[Guidotti et al. 2017]

Explaining Deep Learning Methods

- 1. Explaining Models
  - 1.1. Activation Maximization
  - 1.2. Data Generation
  - 1.3. Model Simplification/ Global Surrogates
- 2. Explaining Outcome
  - 2.1. Perturbation
  - 2.2. Gradient based
  - 2.3. Backpropagation (Decomposition)

Part 3: Interpretable Deep Learning

- **Explaining Models (EM)**
- Explaining Outcome (EO)

* Most of the slides comes in this section comes from

- ICASSP 2017 Tutorial and CVPR'18 Tutorial by W. Samek, G. Montavon and K.R. Müller [ICASSP 2017 Tutorial] [CVPR'18 Tutorial]
- G. Montavon, et al. "Methods for interpreting and understanding deep neural networks," *Digit. Signal Process.*, vol. 73, pp. 1–15, 2018.
- R. Guidotti et al., "A Survey of Methods for Explaining Black Box Models," *ACM Comput. Surv.*, vol. 51, no. 5, pp. 1–42, Aug. 2018.

Class Prototypes (CP)

- *"How does a goose typically look like according to the neural network?"*

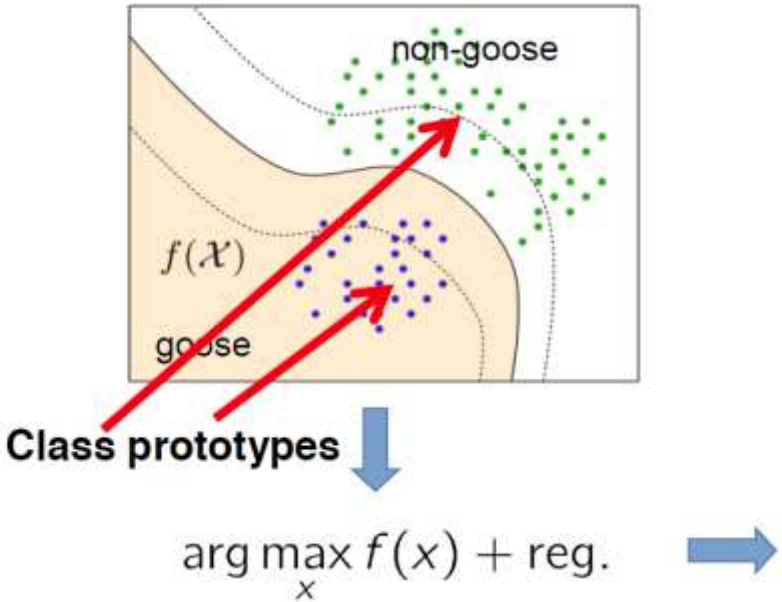
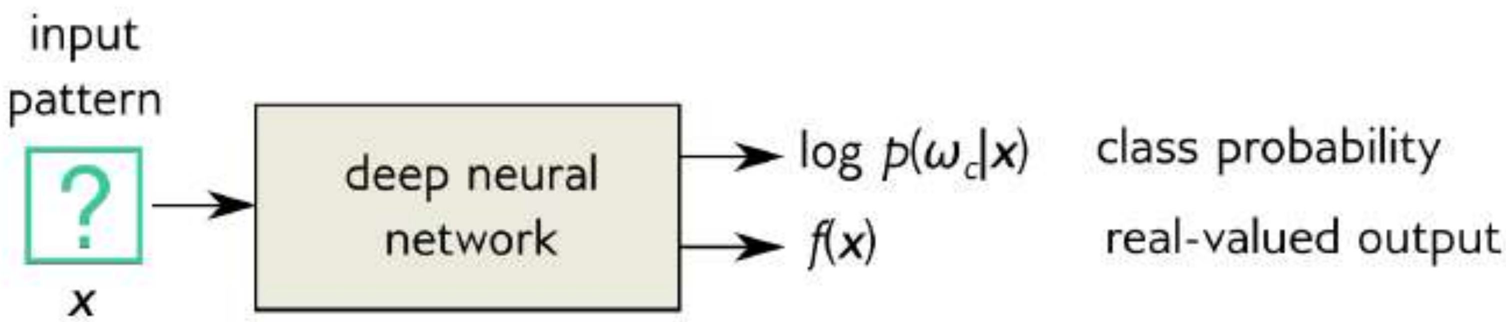


Image from **Symonian'13**

[CVPR'18 Tutorial]

Activation Maximization (AM)

Interpreting concepts predicted by a deep neural net via activation maximization



- Example :
  - Creating class prototype: $argmax_{\boldsymbol{x} \in \chi} \log p(w_c|\boldsymbol{x})$
  - Synthesizing extreme case: $argmax_{\boldsymbol{x} \in \chi} f(\boldsymbol{x})$

Activation Maximization

- [Erhan et al. 2010] – Find image that maximize neuron activity in of interest in Deep Belief Network
- [Le et al. 2012] – Visualize class model in Autoencoder
- [Simonyan et al. 2014] – Saliency map of CNN
- [Nguyen et al. 2016]
- …

Saliency Map via AM

Saliency map of goose and ostrich from **Simonyan et al. 2013**

Problem: Saliency map obtained by AM

1) often not resembling true data,

2) can be uninterpretable to humans

Improving Activation Maximization

- **Idea:** Force the features learned to match the data more closely.
- Now the optimization problem become

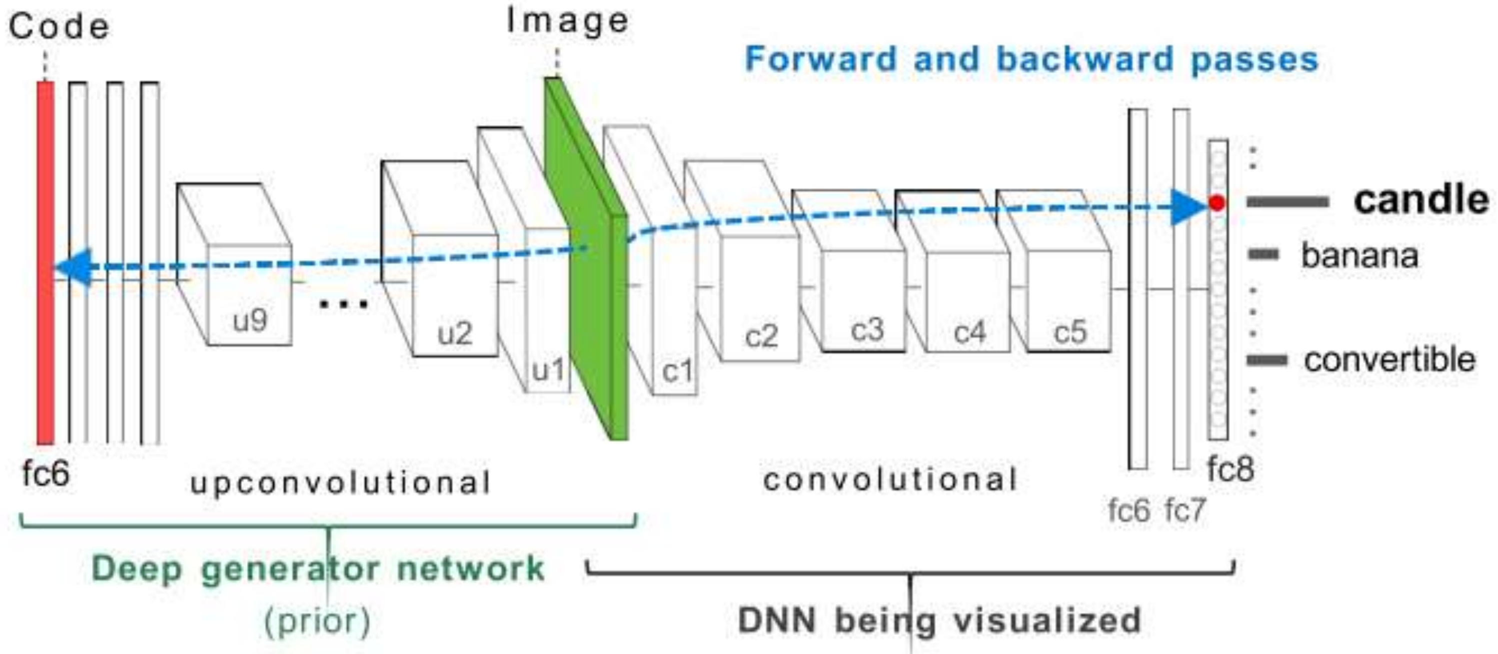
Finding the input pattern that maximizes **class proba bility**. p(**w**|**x**)

Find the **most likely input pattern** for a given class. p(**x**|**w**)

Data Generation

Problem: Activation maximization problem as finding a code $\boldsymbol{y}^l$ such that:

$$\widehat{\boldsymbol{y}^l} = \underset{\boldsymbol{y}^l}{\arg\max}\, \Phi_h\left(G_l(\boldsymbol{y}^l)\right) - \lambda\|\boldsymbol{y}^l\|$$



Deep generator network proposed by Nguyen et al. 2016

Model Simplification/ Global Surrogates

- Model Simplification – AKA Model Compression
  - Applied more for embedded programing then to interpretation
- Global Surrogates – Simple models often fails for DNN cases.

[Watanabe et al 2018]

Modular Representation

- Trained network
- Trained network
- Community structure
- Modular representation
  - bundled connections are defined that summarize multiple connections between pairs of detected communities

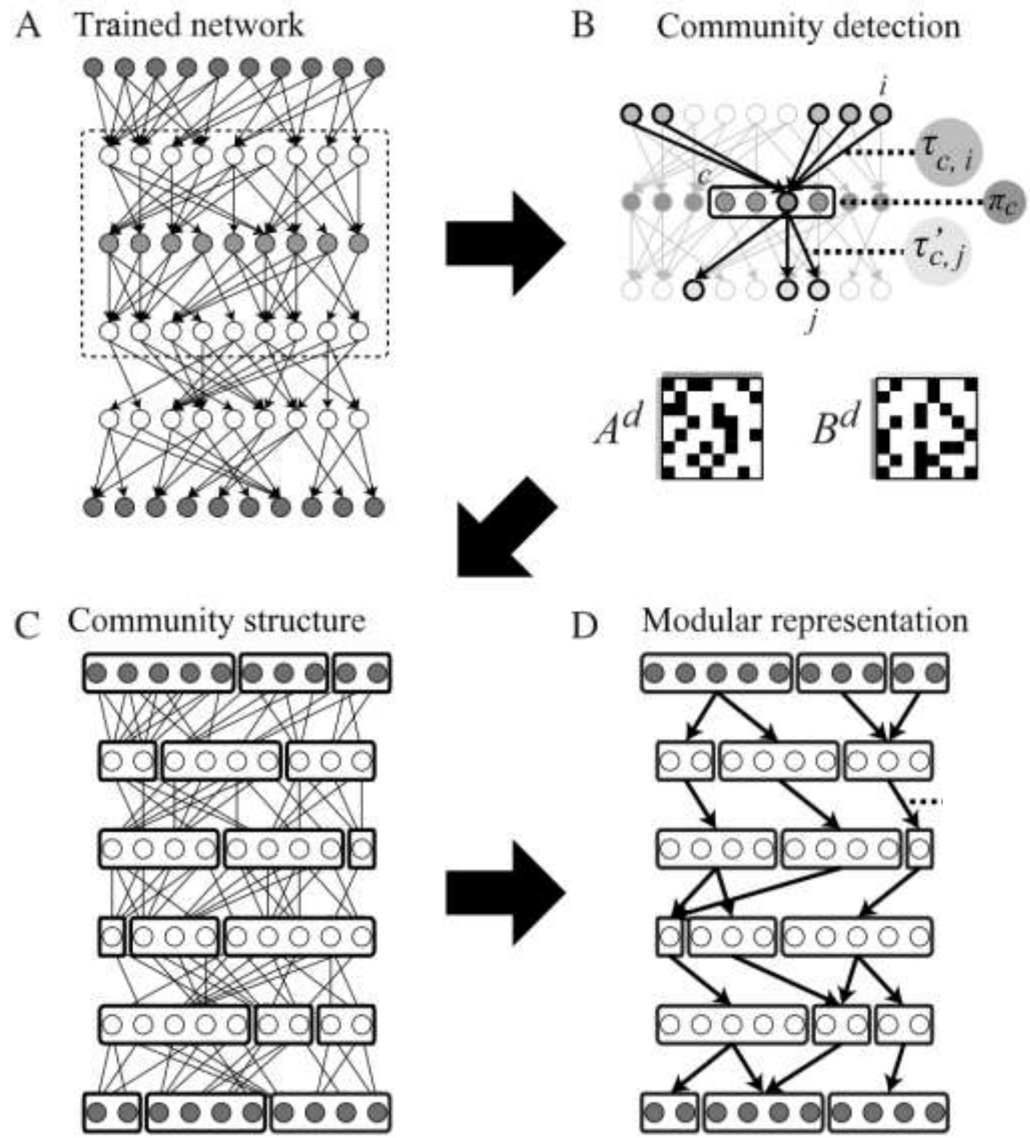


Fig 1. of Watanabe et al. 2018

Part 3: Interpretable Deep Learning

- Explaining Models (EM)
- **Explaining Outcome (EO)**

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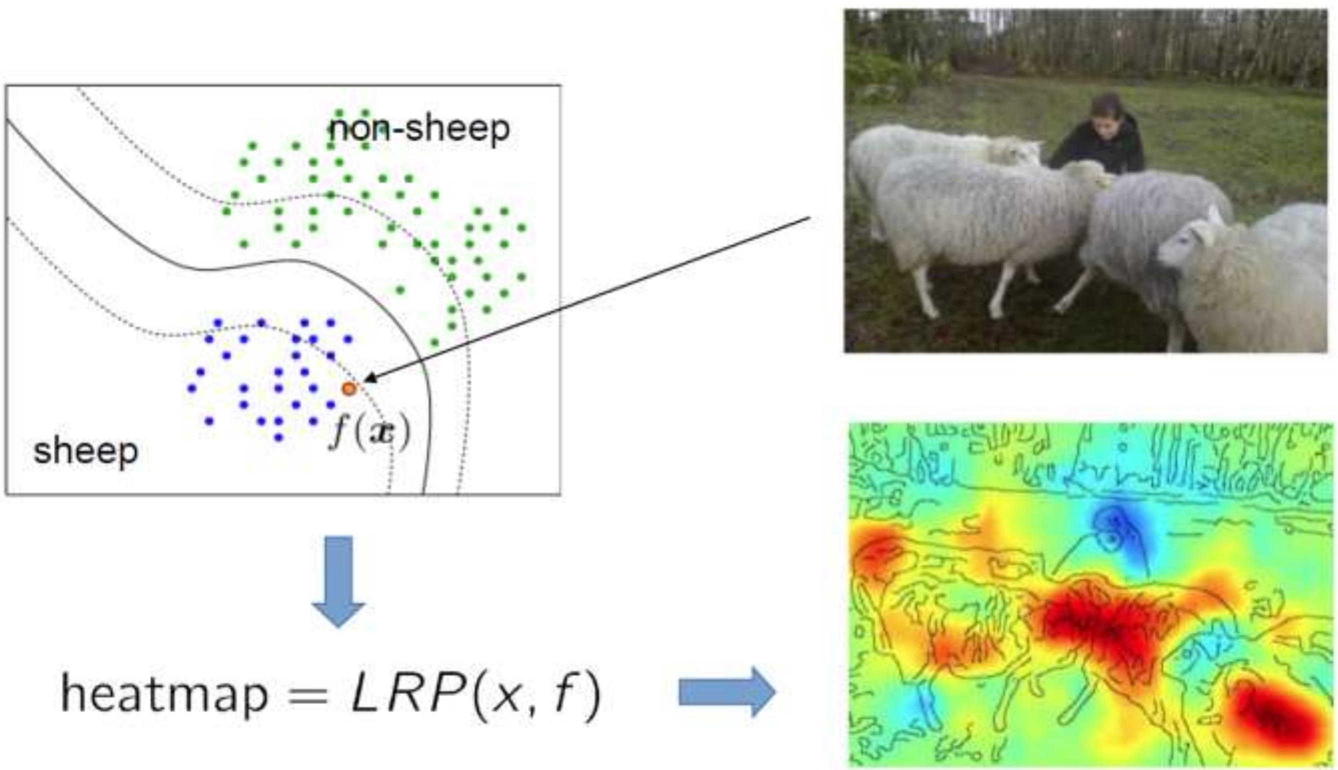
Explaining Outcome

- **Goal:** Determine the relevance of each (set of) input feature for a given decision on an instance, by assigning to these variables **a scores to each (set of) feature.**
- Important for **Personalized Healthcare**
- Most DNN explained via a **Saliency Mask**
  - Feature importance that is presented in a visual form to show subset of the original input which is mainly responsible for the prediction.

Explaining Individual Outcome

- *EX> "Why is a given image classified as a sheep?"*



Images from **Lapuschkin'16**

Saliency Map Examples

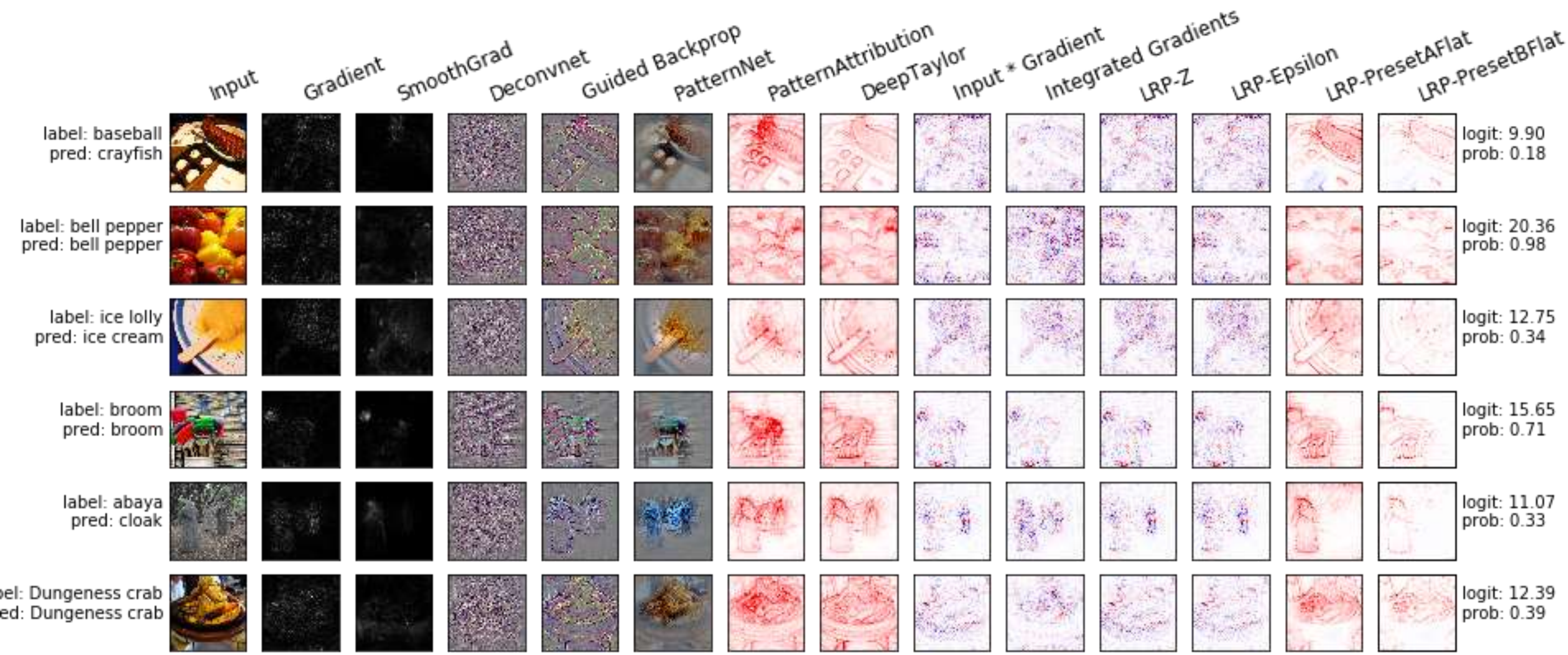


Figure from https://github.com/albermax/innvestigate

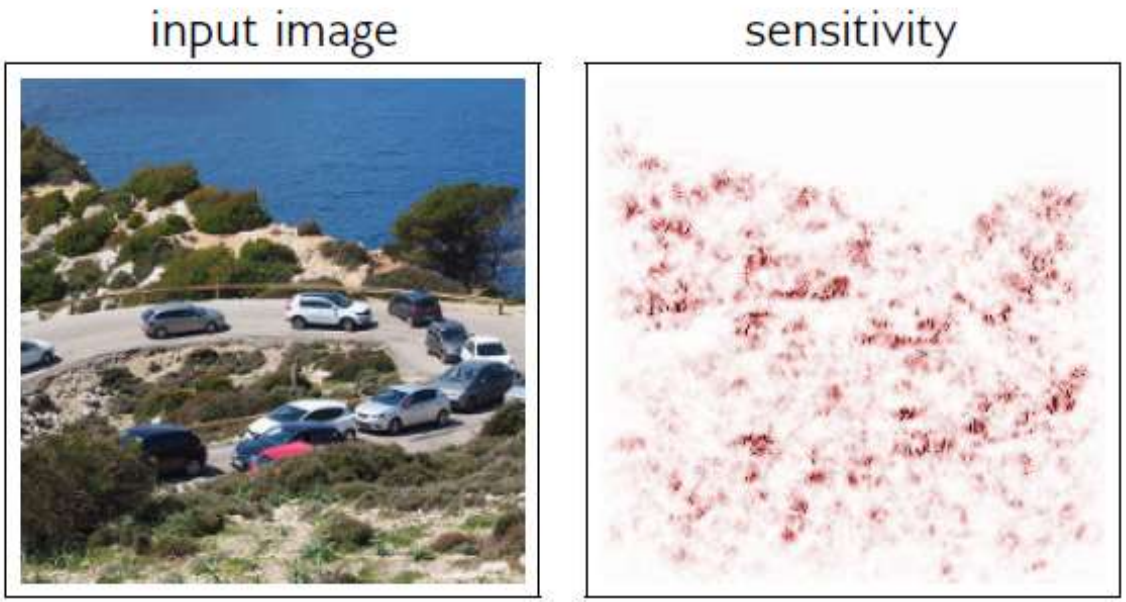
Explaining by Sensitivity Analysis

Given prediction function $f\,(x_1, x_2, \dots, x_d)$ on d dimensional input data $\boldsymbol{x} = (x_1, x_2, \dots, x_d\,)$,

Sensitivity analysis is the measure of local variation of the prediction function f along each input dimension

$$R_i = \left(\frac{\partial f}{\partial x_i}\Big|_{x=x}\right)^2$$

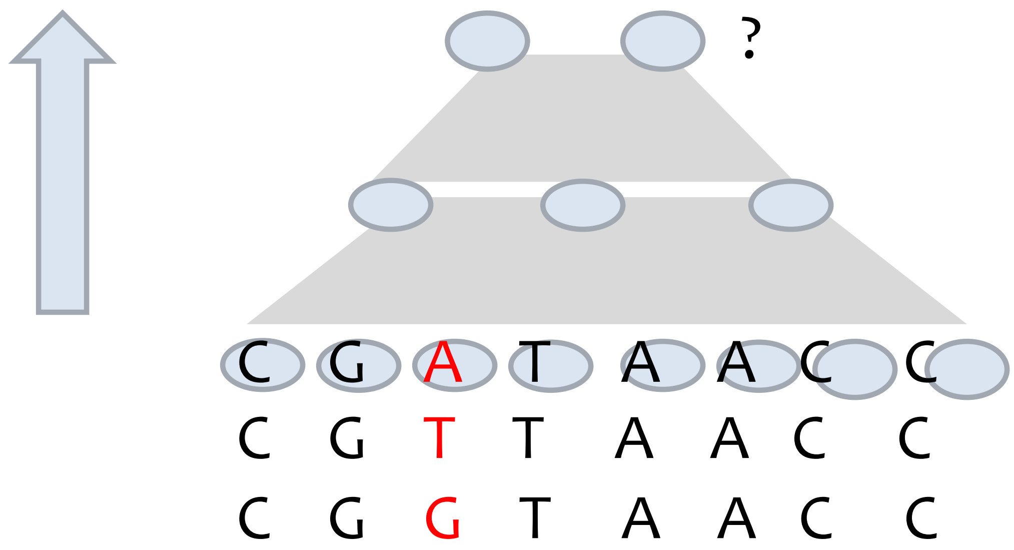
Sensitivity Analysis



- Easy to implement
  - Requires access to the **gradient** of the decision function
  - May not explain the prediction well

Perturbation Approaches

- Make perturbation to input and observe the difference in the output
- ☹ Every time you make a perturbation output needs to be recomputed



[Fong and Vedaldi ICCV'17]

Meaningful Perturbation

The aim of saliency is to identify which regions of an image x are used by the black box to produce the output value f(x) by "deleting" different regions R of x

"deletions":

Class Activation Mapping (CAM)

- linear combination of a late layer's activations and class-specific weights

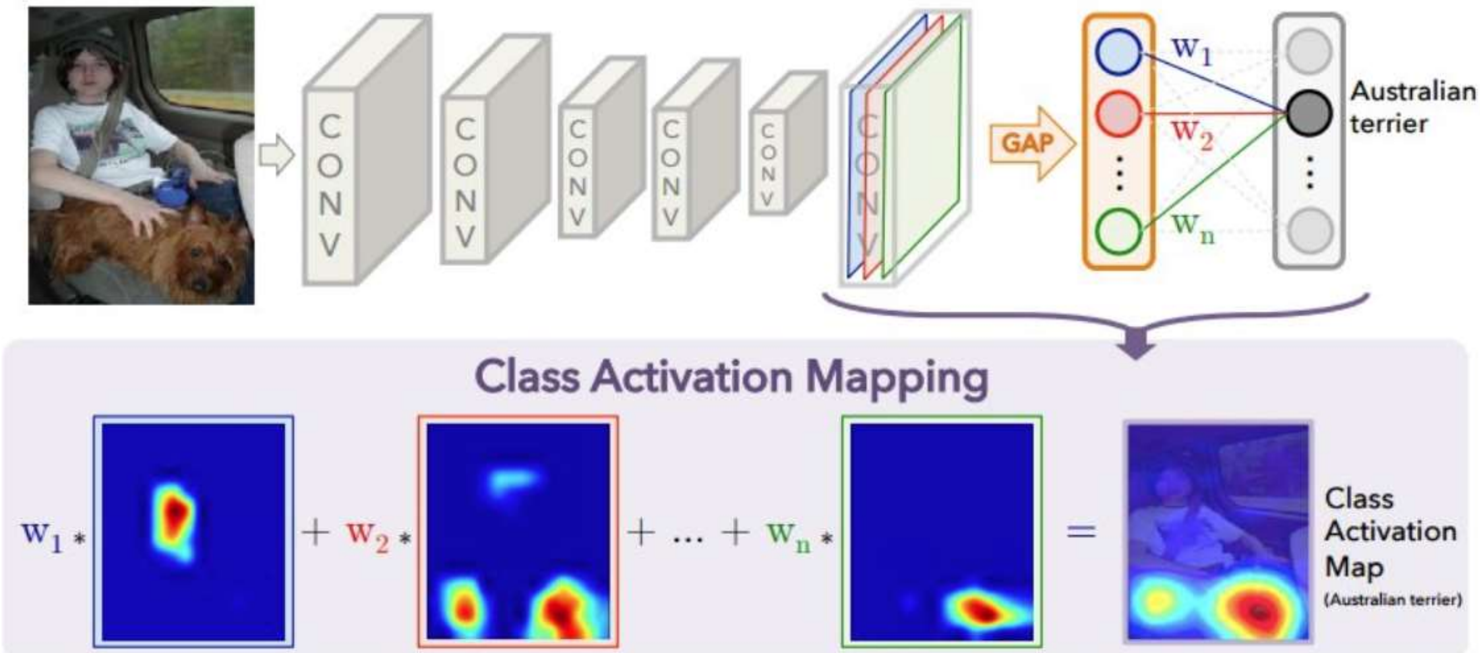


Figure from http://cnnlocalization.csail.mit.edu/

Gradient-Weighted CAM (Grad-CAM)

- Linear combination of a late layer's activations and class-specific gradients

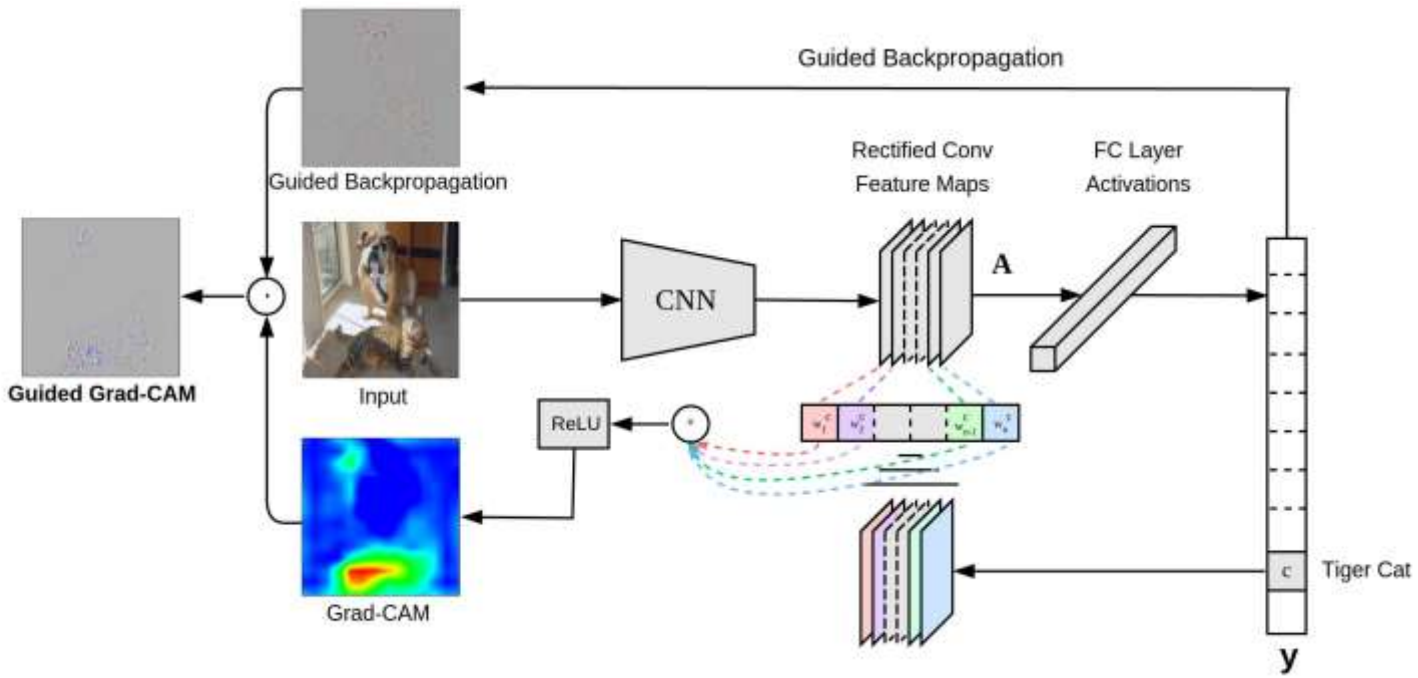
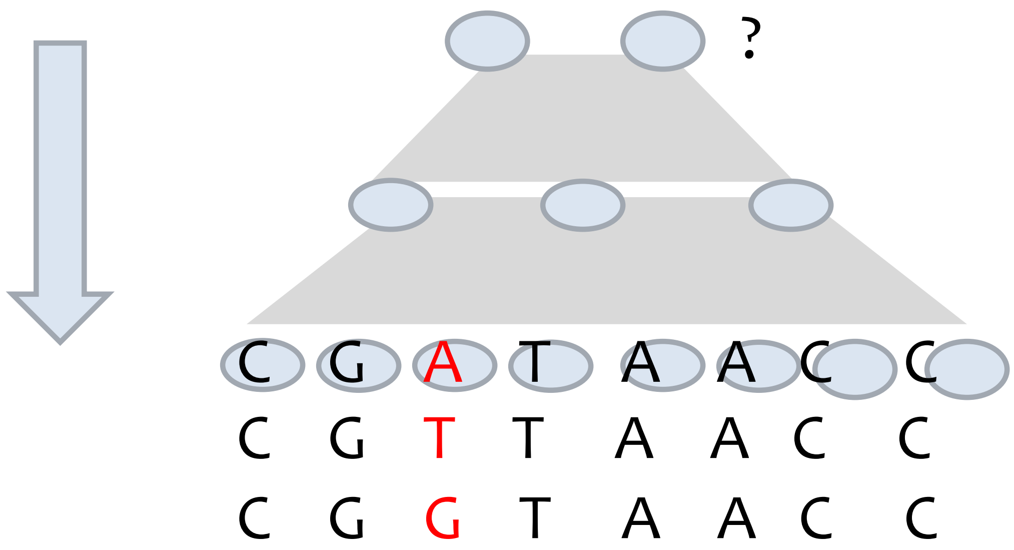


Figure from Selvaraju et al.

Backpropagation methods

- Sensitivity analysis
- Layer-wise relevance propagation (Deep Tylor)
- DeepLIFT



Explaining by Decomposing

Decomposition methods decompose prediction value f(x) to **relevance scores** R_i such that

$$\sum_i R_i = f(x_1, \ldots, x_d)$$

Decomposition **explains the function value** itself.

Sensitivity Analysis in Decomposition View

- Decomposition: $\sum_i R_i = f(x_1, \dots, x_d)$

- Sensitivity Analysis:

$$R_i = \left(\frac{\partial f}{\partial x_i}\Big|_{x=x}\right)^2$$

$$\sum_i R_i = \|\nabla_x f\|^2$$

  - Sensitivity analysis **explains a variation** of the function.

Decomposition on Shallow Nets

- Taylor decomposition of function $f(x_1, \ldots, x_d)$

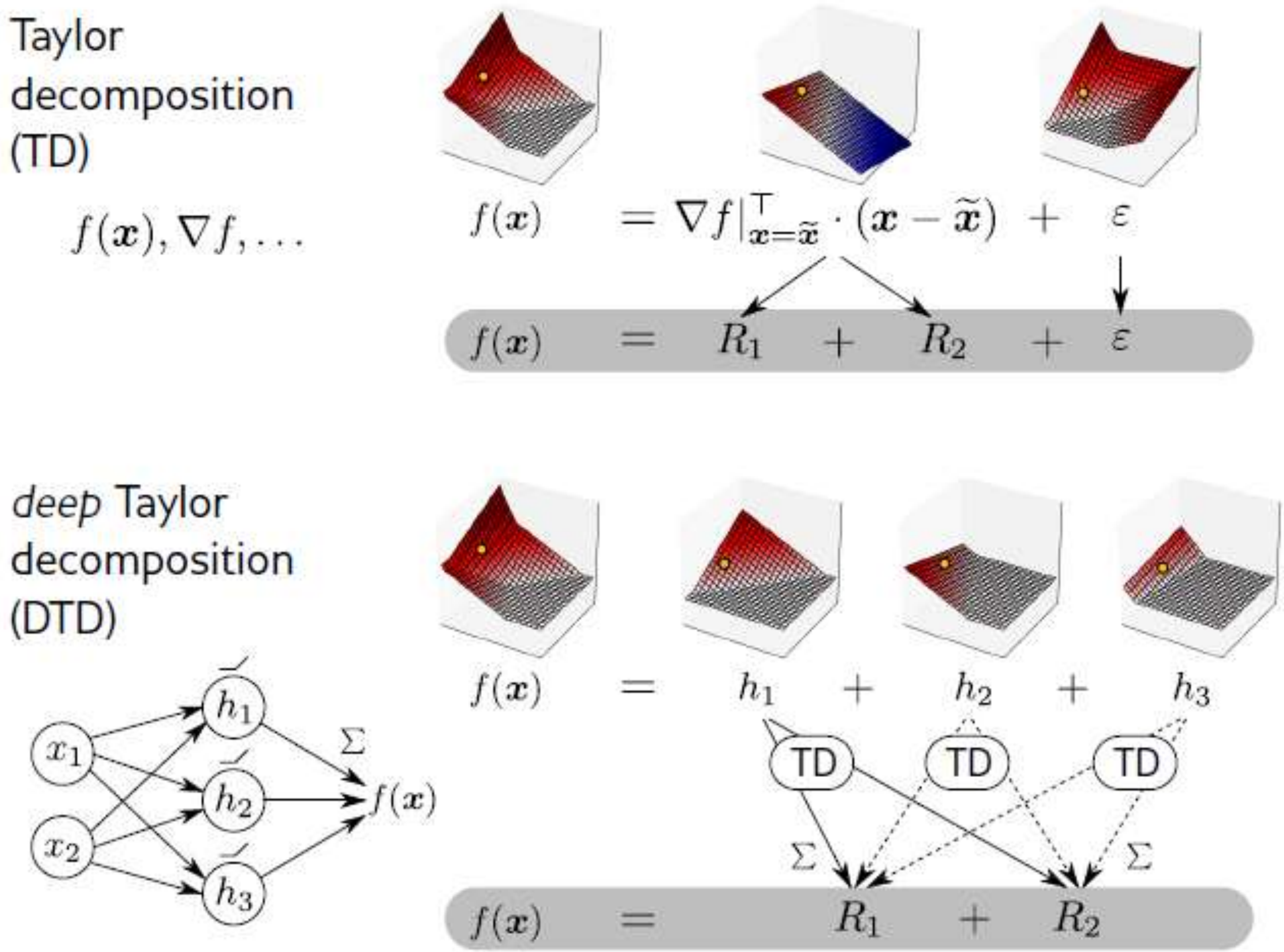
$$f(\mathbf{x}) = \underbrace{f(\widetilde{\mathbf{x}})}_{0} + \sum_{i=1}^{d} \underbrace{\frac{\partial f}{\partial x_i}\Big|_{\mathbf{x}=\widetilde{\mathbf{x}}} (x_i - \widetilde{x}_i)}_{R_i} + \underbrace{O(\mathbf{x}\mathbf{x}^\top)}_{0}$$

- Can it be applied on Deep Learning?
  - Doesn't work well on DNN
  - Also subjected to gradient noise

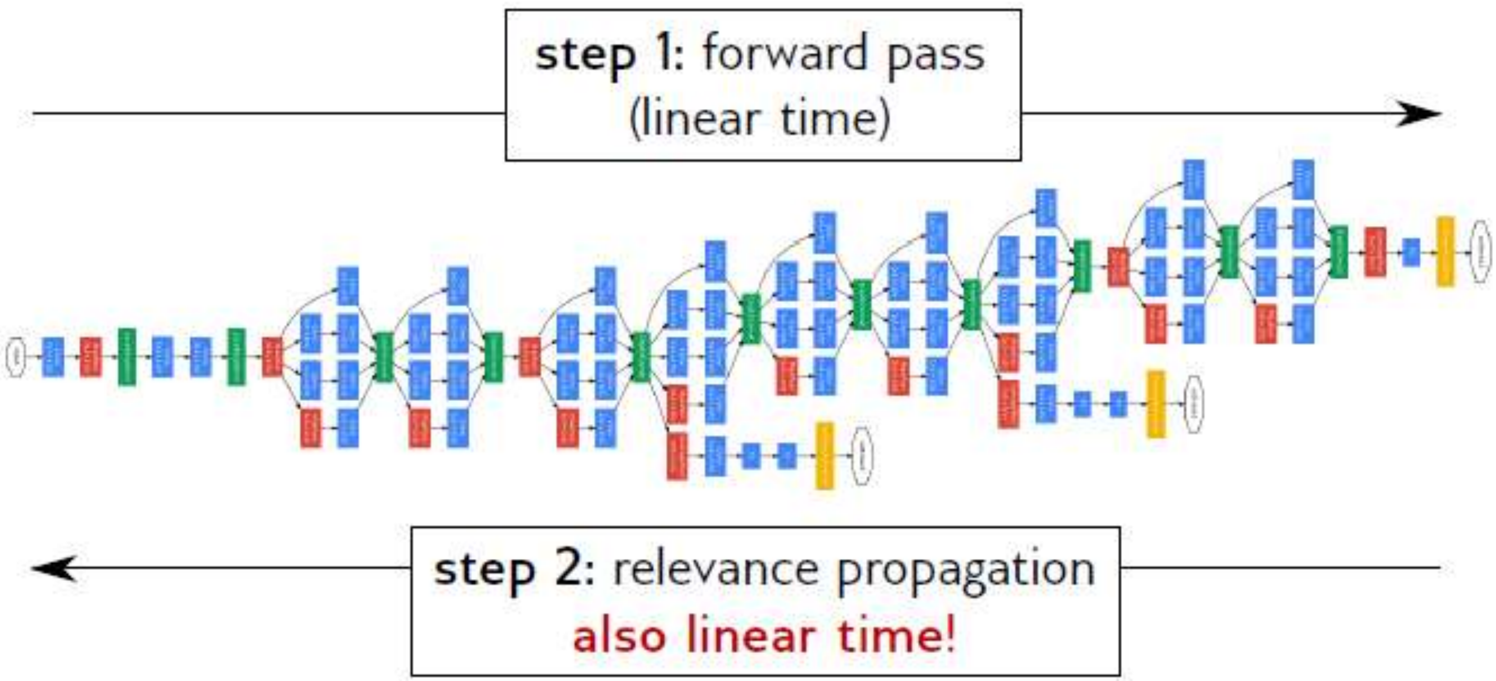
[ICASSP 2017 Tutorial]

[Montavon et al. 2017]

Deep Taylor Decomposition



Layer-Wise Relevance Propagation (LRP)



Propagation rule:

$$R_i = \sum_j q_{ij} R_j \qquad \sum_i q_{ij} = 1$$

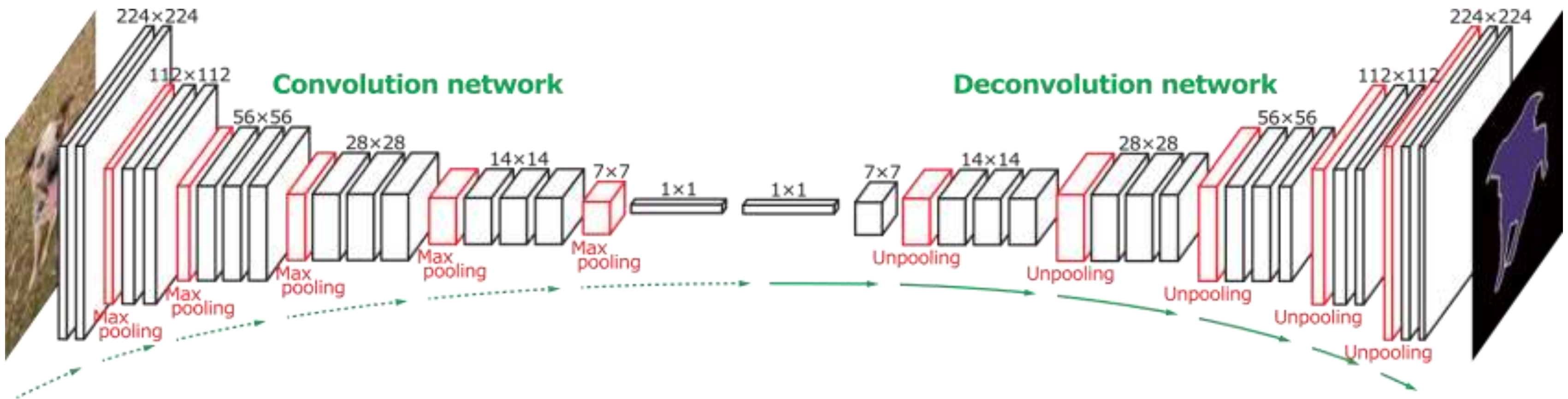
DeepLIFT

- DeepLIFT explains the difference in output from some ‘reference’ output in terms of the difference of the input from some ‘reference’ input.
- The ‘reference’ input represents some default or ‘neutral’ input that is chosen according to what is appropriate for the problem at hand
- **Activation difference** propagated down to input
- Capable to propagate relevance down even when the gradient is zero. (solves saturation problem)

[Zeiler and Fergus ECCV'14]
[Noh et al. ICCV'15]

DeConvNet

- Outputs **probability map** that indicate probability of each pixel belonging to one of the classes



- Convolution Network extract features
- Deconvolution Network generate probability map (same size as the input)

Figure from [Noh et al. ICCV'15]

Summary – What We Have Discussed

- Interpretable ML
- Agonistics methods
- Model-specific methods
- Interpretability in deep learning

Discussion – Current Limitations

- What we have not discussed
  - Interpretable recurrent neural nets
  - Interpretable reinforcement learning
  - Interpretable unsupervised learning models

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Thank you!

Omics Data + Clinical Data

Interpretable **Integrative**

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Better Healthcare

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https://leesael.github.io/