



Fraunhofer

Heinrich Hertz Institute

# Meta-Explanations, Interpretable Clustering & Other Recent Developments

Fraunhofer HHI, Machine Learning Group

Wojciech Samek

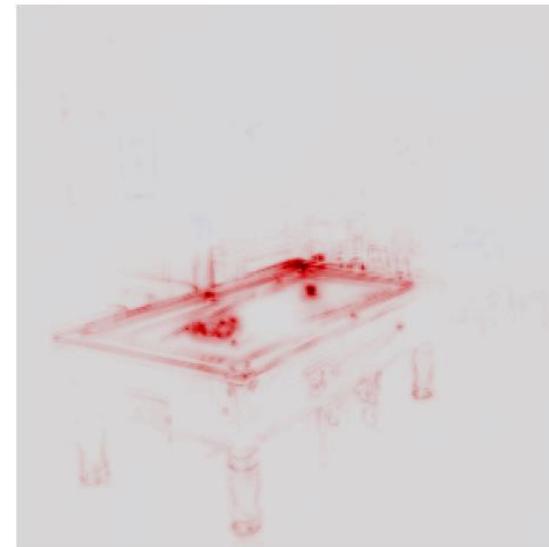


# Explaining Predictions

*“why a given image is classified as a pool table”*



some pool table



why it is classified  
as a pool table

# Today's Talk

## Which one to choose ?

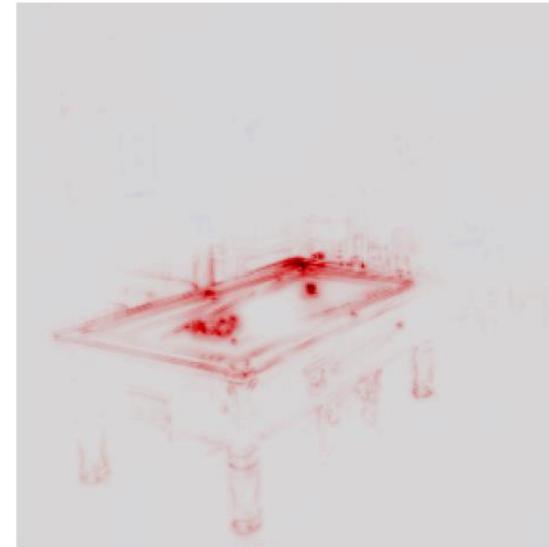


Baehrens'10 Gradient	Sundarajan'17 Int Grad	Zintgraf'17 Pred Diff	Ribeiro'16 LIME	Haufe'15 Pattern
Zurada'94 Gradient	Symonian'13 Gradient	Zeiler'14 Occlusions	Fong'17 M Perturb	Kindermans'17 PatternNet
Poulin'06 Additive	Lundberg'17 Shapley	Bazen'13 Taylor	Montavon'17 Deep Taylor	Shrikumar'17 DeepLIFT
Zeiler'14 Deconv	Landecker'13 Contrib Prop		Bach'15 LRP	Zhang'16 Excitation BP
Caruana'15 Fitted Additive	Springenberg'14 Guided BP		Zhou'16 GAP	Selvaraju'17 Grad-CAM



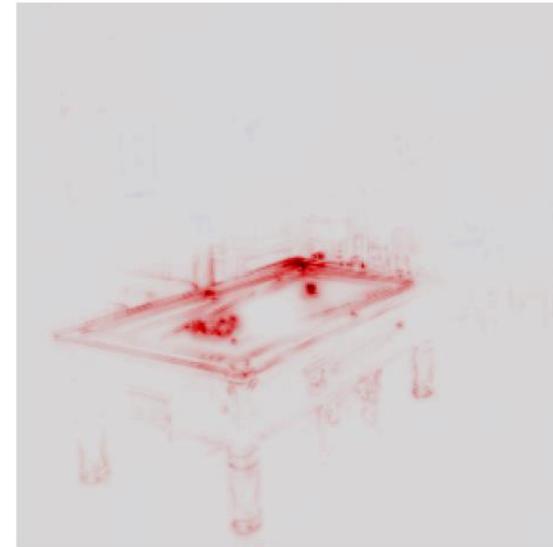
# Today's Talk

From individual explanations to  
common prediction strategies



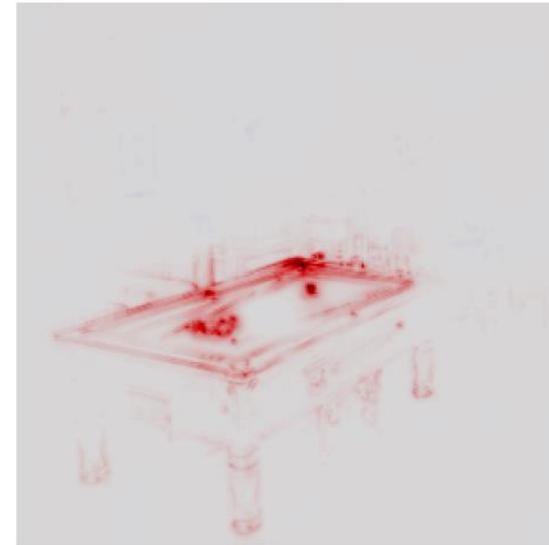
# Today's Talk

What can we do with it ?



# Today's Talk

Explaining more than classifiers



# **Explanation Methods**

# Explanation Methods

## Perturbation-Based

Occlusion-Based (Zeiler & Fergus 14)

Meaningful Perturbations (Fong & Vedaldi 17)

...

## Function-Based

Sensitivity Analysis (Simonyan et al. 14)

(Simple) Taylor Expansions

Gradient x Input (Shrikumar et al. 16)

...

## Surrogate- / Sampling-Based

LIME (Ribeiro et al. 16)

SmoothGrad (Smilkov et al. 16)

...

## Structure-Based

LRP (Bach et al. 15)

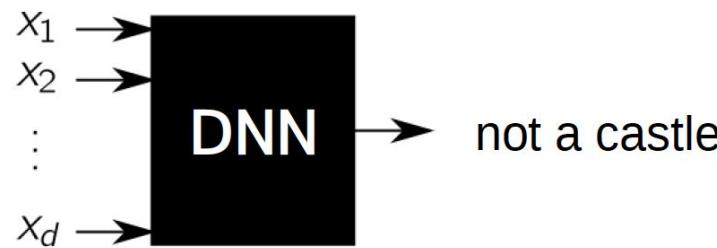
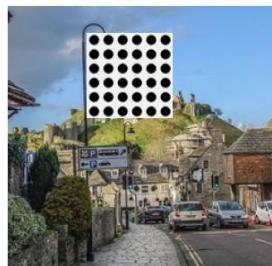
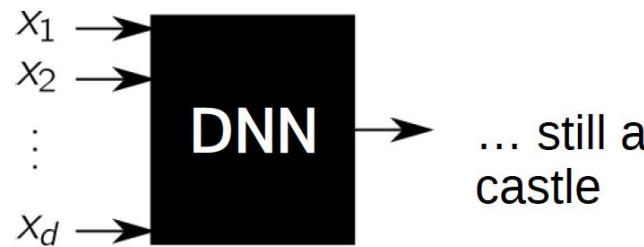
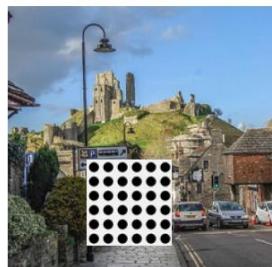
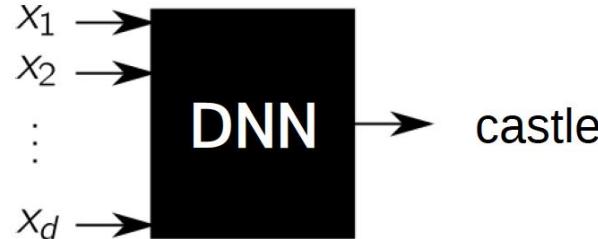
Deep Taylor Decomposition (Montavon et al. 17)

Excitation Backprop (Zhang et al. 16)

...

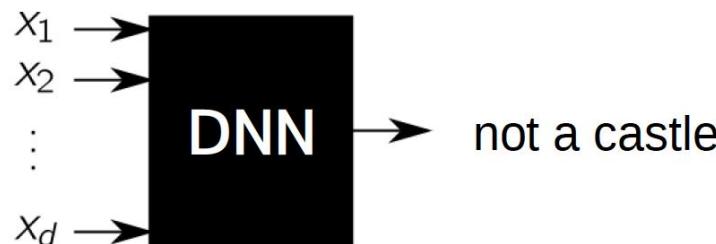
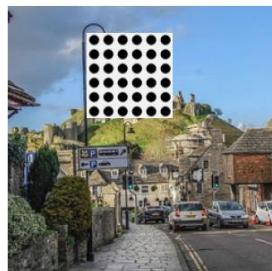
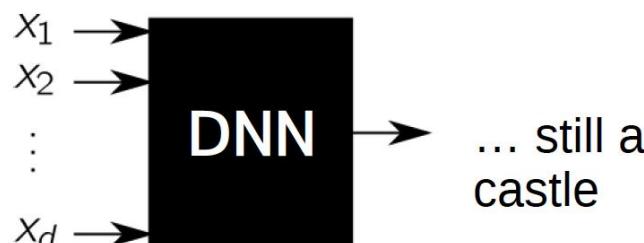
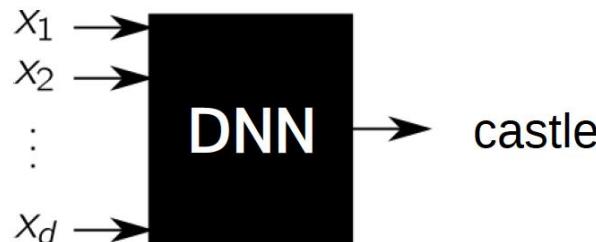
# Approach 1: Perturbation

**Idea:** Assess features relevance by testing the model response to their removal or perturbation.



# Approach 1: Perturbation

**Idea:** Assess features relevance by testing the model response to their removal or perturbation.



## Disadvantages

- slow
  - assumes locality
  - perturbation may introduce artefacts
- > unreliable

# Approach 2: (Simple) Taylor Expansions

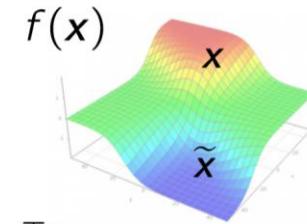
**Idea:** identify the contribution of input features as the first-order terms of a Taylor expansion

Taylor Expansion

$$f(\mathbf{x}) = f(\tilde{\mathbf{x}}) + \sum_{i=1}^d [\nabla f(\tilde{\mathbf{x}})]_i \cdot (x_i - \tilde{x}_i) + \mathcal{O}(\mathbf{x}\mathbf{x}^\top)$$



$R_i$

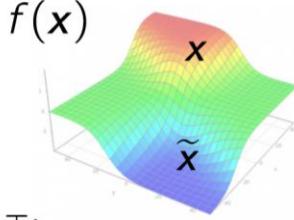


# Approach 2: (Simple) Taylor Expansions

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Taylor Expansion

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$R_i$

## Advantages

- Can be applied to *any* (differentiable and mildly nonlinear) ML model.

## Limitations

- Need to find a meaningful root point where to perform the expansion.

# Approach 3: Gradient x Input

## Motivation

- Compute an explanation in a single pass without having to optimize or search for a root point.

### Gradient x Input

$$\forall_i : R_i = [\nabla f(\mathbf{x})]_i \cdot x_i$$

$$\mathbf{R} = \nabla f(\mathbf{x}) \odot \mathbf{x}$$

**Observation:** Complex analyses reduce to gradient x input for simple cases.

# Approach 3: Gradient x Input

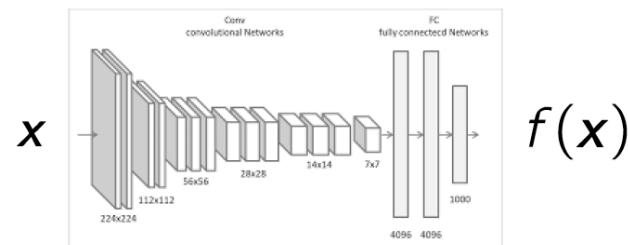
**Input**



$x$

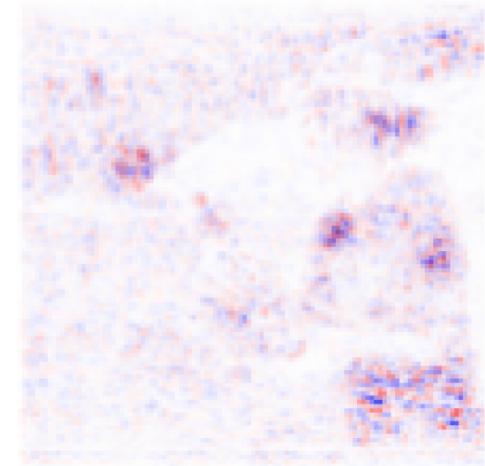
**Prediction**

(class: baseball)



$f(x)$

**Explanation**



$$R = \nabla f(x) \odot x$$

**Observation:** Explanations are noise

# Approach 3: Gradient x Input

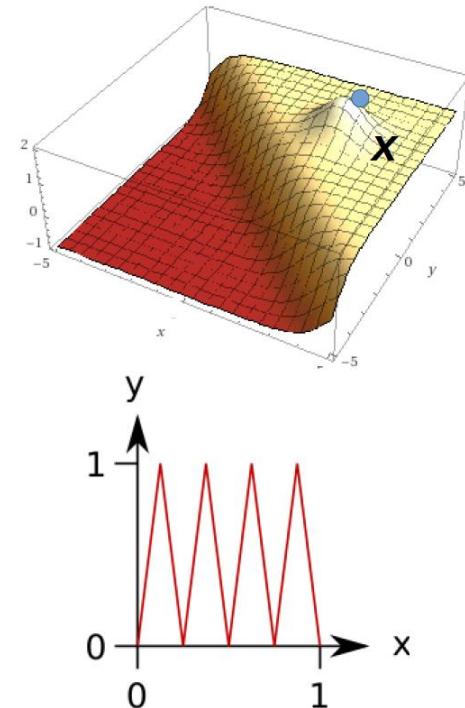
**Two reasons why gradient-based explanation are noisy**

## 1. Local vs. global variations

Global effects are not visible when looking at the function  $f(x)$  locally.

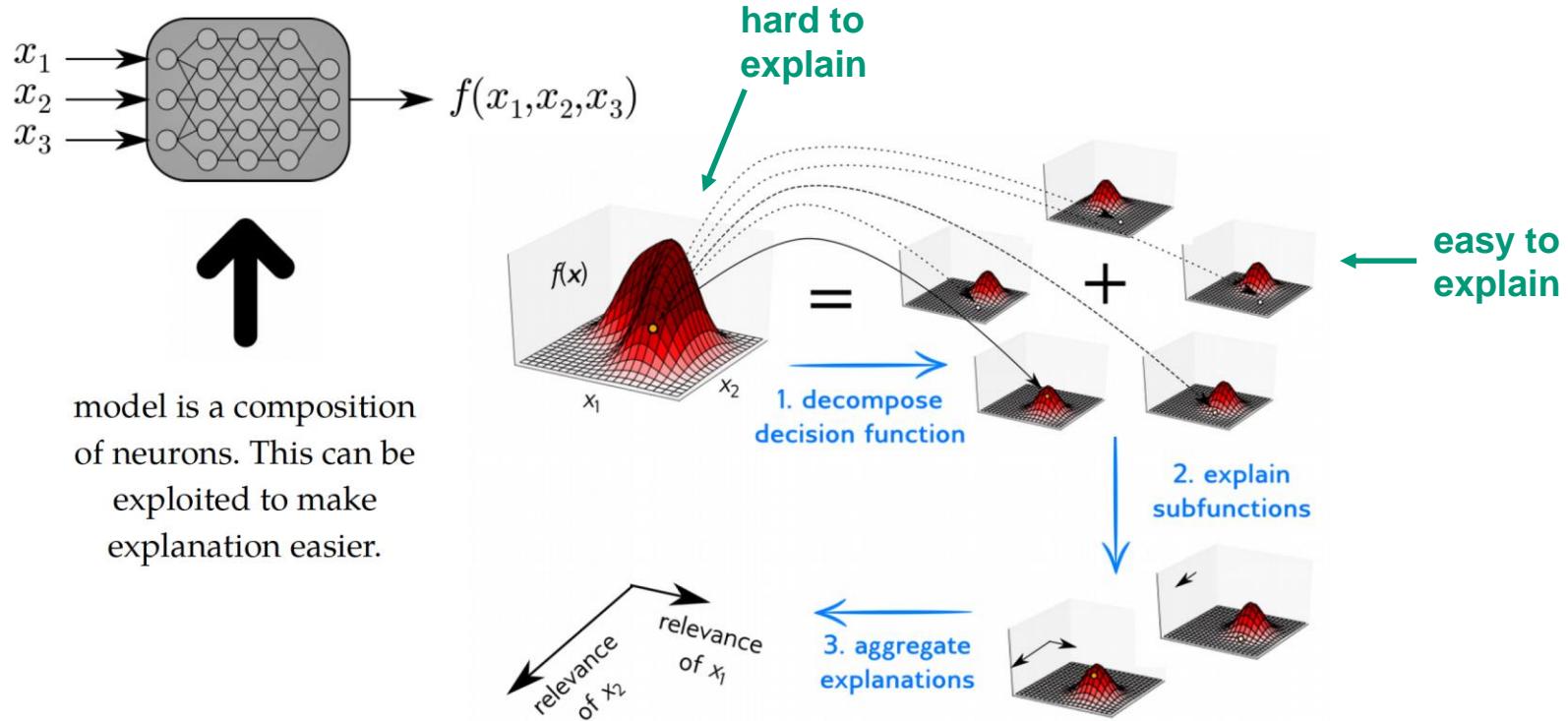
## 2. Shattered gradients

Function local variations grows exponentially with depth.

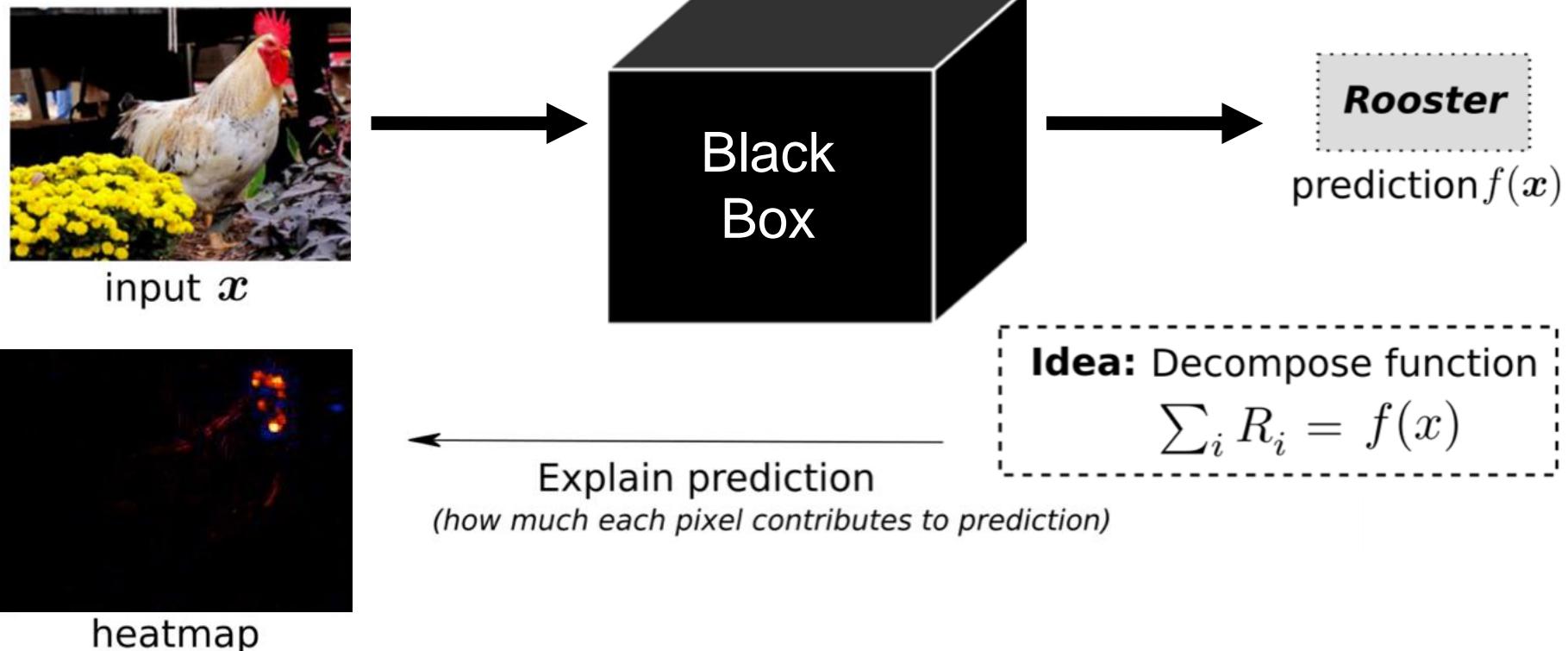


# Layer-wise Relevance Propagation

**LRP's idea:** To robustly explain a model, leverage the neural network structure of the decision function.



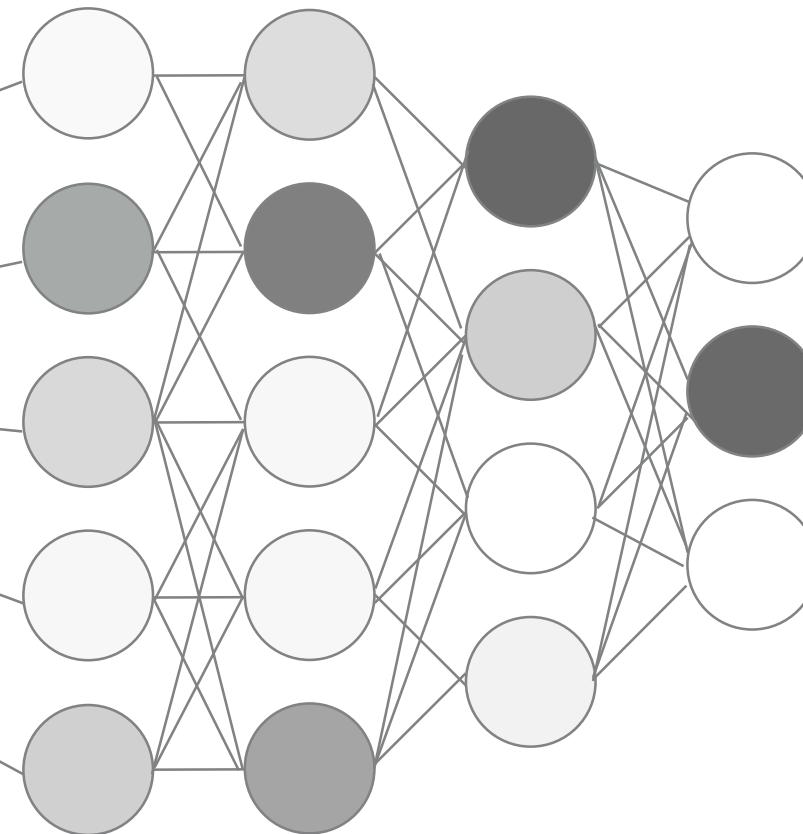
# Layer-wise Relevance Propagation



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

# Layer-wise Relevance Propagation

Classification

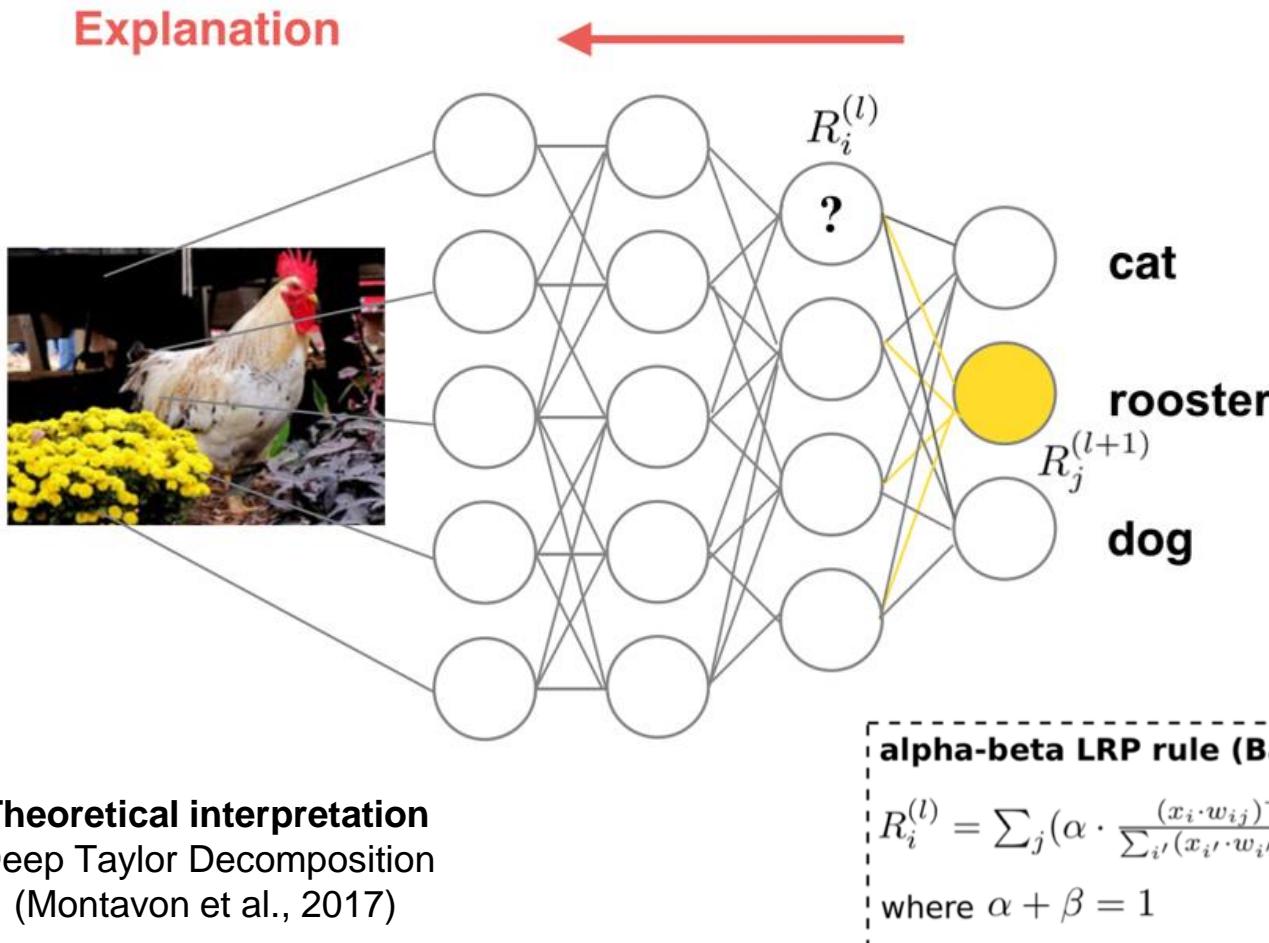


cat

rooster

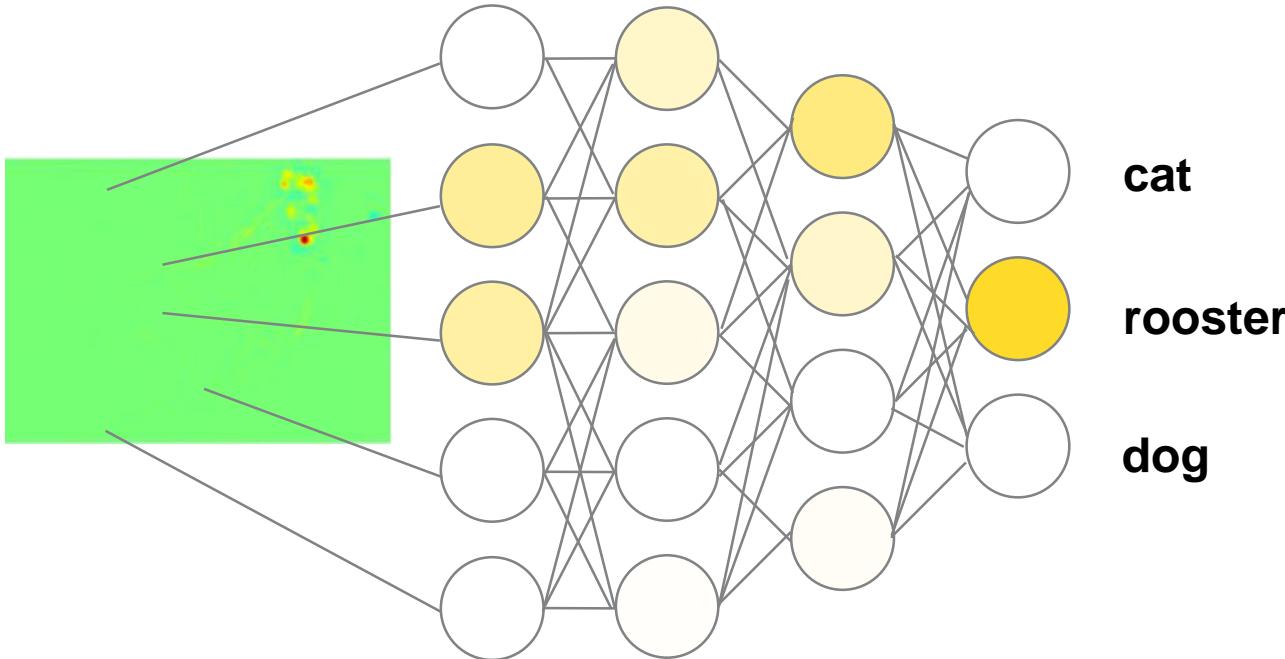
dog

# Layer-wise Relevance Propagation



# Layer-wise Relevance Propagation

Explanation



Layer-wise relevance conservation

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

# Equivalence

LRP- $\alpha_1\beta_0$

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

Layer-wise Relevance Propagation  
(Bach'15)



DTD- $\mathbf{z}^+$

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

Deep Taylor Decomposition  
(Montavon'17, arXiv in 2015)



Marginal Winning Probability

$$P(a_i) = \sum_{a_j \in \mathcal{P}_i} P(a_i|a_j)P(a_j) \quad P(a_i|a_j) = \begin{cases} Z_j \hat{a}_i w_{ij} & \text{if } w_{ij} \geq 0, \\ 0 & \text{otherwise.} \end{cases}$$

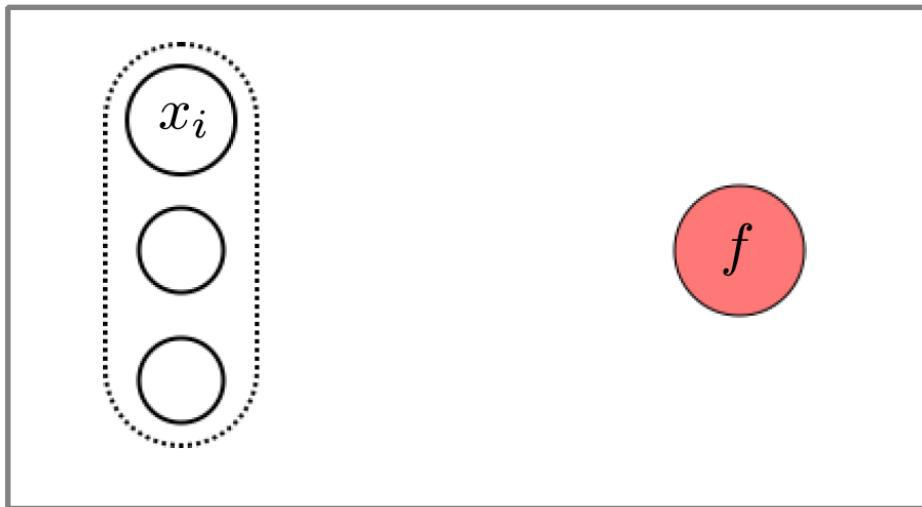
**A1** activations non-negative

$$Z_j = 1 / \sum_{i: w_{ij} \geq 0} \hat{a}_i w_{ij}$$

Excitation Backprop  
(Zhang'16)

# Simple Taylor Decomposition

$$\mathbf{x} \mapsto f(\mathbf{x})$$



$$f(\mathbf{x}) = f(\tilde{\mathbf{x}}) + \sum_{i=1}^d [\nabla f(\tilde{\mathbf{x}})]_i \cdot (x_i - \tilde{x}_i) + \mathcal{O}(\mathbf{x}\mathbf{x}^\top)$$

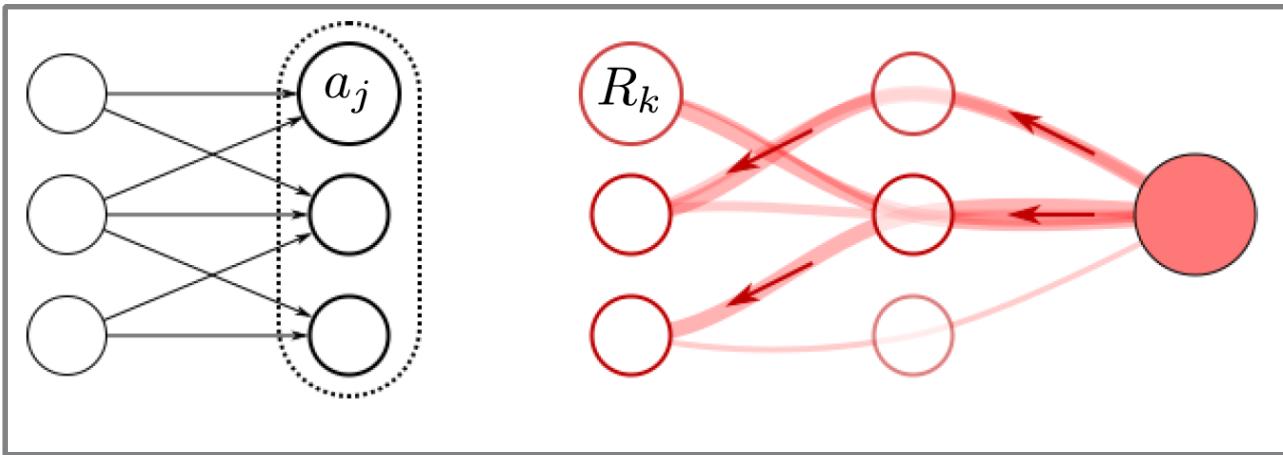
**Idea:** Use Taylor expansion to redistribute relevance from output to input

**Limitations:**

- difficult to find good root point
- gradient shattering

# Deep Taylor Decomposition

$$\mathbf{a} \mapsto R_k(\mathbf{a})$$



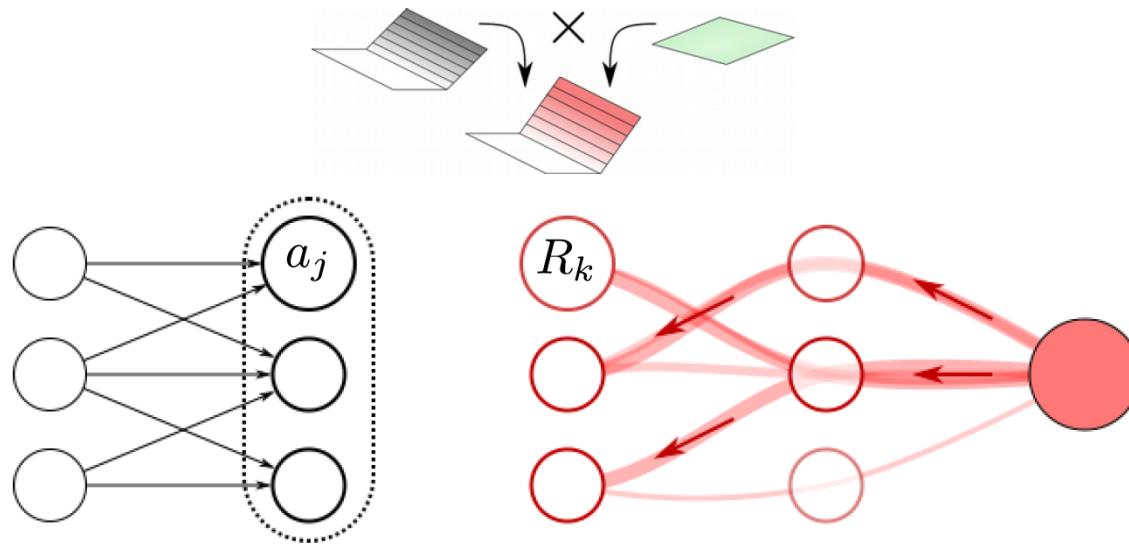
$$R_k(\mathbf{a}) = R_k(\tilde{\mathbf{a}}) + \sum_j [\nabla R_k(\tilde{\mathbf{a}})]_j \cdot (a_j - \tilde{a}_j) + \mathcal{O}(\mathbf{a}\mathbf{a}^\top)$$

**Idea:** Use Taylor expansion to redistribute relevance from one layer to another

## Advantage:

- easy to find good root point
- no gradient shattering

# Deep Taylor Decomposition



**Key Idea:** Use a “relevance model” that is easy to analyze

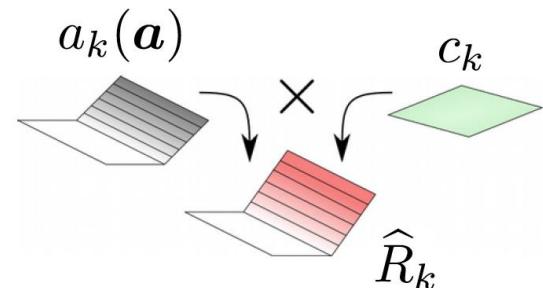
$$\hat{R}_k(\mathbf{a}) = \max(0, \sum_j a_j w_{jk}) c_k$$

(Montavon et al., 2017)

# Deep Taylor Decomposition

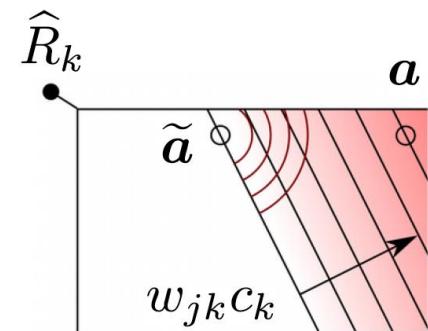
## 1. Relevance model

$$\widehat{R}_k(\mathbf{a}) = \max(0, \sum_j a_j w_{jk}) c_k$$



## 2. Taylor expansion

$$\widehat{R}_k(\mathbf{a}) = \widehat{R}_k(\tilde{\mathbf{a}}) + \sum_j \underbrace{(a_j - \tilde{a}_j) \cdot w_{jk} c_k}_{R_{j \leftarrow k}} + 0$$



## 3. Choosing the reference point

$$\tilde{\mathbf{a}}^{(k)} = \mathbf{0} \quad \leftrightarrow \quad \rho = (\cdot), \epsilon = 0 \quad (\text{LRP-0})$$

$$\tilde{\mathbf{a}}^{(k)} = \mathbf{a} - t \cdot \mathbf{a} \quad \leftrightarrow \quad \rho = (\cdot), \epsilon = (t^{-1} - 1) \cdot a_k \quad (\text{LRP-}\epsilon)$$

$$\tilde{\mathbf{a}}^{(k)} = \mathbf{a} - t \cdot \mathbf{a} \odot \mathbf{1}_{w_k > 0} \quad \leftrightarrow \quad \rho = \max(0, \cdot) \quad (\text{LRP-}\gamma)$$

(Montavon et al., 2017)

# Various LRP Rules

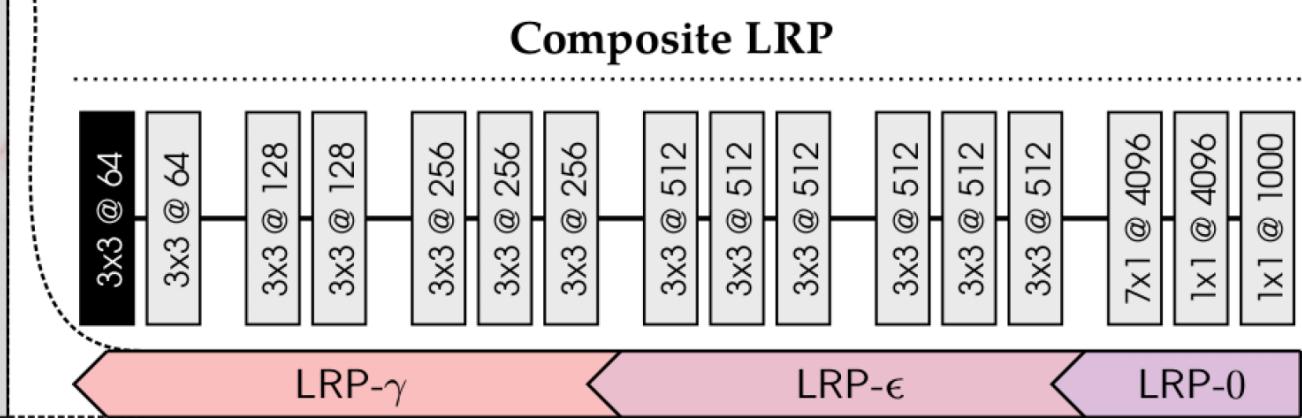
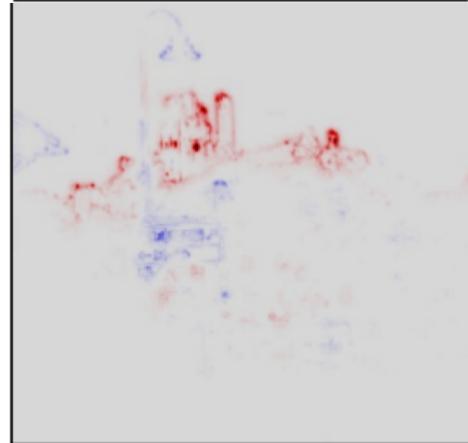
Name	Formula	Usage	DTD
LRP-0 [7]	$R_j = \sum_k \frac{a_j w_{jk}}{\sum_{0,j} a_j w_{jk}} R_k$	upper layers	✓
LRP- $\epsilon$ [7]	$R_j = \sum_k \frac{a_j w_{jk}}{\epsilon + \sum_{0,j} a_j w_{jk}} R_k$	middle layers	✓
LRP- $\gamma$	$R_j = \sum_k \frac{a_j (w_{jk} + \gamma w_{jk}^+)}{\sum_{0,j} a_j (w_{jk} + \gamma w_{jk}^+)} R_k$	lower layers	✓
LRP- $\alpha\beta$ [7]	$R_j = \sum_k \left( \alpha \frac{(a_j w_{jk})^+}{\sum_{0,j} (a_j w_{jk})^+} - \beta \frac{(a_j w_{jk})^-}{\sum_{0,j} (a_j w_{jk})^-} \right) R_k$	lower layers	✗*
flat [30]	$R_j = \sum_k \frac{1}{\sum_j 1} R_k$	lower layers	✗
$w^2$ -rule [36]	$R_i = \sum_j \frac{w_{ij}^2}{\sum_i w_{ij}^2} R_j$	first layer ( $\mathbb{R}^d$ )	✓
$z^B$ -rule [36]	$R_i = \sum_j \frac{x_i w_{ij} - l_i w_{ij}^+ - h_i w_{ij}^-}{\sum_i x_i w_{ij} - l_i w_{ij}^+ - h_i w_{ij}^-} R_j$	first layer (pixels)	✓

(\* DTD interpretation only for the case  $\alpha = 1, \beta = 0.$ )

# Best Practice for LRP



**Principle:** Explain each layer type (input, conv., fully connected layer) with the optimal rule according to DTD.



(Montavon et al., 2019)  
(Kohlbrenner et al., 2019)

# Which one to choose ?

Baehrens'10 Gradient	Sundarajan'17 Int Grad	Zintgraf'17 Pred Diff	Ribeiro'16 LIME	Haufe'15 Pattern
Zurada'94 Gradient	Symonian'13 Gradient	Zeiler'14 Occlusions	Fong'17 M Perturb	Kindermans'17 PatternNet
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Caruana'15 Fitted Additive	Springenberg'14 Guided BP		Zhou'16 GAP	Selvaraju'17 Grad-CAM

# Evaluating Explanations

Perturbation Analysis

[Bach'15, Samek'17, Arras'17, ...]

Pointing Game  
[Zhang'16]

Using Axioms

[Montavon'17, Sundararajan'17, Lundberg'17, ...]

Task Specific Evaluation  
[Poerner'18]

Solve other Tasks  
[Arras'17, Arjona-Medina'18, ...]

Using Ground Truth  
[Arras'19]

Human Judgement  
[Ribeiro'16, Nguyen'18 ...]

# **Applications of XAI**

# LRP Applied to Different Problems

General Images (Bach' 15, Lapuschkin'16)



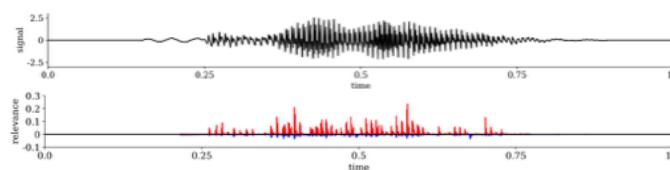
Games (Lapuschkin'19)



Faces (Lapuschkin'17)



Speech (Becker'18)



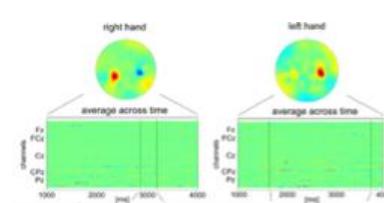
VQA (Samek'19)



Video (Anders'19)



EEG (Sturm'16)



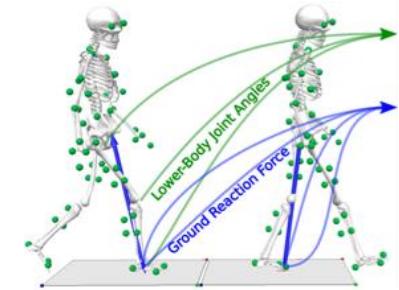
Text Analysis (Arras'16 & 17)

do n't waste your money  
neither funny nor susper

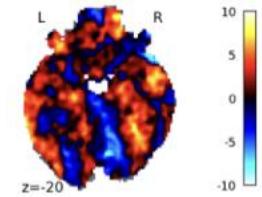
Morphing Attacks (Seibold'18)



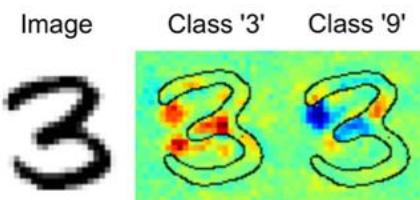
Gait Patterns (Horst'19)



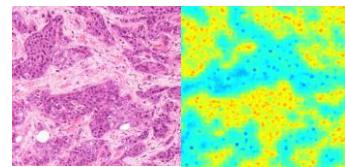
fMRI (Thomas'18)



Digits (Bach' 15)

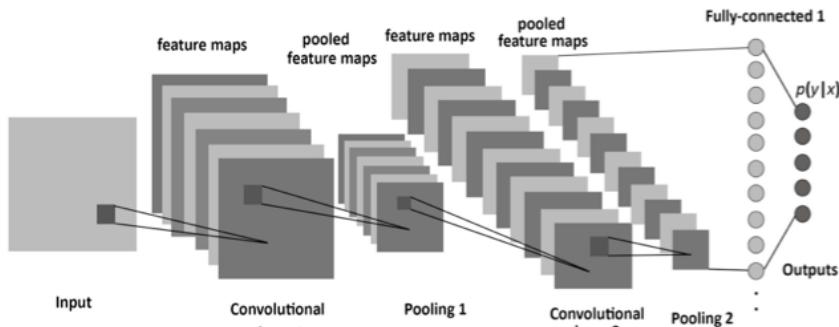


Histopathology (Hägele'19)

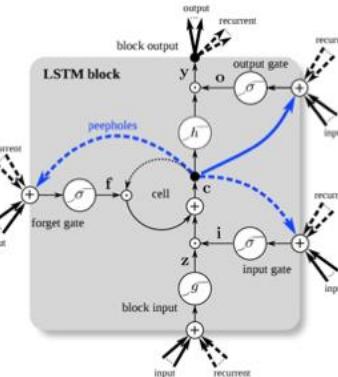


# LRP Applied to Different Models

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

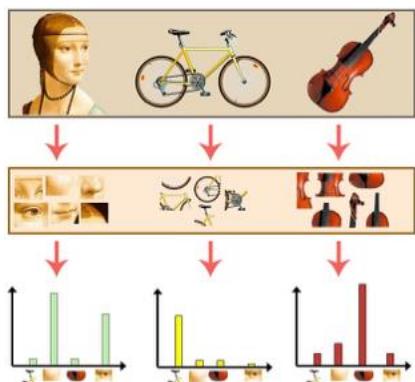


LSTM (Arras'17, Arras'19)

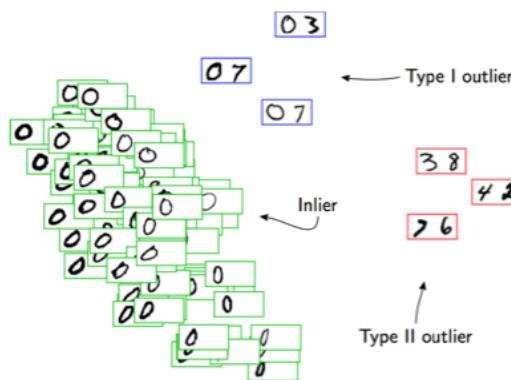


"Explaining and  
Interpreting LSTMs"  
(with S. Hochreiter)

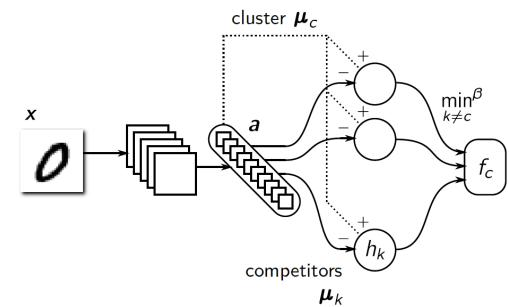
BoW / Fisher Vector models  
(Bach'15, Arras'16, Lapuschkin'16 ...)



One-class SVM (Kauffmann'18)



Clustering (Kauffmann'19)



# Unmasking Clever Hans Predictors

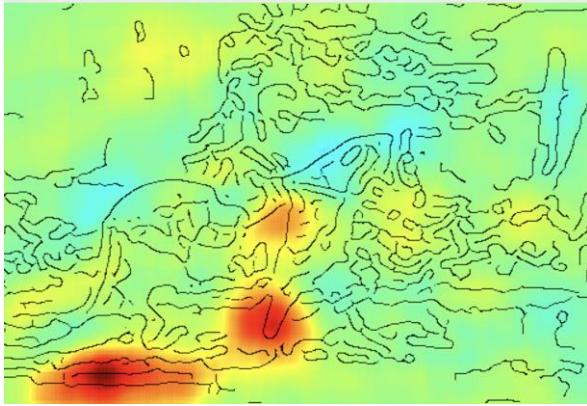
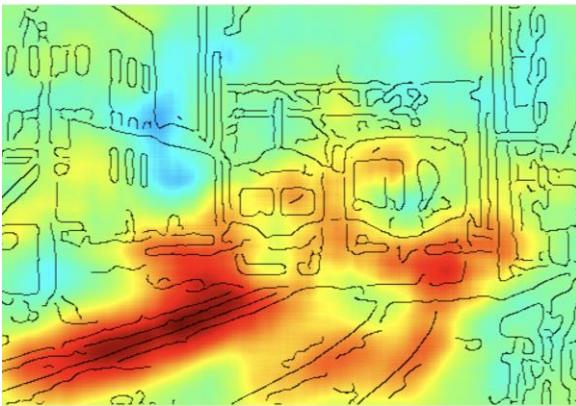
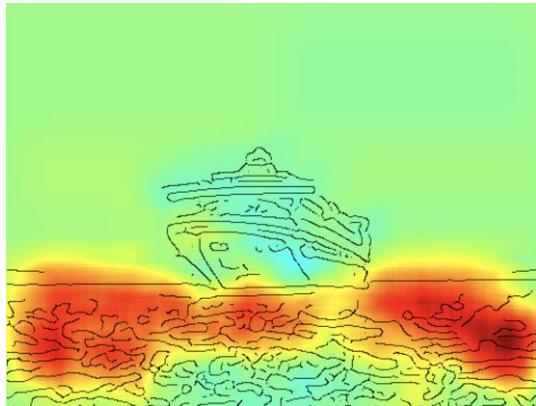
Leading method (Fisher-Vector / SVM Model) of PASCAL VOC challenge



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

# Unmasking Clever Hans Predictors

Leading method (Fisher-Vector / SVM Model) of PASCAL VOC challenge



Unmasking Clever Hans predictors and  
assessing what machines really learn

# Unmasking Clever Hans Predictors



'horse' images in PASCAL VOC 2007

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# Identifying Biases

## Smiling as a contradictor of age



### Predictions

25-32 years old

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

60+ years old

pretraining on

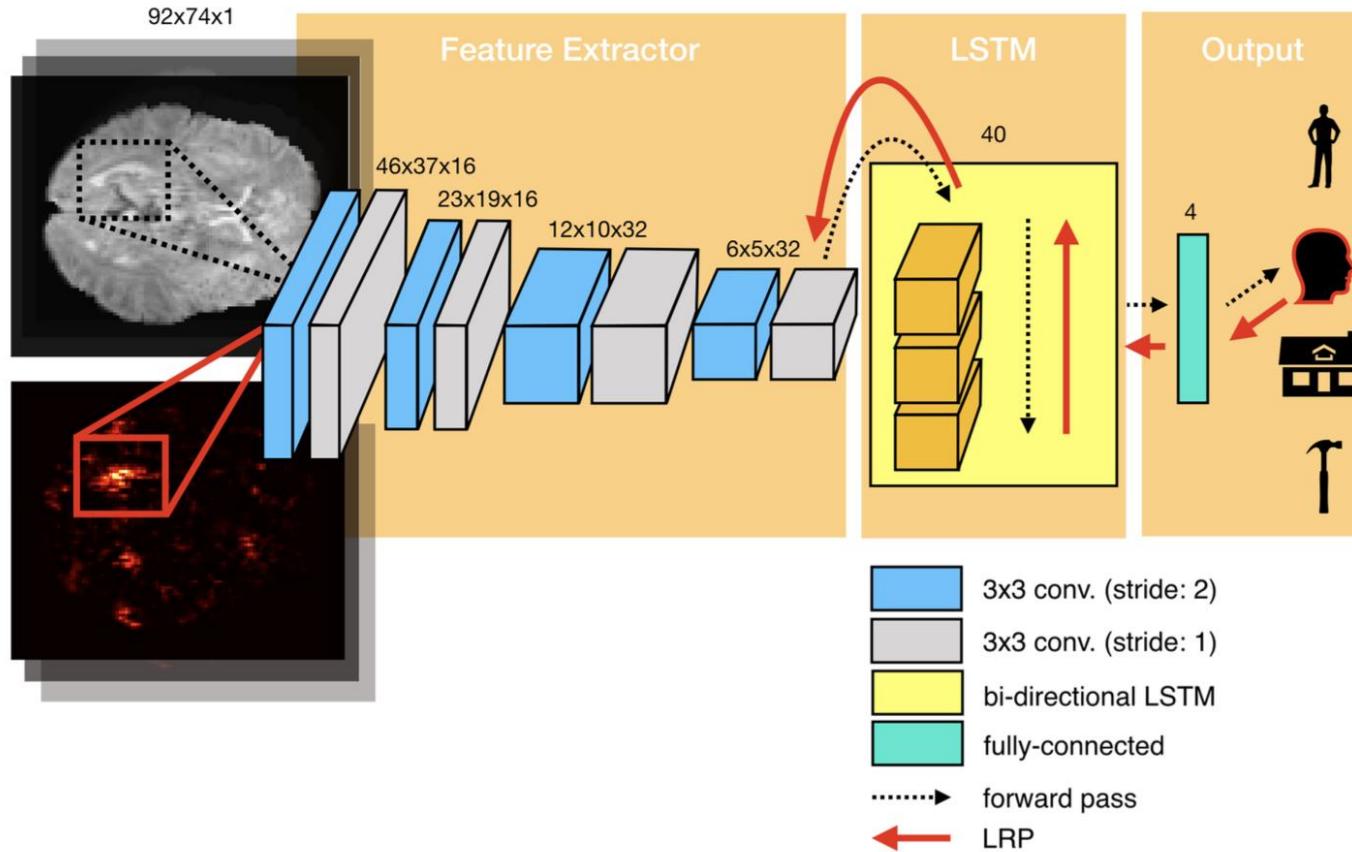
ImageNet

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

State-of-the-art DNN model, Adience Dataset (26k faces)

(Lapuschkin et al. 2017)

# Scientific Insights

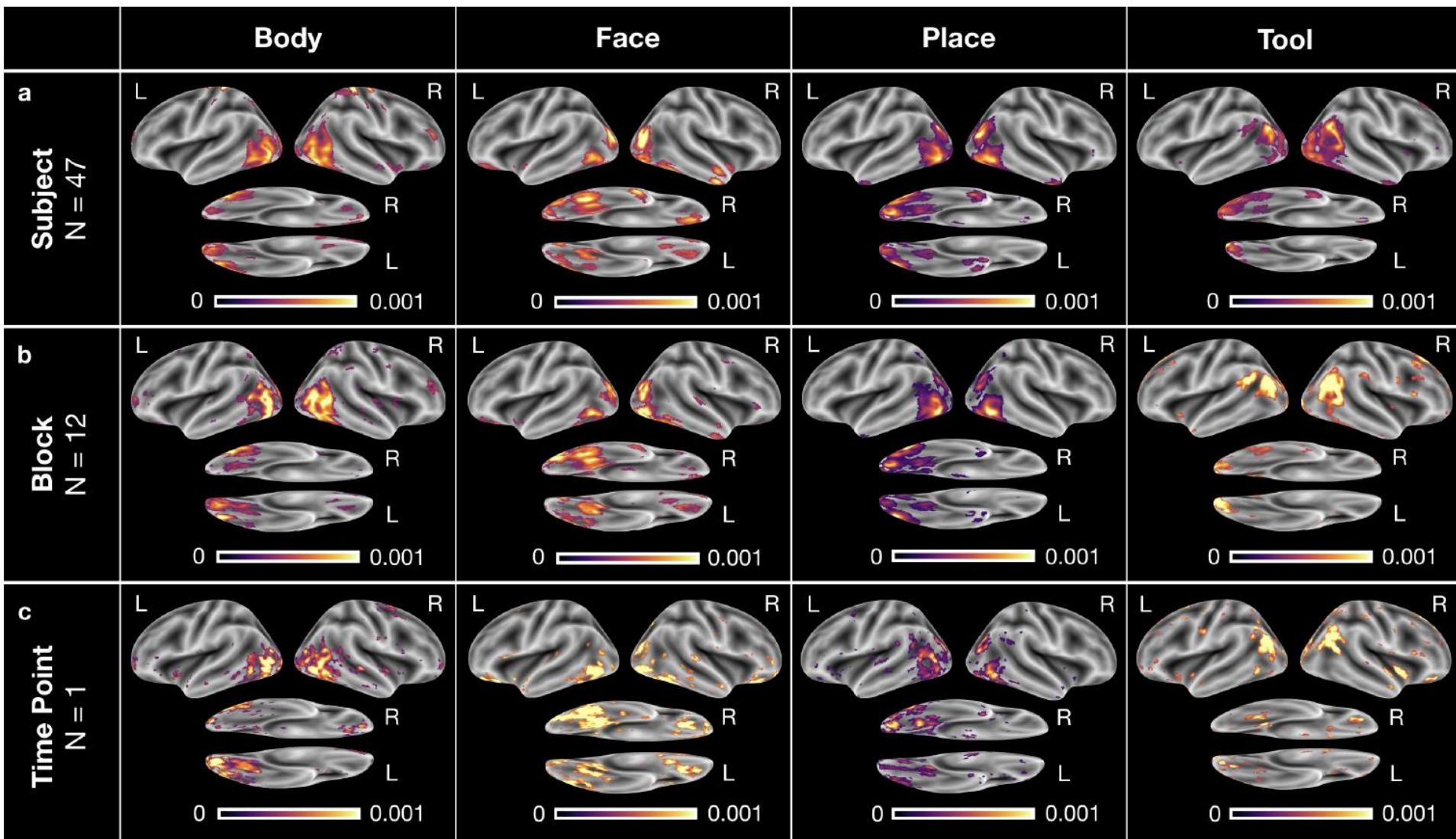


## Our approach:

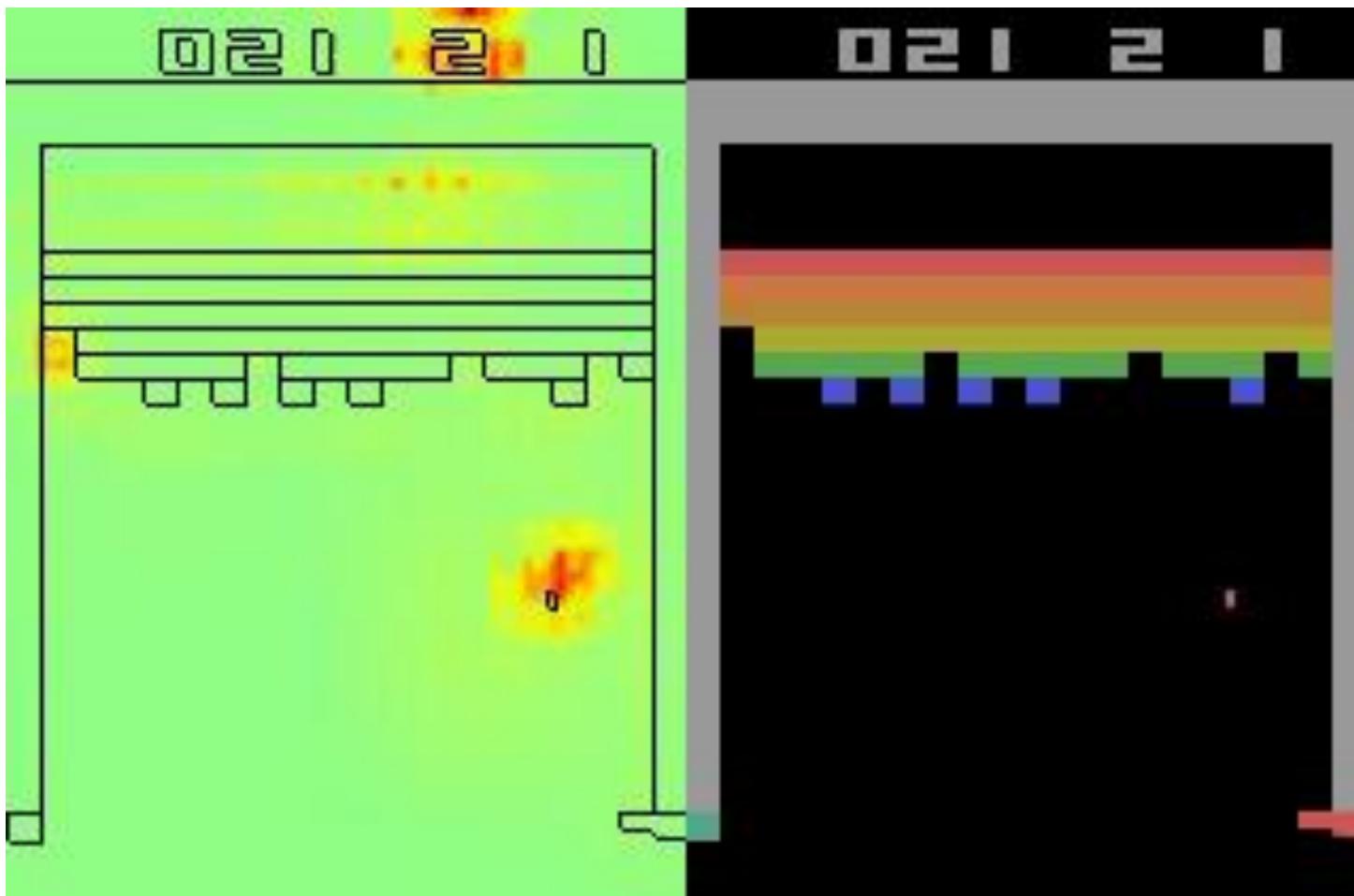
- Recurrent neural networks (CNN + LSTM) for whole-brain analysis
- LRP allows to interpret the results

(Thomas et al. 2018)

# Scientific Insights

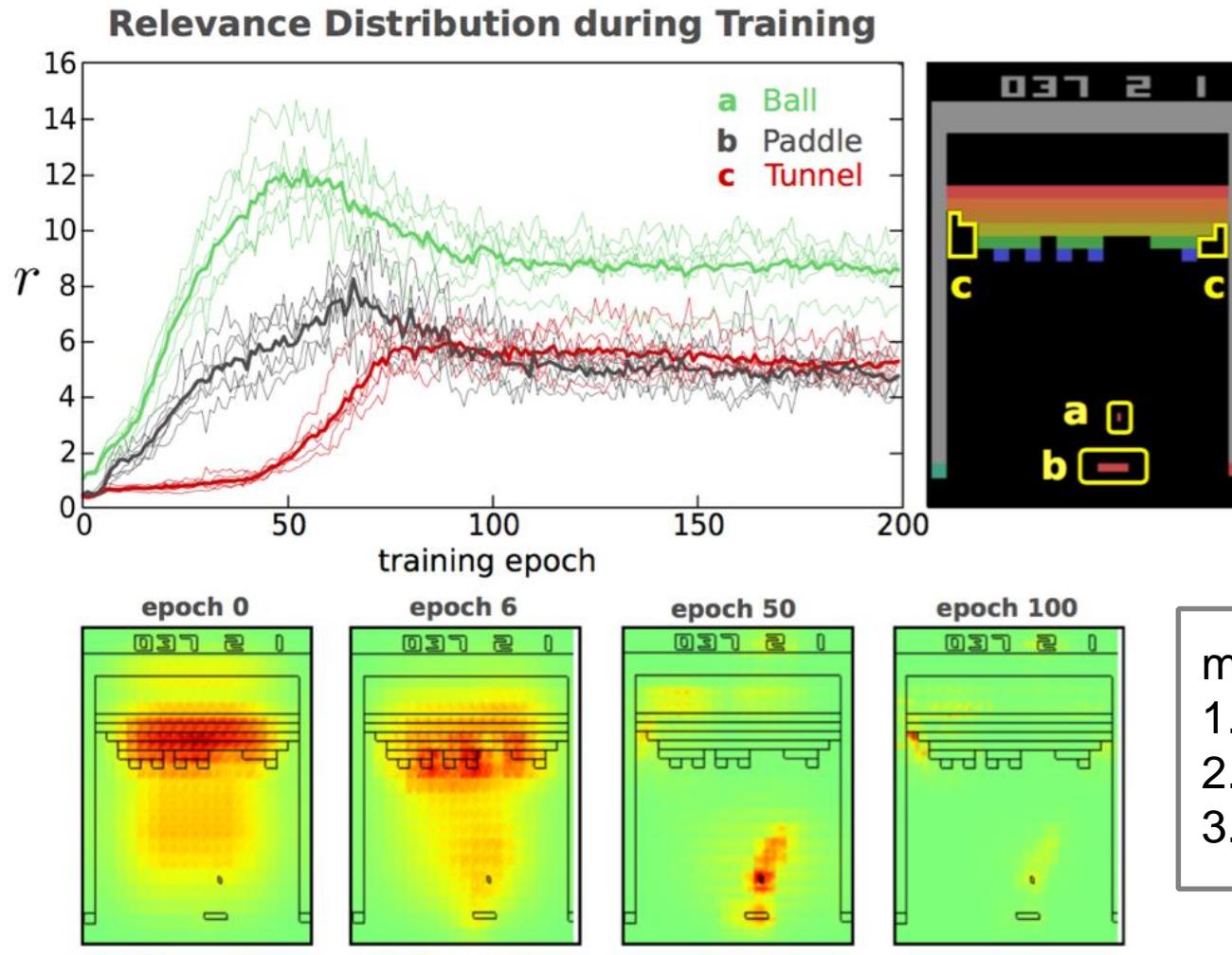


# Understanding Learning Behaviour



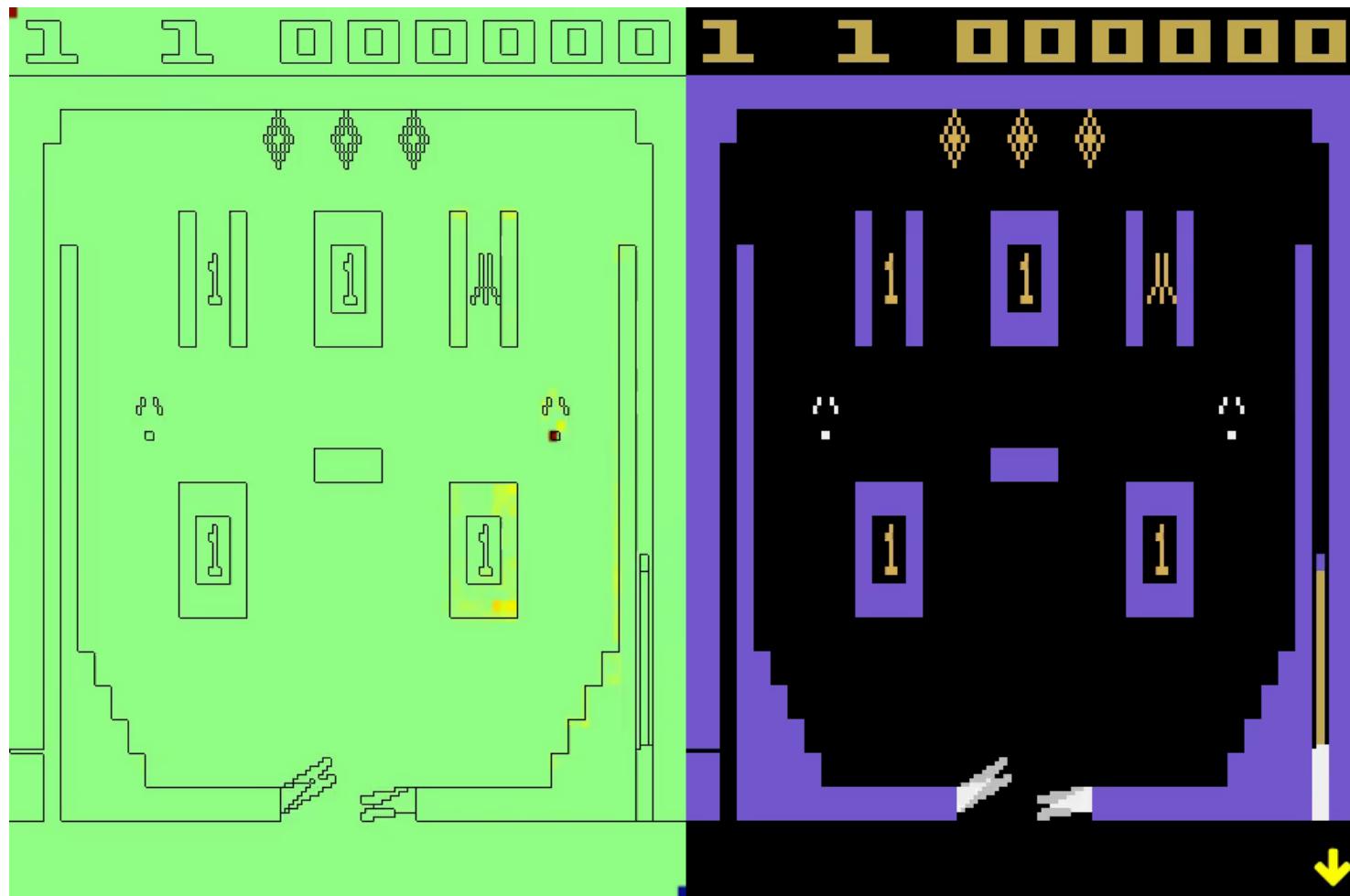
(Lapuschkin et al., 2019)

# Understanding Learning Behaviour



(Lapuschkin et al., 2019)

# Understanding Learning Behaviour

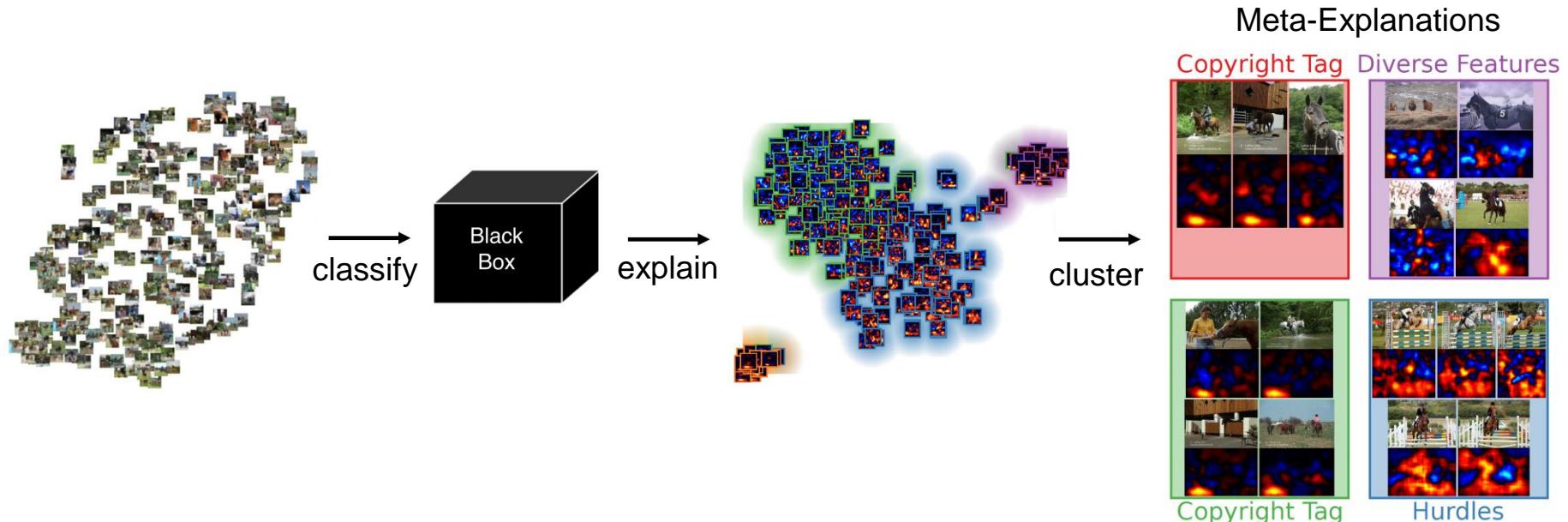


(Lapuschkin et al., 2019)

# **Meta-Explanations**

# Meta-Explanations

**SpRAY's idea:** Explain *whole dataset* decisions of a ML model by systematically analyzing distributions of LRP heatmaps.

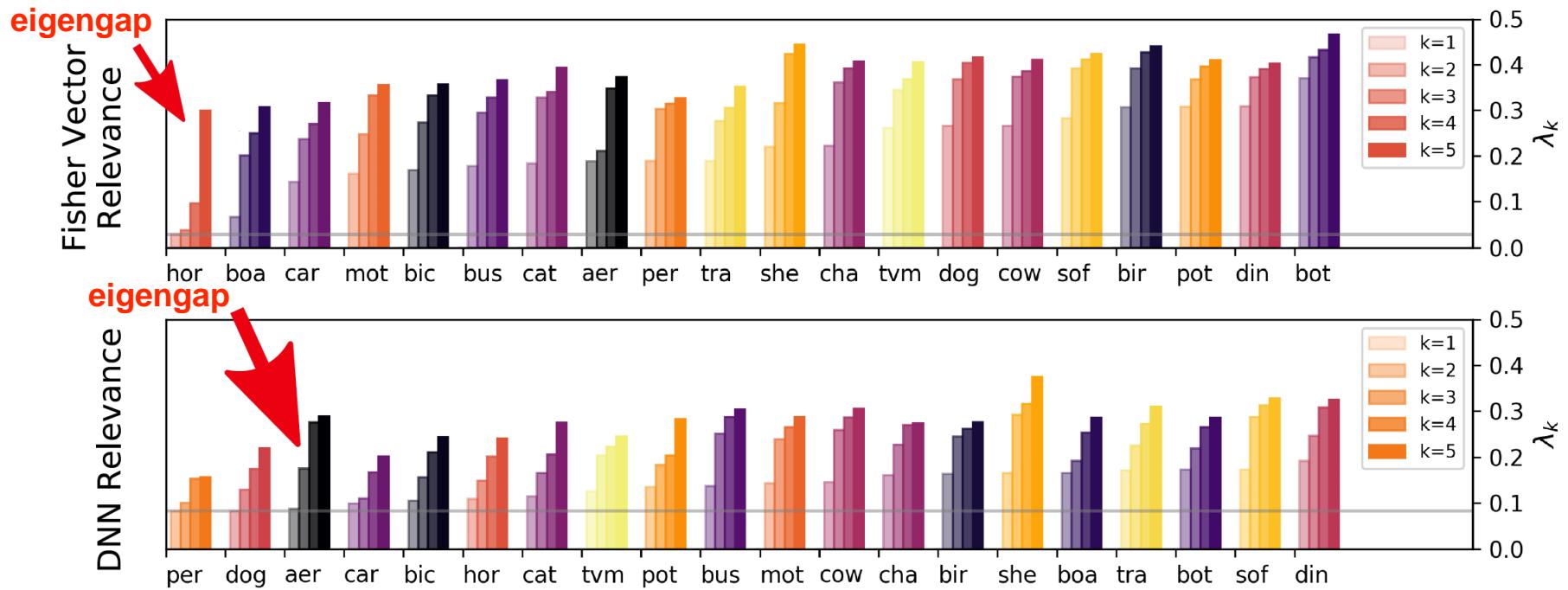


Unmasking Clever Hans predictors and assessing what machines really learn

(Lapuschkin et al., 2019)

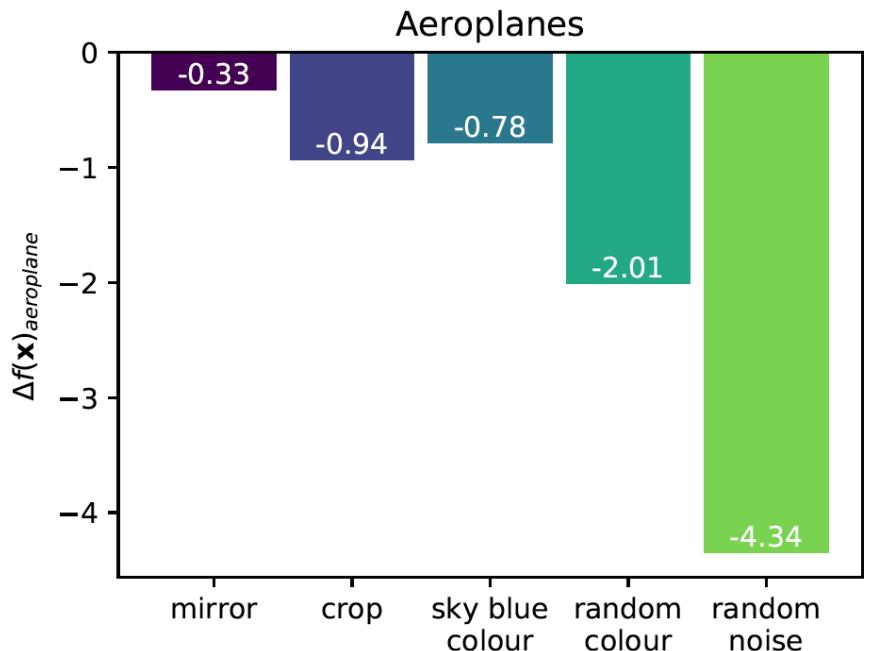
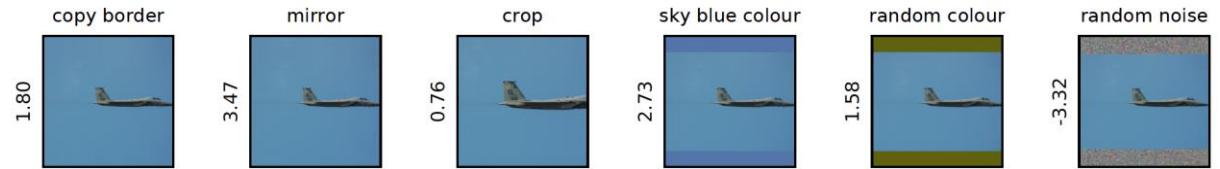
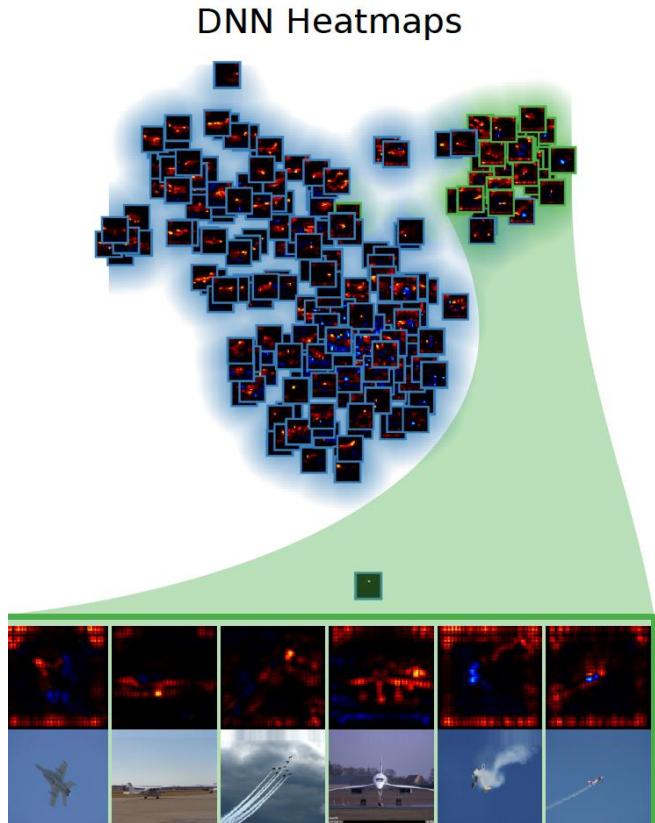
# Spectral Relevance Analysis (SpRAY)

SpRAY for Fisher Vector and DNN classifiers on PASCAL VOC 2017.



(Lapuschkin et al., 2019)

# Spectral Relevance Analysis (SpRAY)



# **Beyond Explaining Classifiers**

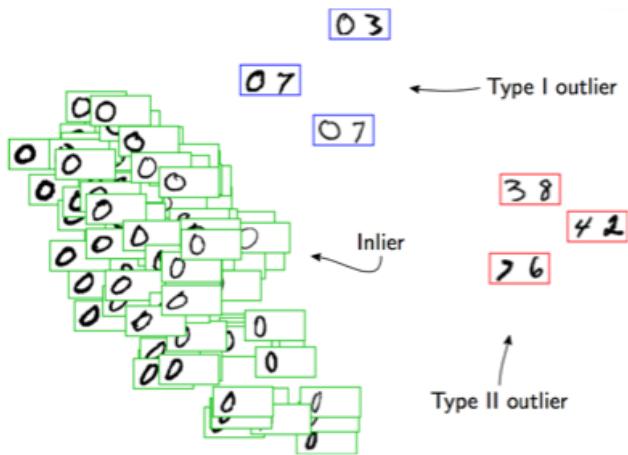
# The “Neuralization” Trick

## NEON (Neuralization-Propagation)

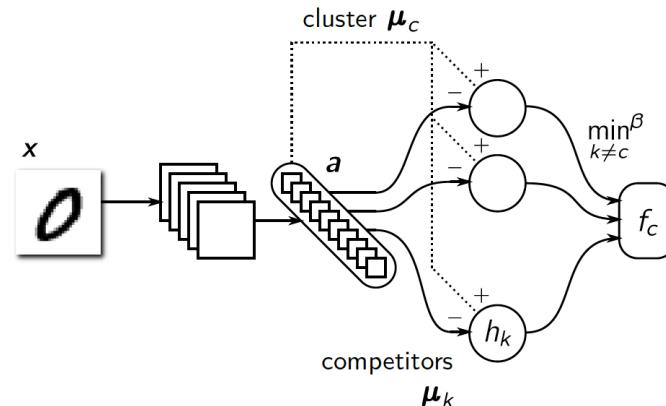
Explain ML algorithm (e.g., SVM, k-Means) in two steps:

1. Convert it into a neural network ('neuralize it')
2. Explain the neural network with propagation methods (LRP)

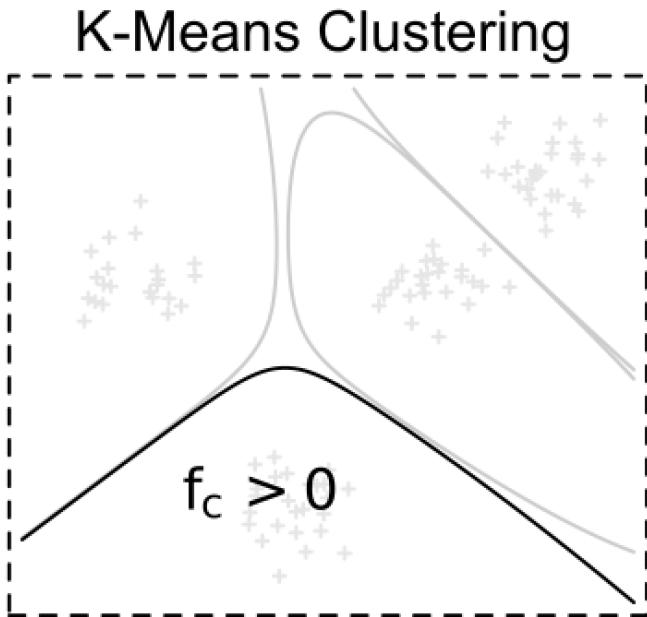
One-class SVM (Kauffmann'18)



Clustering (Kauffmann'19)



# Neuralizing K-means



Represent evidence for cluster membership using logit

$$f_c(\mathbf{x}) = \log \left( \frac{P(\omega_c | \mathbf{x})}{1 - P(\omega_c | \mathbf{x})} \right)$$

with

$$P(\omega_c | \mathbf{x}) = \frac{\exp(-\beta \cdot o_c(\mathbf{x}))}{\sum_k \exp(-\beta \cdot o_k(\mathbf{x}))}$$

$$o_k(\mathbf{x}) = \|\mathbf{x} - \boldsymbol{\mu}_k\|^2$$

**Proposition 1.** *The logit that quantifies cluster membership can be written as a soft min-pooling layer*

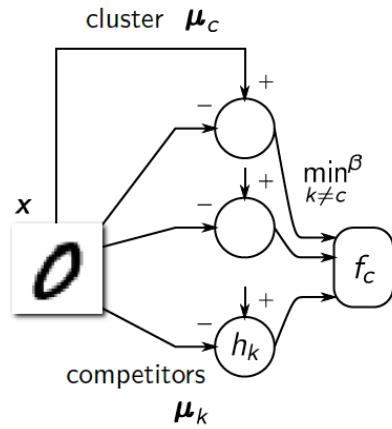
$$f_c(\mathbf{x}) = \beta \cdot \min_{k \neq c}^{\beta} \{o_k(\mathbf{x}) - o_c(\mathbf{x})\},$$

where we define  $\min^{\beta}\{\cdot\} = -\beta^{-1} \log \sum \exp(-\beta(\cdot))$ .

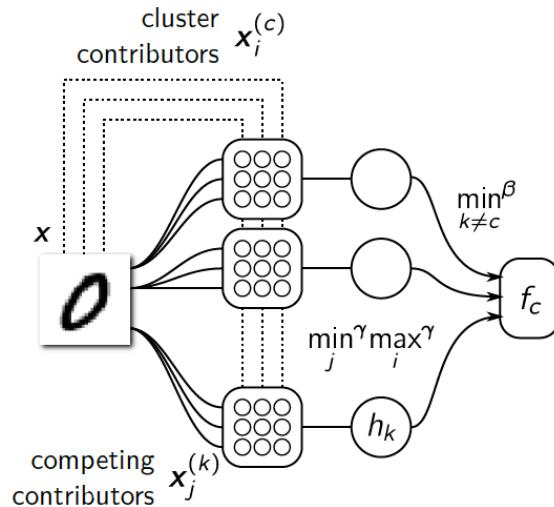
(Kauffmann et al. 2019)

# Neuralizing K-means

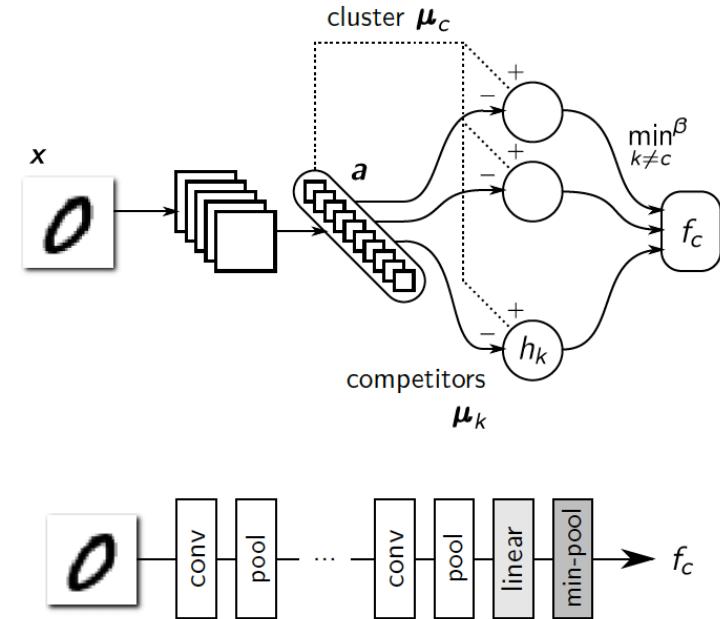
Standard K-Means



Kernel K-Means

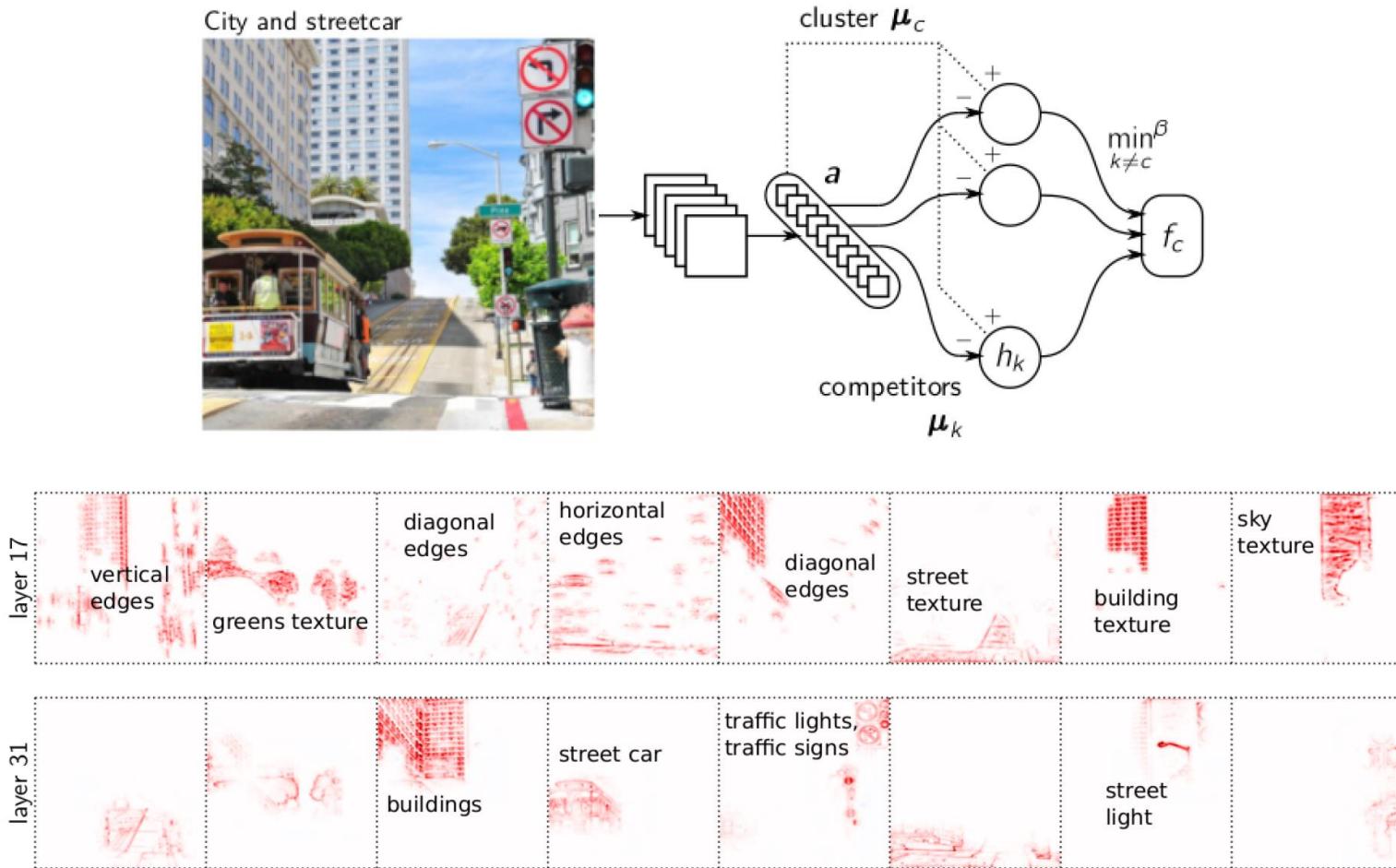


Deep K-Means



(Kauffmann et al. 2019)

# K-Means on VGG-16 Features



(Kauffmann et al. 2019)

# Summary

Decisions functions of ML models are often complex, and analyzing them directly can be difficult.

Levering the model's structure largely simplifies the explanation problem.

Layer type dependent redistribution rules exist and should be used.

Explanations and Meta-Explanations can be used for various purposes.

Common ML models (e.g. OC-SVM, k-means) can often be decomposed as a sequence of explainable layers (“neuralization”).

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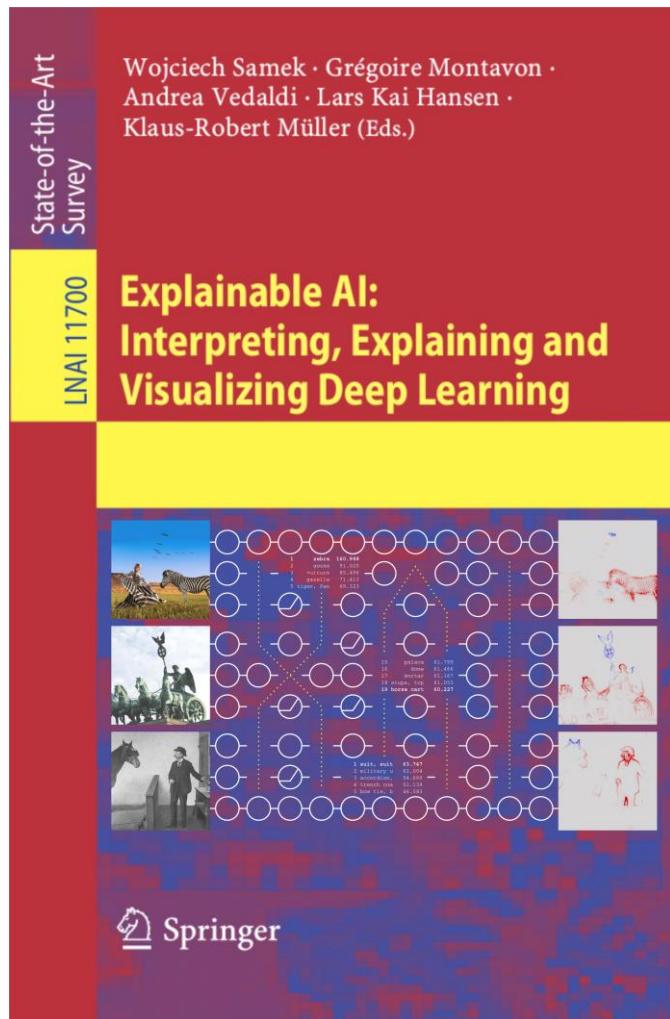
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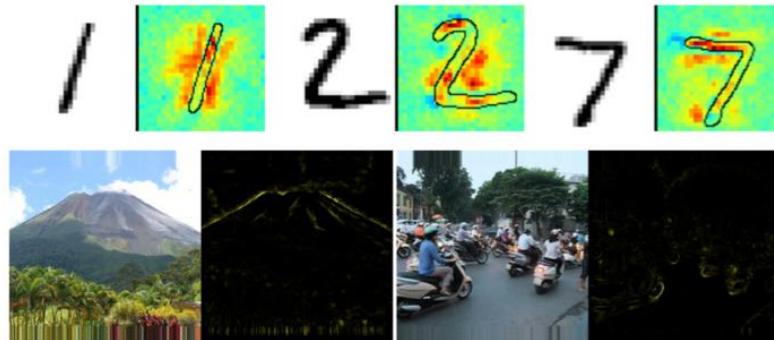
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Alexander Binder (SUTD)

...

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Digital Signal Processing, 73:1-5, 2018

## Keras Explanation Toolbox

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