Explaining NonLinear Classification Decisions with Deep Taylor Decomposition by Montavon et al.

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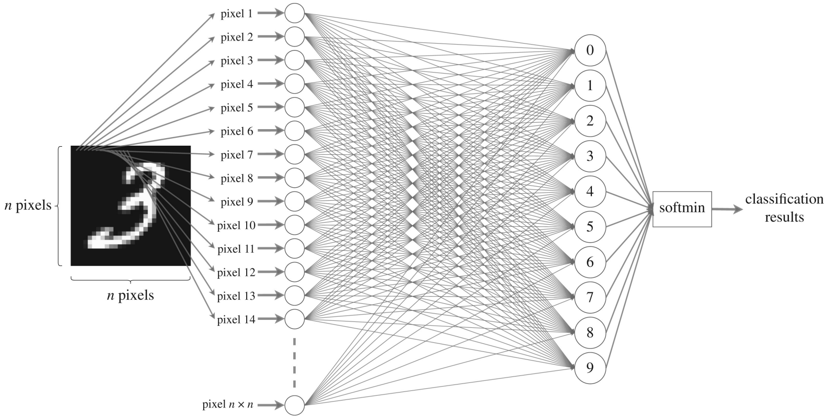
Explainability



Deep neural networks perform great on a variety of problems
but how can we explain decisions made by complex deep architectures?

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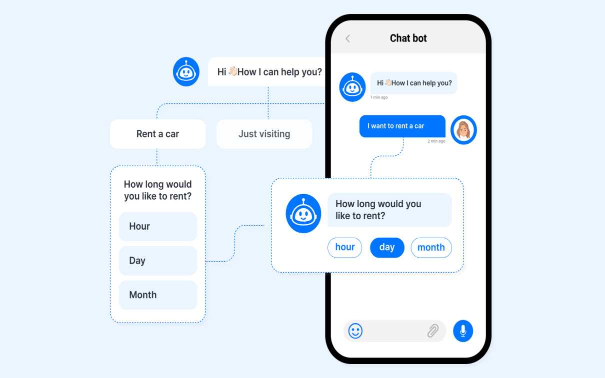
Introduction

Deep neural networks revolutionized amongst others the field of



- Image recognition
- Natural language processing
- Human action recognition
- Physics
- Finance
- ...

Introduction

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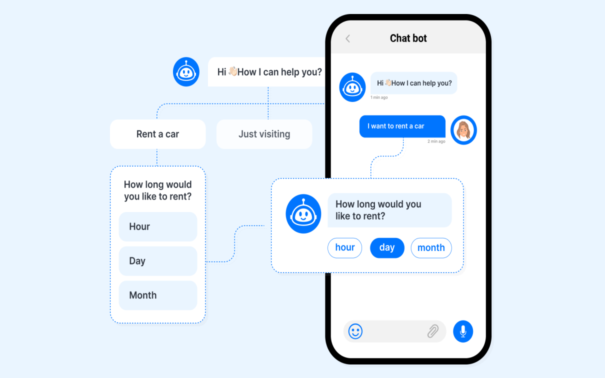

- Image recognition
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With one major drawback → **lack of transparency**

General Idea

To accomplish the task of explainability we map relevance from the output to the input features

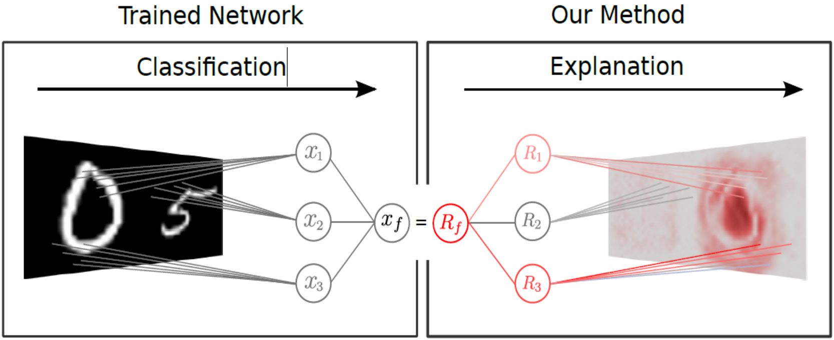

Figure 1: Neural Network Detecting 0 while Distracted by 5

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Mathematical Framework

In the context of image classification we define the following mathematical framework

- Positive valued function $f : \mathbb{R}^d \to \mathbb{R}^+$, where the output $f(x)$ defines either the probability that the object is present or the quantity of the object in question

$\rightarrow$ $f(x) > 0$ expresses the presence of the object

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$\rightarrow$ $f(x) > 0$ expresses the presence of the object

- Input $x \in \mathbb{R}^d$, decomposable in a set of pixel values $x = \{x_p\}$
- Relevance score $R_p(x)$ indicating the relevance of each pixel

$\rightarrow$ The relevance score can be displayed in a heatmap denoted by $R(x) = \{R_p(x)\}$

Definitions

Definition 1

A heatmapping $R(x)$ is <u>conservative</u> if the sum of assigned relevances in the pixel space corresponds to the total relevance detected by the model, that is

$$\forall x : f(x) = \sum_p R_p(x) \quad (1)$$

Definitions

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A heatmapping $R(x)$ is <u>conservative</u> if the sum of assigned relevances in the pixel space corresponds to the total relevance detected by the model, that is

$$\forall x : f(x) = \sum_p R_p(x) \tag{1}$$

Definition 2

A heatmapping $R(x)$ is <u>positive</u> if all values forming the heatmap are greater or equal to zero, that is:

$$\forall x, p : R_p(x) \geq 0 \tag{2}$$

Definitions

All algorithms are shall comply with definition 1 and 2

Definition 3

A heatmapping $R(x)$ is consistent if it is *conservative* and *positive*. That is, it is consistent if it complies with Definitions 1 and 2.

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Definition 3

A heatmapping $R(x)$ is consistent if it is *conservative* and *positive*. That is, it is consistent if it complies with Definitions 1 and 2.

But consistency is not a measure of quality which can be seen on the following example which complies with definition 3

$$\forall p : R_p(x) = \frac{1}{d} \cdot f(x),$$

where d denotes the number of pixels

Taylor Expansion

First order Taylor expansion at root point $\tilde{x}$

$$\begin{aligned} f(x) &= f(\tilde{x}) + \left(\frac{\partial f}{\partial x}\bigg|_{x=\tilde{x}} \right)^T \cdot (x - \tilde{x}) + \epsilon \\ &= 0 + \sum_p \underbrace{\frac{\partial f}{\partial x_p}\bigg|_{x=\tilde{x}} \cdot (x_p - \tilde{x}_p)}_{R_p(x)} + \epsilon \end{aligned}$$

Taylor Expansion

First order Taylor expansion at root point $\tilde{x}$

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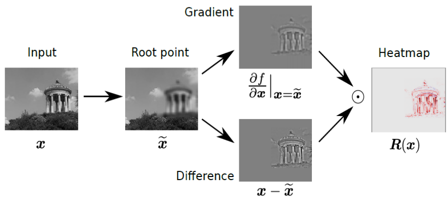
The challenge of finding a root point



- Potentially more than one root point
- Remove object but deviate as few as possible

$\rightarrow$ $\min_\xi \|\xi - x\|^2$ subject to $f(\xi) = 0$

Sensitivity Analysis

Choose a point at infinitesimally small distance from the actual point, i.e. $\xi = x - \delta \frac{\partial f}{\partial x}$, where δ is small

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If we assume a locally constant function we get

$$\begin{aligned}
f(x) &= f(\xi) + \left(\frac{\partial f}{\partial x}\bigg|_{x=\xi} \right)^T \cdot (x - (x - \delta \frac{\partial f}{\partial x})) + 0 \\
&= f(\xi) + \delta \left(\frac{\partial f}{\partial x} \right)^T \cdot \frac{\partial f}{\partial x} + 0 \\
&= f(\xi) + \sum_p \underbrace{\delta \left(\frac{\partial f}{\partial x} \right)^2}_{R_p} + 0
\end{aligned}$$

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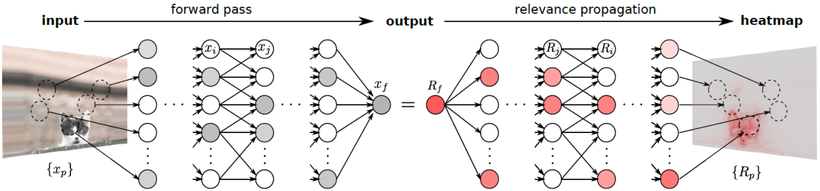
&= f(\xi) + \sum_p \underbrace{\delta\left(\frac{\partial f}{\partial x}\right)^2}_{R_p} + 0
\end{aligned}
$$

- The heatmap is positive but not conservative
- The heatmap only measures a local effect

Deep Taylor Decomposition



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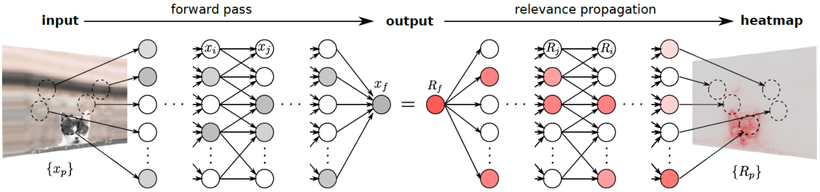
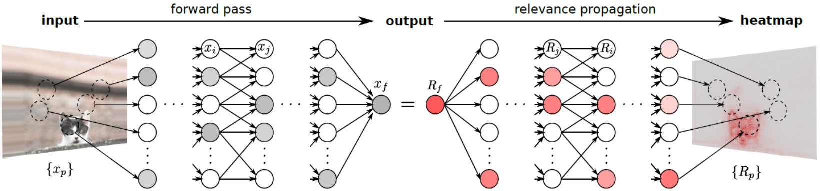


We view each layer as a separate function and write the Taylor decomposition of $\sum_j R_j$ at $\{x_i\}$ as

$$\sum_j R_j = \left(\frac{\partial(\sum_j R_j)}{\partial\{x_i\}} \bigg|_{\{\tilde{x}_i\}} \right)^T \cdot (\{x_i\} - \{\tilde{x}_i\}) + \epsilon$$

$$= \sum_i \underbrace{\sum_j \frac{\partial R_j}{\partial x_i} \bigg|_{\tilde{x}_i} \cdot (x_i - \tilde{x}_i)}_{R_i} + \epsilon$$

Deep Taylor Decomposition



- If each local Taylor decomposition is *conservative* then the chain of equalities is also *conservative* (layer-wise relevance conservation)

$\rightarrow$ $R_f = ... = \sum_i R_i = ... = \sum_p R_p$

- If each local Taylor decomposition is *positive* then the chain of equalities is also *positive*

$\rightarrow$ $R_f, ..., \{R_i\}, ..., \{R_p\} \geq 0$

- If each local Taylor decomposition is *consistent* then the chain of equalities is also *consistent*

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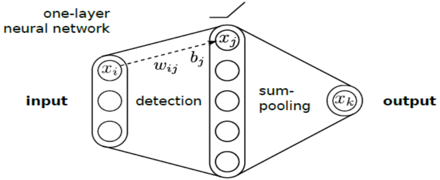
Setting

Consider a simple detection-pooling one layer neural network with

$$x_j = \max(0, \sum_i x_i w_{ij} + b_j)$$

$$x_k = \sum_j x_j, \;\; b_j \leq 0, \forall j$$



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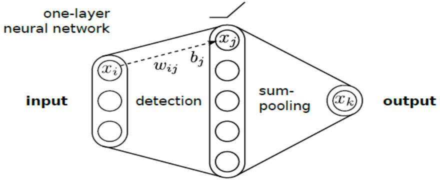

1. $R_k = x_k$ and thus $R_k = \sum_j x_j$
2. Chose a root point and redistribute R_k on neurons x_j
   $\rightarrow R_j = \frac{\partial R_k}{\partial x_j}\Big|_{\{\tilde{x}_j\}} \cdot (x_j - \tilde{x}_j)$, with $\{\tilde{x}_j\} = 0$
3. Since $\frac{\partial R_k}{\partial x_j}\Big|_{\{\tilde{x}_j\}} = 1$ we obtain $R_j = x_j$
4. Apply Taylor decomposition another time and get
   $R_i = \sum_j \frac{\partial R_j}{\partial x_i}\Big|_{\{\tilde{x}_i\}^{(j)}} \cdot (x_i - \tilde{x}_i^{(j)})$

Derivation of Propagation Rules

Given $R_j = \max(0, \sum_i x_i w_{ij} + b_j)$ and $b_j \leq 0$ and a search direction $\{v_i\}^{(j)}$

$$\tilde{x}_i^{(j)} = x_i + t v_i^{(j)} \Leftrightarrow t = \frac{\tilde{x}_i^{(j)} - x_i}{v_i^{(j)}} \tag{3}$$

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If $\sum_i x_i w_{ij} + b_j > 0$ the nearest root along the search direction $\{v_i\}^{(j)}$ is given by the intersection of equation (3) and $\sum_i \tilde{x}_i^{(j)} w_{ij} + b_j = 0$

$$\begin{aligned} & & 0 &= \sum_i x_i w_{ij} + b_j + \sum_i v_i^{(j)} t w_{ij} \\ &\Leftrightarrow & -t &= \frac{\sum_i x_i w_{ij} + b_j}{\sum_i v_i^{(j)} w_{ij}} \\ &\Leftrightarrow & x_i - \tilde{x}_i^{(j)} &= \frac{\sum_i x_i w_{ij} + b_j}{\sum_i v_i^{(j)} w_{ij}} v_i^{(j)} \end{aligned}$$

Derivation of Propagation Rules

Starting from the Taylor expansion we can plug in

$$x_i - \tilde{x}_i^{(j)} = \frac{\sum_i x_i w_{ij} + b_j}{\sum_i v_i^{(j)} w_{ij}} v_i^{(j)}$$

To get

$$R_i = \sum_j \frac{\partial R_j}{\partial x_i}\bigg|_{\{\tilde{x}_i^{(j)}\}} \cdot (x_i - \tilde{x}_i^{(j)}) = \sum_j w_{ij} \frac{\sum_i x_i w_{ij} + b_j}{\sum_i v_i^{(j)} w_{ij}} v_i^{(j)}$$

$$= \sum_j \frac{v_i^{(j)} w_{ij}}{\sum_i v_i^{(j)} w_{ij}} R_j \tag{4}$$

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The relevance propagation rule can be calculated with the following steps

1. Define a segment with search direction $\{v_i\}^{(j)}$
2. The line lies inside the input domain and contains a root point
3. Inject search direction in equation (4)

ω^2-rule $\mathcal{X} = \mathbb{R}^d$

Choose a root point which is nearest in the euclidean sense

1. Search direction $\{v_i\}^{(j)} = w_{ij}$ (gradient of R_j)
2. No domain restriction and for $\tilde{x}_i^{(j)} = x_i - \frac{R_j(x_i)}{\sum_{i'} w_{i'j}^2} w_{ij}$

$$R_j(\{\tilde{x}_i^{(k)}\}) = \max(0, \sum_i (x_i - \frac{R_j(x_i) w_{ij}}{\sum_{i'} w_{i'j}^2}) w_{ij} + b_j)$$

$$= \max(0, \underbrace{\sum_i (x_i w_{ij} + b_j)}_{=R_j(x_i)} - R_j(x_i) \underbrace{\frac{\sum_i w_{ij}^2}{\sum_{i'} w_{i'j}^2}}_{=1}) = 0$$

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ω^2-rule

$$R_i = \sum_j \frac{\partial R_j}{\partial x_i}\bigg|_{\{\tilde{x}_i\}^{(j)}} \cdot (x_i - \tilde{x}_i^{(j)}) = \sum_j \frac{w_{ij}^2}{\sum_{i'} w_{i'j}^2} R_j$$

w^2-rule $\mathcal{X} = \mathbb{R}^d$

Proposition 1

For all functions $g \in G$, the deep Taylor decomposition with the ω^2-rule is consistent.

w^2-rule $\mathcal{X} = \mathbb{R}^d$

Proposition 1

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Proof

1. *Conservative*

$$\sum_i R_i = \sum_i \Big(\sum_j \frac{w_{ij}^2}{\sum_{i'} w_{i'j}^2} R_j \Big)$$

$$= \sum_j \underbrace{\frac{\sum_i w_{ij}^2}{\sum_{i'} w_{i'j}^2}}_{=1} R_j = \sum_j R_j = \sum_j x_j = f(x)$$

2. *Positive*

$$R_i = \sum_j \frac{w_{ij}^2}{\sum_{i'} w_{i'j}^2} R_j = \sum_j \underbrace{w_{ij}^2}_{\geq 0} \underbrace{\frac{1}{\sum_{i'} w_{i'j}^2}}_{>0} \underbrace{R_j}_{\geq 0} \geq 0$$

z^+-rule $\mathcal{X} = \mathbb{R}^d_+$

Search for a root point on the segment $(\{x_i 1_{w_{ij}<0}\}, \{x_i\}) \subset \mathbb{R}^d_+$

1. Search direction $\{v_i\}^{(j)} = x_i - x_i 1_{w_{ij}<0} = x_i 1_{w_{ij}\geq 0}$
2. If $\{x_i\} \in \mathbb{R}^d_+$ so is the whole domain, further for $w_{ij}^- = \min(0, w_{ij})$ and $w_{ij}^+ = \max(0, w_{ij})$

$$\begin{aligned} R_j(\{x_i 1_{w_{ij}<0}\}) &= \max(0, \sum_i x_i 1_{w_{ij}<0} w_{ij} + b_j) \\ &= \max(0, \underbrace{\sum_i x_i w_{ij}^-}_{\leq 0} + b_j) = 0 \end{aligned}$$

3. Inject search direction in equation (4)

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2. If $\{x_i\} \in \mathbb{R}^d_+$ so is the whole domain, further for $w^-_{ij} = \min(0, w_{ij})$ and $w^+_{ij} = \max(0, w_{ij})$

$$\begin{aligned} R_j(\{x_i 1_{w_{ij}<0}\}) &= \max(0, \sum_i x_i 1_{w_{ij}<0} w_{ij} + b_j) \\ &= \max(0, \underbrace{\sum_i x_i w^-_{ij}}_{\leq 0} + b_j) = 0 \end{aligned}$$

3. Inject search direction in equation (4)

z^+-rule

$$R_i = \sum_j \frac{x_i w^+_{ij}}{\sum_{i'} x_{i'} w^+_{i'j}} R_j$$

z^+-rule $\mathcal{X} = \mathbb{R}_+^d$

Proposition 2

For all functions $g \in G$ and data points $\{x_i\} \in \mathbb{R}_+^d$, the deep Taylor decomposition with the z^+-rule is consistent.

z^+-rule $\mathcal{X} = \mathbb{R}_+^d$

Proposition 2

For all functions $g \in G$ and data points $\{x_i\} \in \mathbb{R}_+^d$, the deep Taylor decomposition with the z^+-rule is consistent.

Proof

If $\sum_i x_i w_{ij}^+ > 0$ the same proof as for the w^2-rule applies, if $\sum_i x_i w_{ij}^+ = 0$ it follows that $\forall i : x_i w_{ij} \leq 0$ and

$$R_j = x_j = \max(0, \underbrace{\sum_i x_i w_{ij}}_{\leq 0} + b_j) = 0$$

and there is no relevance to redistribute to the lower layers.

z^b-rule $\mathcal{X} = \mathcal{B}$

Given a bounded input space $\mathcal{B} = \{\{x_i\} : \forall_{i=1}^{d} l_i \leq x_i \leq h_i\}$, with $l_i \leq 0$ and $h_i \geq 0$ and we search on the segment $(\{l_i 1_{w_{ij}>0} + h_i 1_{w_{ij}<0}\}, \{x_i\}) \subset \mathcal{B}$

1. Search direction $\{v_i\}^{(j)} = x_i - l_i 1_{w_{ij}>0} - h_i 1_{w_{ij}<0}$
2. If $\{x_i\} \in \mathcal{B}$ so is the whole domain and for $w_{ij}^- = \min(0, w_{ij})$, $w_{ij}^+ = \max(0, w_{ij})$

$$
\begin{aligned}
R_j(\{l_i 1_{w_{ij}>0} + h_i 1_{w_{ij}<0}\}) &= \max(0, \sum_i l_i 1_{w_{ij}>0} w_{ij} + h_i 1_{w_{ij}<0} w_{ij} + b_j) \\
&= \max(0, \sum_i \underbrace{l_i w_{ij}^+}_{\leq 0} + \underbrace{h_i w_{ij}^-}_{\leq 0} + b_j) = 0
\end{aligned}
$$

3. Inject search direction in equation (4)

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2. If $\{x_i\} \in \mathcal{B}$ so is the whole domain and for $w_{ij}^- = \min(0, w_{ij})$, $w_{ij}^+ = \max(0, w_{ij})$

$$R_j(\{l_i 1_{w_{ij}>0} + h_i 1_{w_{ij}<0}\}) = \max(0, \sum_i l_i 1_{w_{ij}>0} w_{ij} + h_i 1_{w_{ij}<0} w_{ij} + b_j)$$

$$= \max(0, \sum_i \underbrace{l_i w_{ij}^+}_{\leq 0} + \underbrace{h_i w_{ij}^-}_{\leq 0} + b_j) = 0$$

3. Inject search direction in equation (4)

z^b-rule

$$R_i = \sum_j \frac{x_i w_{ij} - l_i w_{ij}^+ - h_i w_{ij}^-}{\sum_{i'} x_{i'} w_{i'j} - l_i w_{i'j}^+ - h_i w_{i'j}^-} R_j$$

z^b-rule $\mathcal{X} = \mathcal{B}$

Proposition 3

For all function $g \in G$ and data points $\{x_i\} \in \mathcal{B}$, the deep Taylor decomposition with the z^b-rule is consistent.

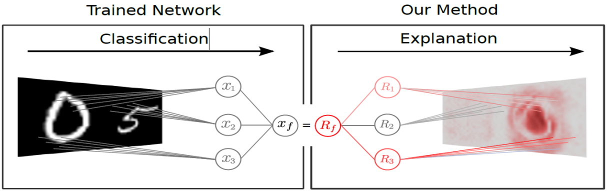
Proof

Since the proof is similar to the proofs of proposition 1 and 2 but lengthy I refer to the literature.

Example MNIST: Setting

Training of a neural network to detect a handwritten digit between 0-3 next to a distracting digit from 4-9 given the following setting:

- Images of size 28 x 56 pixels and 1568 input neurons $\{x_i\}$
- One hidden layer with 400 neurons $\{x_j\}$ and one output x_k
- Random initialized weights $\{w_{ij}\}$ and non-positive bias $\{b_j\}$ initialized to zero
- Training with 300000 iterations of stochastic gradient descent with a batch size of 20



Example MNIST: Heatmaps

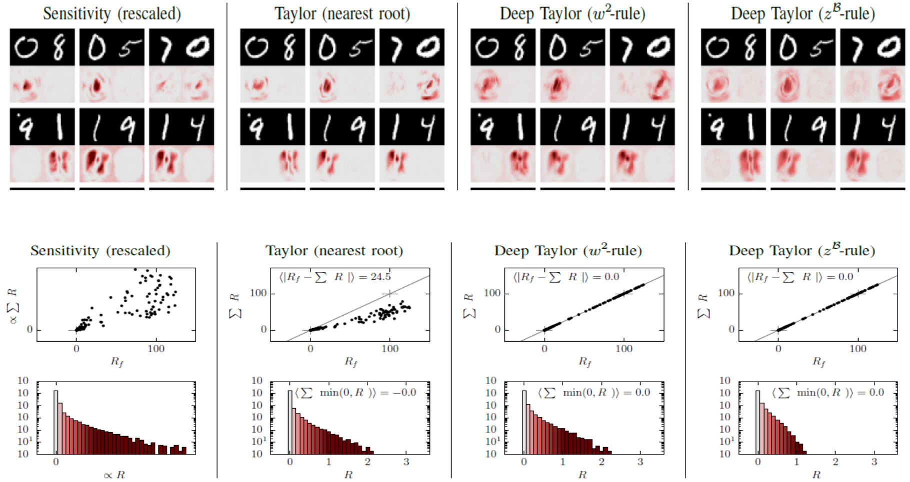


Figure 2: Heatmap and Empirical Results of Consistency

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Deep Networks

Many problems require very complex deep architectures

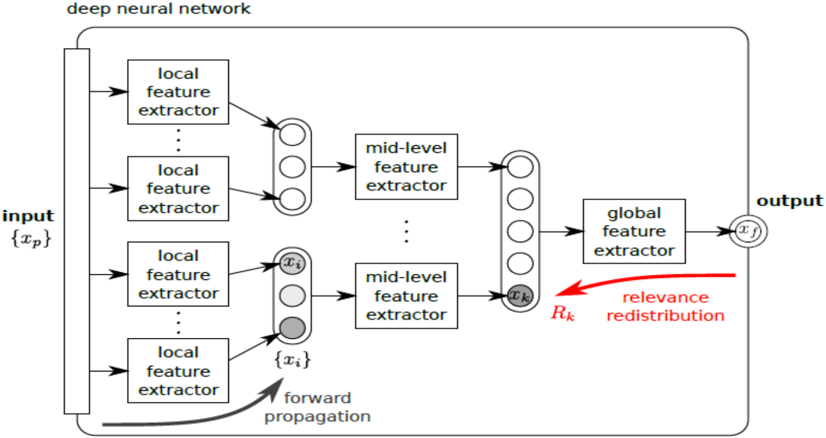


Figure 3: Example Deep Network

Min-Max Relevance Model

Trainable relevance model defined as

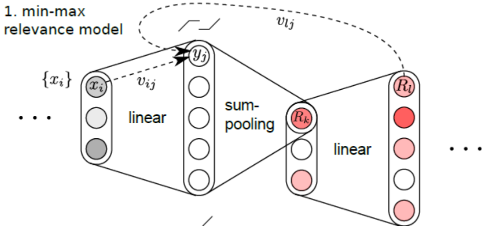
$$y_j = \max(0, \sum_i x_i v_{ij} + a_j)$$

$$\hat{R}_k = \sum_j y_j,$$

where $a_j = \min(0, \sum_l R_l v_{lj} + d_j)$ is a negative bias

$\rightarrow$ Compute $\{v_{ij}, v_{lj}, d_j\}$ by minimizing

$$\min \langle (\hat{R}_k - R_k)^2 \rangle \rangle$$



Min-Max Relevance Model

Due to the similar structure we can apply the propagation rules for the one-layer neural network

- Pooling layer

$$R_j = y_j$$

- Detection layer

$$R_i = \sum_j \frac{q_{ij}}{\sum_{i'} q_{i'j}} R_j$$

where $q_{ij} = v_{ij}^2$, $q_{ij} = x_i v_{ij}^+$ or $q_{ij} = x_i v_{ij} - l_i v_{ij}^+ - h_i v_{ij}^-$ for the w^2-rule, z^+-rule and the z^b- rule respectively

$\rightarrow$ The Min-Max relevance model is due to the minimization only approximately consistent

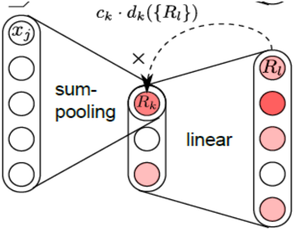
Training-Free Relevance Model

Consider the original network structure

$$x_j = \max(0, \sum_i x_i w_{ij} + b_j)$$
$$x_k = \|\{x_j\}\|_p$$

If the upper layer was explained by the z^+-rule, relevance R_k can be written as

$$R_k = \sum_l \frac{x_k w_{kl}^+}{\sum_{k'} x_{k'} w_{k'l}^+} R_l$$
$$= (\sum_j x_j) \cdot \frac{\|\{x_j\}\|_p}{\|\{x_j\}\|_1} \sum_l \frac{w_{kl}^+ R_l}{\sum_{k'} x_{k'} w_{k'l}^+}$$



Training-Free Relevance Model

As before we can apply the propagation rules for the one-layer neural network

- Pooling layer

$$R_j = \frac{x_j}{\sum_{j'} x_{j'}} R_k$$

- Detection layer

$$R_i = \sum_j \frac{q_{ij}}{\sum_{i'} q_{i'j}} R_j$$

where $q_{ij} = w_{ij}^2$, $q_{ij} = x_i w_{ij}^+$ or $q_{ij} = x_i w_{ij} - l_i w_{ij}^+ - h_i w_{ij}^-$ for the w^2-rule, z^+-rule and the z^b- rule respectively

$\rightarrow$ The training-free relevance model is consistent

When using the training-free model for the whole network all but the first layer need to be decomposed using the z^+-rule

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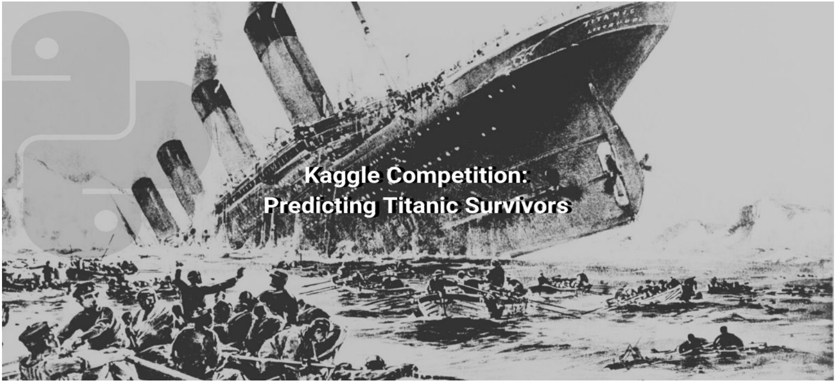
Relevance Distribution on the Titanic Dataset



https://github.com/mpommer/Deep-Taylor-Decomposition-Python

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