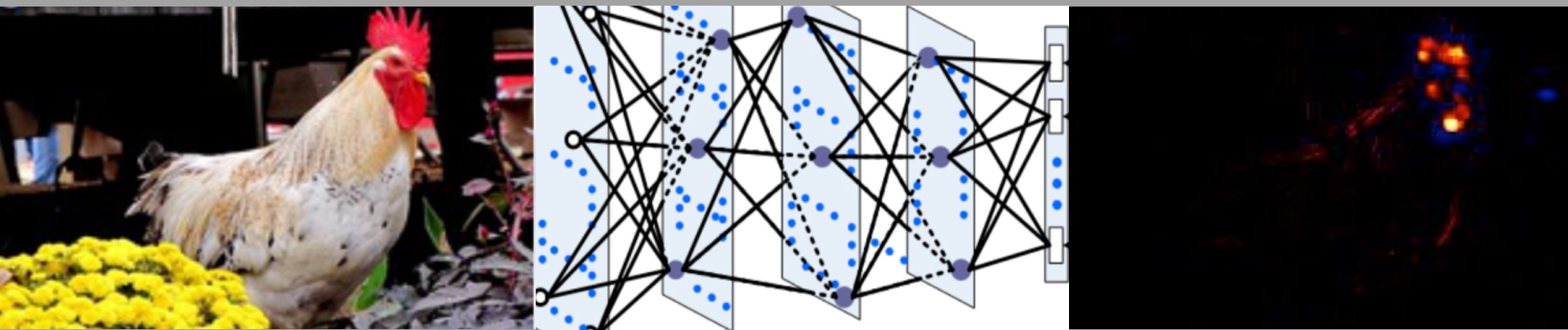
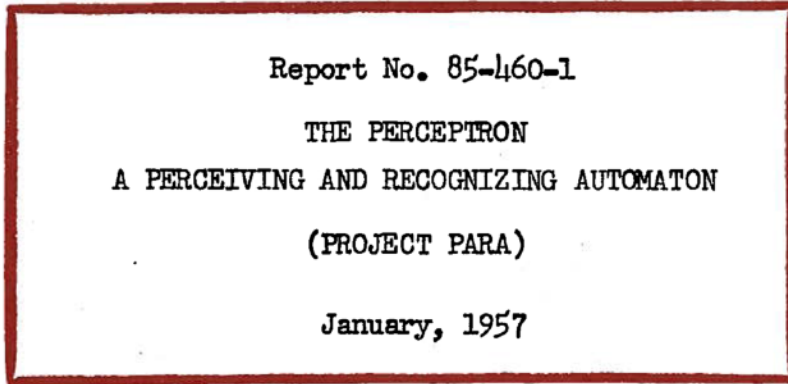


# XXAI: eXtending XAI towards Actionable Interpretability

Wojciech Samek  
AI Department, Fraunhofer HHI



# ML Models = Black Boxes ?



Prepared by: Frank Rosenblatt  
Frank Rosenblatt,  
Project Engineer

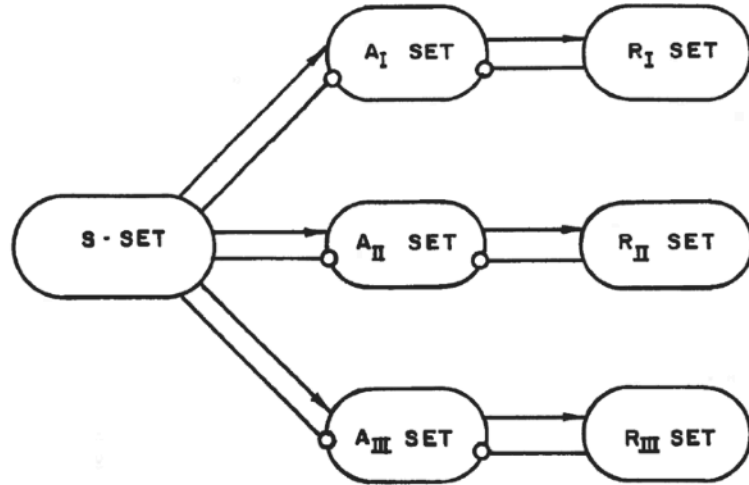
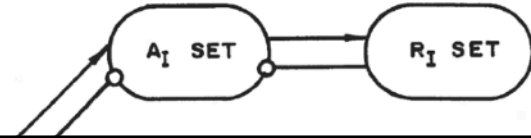


FIGURE 2  
ORGANIZATION OF A PERCEPTRON WITH  
THREE INDEPENDENT OUTPUT-SETS

# ML Models = Black Boxes ?



## II. GENERAL DESCRIPTION OF A PHOTOPERCEPTRON

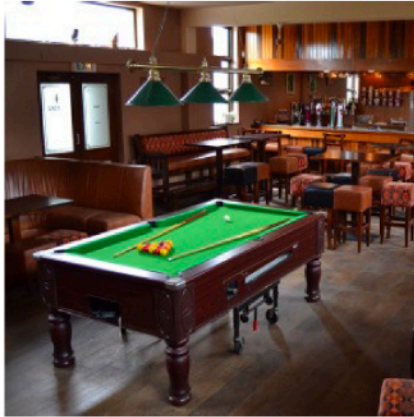
We might consider the perceptron as a black box, with a TV camera for input, and an alphabetic printer or a set of signal lights as output. Its performance can then be described as a process

Frank Rosenblatt,  
Project Engineer

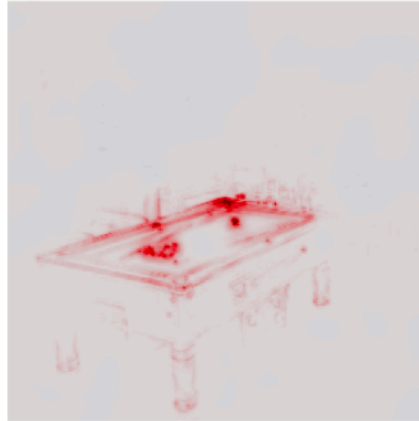
ORGANIZATION OF A PERCEPTRON WITH  
THREE INDEPENDENT OUTPUT-SETS

# Today: Post-hoc XAI

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



some pool table



why it is classified as a pool table

# Brief History

Visualization of neural networks using saliency maps

NJS **Morch**, U Kjems, [LK Hansen](#)... - Proceedings of ICNN ..., 1995

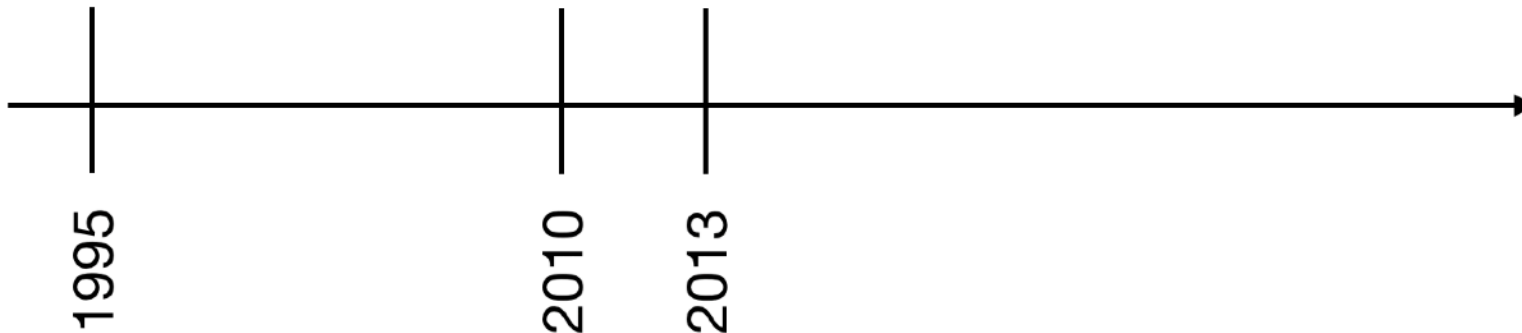
[\[PDF\]](#) How to explain individual classification decisions

D **Baehrens**, T Schroeter, [S Harmeling](#)... - The Journal of Machine ..., 2010 - jmlr.org

Deep inside convolutional networks: Visualising image classification models and saliency maps

K Simonyan, A Vedaldi, [A Zisserman](#) - arXiv preprint arXiv:1312.6034, 2013 - arxiv.org

sensitivity analysis



# Brief History

[HTML] On pixel-wise explanations for non-linear classifier decisions by layer-wise relevance propagation

[S Bach, A Binder, G Montavon, F Klauschen...](#) - PloS one, 2015 - journals.plos.org

" Why should I trust you?" **Explaining** the predictions of any classifier

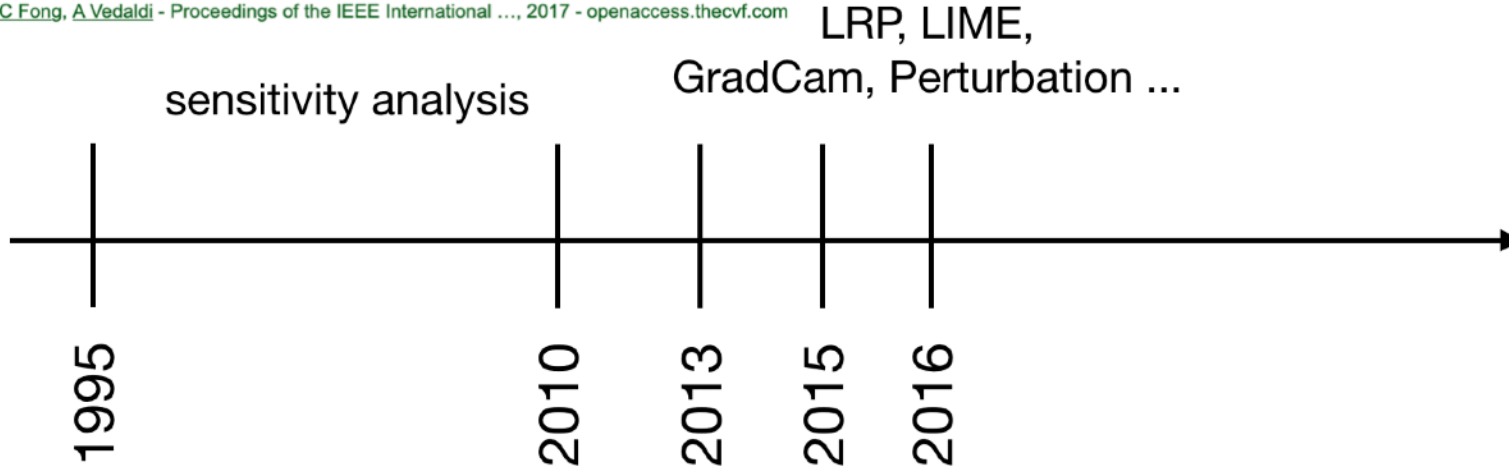
[MT Ribeiro, S Singh, C Guestrin](#) - Proceedings of the 22nd ACM ..., 2016 - dl.acm.org

**Grad-CAM: Why did you say that?**

[RR Selvaraju, A Das, R Vedantam, M Cogswell...](#) - arXiv preprint arXiv ..., 2016 - arxiv.org

Interpretable explanations of black boxes by **meaningful perturbation**

[RC Fong, A Vedaldi](#) - Proceedings of the IEEE International ..., 2017 - openaccess.thecvf.com



# Brief History

[HTML] Explaining nonlinear classification decisions with **deep taylor decomposition**

[G Montavon](#), [S Lapuschkin](#), [A Binder](#), [W Samek](#)... - Pattern Recognition, 2017 - Elsevier

A unified approach to interpreting model predictions

[SM Lundberg](#), [SI Lee](#) - Advances in neural information processing ..., 2017 - papers.nips.cc

Explaining recurrent neural network predictions in sentiment analysis

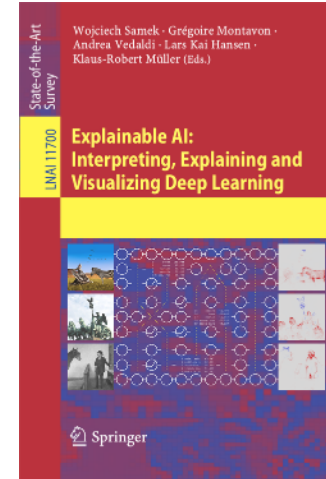
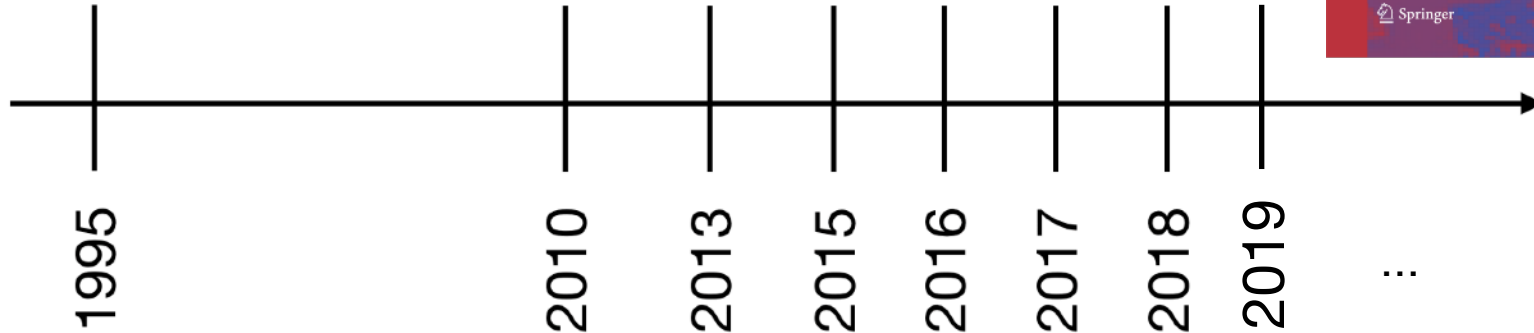
[L Arras](#), [G Montavon](#), [KR Müller](#), [W Samek](#) - arXiv preprint arXiv ..., 2017 - arxiv.org

XAI for LSTMs

Theoretical frameworks  
for XAI

LRP, LIME,  
GradCam, Perturbation ...

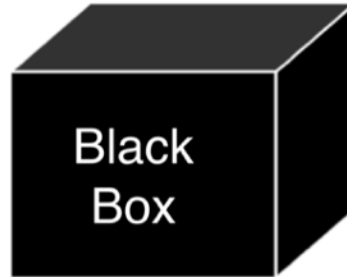
sensitivity analysis



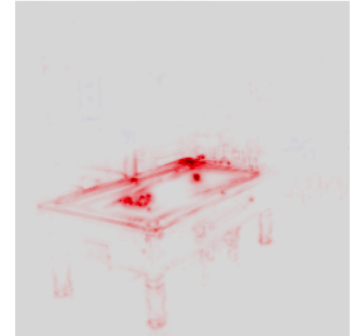
# Explain? Yes We Can



*classify*



*explain*

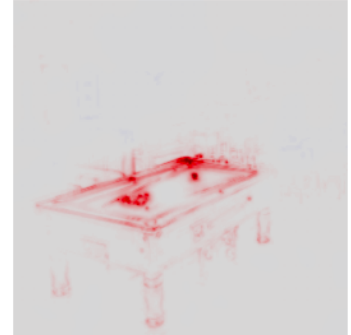




# Explain? Yes We Can



And now ?



**Are Our Explanations Good Enough?**

# What are good Explanations ?

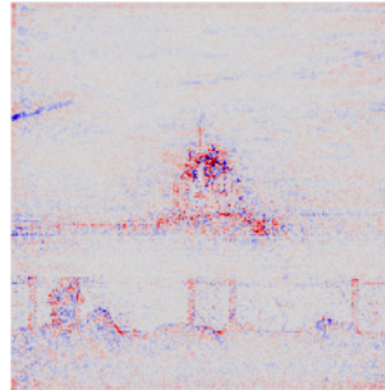
input



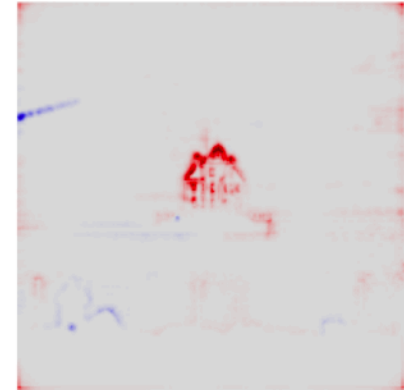
Occlusion



Smooth IG



LRP



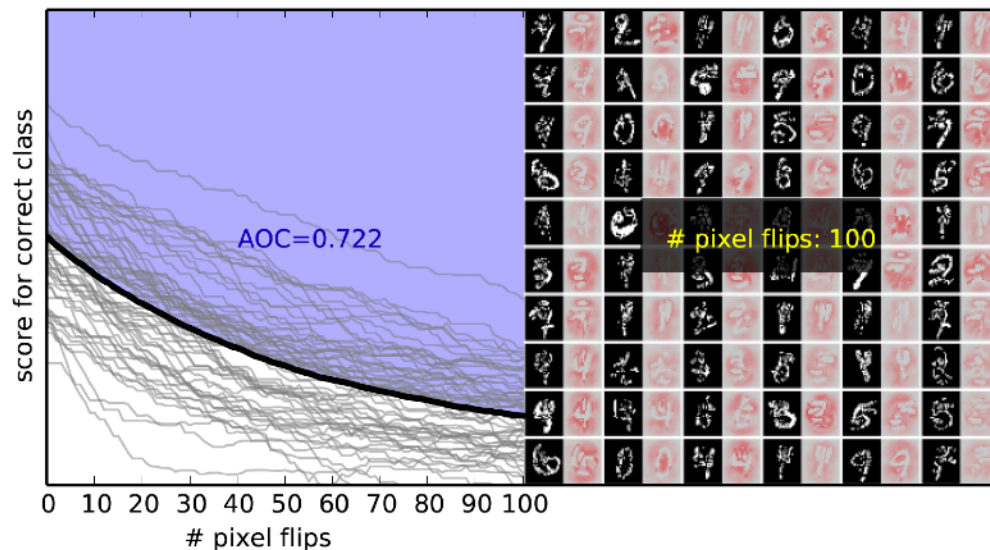
Which explanation technique should be preferred?

# Some Desiderata for Explanations

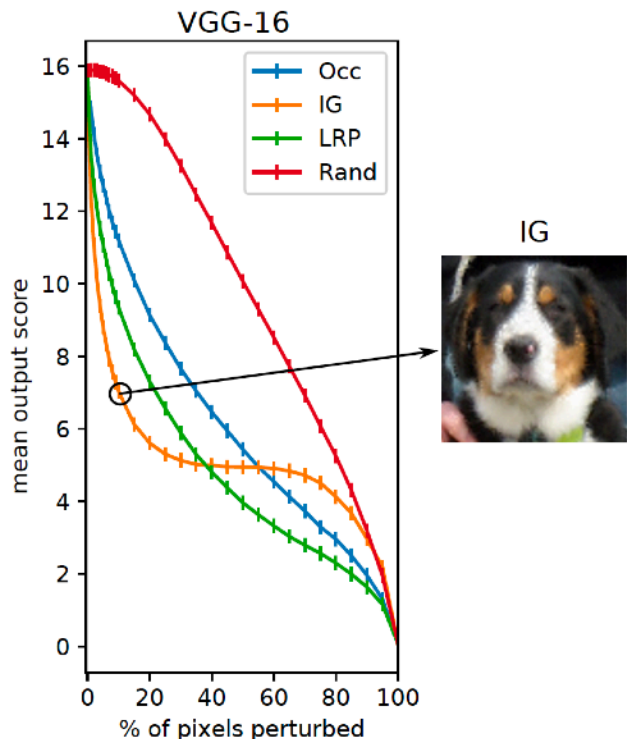
1. **Fidelity:** The explanation should reflect the quantity being explained and not something else.
2. **Understandability:** The explanation must be easily understandable by its receiver.
3. **Sufficiency:** The explanation should provide sufficient information on how the model came up with its prediction.
4. **Low Overhead:** The explanation should not cause the prediction model to become less accurate or less efficient.
5. **Runtime Efficiency:** Explanations should be computable in reasonable time.

# Evaluating Fidelity: Pixel-Flipping

- ▶ The pixel-flipping procedure [9] destroys pixels from most to least relevant according to the explanation, and keeps track of the neural network output.
- ▶ The faster the output decreases, the better the explanation.



# Evaluating Fidelity: Pixel-Flipping

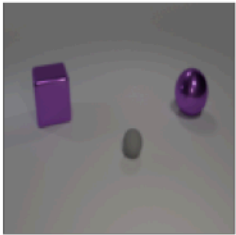



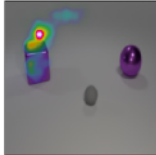
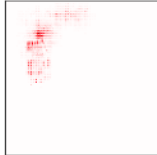
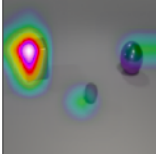



- ▶ All explanation methods are more faithful than a random explanation.
- ▶ IG is the most faithful for the first few most relevant pixels, and then stagnates.
- ▶ Although not detected by VGG-16 anymore, the class-relevant patterns are still there after flipping (e.g. we can still see the dog). Did IG actually explain a *vulnerability* of VGG-16 instead of its typical behavior?

[Samek et al. 2021]

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# Evaluating Fidelity: Comparison with Ground Truth

			GT Unique First-non-empty
What material is the large object that is left of the big purple metallic ball? <i>metal</i>			
LRP [20]			0.97
SmoothGrad [43]			0.42
Grad-CAM [42]			0.38

[Arras et al. 2020]

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# Evaluating Sufficiency

- ▶ Example of a faithful, understandable, but *insufficient* explanation

**Q:** *Why did the classifier predict this image to be a 'lighthouse'?*

**A:** *Because the classifier found a lighthouse in the image.*

- ▶ Evaluating sufficiency:
  - ▶ Is the explanation actionable? (e.g. can we improve a model from the produced explanations).
  - ▶ Can we learn something general about the classifier? (e.g. what kind of features it uses).
- ▶ Is it sufficient to explain a prediction in terms of individual pixels, or should we identify higher-order interactions?

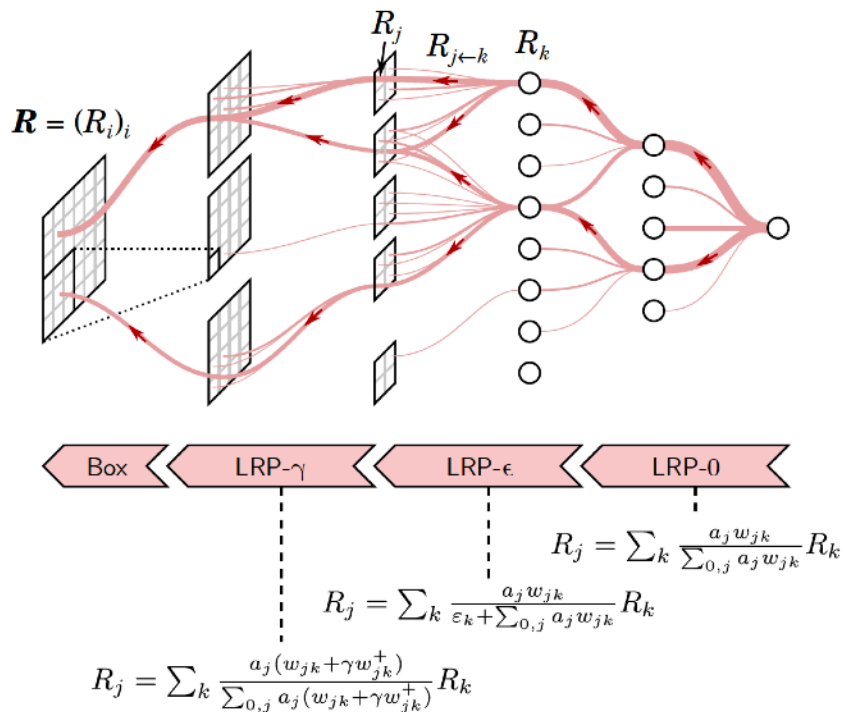


# Utilitarian Perspective

Explanations are good if they provide some additional (measurable) advantage.

# **Layer-wise Relevance Propagation**

# Layer-wise Relevance Propagation



## Ideas:

- ▶ Use the structure of the neural network to robustly compute relevance scores for the input features.
- ▶ Propagate the output of the network backwards by means of propagation rules.
- ▶ Propagation rules can be tuned for explanation quality. E.g. sensitive in top-layers, robust in lower layers.

[Bach et al. 2015]

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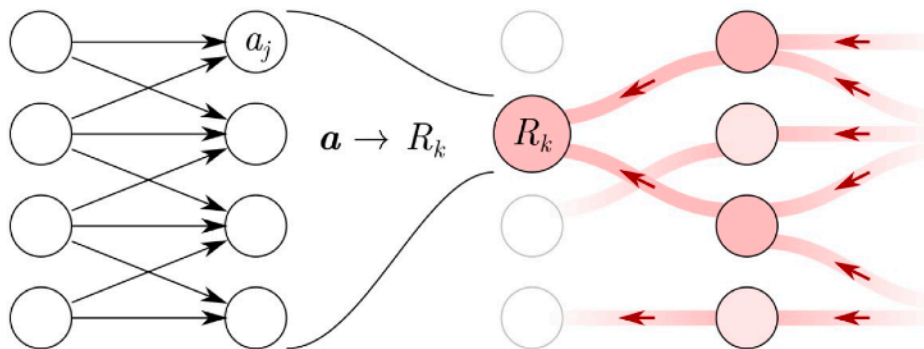
# Can LRP be Justified Theoretically?

$$R_j = \sum_k \frac{a_j \cdot \rho(w_{jk})}{\epsilon + \sum_{0,j} a_j \cdot \rho(w_{jk})} R_k$$

**Answer:** Yes, using the deep Taylor decomposition framework.



# Deep Taylor Decomposition



**Key idea:** Taylor expansions at each layer

$$R_k(\mathbf{a}) \approx \hat{R}_k(\tilde{\mathbf{a}}) + \underbrace{\sum_j [\nabla \hat{R}_k(\tilde{\mathbf{a}})]_j \cdot (a_j - \tilde{a}_j)}_{\text{LRP}} + \dots$$

**LRP**

[Montavon et al. 2017]

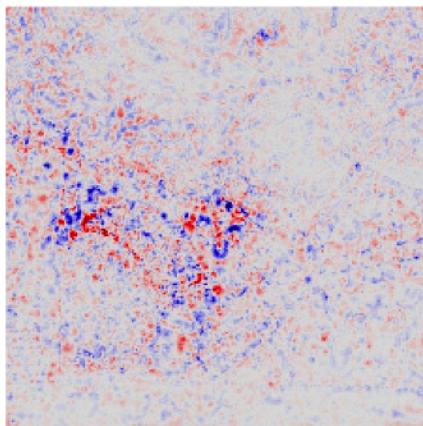
21

# LRP is More Stable than Gradient

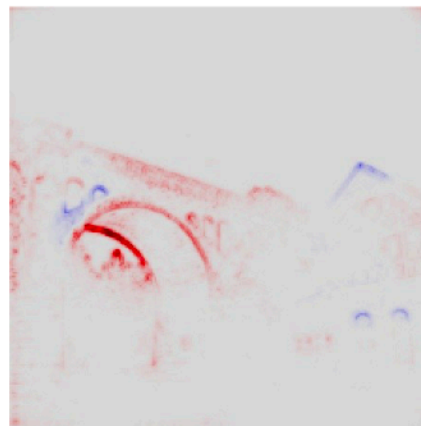
Image classified by a DNN as a viaduct.



**Gradient** explanation



**LRP** explanation



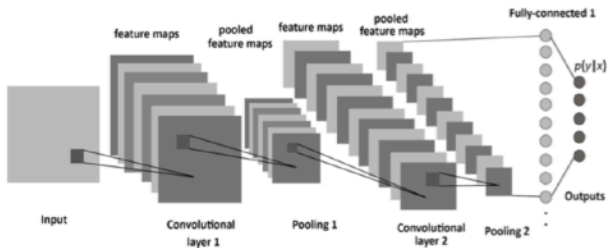
DNN gradients are **shattered**

[Samek et al. 2021]

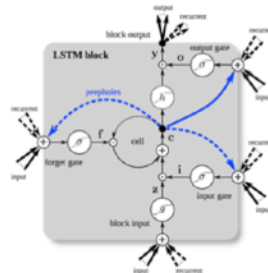
22

# LRP for Different Types of Models

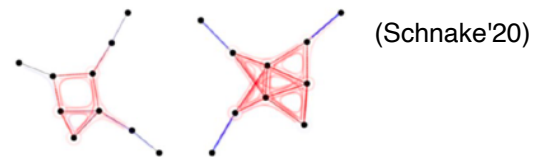
Convolutional NNs (Bach'15, Arras'17 ...)



LSTM (Arras'17, Arras'19)



Graph neural networks (GNN-LRP)

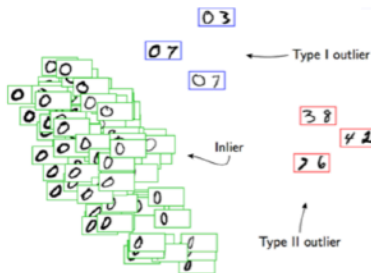


(Schnake'20)

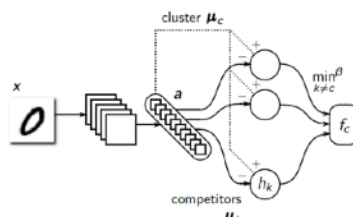
BoW / Fisher Vector models  
(Bach'15, Arras'16, Lapuschkin'16 ...)



One-class SVM (Kauffmann'18)



Clustering (Kauffmann'19)



Similarity models (BiLRP)



(Eberle'20)

# **Towards Actionable Explanations with LRP**



# PASCAL VOC Challenge (2005 - 2012)



(a) Aero plane



(b) Bicycle



(c) Boat



(d) Bus



(e) Bird



(f) Bottle



(g) Cat



(h) Cow



(i) Car



(j) Chair



(k) Dog



(l) Dining table



(m) Horse



(n) Motorbike



(o) Person



(p) Potted Plant



(q) Sheep



(r) Sofa



(s) TV monitor

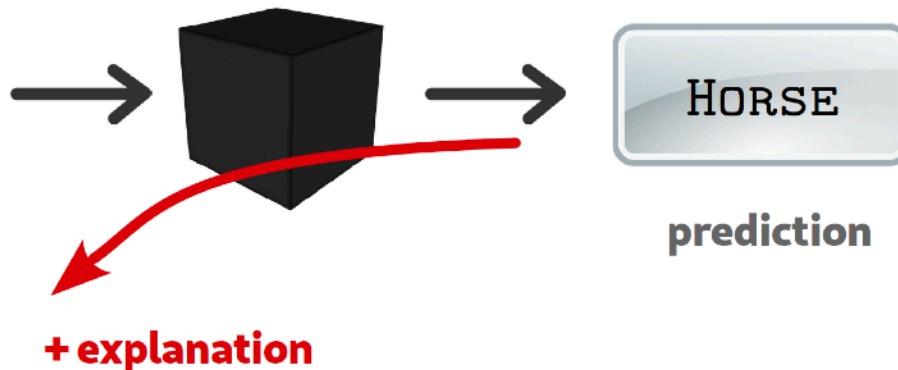
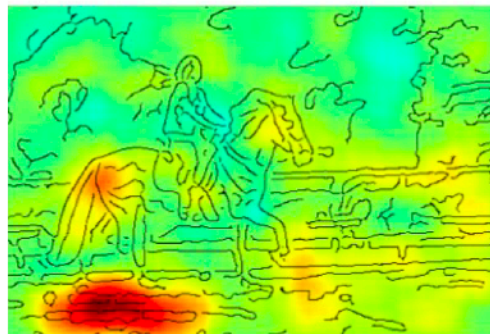


(t) Train

average precision of the Fisher Vector model on the PascalVOC dataset

aer	bic	bir	boa	bot
79.08	66.44	45.90	70.88	27.64
bus	car	cat	cha	cow
69.67	80.96	59.92	51.92	47.60
din	dog	hor	mot	per
58.06	42.28	80.45	69.34	85.10
pot	she	sof	tra	tvm
28.62	49.58	49.31	82.71	54.33

# Detecting Clever Hans



**Unexpected:** The classifier predicts correctly based on an **artifact** in the data (aka. '**Clever Hans**').

[Lapuschkin et al. 2019]

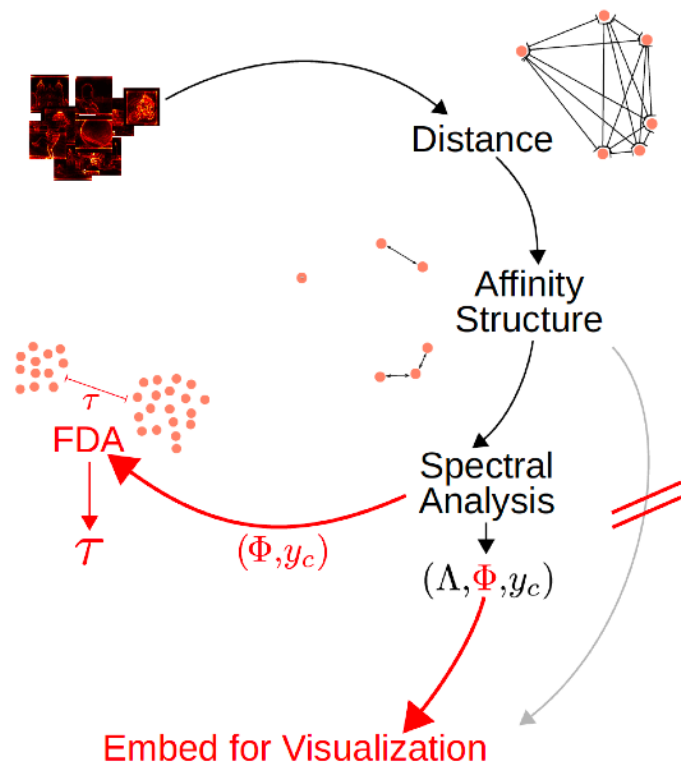
26

# Detecting Clever Hans



**Reason:** This strategy works on the current data (many horses images have a copyright tag) → **spurious correlation**.

# Automating Clever Hans Detection

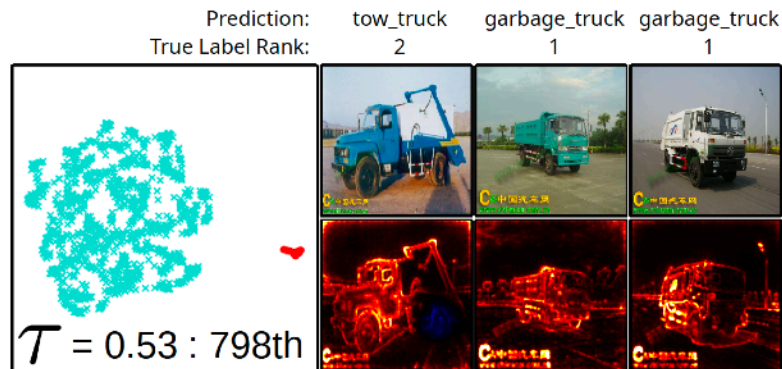
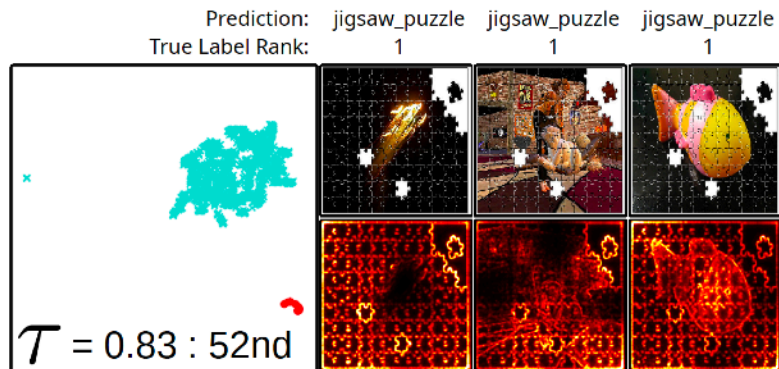
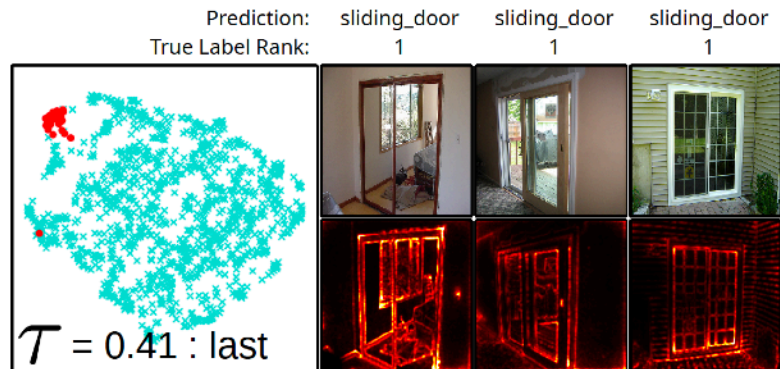
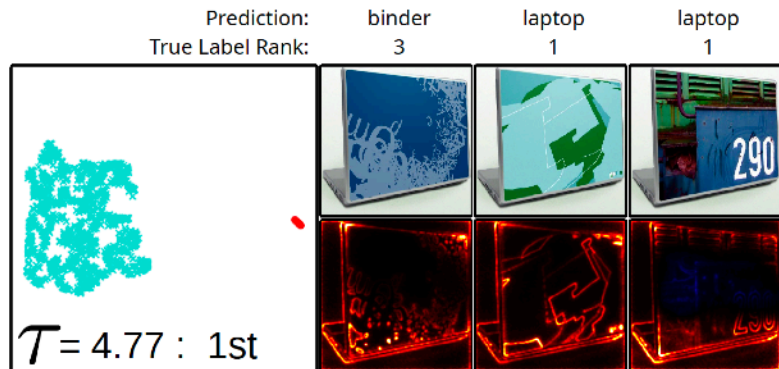


## Extending SpRAy from [4]

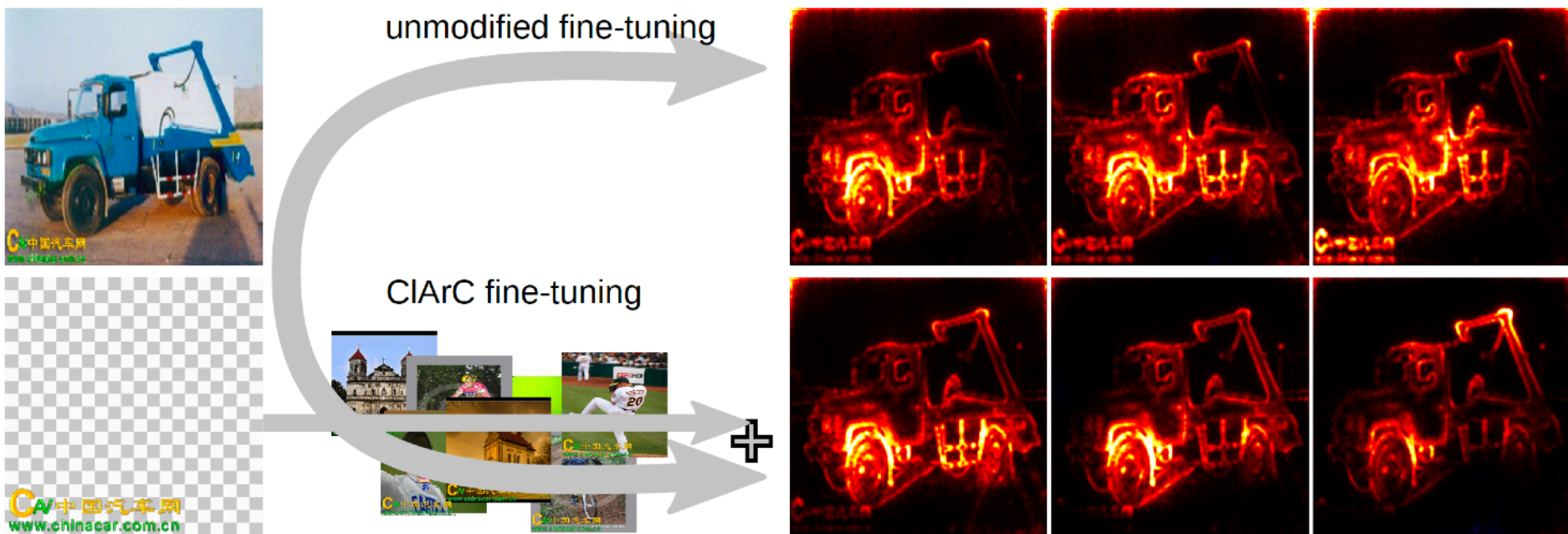
- Further automating spurious cluster/class discovery by analyzing  $\Phi$  with FDA<sup>7</sup>
- Visualizing the spectral embedding  $\Phi$ , instead of affinity structure

$$J(w) = \frac{w^T S_b w}{w^T S_w w} \quad (\text{Anders et al. 2019})$$

# Automating Clever Hans Detection



# XAI-Based Model Improvement



Isolate artefact, add to *other/all* classes, re-train model.

# XAI-Based Model Improvement

1 epoch

5 epochs

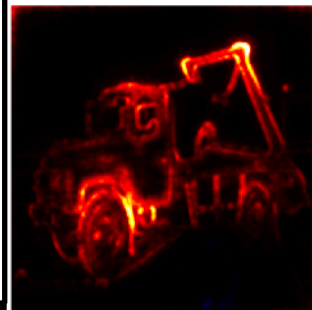
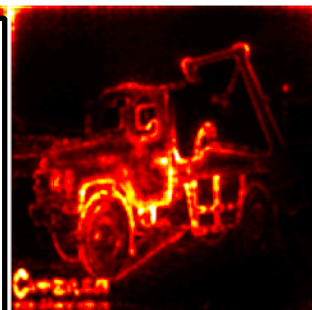
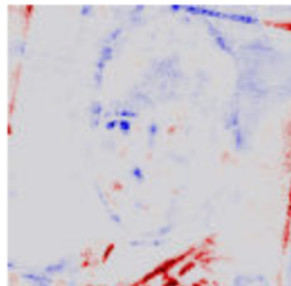
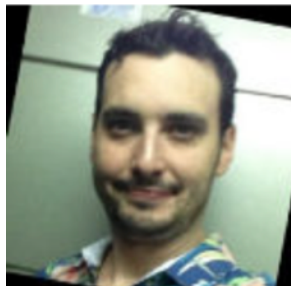
10 epochs

## P-CIArC Projective Class Artifact Compensation

Detect problem in CAV space -> project out (no retraining)

CAV-Predictor

CAV-Predictor



Isolate artefact, add to *other/all* classes, re-train model.

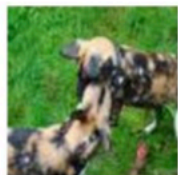
[Anders et al. 2019]

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# Explanation-Guided Training

Cross-domain few-shot classification task (CD-FSC)

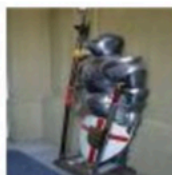
examples of  
support images



dog



crate



cuirass

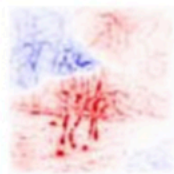
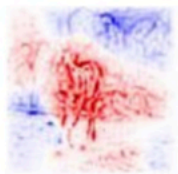


lion

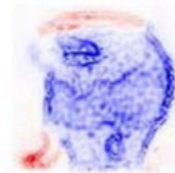
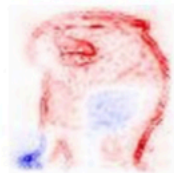
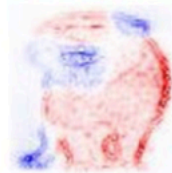
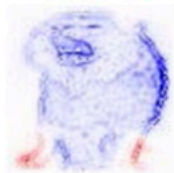


vase

Q1  
pred: dog



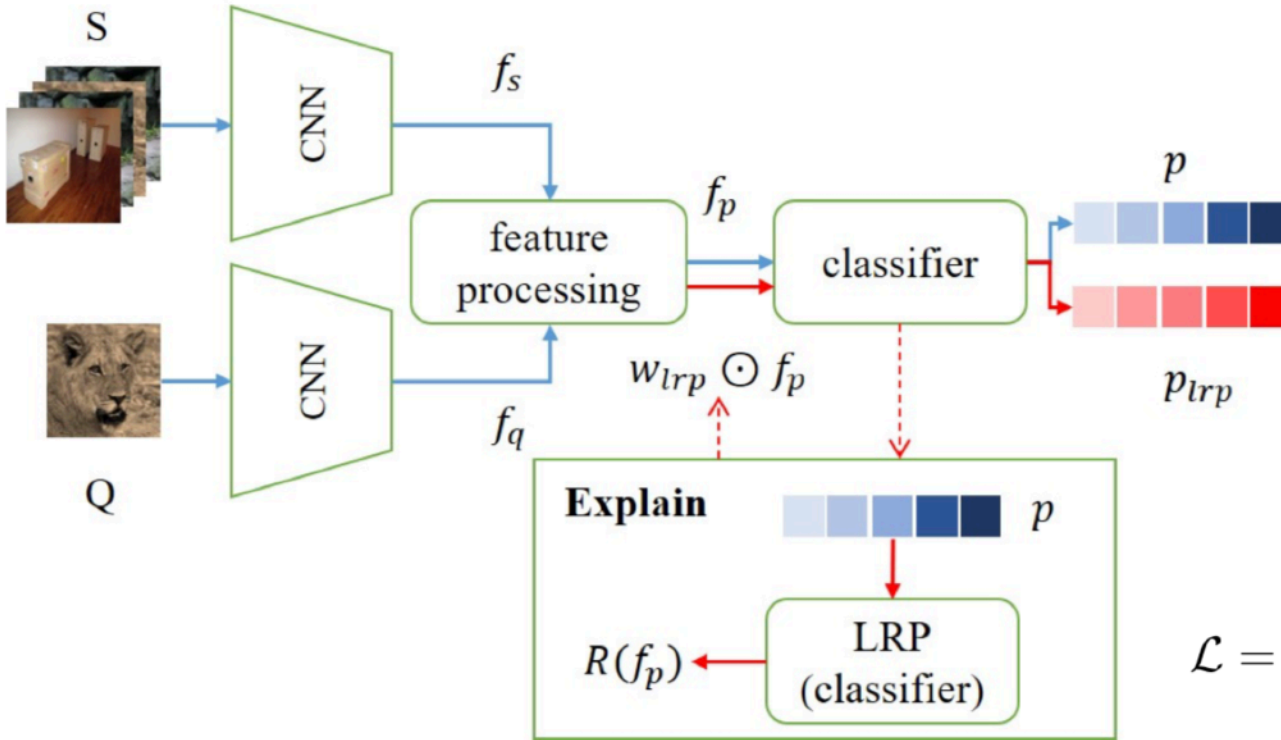
Q2  
pred: lion



[Sun et al. 2021]



# Explanation-Guided Training

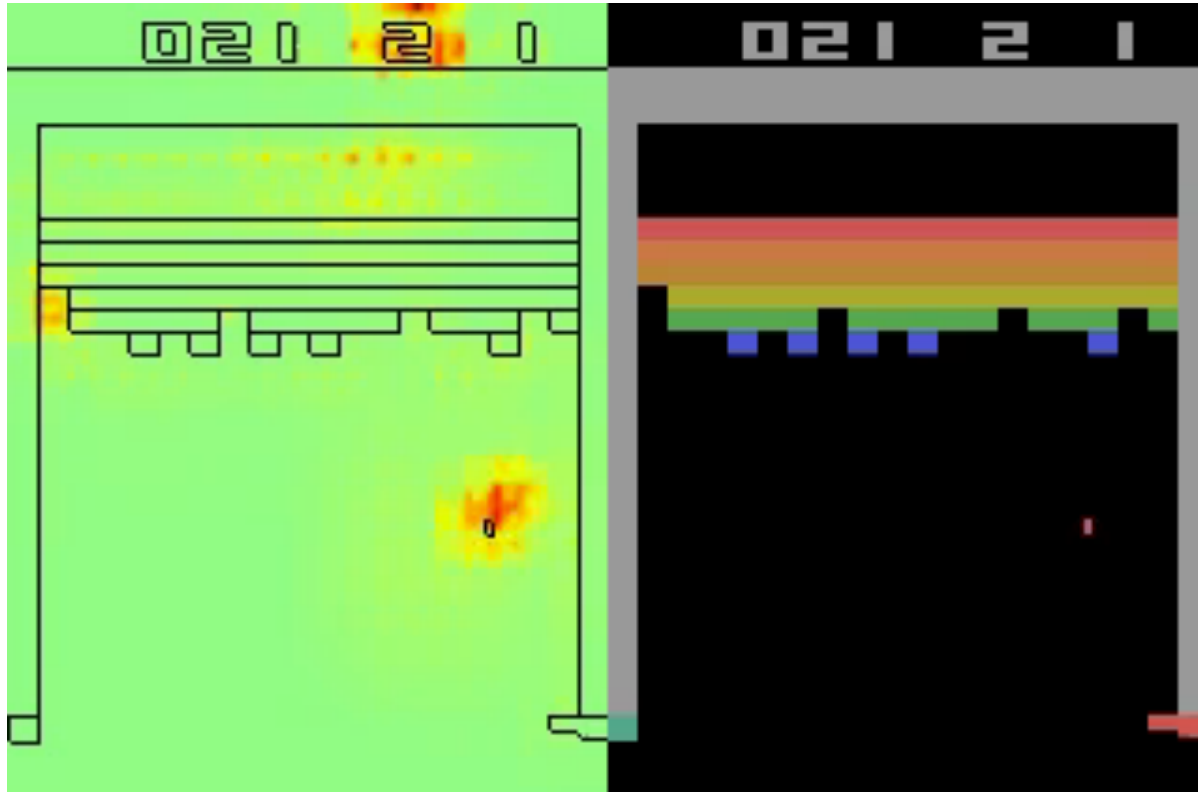


$$w_{lrp} = 1 + R(f_p)$$

$$f_{p-lrp} = w_{lrp} \odot f_p$$

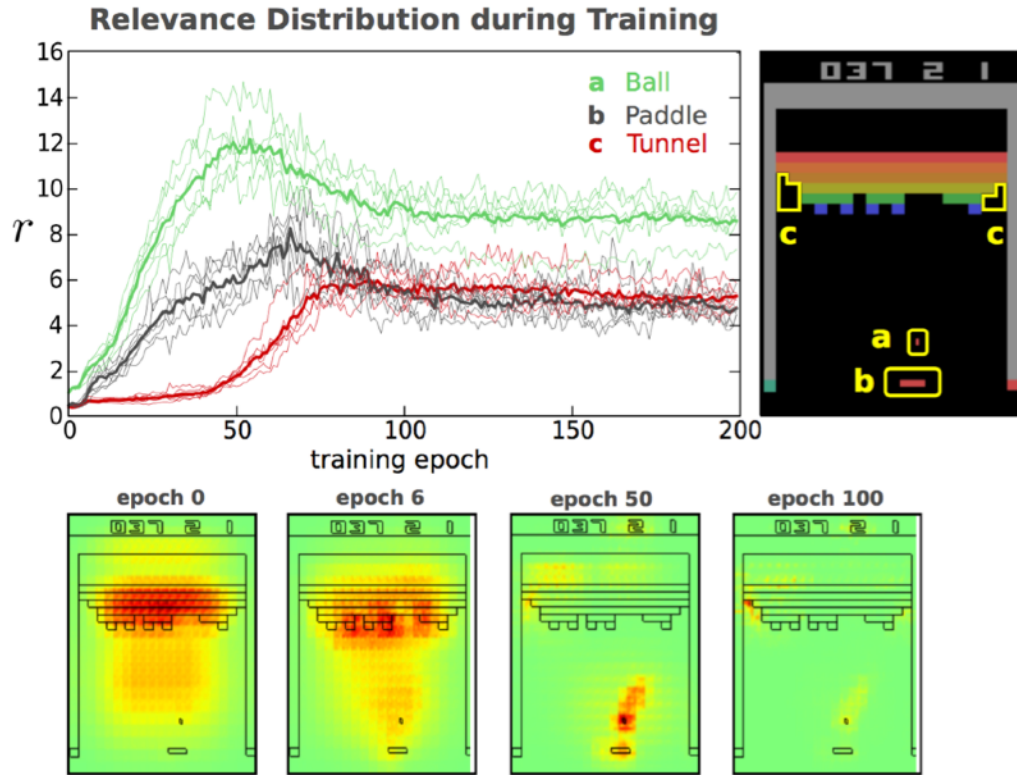
$$\mathcal{L} = \xi \mathcal{L}_{ce}(y, p) + \lambda \mathcal{L}_{ce}(y, p_{lrp})$$

# Understanding Learning Behaviour



*(Lapuschkin et al., 2019)*

# Understanding Learning Behaviour



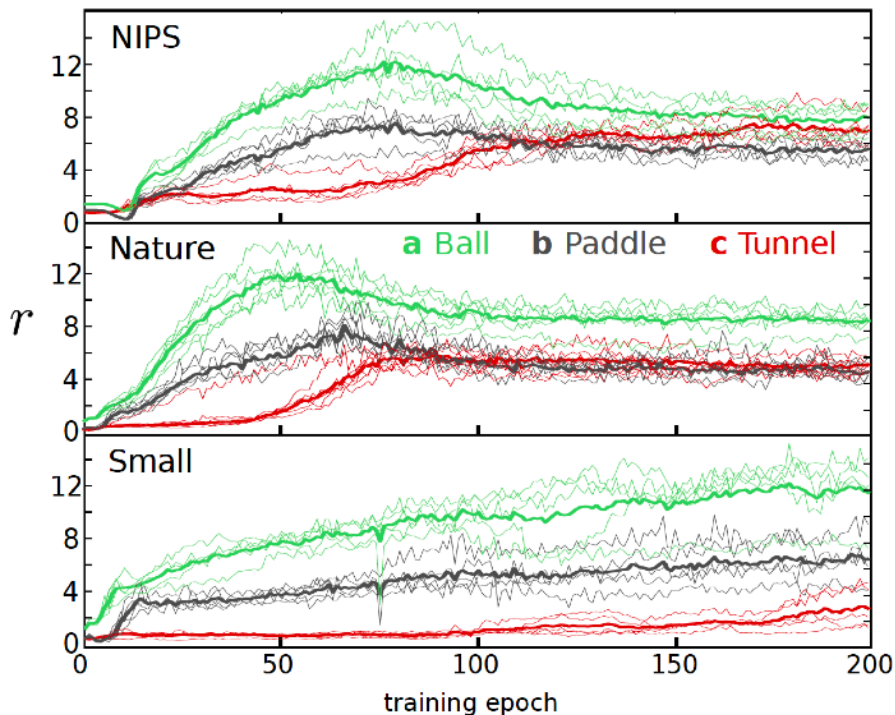
- model learns
1. track the ball
  2. focus on paddle
  3. focus on the tunnel



Unmasking Clever Hans predictors and assessing what machines really learn

# Understanding Learning Behaviour

Relevance Distribution during Training



NIPS architecture

C1  $(4 \times 8 \times 8) \rightarrow (16), [4 \times 4]$   
 C2  $(16 \times 4 \times 4) \rightarrow (32), [2 \times 2]$

F1  $(2592) \rightarrow (256)$   
 F2  $(256) \rightarrow (4)$

Nature architecture

C1  $(4 \times 8 \times 8) \rightarrow (32), [4 \times 4]$   
 C2  $(32 \times 4 \times 4) \rightarrow (64), [2 \times 2]$   
 C3  $(64 \times 3 \times 3) \rightarrow (64), [1 \times 1]$

F1  $(3136) \rightarrow (512)$   
 F2  $(512) \rightarrow (4)$

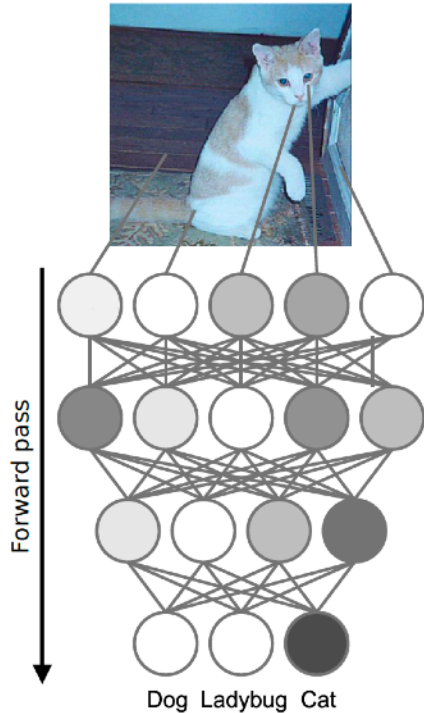
Small architecture

C1  $(4 \times 8 \times 8) \rightarrow (32), [4 \times 4]$   
 C2  $(32 \times 4 \times 4) \rightarrow (64), [2 \times 2]$   
 C3  $(64 \times 3 \times 3) \rightarrow (64), [1 \times 1]$   
 F1  $(3136) \rightarrow (4)$

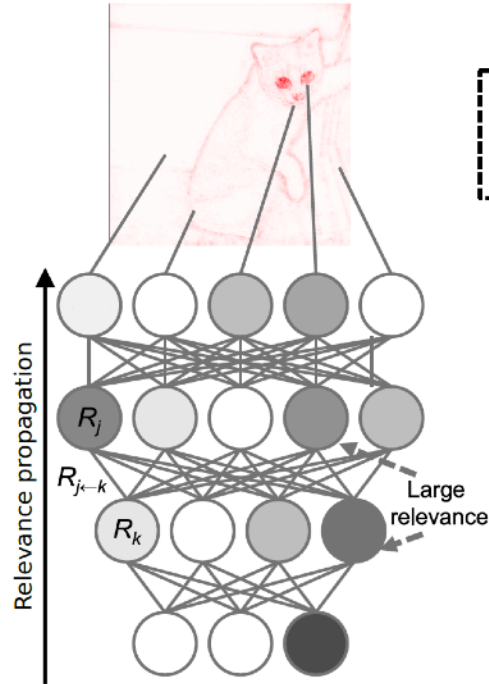
(Lapuschkin et al., 2019)

# XAI-Based Pruning

A. Forward Propagation with given image



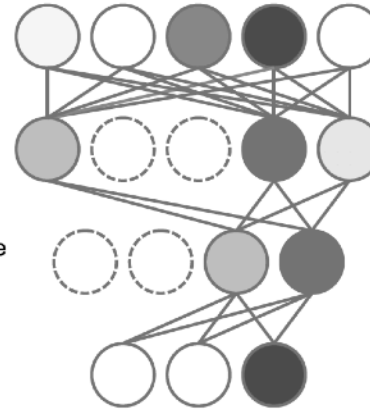
B. Evaluation on relevance of neurons/filters using LRP



C. Iterative pruning of the irrelevant neurons/filters and fine-tuning

Relevance conservation property

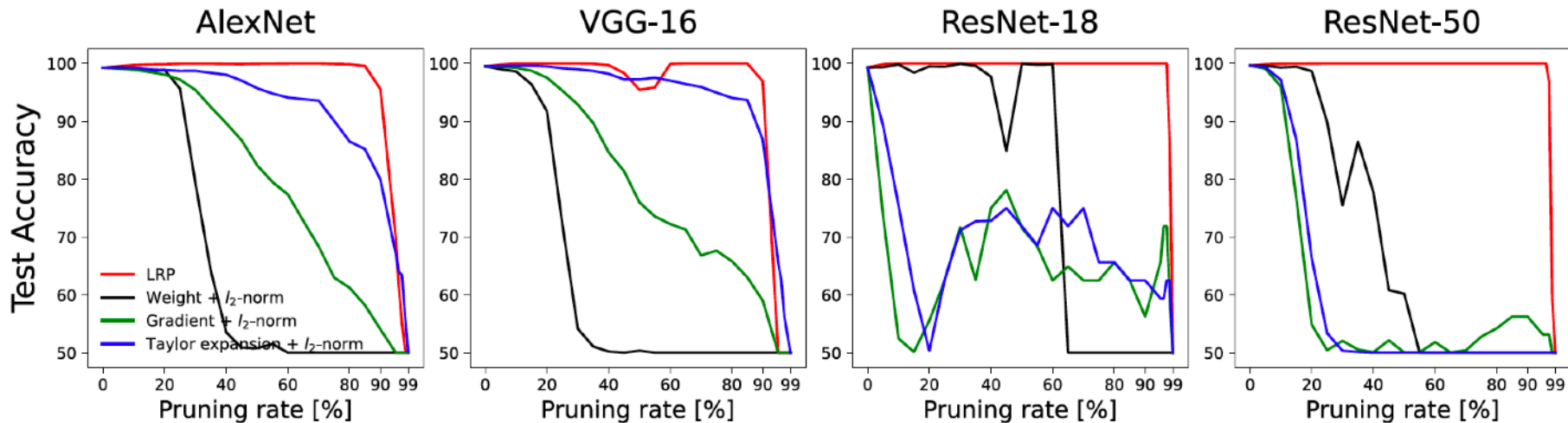
$$\sum_{i=1}^d R_i = f(x)$$



(Yeom et al. 2021)

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# XAI-Based Pruning

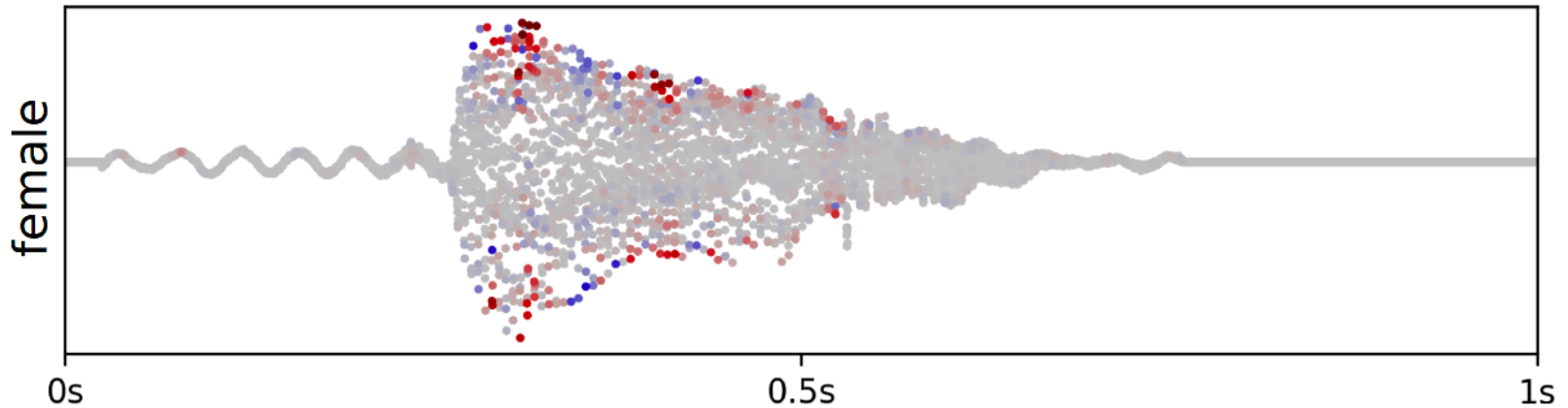


No fine-tuning

only 10 samples per class  
(domain adaptation scenario)

**So are we done ?**

# Is This Explanation Actionable ?

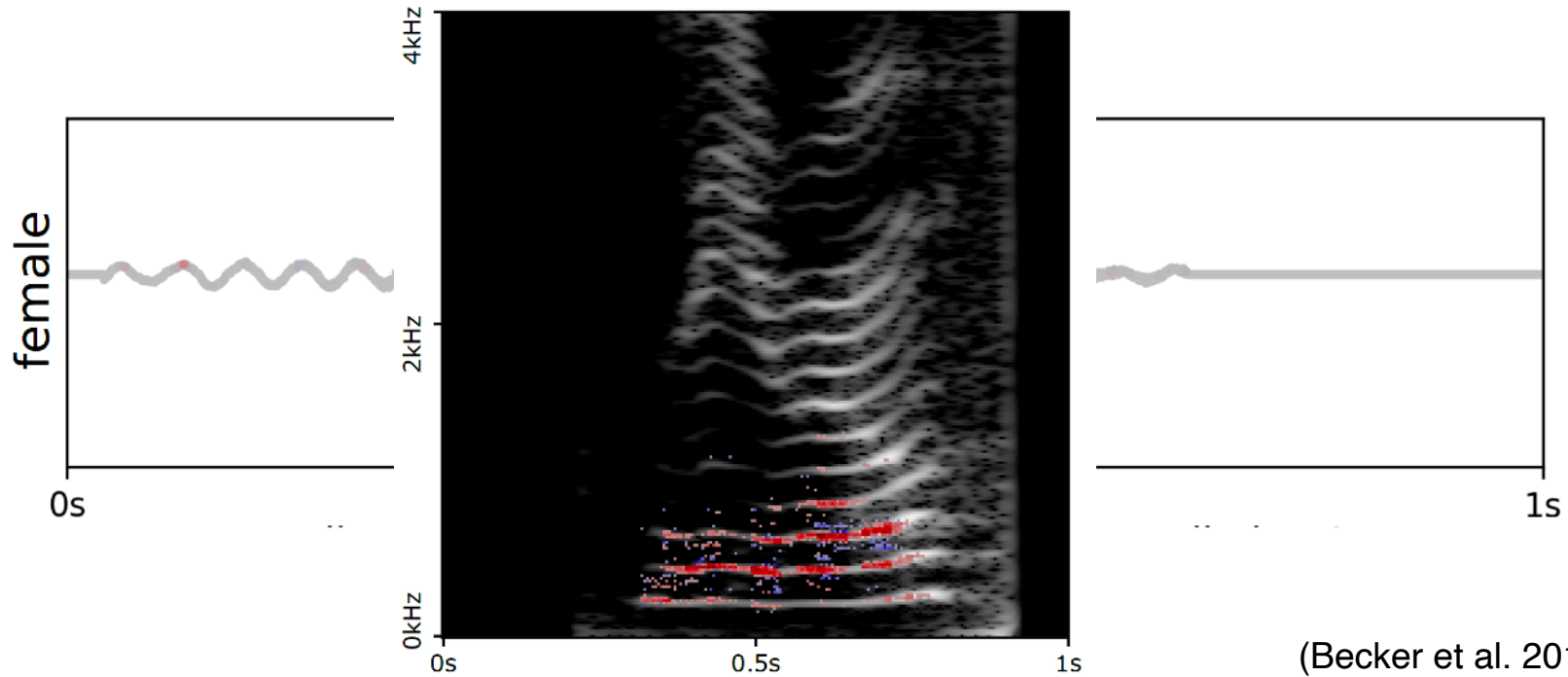


(Becker et al. 2018)

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# Is This Explanation Actionable ?



(Becker et al. 2018)

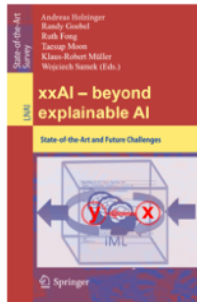
# Conclusion

Explanations can be used beyond visualization purposes

Theoretical approaches to XAI exist (e.g. Deep Taylor, Shapley). That allows to compute meaningful explanations, also beyond deep nets.

Explanations need to be actionable (e.g. in scientific applications)

New book to come soon ...



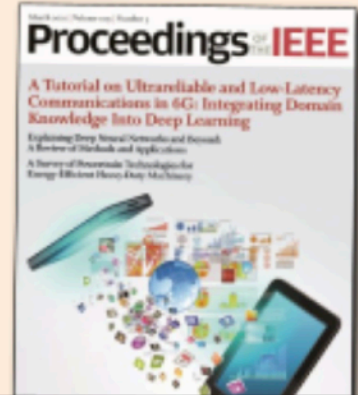
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W Samek, G Montavon, S Lapuschkin, C Anders, KR Müller

## [Explaining Deep Neural Networks and Beyond: A Review of Methods and Applications](#)

Proceedings of the IEEE, 109(3):247-278, 2021

With the broader and highly successful usage of machine learning (ML) in industry and the sciences, there has been a growing demand for explainable artificial intelligence (XAI). Interpretability and explanation methods for gaining a better understanding of the problem-solving abilities and strategies of nonlinear ML, in particular, deep neural networks, are, therefore, receiving increased attention. In this work, we aim to: 1) provide a timely overview of this active emerging field, with a focus on “post hoc” explanations, and explain its theoretical foundations; 2) put interpretability algorithms to a test both from a theory and comparative evaluation perspective using extensive simulations; 3) outline best practice aspects, i.e., how to best include interpretation methods into the standard usage of ML; and 4) demonstrate successful usage of XAI in a representative selection of application scenarios. Finally, we discuss challenges and possible future directions of this exciting foundational field of ML.



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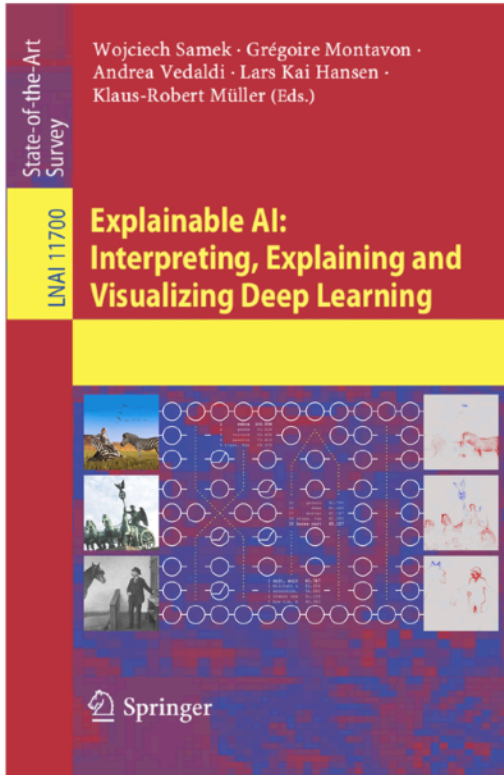
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