Tutorial on Interpreting and Explaining Deep Models in Computer Vision


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08:30 - 09:15	Introduction KRM
09:15 - 10:00	Techniques for Interpretability GM
10:00 - 10:30	Coffee Break ALL
10:30 - 11:15	Applications of Interpretability WS
11:15 - 12:00	Further Applications and Wrap-Up KRM

Overview of Explanation Methods

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

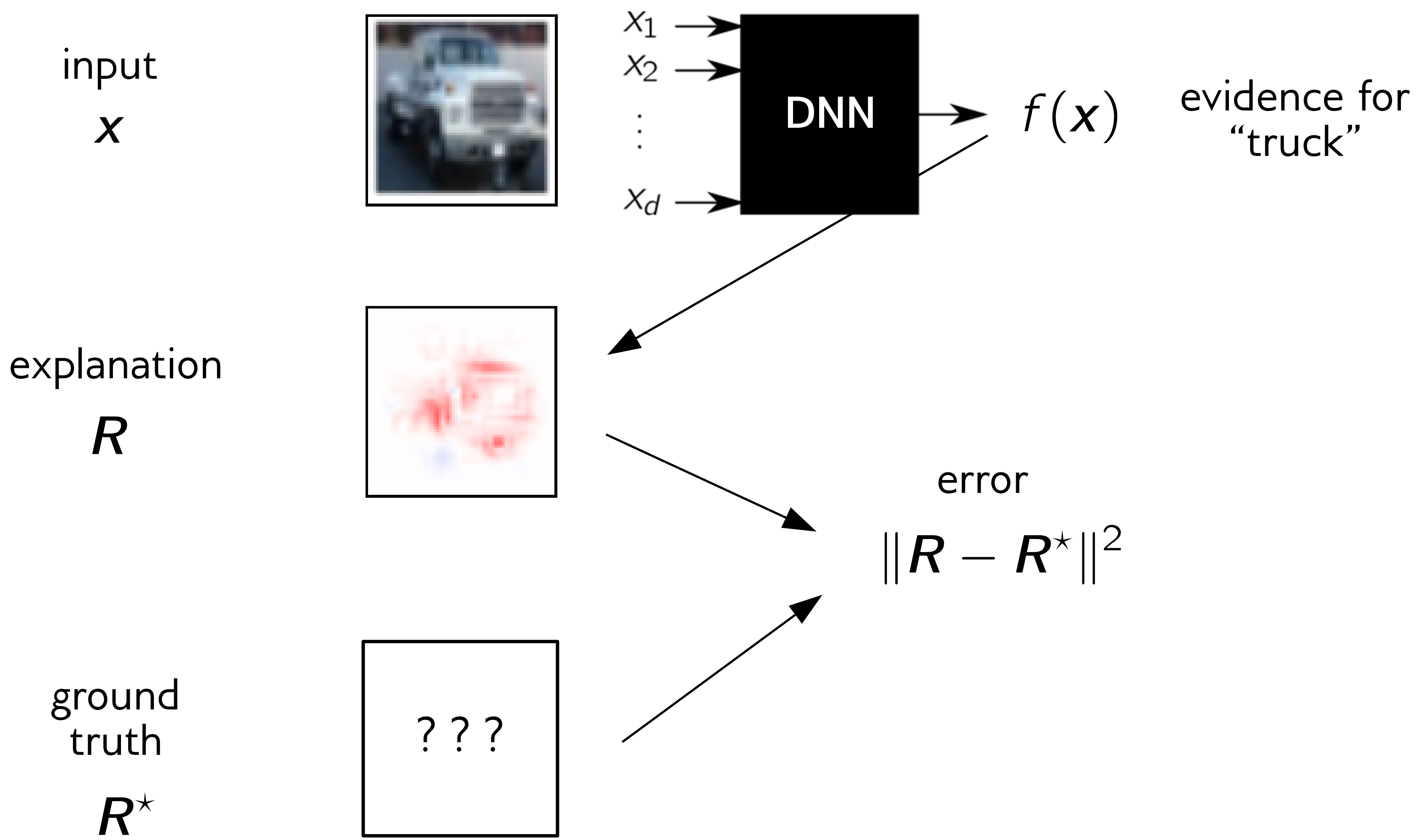
Springenberg'14
Guided BP

Zhou'16
GAP

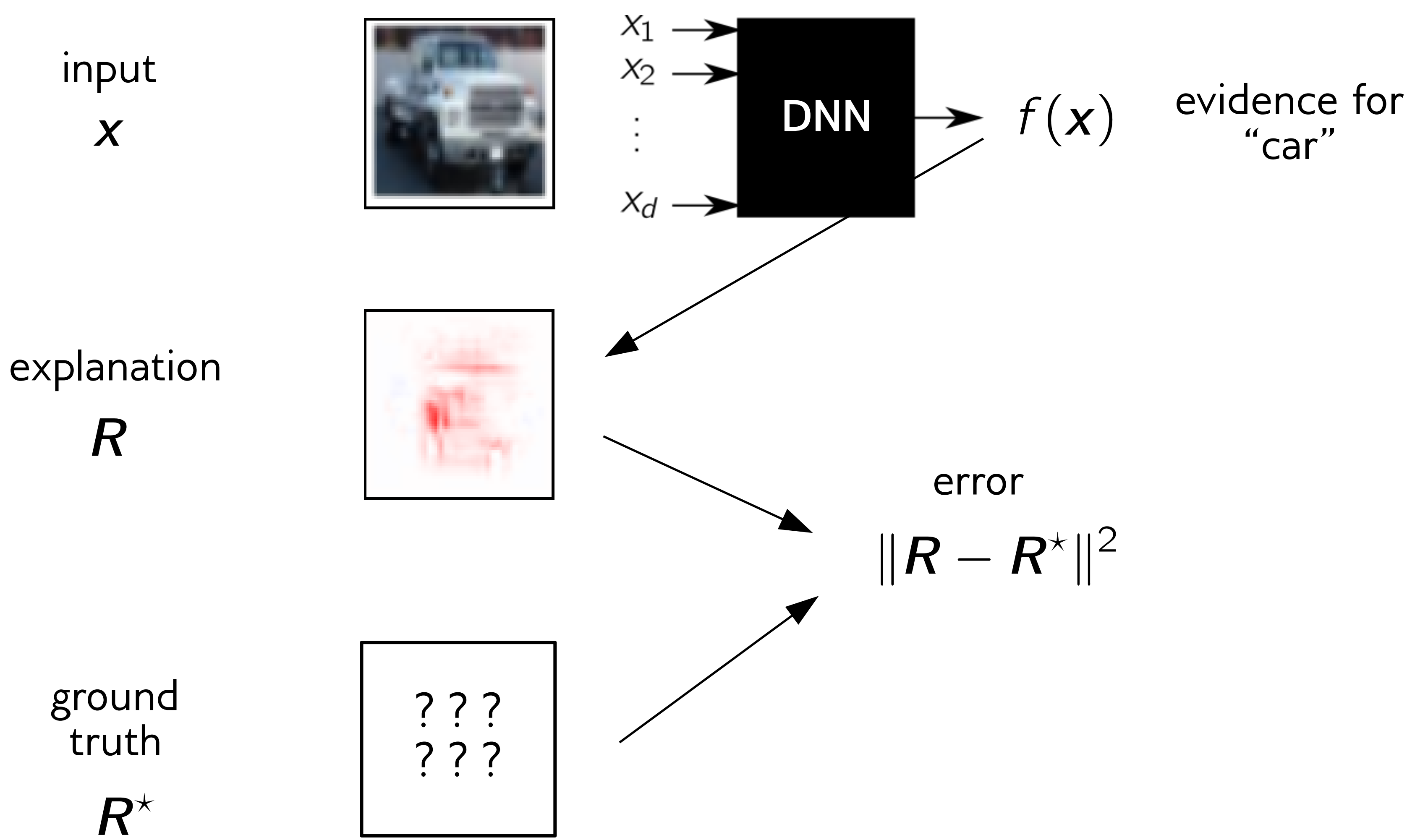
Selvaraju'17
Grad-CAM

Question: Which one to choose ?

First Attempt: Distance to Ground Truth



First Attempt: Distance to Ground Truth

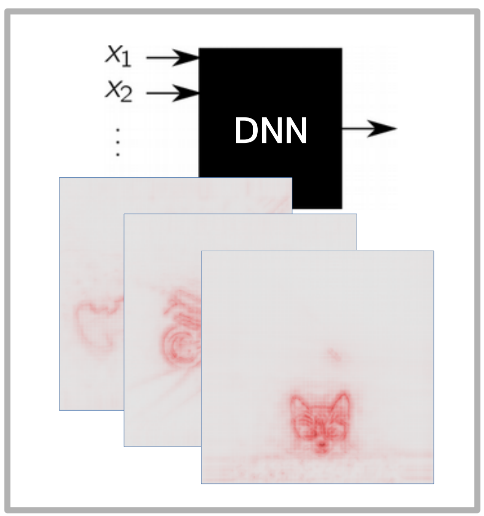


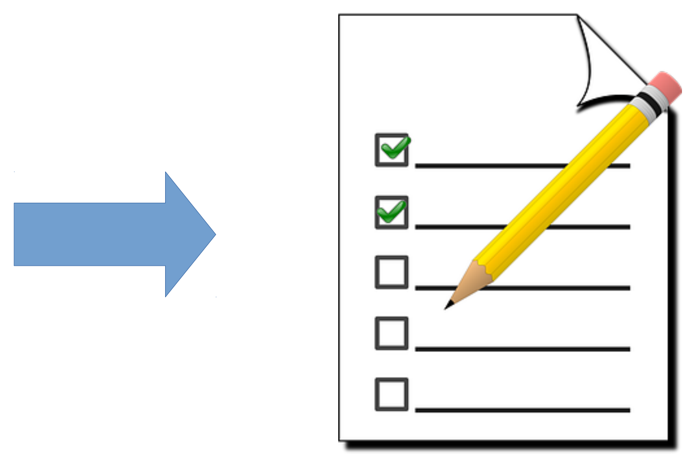
From Ground Truth Explanations to Axioms

Idea: Evaluate the explanation technique axiomatically, i.e. it must pass a number of predefined "unit tests".

[Sun'11, Bach'15, Montavon'17, Samek'17, Sundarajan'17, Kindermans'17, Montavon'18].

explanation technique

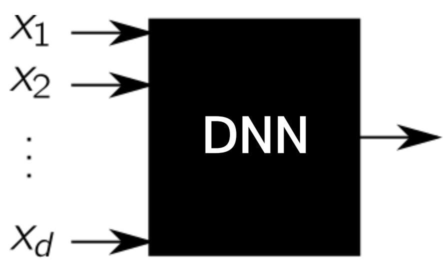




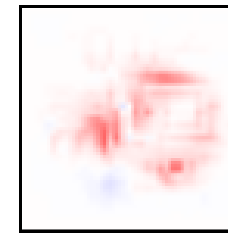
Properties 1-2: Conservation and Positivity

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

explanation



$f(\boldsymbol{x}) = f_{\text{exp}}(\boldsymbol{x}) + \varepsilon$



$R_1, \ldots, R_d$

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

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

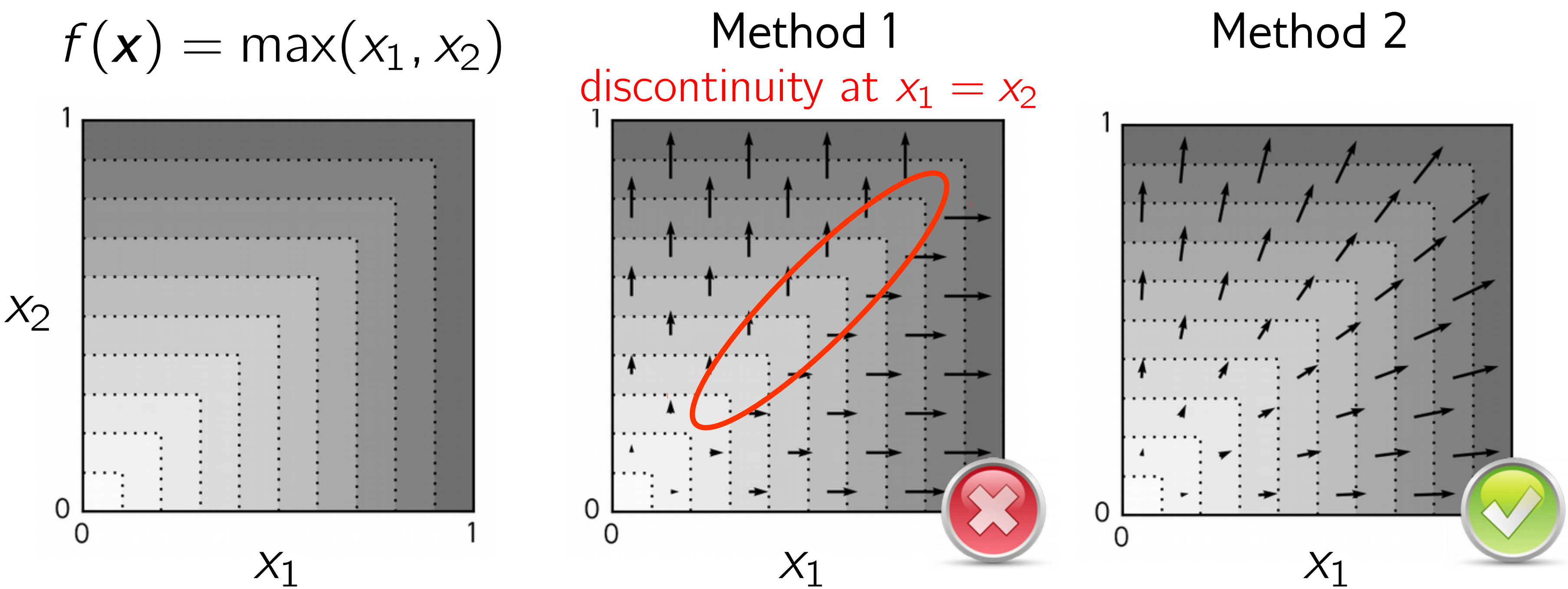
Positivity: If the neural network is certain about its prediction, input features are either relevant (positive) or irrelevant (zero).

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

Property 3: Continuity [Montavon'18]

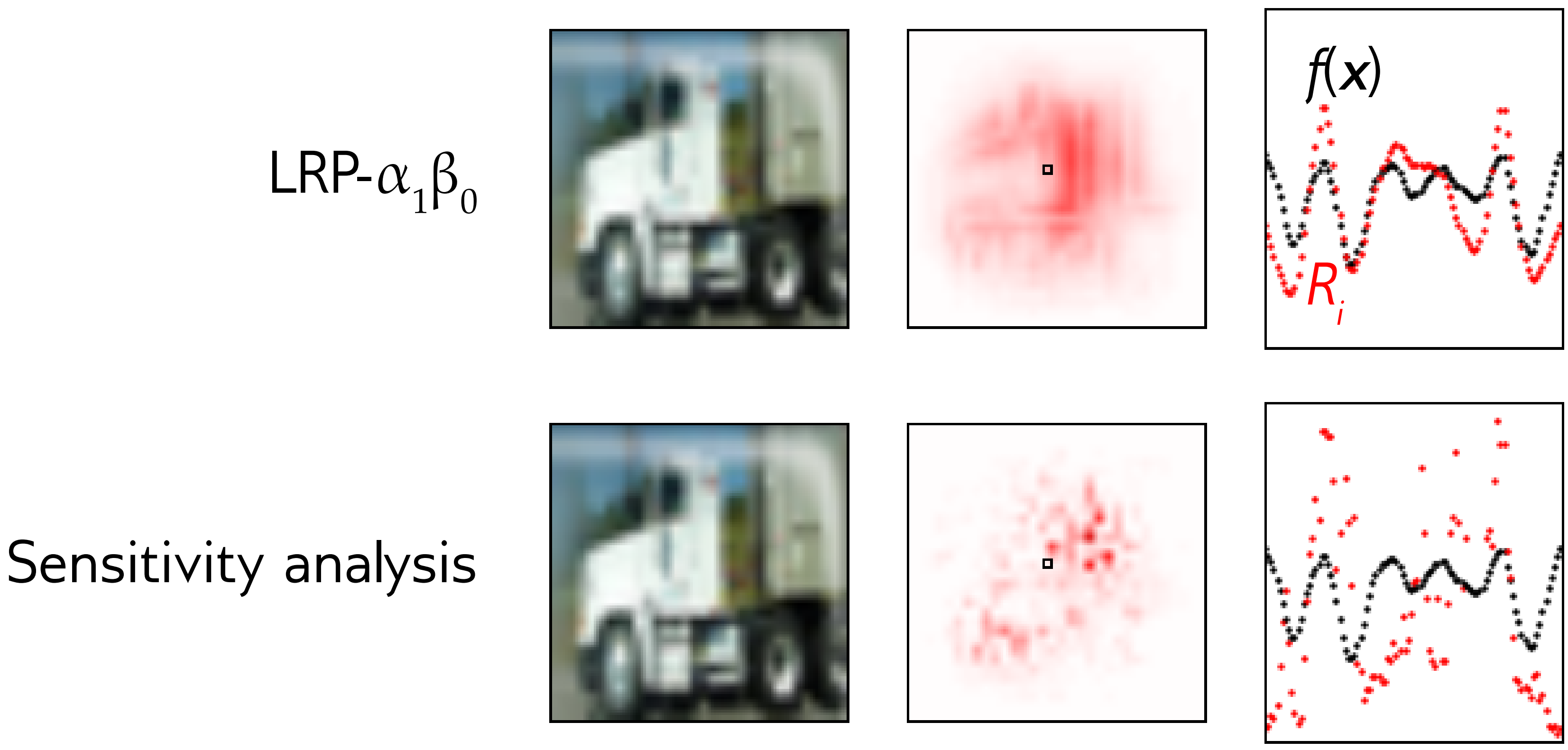
If two inputs are the almost the same, and the prediction is also almost the same, then the explanation should also be almost the same.

Example:



Testing Continuity

input | explanation scores



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.

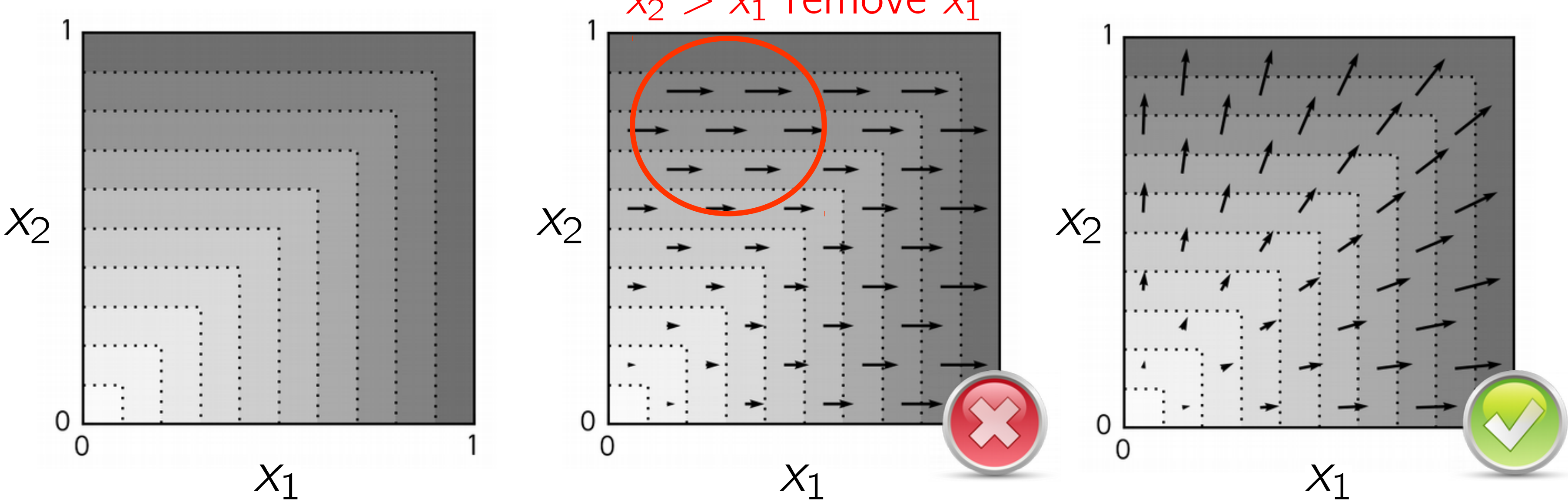
Example:

$f(\boldsymbol{x}) = \max(x_1, x_2)$

Method 1

$x_2 > x_1$ remove x_1

Method 2



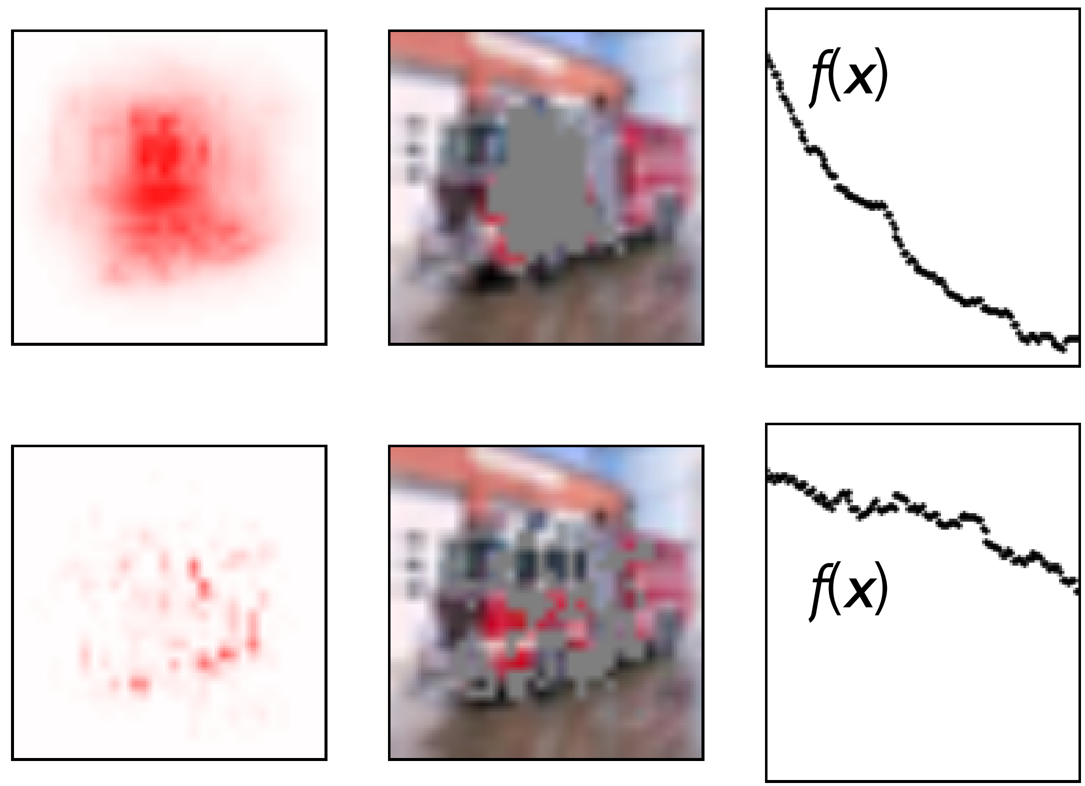
Testing Selectivity with Pixel-Flipping

[Bach'15, Samek'17]

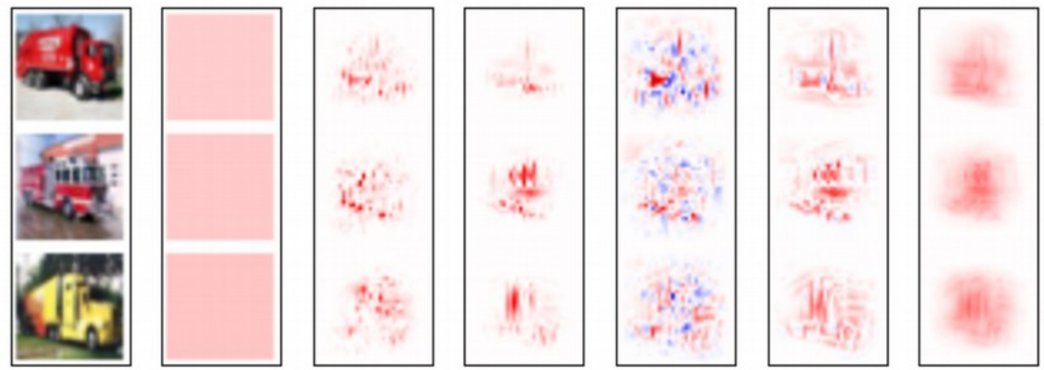
explanation scores | input

LRP-$\alpha_1\beta_0$

Sensitivity analysis



Explanation techniques



Properties	Uniform	$(\text{Gradient})^2$	$(\text{Guided BP})^2$	Gradient x Input	Guided BP x Input	LRP-$\alpha_1\beta_0$	...
1. Conservation	✔			✔	✔	✔	
2. Positivity	✔	✔	✔		✔	✔	
3. Continuity	✔		✔		✔	✔	
4. Selectivity		✔	✔	✔	✔	✔	
...							

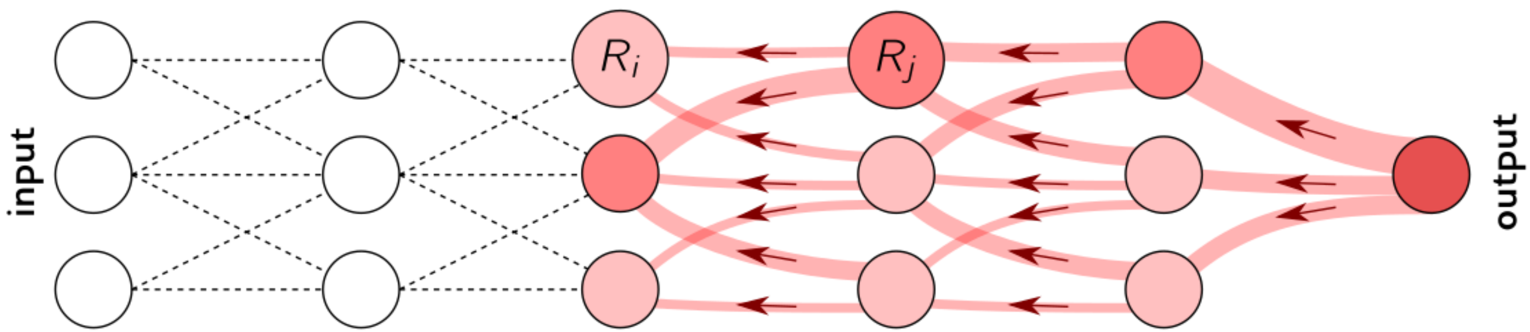
Question: Can we deduce some properties without experiments, directly from the equations?

Reminder

Backprop internals (for propagating gradient)

$$a_j = \max\left(0, \textstyle\sum_i a_i w_{ij} + b_j\right) \qquad \delta_i = \textstyle\sum_j w_{ij} \cdot 1_{z_j>0} \cdot \delta_j$$

LRP-$\alpha_1\beta_0$ internals (for propagating relevance)



$$a_j = \max\left(0, \textstyle\sum_i a_i w_{ij} + b_j\right) \qquad R_i = \sum_j \frac{a_i w_{ij}^+}{\sum_i a_i w_{ij}^+} R_j$$

Example: Deducing Conservation

LRP-$\alpha_1\beta_0$ propagation rule

$$R_i = \sum_j \frac{a_i w_{ij}^+}{\sum_i a_i w_{ij}^+} R_j$$

Summing gives the property

$$\sum_i R_i = \sum_j \frac{\sum_i a_i w_{ij}^+}{\sum_i a_i w_{ij}^+} R_j$$

vs. grad × input

$$\delta_i = \sum_j w_{ij} 1_{z_j > 0} \delta_j$$

× input

$$\sum_i a_i \delta_i = \sum_j \frac{\sum_i a_i w_{ij}}{\sum_i a_i w_{ij} + b_j} a_j \delta_j$$

When bias is negative, grad × input will tend to inflate scores.

$$\sum_{p=1}^d R_p = \cdots = \sum_i R_i = \sum_j R_j = \ldots = f(\boldsymbol{x})$$

Example: Deducing Continuity

LRP-$\alpha_1\beta_0$ propagation rule

$$R_i = \sum_j \frac{a_i w_{ij}^+}{\sum_i a_i w_{ij}^+} R_j$$

$$\Rightarrow \quad \underbrace{a_i c_i}_{R_i} = \sum_j \frac{a_i w_{ij}^+}{\sum_i a_i w_{ij}^+} \underbrace{a_j c_j}_{R_j}$$

$$\Rightarrow \quad c_i = \sum_j w_{ij}^+ \frac{\left(\sum_i a_i w_{ij} + b_j\right)^+}{\sum_i a_i w_{ij}^+} c_j$$

(when bias negative, continuity due to denominator upper-bounding numerator.)

vs. grad × input

$$\delta_i = \sum_j w_{ij} \cdot 1_{z_j > 0} \cdot \delta_j$$

$$\cdots \Leftarrow c_i(\boldsymbol{a}, (c_j)_j) \text{ continuous} \Leftarrow \cdots \Leftarrow 1 \text{ continuous}$$

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Intermediate Conclusion

1. Ground-truth explanations are elusive. In practice, we are reduced to visual assessment or to test the explanation for a number of axioms.

2. Some properties can be deduced from the structure of the explanation method. Other can be tested empirically.

3. LRP-$\alpha_1\beta_0$ satisfies key properties of an explanation. Sensitivity analysis and gradient × input have crucial limitations.

From LRP to Deep Taylor Decomposition

The LRP-$\alpha_1\beta_0$ rule

$$R_i = \sum_j \frac{a_i w_{ij}^+}{\sum_i a_i w_{ij}^+} R_j$$

can be seen as

a deep Taylor decomposition (DTD)

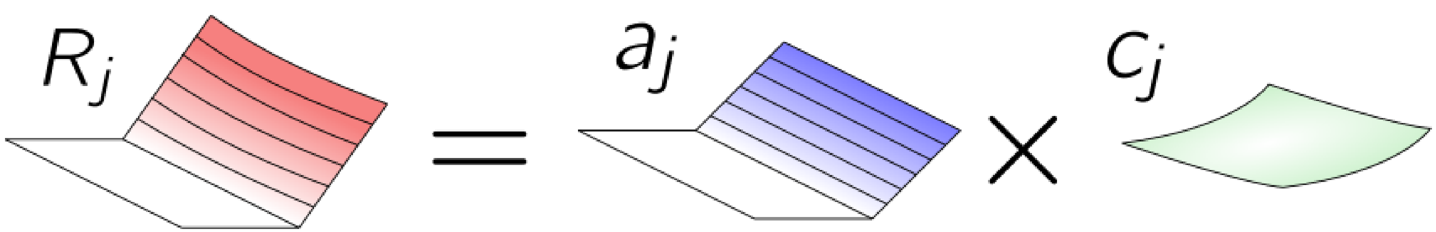
[Montavon'17]

which then yields

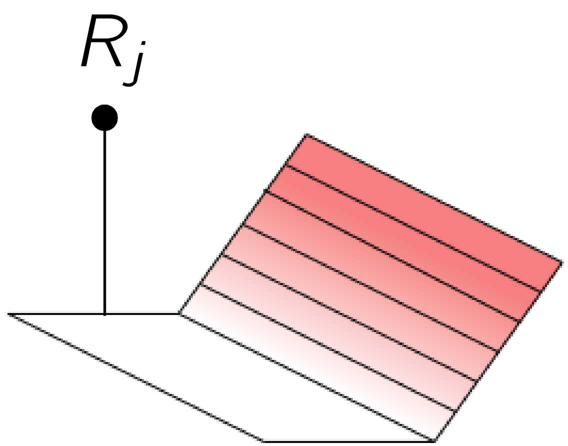
domain- and layer-specific rules

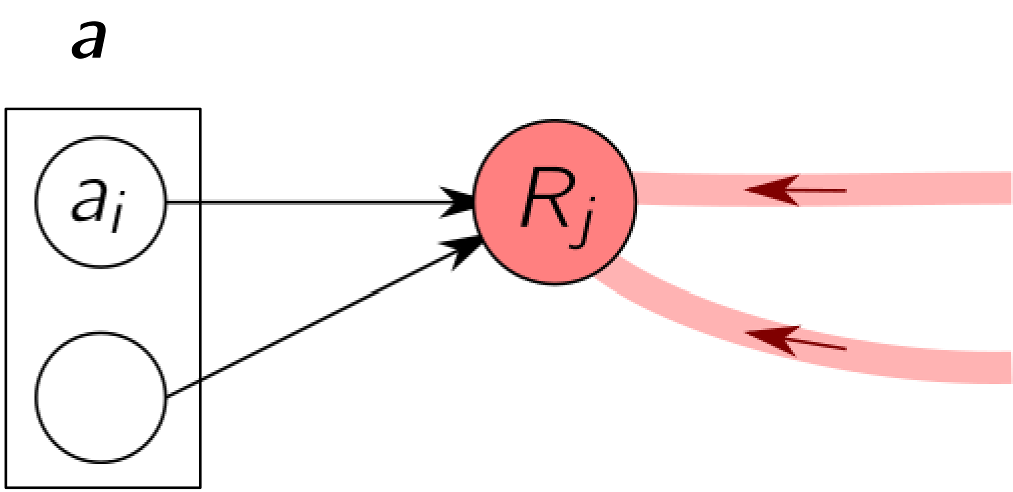
DTD: The Structure of Relevance

Proposition: Relevance at each layer is a product of the activation and an approximately constant term.



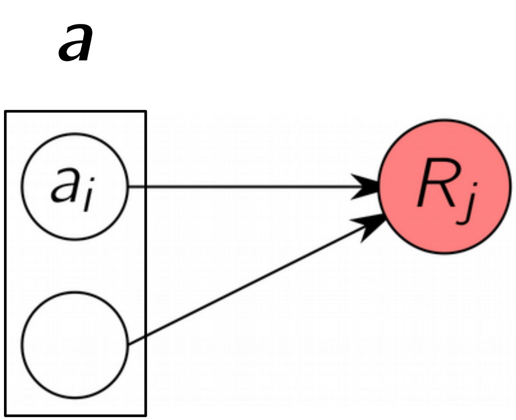
DTD: The Relevance as a Neuron

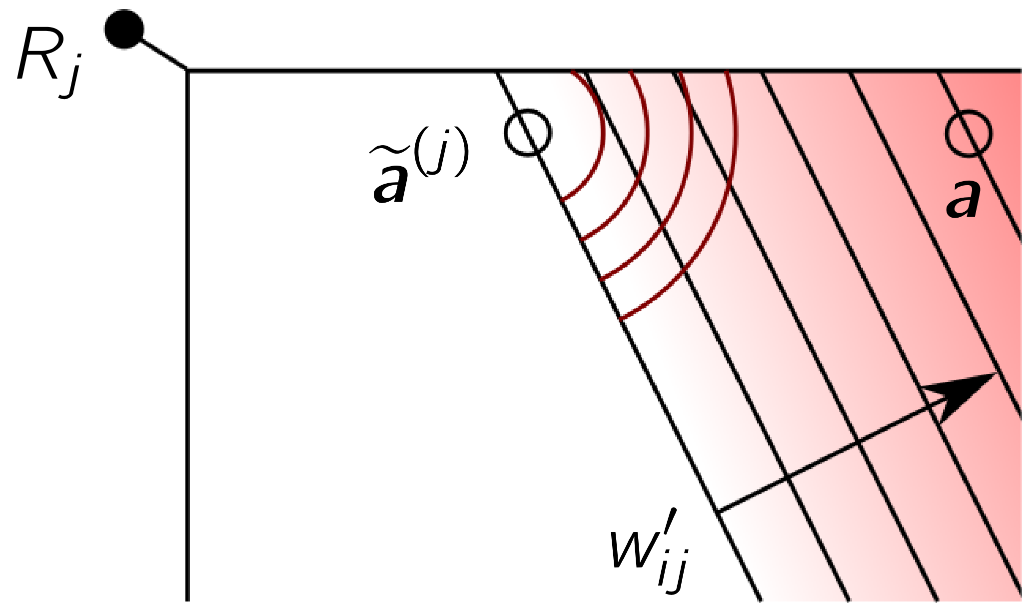




$$
\begin{aligned}
R_j(\boldsymbol{a}) &= \max(0, \textstyle\sum_i a_i w_{ij} + b_j) \cdot c_j \\
&= \max(0, \textstyle\sum_i a_i \underbrace{w_{ij} c_j}_{w'_{ij}} + \underbrace{b_j c_j}_{b'_j})
\end{aligned}
$$

DTD: Taylor Expansion of the Relevance





$$R_j(\boldsymbol{a}) = R_j(\widetilde{\boldsymbol{a}}^{(j)}) + \sum_i \frac{\partial R_j}{\partial a_i}\bigg|_{\widetilde{\boldsymbol{a}}^{(j)}} \cdot (a_i - \widetilde{a}_i^{(j)}) + \varepsilon$$

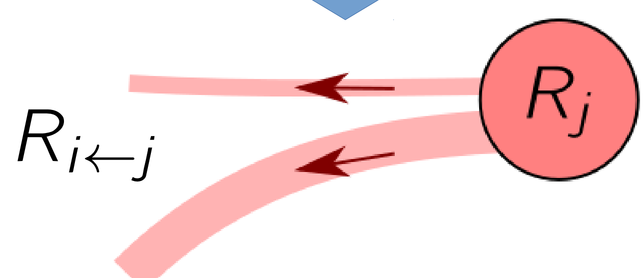
DTD: Decomposing the Relevance

Taylor expansion at root point:

$$R_j(\boldsymbol{a}) = R_j(\widetilde{\boldsymbol{a}}^{(j)}) + \sum_i \underbrace{\frac{\partial R_j}{\partial a_i}\bigg|_{\widetilde{\boldsymbol{a}}^{(j)}} \cdot (a_i - \widetilde{a}_i^{(j)})} + \varepsilon$$

$$0 \qquad \frac{(a_i - \widetilde{a}_i^{(j)})w_{ij}}{\sum_i (a_i - \widetilde{a}_i^{(j)})w_{ij}} R_j \qquad 0$$

Relevance can now be backward propagated



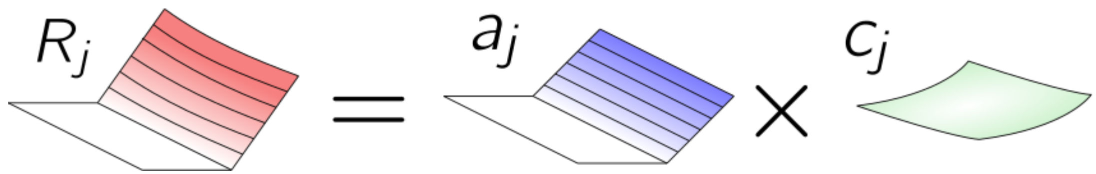
DTD: Choosing the Root Point

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

Choice of root point		$\widetilde{\boldsymbol{a}}^{(j)} \in \mathcal{D}$	$\lVert \boldsymbol{a} - \widetilde{\boldsymbol{a}}^{(j)} \rVert$
1. nearest root	$\widetilde{\boldsymbol{a}}^{(j)} = \boldsymbol{a} - t \cdot \boldsymbol{w}_j$		✔
2. rescaled activation	$\widetilde{\boldsymbol{a}}^{(j)} = \boldsymbol{a} - t \cdot \boldsymbol{a}$	✔	
3. rescaled excitations	$\widetilde{\boldsymbol{a}}^{(j)} = \boldsymbol{a} - t \cdot \boldsymbol{a} \odot \mathbf{1}_{\boldsymbol{w}_j \succ 0}$	✔	✔

$$R_{i \leftarrow j} = \frac{a_i w_{ij}^+}{\sum_i a_i w_{ij}^+} R_j$$ (LRP-$\alpha_1\beta_0$)

DTD: Verifying the Product Structure



But was it true?

1. assume it holds in higher-layer

$$R_j = \sum_k \frac{a_j w_{jk}^+}{\sum_j a_j w_{jk}^+} a_k c_k = a_j \underbrace{\sum_k w_{jk}^+ \frac{(\sum_j a_j w_{jk} + b_k)^+}{\sum_j a_j w_{jk}^+} c_k}_{c_j}$$

2. apply LRP-$\alpha_1\beta_0$ rule

3. observe it also holds in lower-layer

From LRP to Deep Taylor Decomposition

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can be seen as

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[Montavon'17]

which then yields

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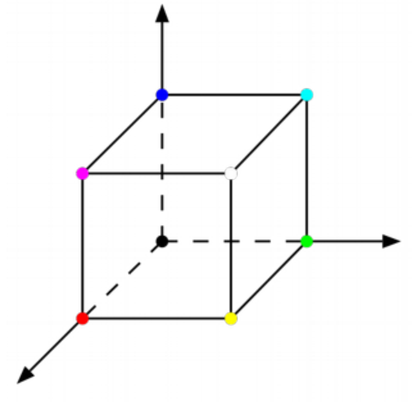
DTD: Application to Input Layers

Pixels:

$$x \in [l, h]^{3\times d}$$



Embeddings:

$$x \in \mathbb{R}^d$$

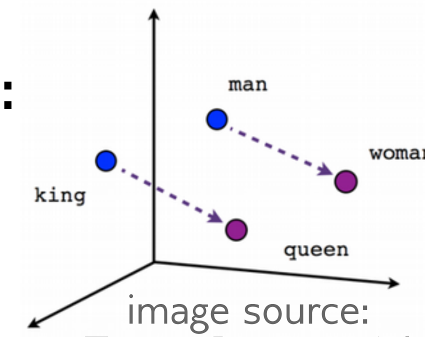


image source:
Tensorflow tutorial

1. Choose a root point that is nearby and satisfies domain constraints

$$(\boldsymbol{x} - \widetilde{\boldsymbol{x}}^{(j)}) = t \cdot (\boldsymbol{x} - \boldsymbol{l} \odot 1_{\boldsymbol{w}_j \succ 0} - \boldsymbol{h} \odot 1_{\boldsymbol{w}_j \prec 0})$$

$$(\boldsymbol{x} - \boldsymbol{x}^{(j)}) = t \cdot \boldsymbol{w}_j$$

2. Inject it in the generic DTD rule to get the specific rule

$$R_p = \sum_j \frac{x_{pj} w_{pj} - l_p w_{pj}^+ - h_p w_{pj}^-}{\sum_p x_{pj} w_{pj} - l_p w_{pj}^+ - h_p w_{pj}^-} R_j$$

$$R_p = \sum_j \frac{w_{pj}^2}{\sum_p w_{pj}^2} R_j$$

DTD: Application to Pooling Layers

A sum-pooling layer over positive activations is equivalent to a ReLU layer with weights 1.

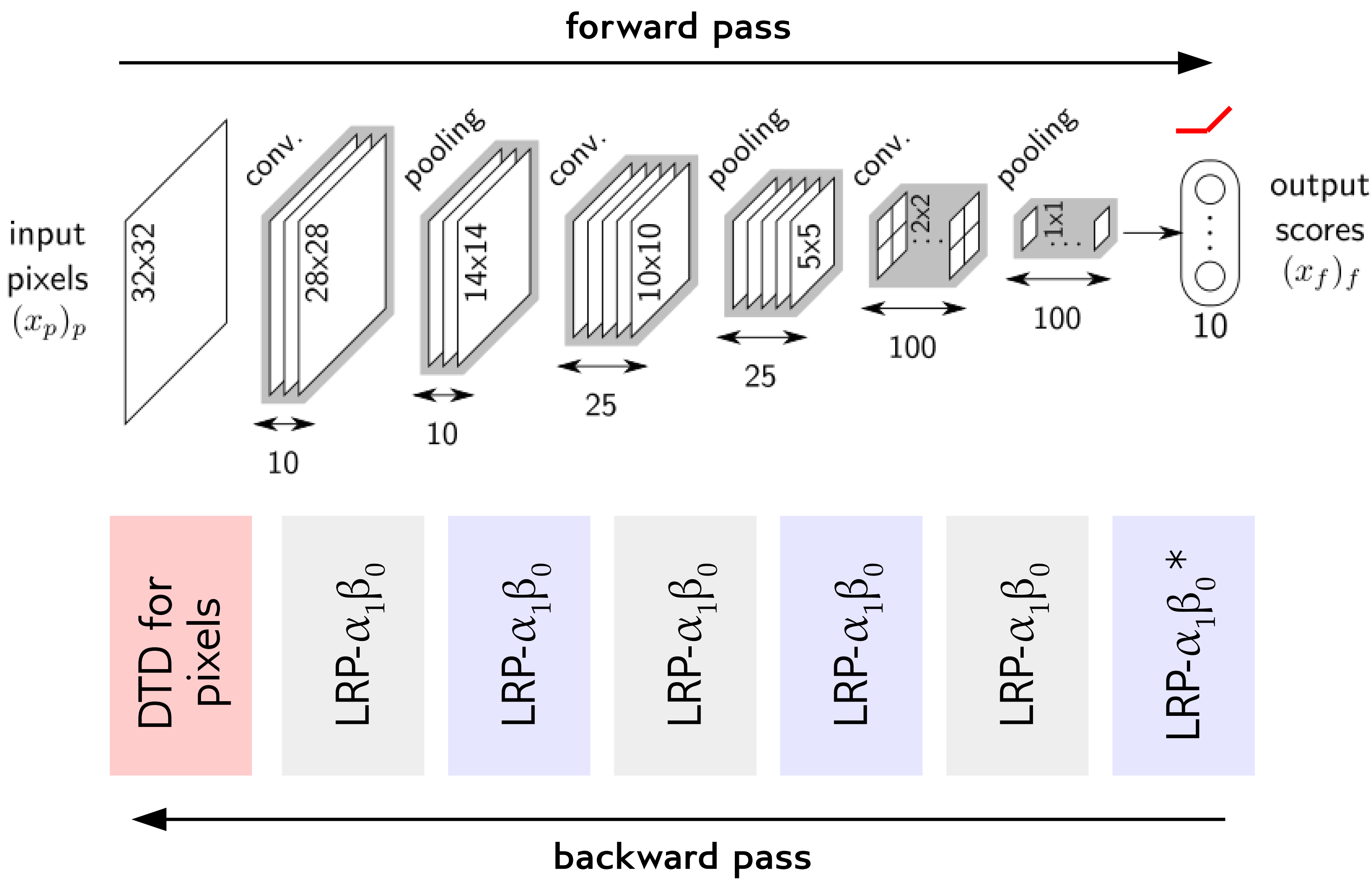
$$a_j = \left(\sum_i a_i \right) = \max\left(0, \sum_i a_i 1_{ij} + 0_j\right)$$

A p-norm pooling layer can be approximated as a sum-pooling layer multiplied by a ratio of norms that we treat as constant [Montavon'17].

$$a_j = \left(\sum_i a_i \right) \cdot \frac{\|(a_i)_i\|_p}{\|(a_i)_i\|_1}$$

→ Treat pooling layers as ReLU detection layers

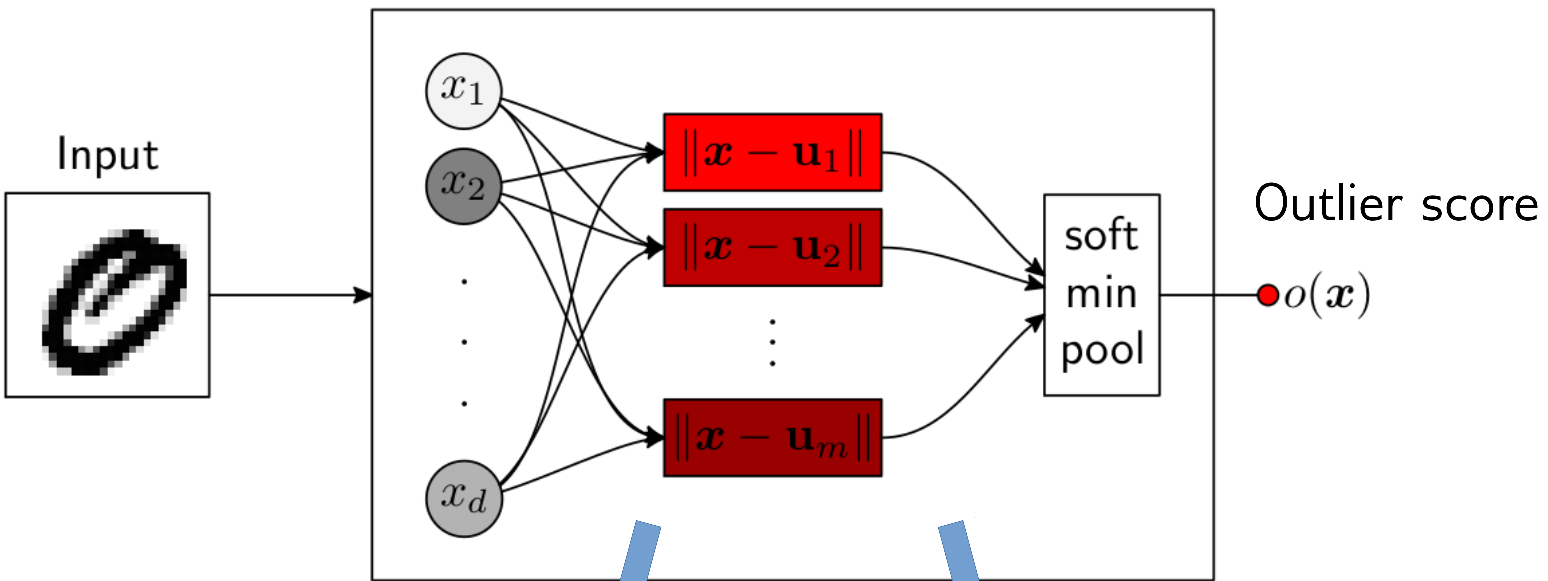
Basic Recommendation for CNNs



* For top-layers, other rules may improve selectivity

DTD for Kernel Models [Kauffmann'18]

1. Build a neural network equivalent of the One-Class SVM:



2. Computes its deep Taylor decomposition

$$R_i = \sum_j \frac{(x_i - u_{ij})^2}{\|\boldsymbol{x} - \boldsymbol{u}_j\|_2^2}(R_j - D_j^+)$$

Gaussian/Laplace Kernel

$$R_j = (a_j + \varepsilon_j) \cdot \frac{\exp(-a_j)}{\sum_j \exp(-a_j)}$$

Student Kernel

$$R_j = a_j \cdot \mathbb{H}[(h_{j'}/h_j)_{j'}]$$

Implementing the LRP-$\alpha_1\beta_0$ rule

Propagation rule to implement:

$$\boxed{R_i = \sum_j \frac{a_i w_{ij}^+}{\sum_i a_i w_{ij}^+} R_j}$$

Sequence of element-wise computations	Sequence of vector computations
$z_j \rightarrow \sum_i a_i w_{ij}^+$	$\boldsymbol{z} \rightarrow W_+^\top \cdot \boldsymbol{a}$
$s_j \rightarrow R_j / z_j$	$\boldsymbol{s} \rightarrow \boldsymbol{R} \oslash \boldsymbol{z}$
$c_i \rightarrow \sum_j w_{ij}^+ s_j$	$\boldsymbol{c} \rightarrow W_+ \cdot \boldsymbol{s}$
$R_i \rightarrow a_i c_i$	$\boldsymbol{R} \rightarrow \boldsymbol{a} \odot \boldsymbol{c}$

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Implementing the LRP-$\alpha_1\beta_0$ rule

Propagation rule to implement:

$$\boxed{R_i = \sum_j \frac{a_i w_{ij}^+}{\sum_i a_i w_{ij}^+} R_j}$$

Code that reuses forward and gradient computations:

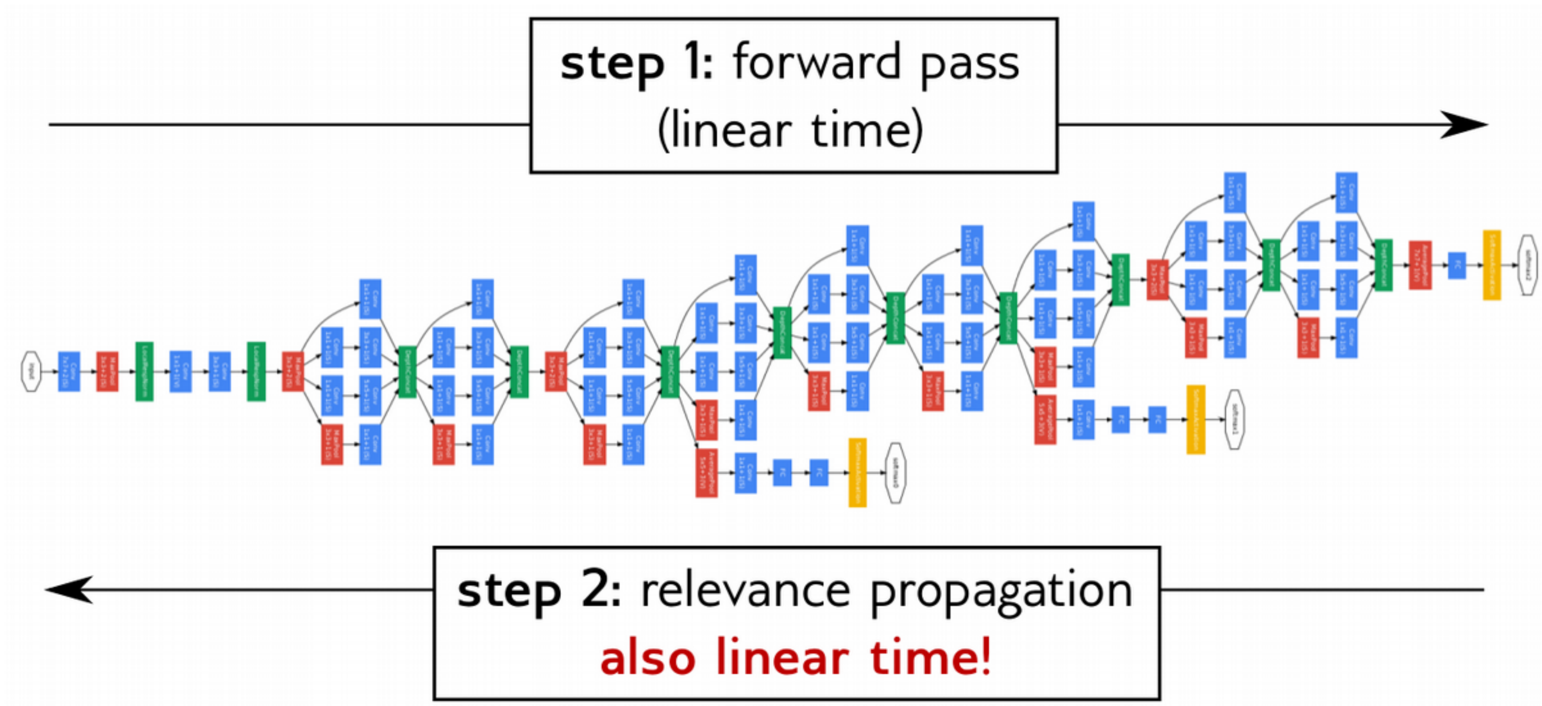
```
def lrp(layer,a,R):

    clone = layer.clone()
    clone.W = maximum(0,layer.W)
    clone.B = 0

    z = clone.forward(a)
    s = R / z
    c = clone.backward(s)

    return a * c
```

How LRP Scales



No need for much computing power. GoogleNet explanation for single image can be done on the CPU.

Linear time scaling allows to use LRP for real-time processing, or as part of training.

Conclusion

1. Ground-truth explanations are elusive. In practice, we are reduced to visual assessment or to test the explanation for a number of axioms.
2. Some properties can be deduced from the structure of the explanation method. Other can be tested empirically.
3. LRP-$\alpha_1\beta_0$ satisfies key properties of an explanation. Sensitivity analysis and gradient × input have crucial limitations.
4. This suitable LRP-$\alpha_1\beta_0$ propagation rule can be seen as performing a <u>deep Taylor decomposition</u> for deep ReLU nets.
5. The deep Taylor decomposition allows to consistently extend the framework to <u>new models</u> and <u>new types of data</u>.

References

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