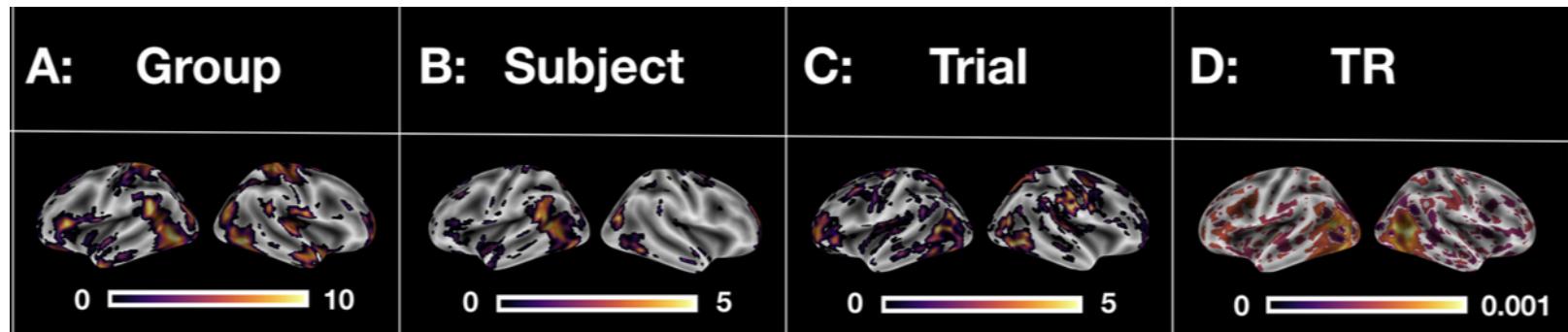
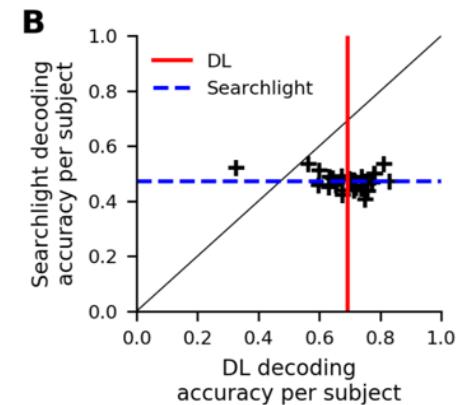
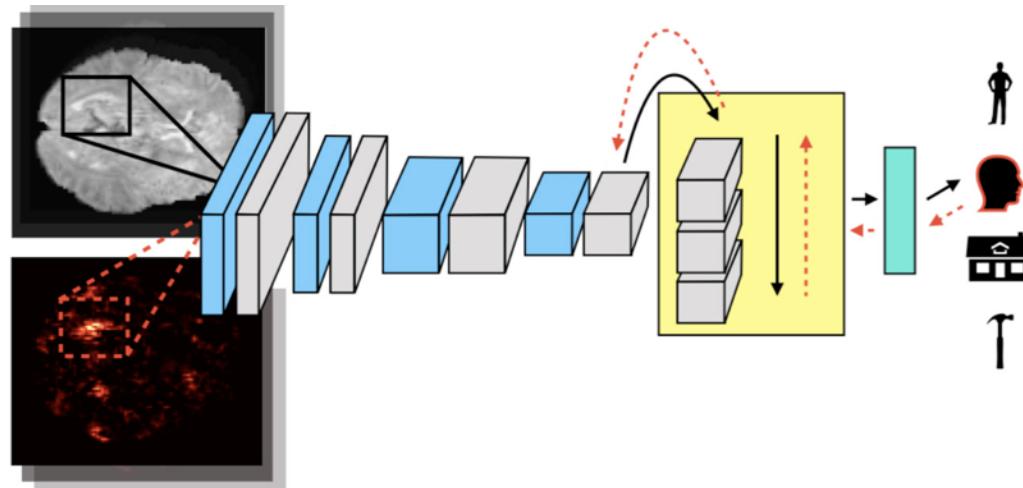
--	--	1. do n't waste your money . 2. neither funny nor suspenseful nor particularly well-drawn . 3. it 's not horrible , just horribly mediocre . 4. ... too slow , too boring , and occasionally annoying . 5. it 's neither as romantic nor as thrilling as it should be .
----	----	---

### Positive sentiment

++	++	19. a worthy entry into a very difficult genre . 20. it 's a good film -- not a classic , but odd , entertaining and authentic .
	--	21. it never fails to engage us .

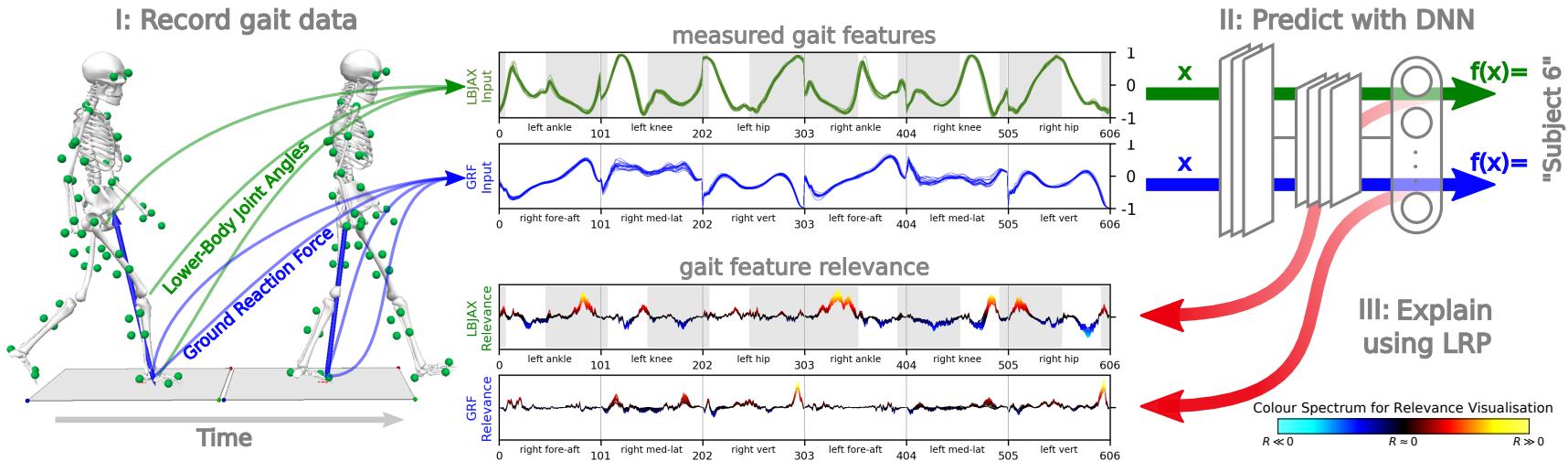
(Arras et al., 2017)

# Application: fMRI Analysis



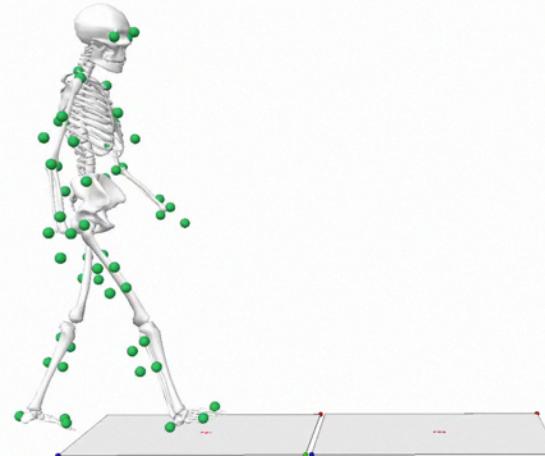
(Thomas et al. 2018)

# Application: Gait Analysis



## Our approach:

- Classify & explain individual gait patterns
- Important for understanding diseases such as Parkinson

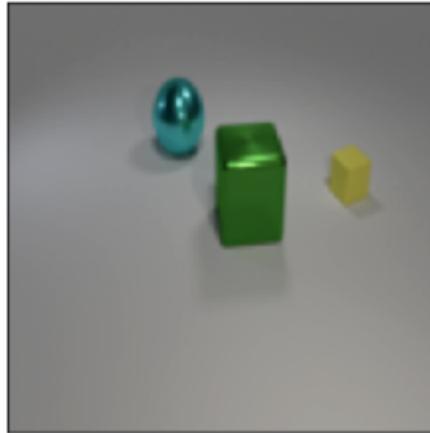


(Horst et al. 2018)

# Application: Understand the model

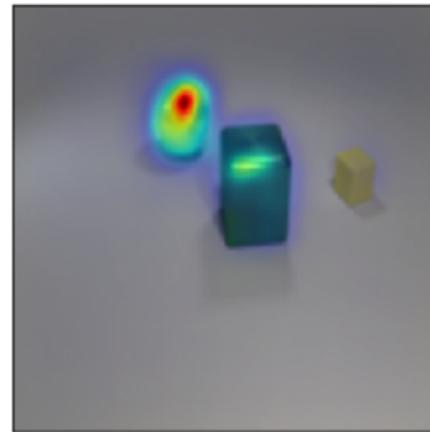
## Question

there is a metallic cube ; are  
there any large cyan metallic  
objects behind it ?



## LRP

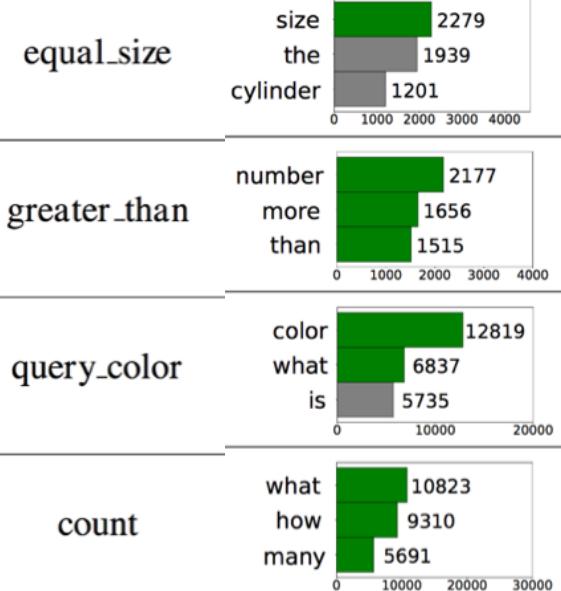
there is a metallic cube ; are  
there any large cyan metallic  
objects **behind** it ?



model understands the question and correctly identifies  
the object of interest

## Question Type

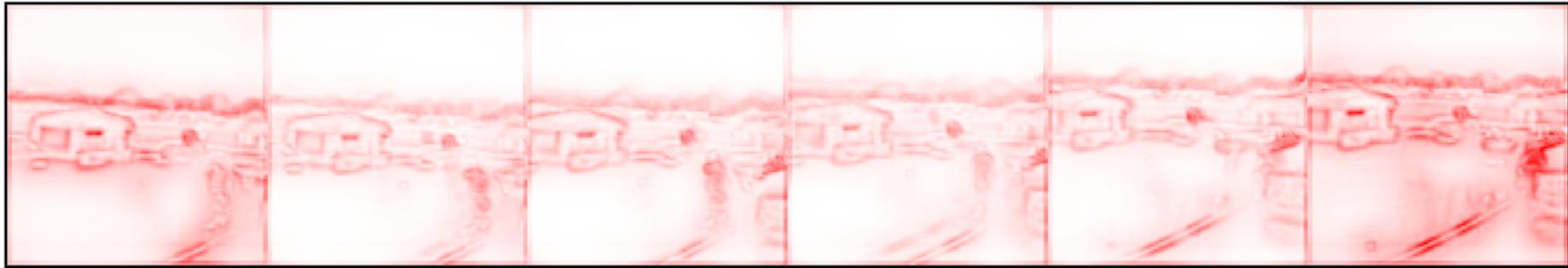
## LRP



(Arras et al., 2018)

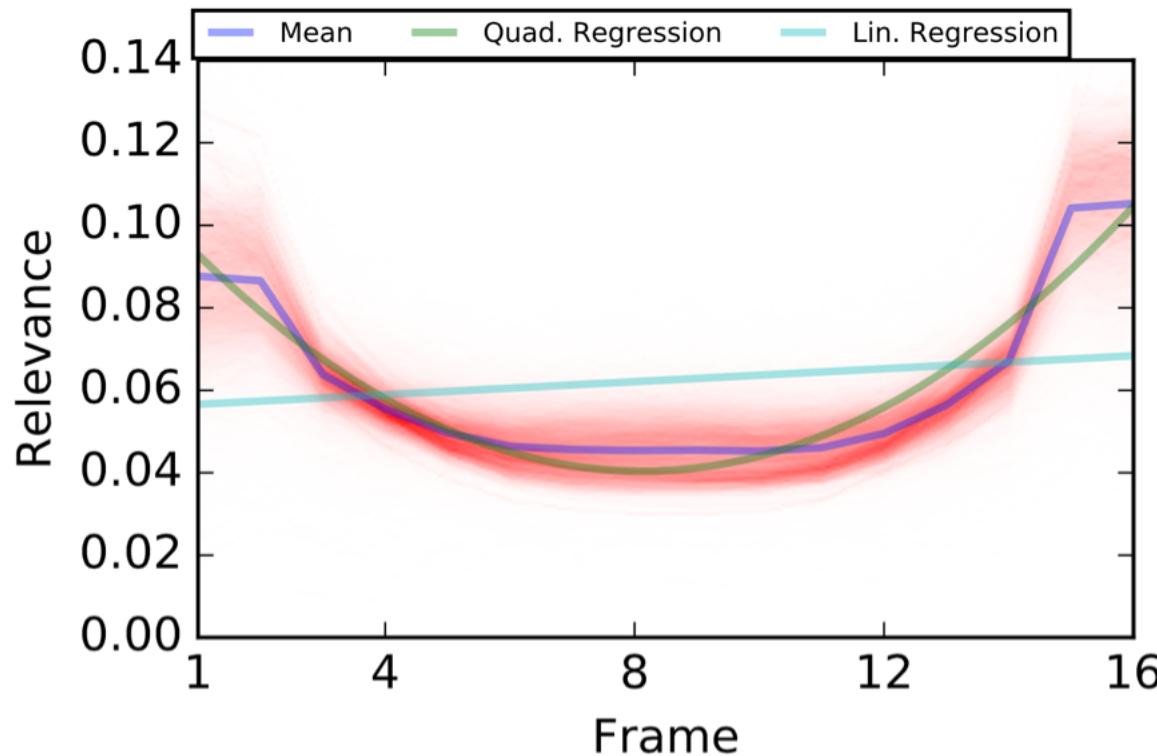
# Application: Understand the model

frame 1      frame 4      frame 7      frame 10      frame 13      frame 16



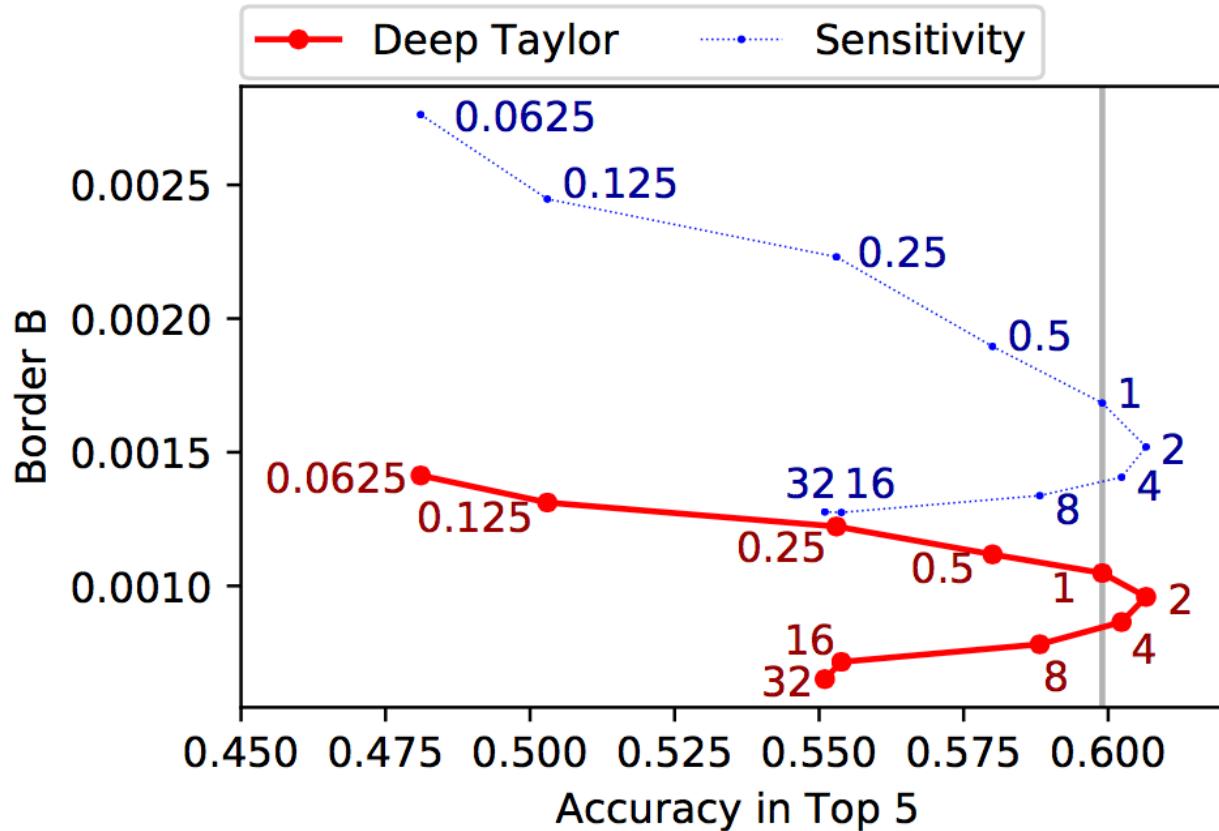
(Anders et al., 2018)

# Application: Understand the model



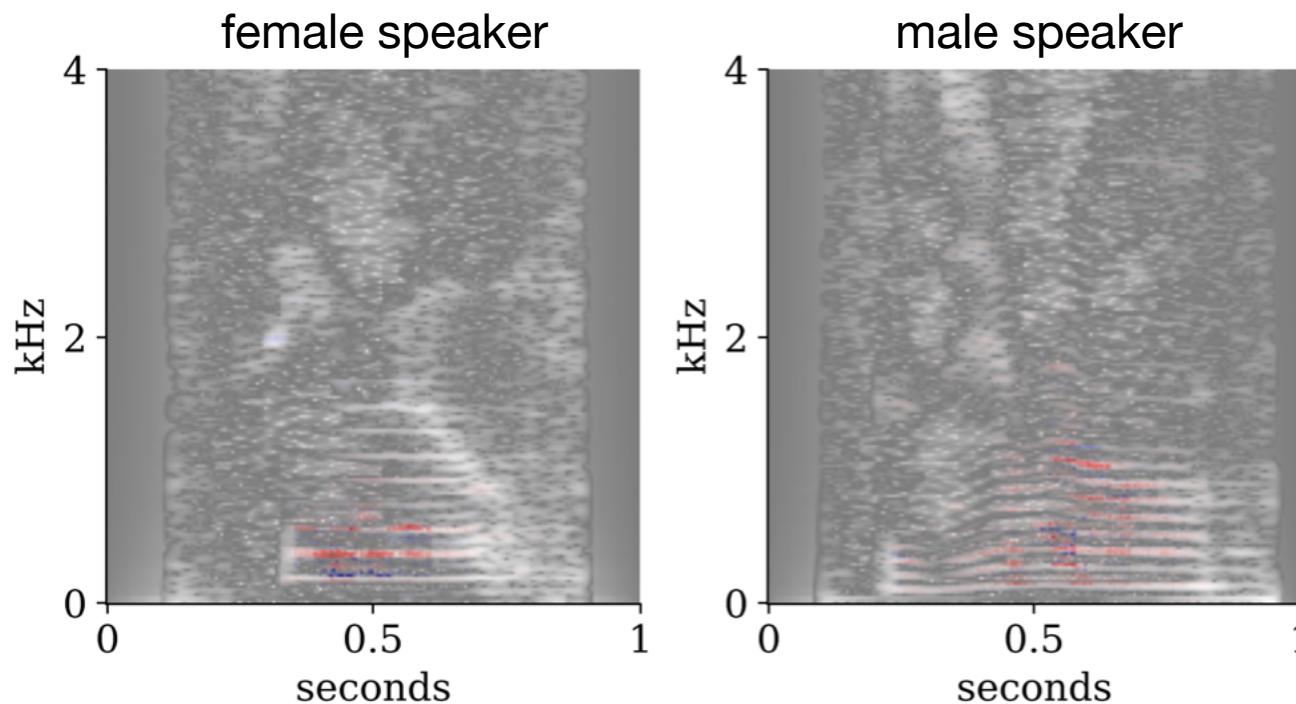
**Observation:** Explanations focus on the bordering of the video, as if it wants to watch more of it.

# Application: Understand the model



**Idea:** Play video in fast forward (without retraining) and then the classification accuracy improves.

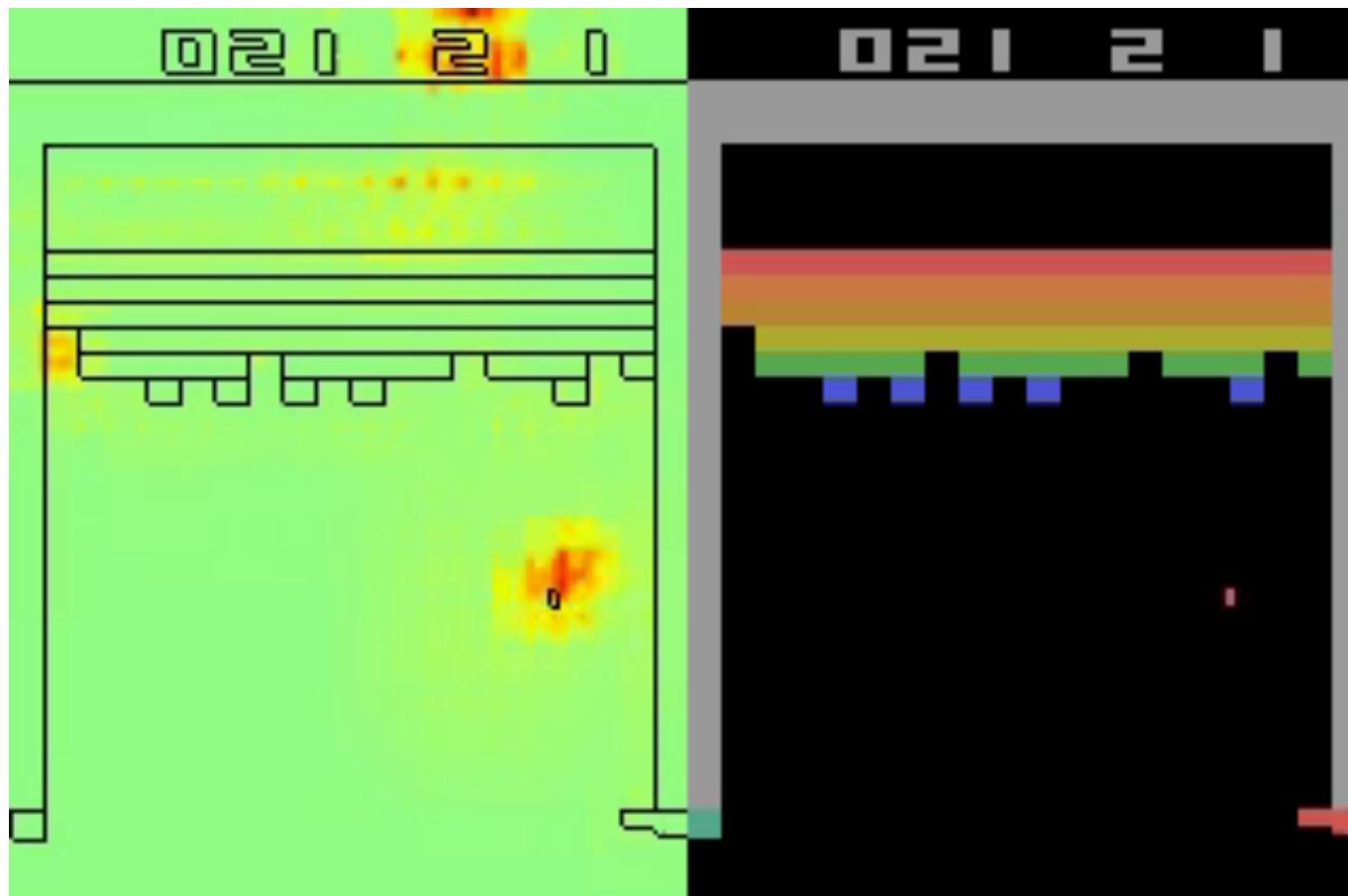
# Application: Understand the model



model classifies gender based on the fundamental frequency and its immediate harmonics (see also Traunmüller & Eriksson 1995)

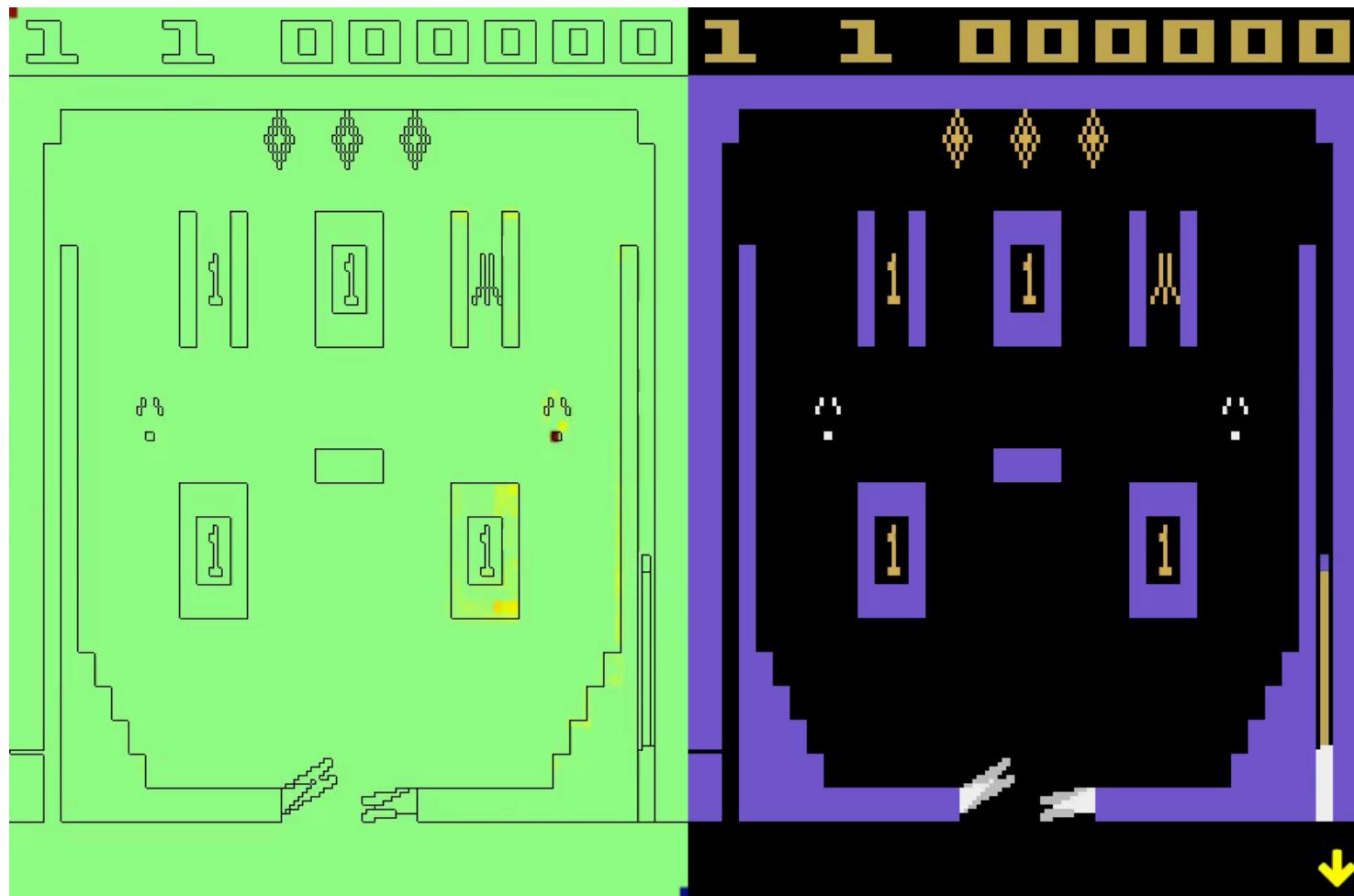
(Becker et al., 2018)

# Application: Understand the model



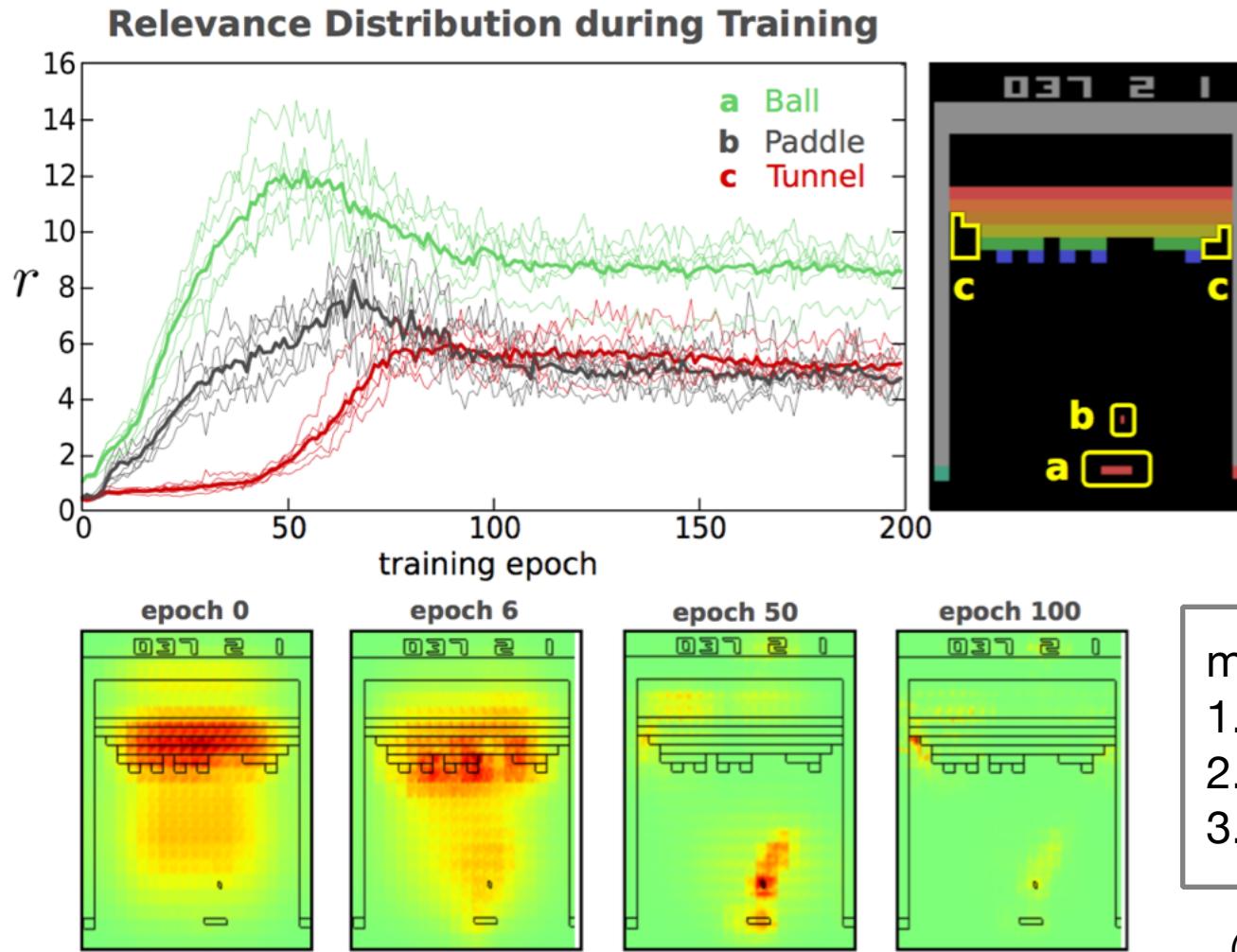
(Lapuschkin et al., in prep.)

# Application: Understand the model



(Lapuschkin et al., in prep.)

# Application: Understand the model



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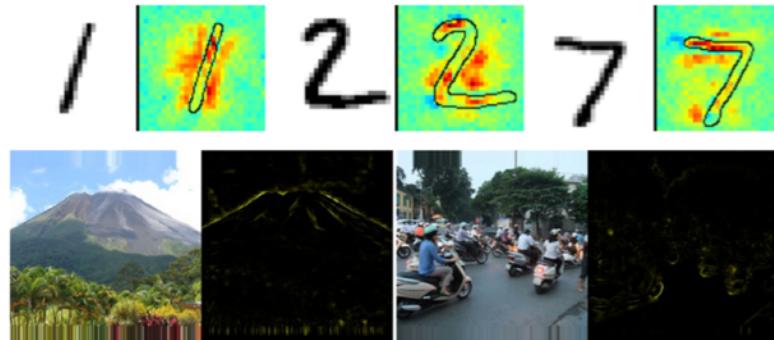
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# Thank you for your attention

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...

## Tutorial Paper

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Digital Signal Processing, 73:1-5, 2018

## Keras Explanation Toolbox

<https://github.com/albermax/innvestigate>