Layer-wise Relevance Propagation (LRP) Machine Learning for Health Informatics

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26.03.2019



Outline

Taylor decomposition

Example

Task description

Taylor Decomposition

► Taylor expansion of a function f(x) at point a: $f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f'''(a)}{2!}(x-a)^2 + \frac{f''''(a)}{3!}(x-a)^3 + \cdots$

▶ Classification (output) f(x) of input x (1st order only):

$$f(\mathbf{x}) = f(\tilde{\mathbf{x}}) + \left(\frac{\partial f}{\partial \mathbf{x}}\Big|_{\mathbf{x} = \tilde{\mathbf{x}}}\right)^{T} (\mathbf{x} - \tilde{\mathbf{x}}) + \epsilon$$
$$0 + \sum_{p} \underbrace{\frac{\partial f}{\mathbf{x}_{p}}\Big|_{\mathbf{x} = \tilde{\mathbf{x}}} (\mathbf{x}_{p} - \tilde{\mathbf{x}}_{p})}_{\mathbf{x} = \tilde{\mathbf{x}}} + \epsilon$$

where p is the index of the pixel.

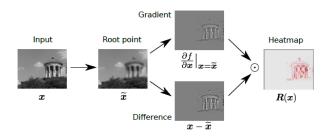
Find a neighbouring point $\tilde{\mathbf{x}}$, for which $f(\tilde{\mathbf{x}}) = 0$

$$\sum_{j} R_{j} = \left(\frac{\partial (\sum_{j} R_{j})}{\partial \{x_{i}\}} \bigg|_{\partial \{\tilde{x}_{i}\}} \right)^{T} (\{x_{i}\} - \{\tilde{x}_{i}\}) + \epsilon =$$

$$\sum_{i} \sum_{j} \frac{\partial R_{j}}{\partial x_{i}} \bigg|_{\partial \{\tilde{x}_{i}\}} (x_{i} - \tilde{x}_{i}) + \epsilon$$

Pixel-wise decomposition of a function

- ▶ Goal: redistribute the neural network output onto the input variables; the relevance R_i to lower-level relevances $\{R_i\}$
- ▶ How to choose the neighbouring point \tilde{x} ?
- Similar image, object not recognizable from the classifier hence the output $f(\tilde{\mathbf{x}}) = 0$

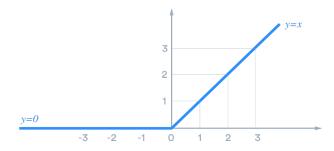


Properties

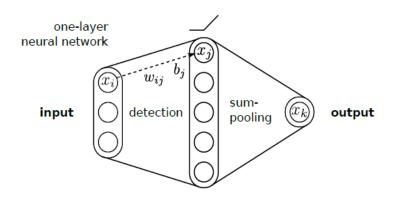
Conservation: $\forall \mathbf{x} : f(\mathbf{x}) = \sum_{p} R_{p}(\mathbf{x})$ $\sum_{j} R_{j} = \sum_{i} R_{i} \ (i \text{ and } j \text{ are layers})$

Positivity: $\forall \mathbf{x}, p : R_p(\mathbf{x}) \geq 0$

► Rectified Linear Unit:



Example (1/2)



- $ightharpoonup x_j = max(0, \sum_i x_i w_{ij} + b_j)$ (ReLU nonlinearity)
- $ightharpoonup x_k = \sum_j x_j$ (Sum pooling)

Example (2/2)

 R_k of output layer: Total relevance that must be backpropagated:

$$ightharpoonup R_k = x_k = \sum_j x_j$$

 R_j of hidden layer: Taylor decomposition on $\{\tilde{x}_j\} = 0$:

$$P_j = R_k(\tilde{\mathbf{x}}) + \frac{\partial R_k}{\partial x_j} \bigg|_{\{\tilde{x}_j\}} \cdot (x_j - \tilde{x}_j) = x_j = \max(0, \sum_i x_i w_{ij} + b_j)$$

For which $\tilde{\mathbf{x}}$ is $R_k(\tilde{\mathbf{x}}) = 0$? Since ReLU ensures that $\{\forall j : \tilde{x_j} \geq 0\}$ and $\frac{\partial R_k}{\partial x_i} = \frac{\partial \sum_j x_j}{\partial x_i} = 1$

 R_i of input layer:

$$\blacktriangleright R_i = \sum_j \frac{\partial R_j}{\partial x_i} \bigg|_{\{\tilde{x}_i\}^{(j)}} \cdot (x_i - \tilde{x}_i^{(j)})$$

$$\blacktriangleright R_i = \sum_j \frac{w_{ij}^2}{\sum_{i'} w_{i'i}^2} R_j$$

Task (1/2)

The task contains two parts

1. Numerical task

- Use the equations above to compute numerically the relevance of all layers of the network depicted in the figure.
- Use your own weight values (w_{ij}), but think on weighting schemes that are typically used in neural networks. See https://keras.io/initializers/
- Verify that the conservation and positivity rules properties apply.
- Provide descriptions of the interpretations

2. Programmatic task

- ▶ Install Python 3.5.+ and the relevant libraries.
- Provide descriptions of the interpretations of the relevance images with respect to the input images as well as their differences

Task (2/2)

1. Python libraries

- https://www.tensorflow.org/,
 https://mxnet.apache.org/
- https://keras.io/
- https://github.com/albermax/innvestigate
- Run the examples/readme_code_snippet.py with any of the .jpg figures in the examples/images folder (line 37)
- Adapt line 54 to select a different analyzer
- Python IDE: https://www.jetbrains.com/pycharm/

Literature

▶ Montavon, Grégoire, et al. "Explaining nonlinear classification decisions with deep taylor decomposition." Pattern Recognition 65 (2017): 211-222.