Explaining neural networks

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Overview

- Linear classifiers
  - Interpretation by examination
  - Case Study: Deepfake detection
- Input Optimization
  - The problem with deep CNN
  - Saliency Maps and Integrated Gradients
- Literature

Motivation

- Neural networks are potent black-box methods.
- Some very deep convolutional neural networks have hundreds of layers and use up to 600mb of disk storage.
- Let's do what we can to open the box!!

Linear classifiers

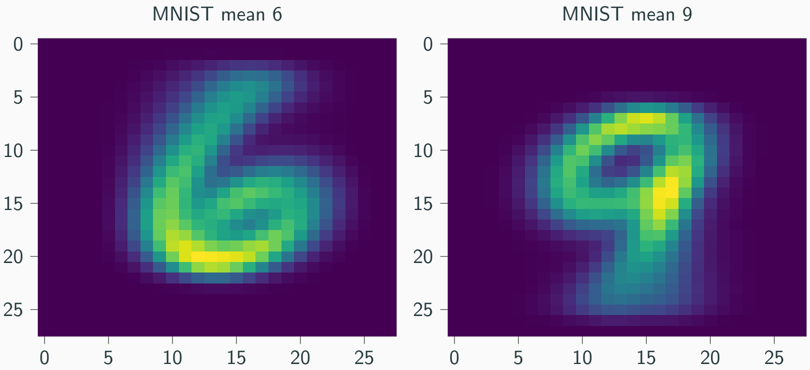
Definition of a linear classifier

Linear classifiers consist of a dense layer without an activation,

$$\mathbf{o} = \mathbf{A}\mathbf{x} + \mathbf{b}. \tag{1}$$

With $\mathbf{A} \in \mathbb{R}^{m,n}, \mathbf{x} \in \mathbb{R}^n$ and $\mathbf{b} \in \mathbb{R}^n$. Linear only works on simple problems that are linearly separable.

Binary MNIST



Cross-Entropy

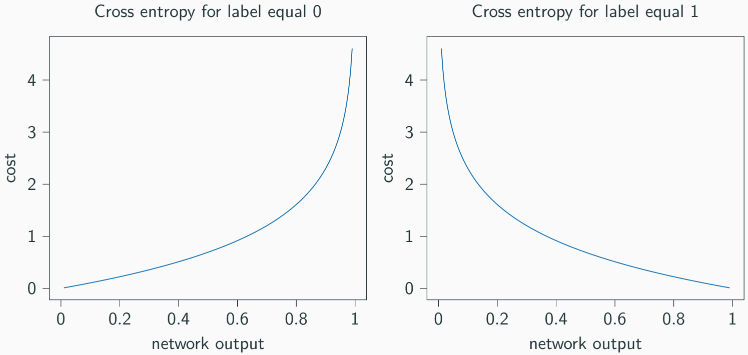
Recall the definition of the cross entropy

$$C_{\text{ce}}(\mathbf{y}, \mathbf{o}) = -\sum_{k}^{n_o} (\mathbf{y}_k \ln \mathbf{o}_k) + (\mathbf{1} - \mathbf{y}_k) \ln(\mathbf{1} - \mathbf{o}_k). \tag{2}$$

With $\mathbf{y}, \mathbf{o} \in \mathbb{R}^{n_o}$ defined as vectors of length n_o.

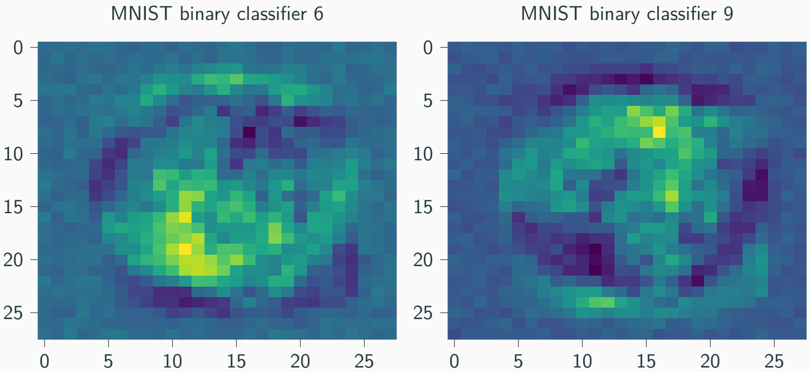
Cross-Entropy

To understand what is going on lets consider the two cases $y_k = 0$ and $y_k = 1$.



Cross-entropy pushes the output towards the label.

Interpretation by examination

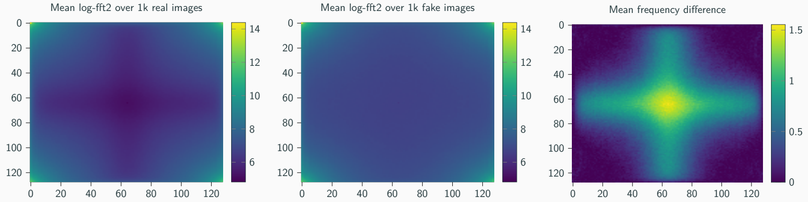


If linear is possible linear is great!!

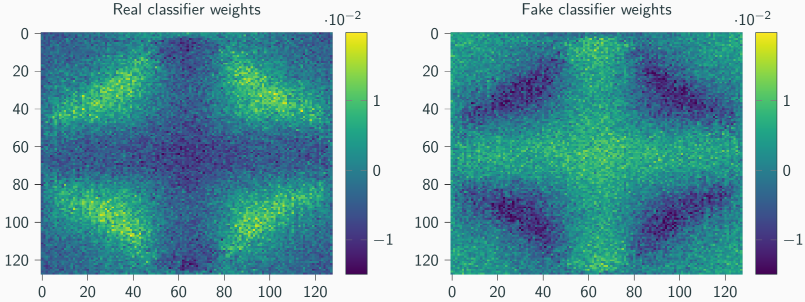
Generative models can generate images. Consider the samples below:



What blows the con?



Fake detectors



StyleGan-generated fakes can be classified with around 99% accuracy this way [Fra+20].

Summary

- For linearly separable binary problems weight inspection works great!
- Engineered features allow the inspection to reveal something about the data.

Input Optimization

Motivation

Let's be honest. Most linearly separable binary problems are academic.

An input CNN-Layer

Kernel-shape: (3, 3, 1, 32)

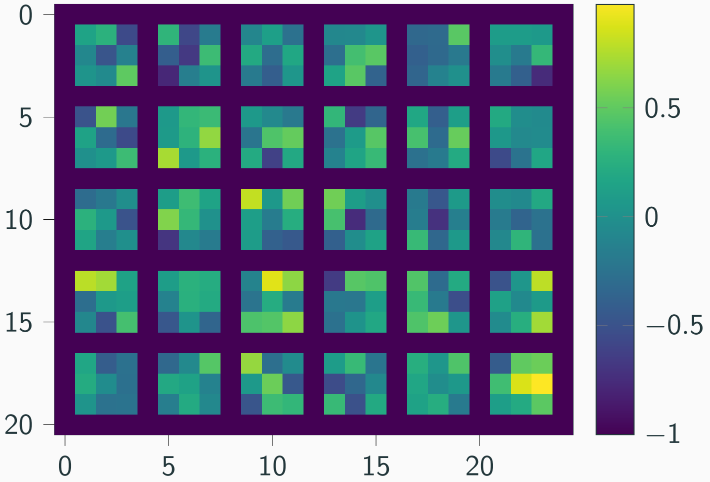


Figure: Plot of the input layer kernel weights trained on MNSIT.

Motivation Reloaded

- How do we verify the correct operation of deep nonlinear networks?
- It is *very* hard to interpret the weights of deep networks directly.
- Unit tests would require extensive re-training.

How to make a single neuron extremely happy

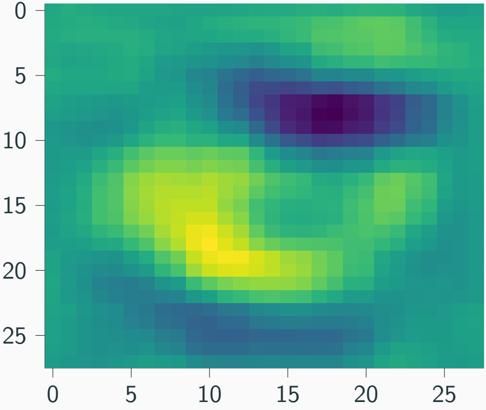
What if we turned the optimization problem around and optimized the input instead of the weights? Consider

$$\max_{\mathbf{x}} y_i = f(\mathbf{x}, \theta), \tag{3}$$

with network weights θ, input $\mathbf{x}$, and y_i, the activation of the i-th output neuron!

The 6-neurons favorite input

Starting from $\mathbf{x} = \mathbf{1} \in \mathbb{R}^{1,28,28,1}$ using image μ-σ-normalization after every step with a step size of one and a positive update yields:



The image net dataset

Figure: Image Net sample images as shown in [Rus+15]. Today 14,197,122 annotated images. Typically with 1000 object categories.

Figure 2. An illustration of the architecture of our CNN, explicitly showing the delineation of responsibilities between the two GPUs. One GPU runs the layer-parts at the top of the figure while the other runs the layer-parts at the bottom. The GPUs communicate only at certain layers. The network's input is 150,528-dimensional, and the number of neurons in the network's remaining layers is given by 290,400–186,624–64,896–64,896–43,264–4096–4096–1000.

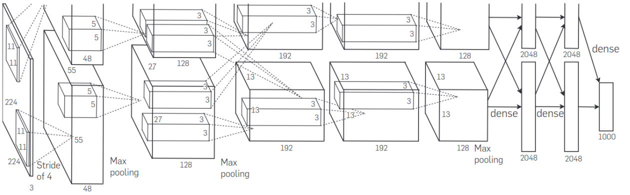


Figure: The Alexnet-architecture used for classify imagenet in 2010 [KSH17]

Early Alexnet layers

Figure 3. Ninety-six convolutional kernels of size 11 × 11 × 3 learned by the first convolutional layer on the 224 × 224 × 3 input images. The top 48 kernels were learned on GPU 1 while the bottom 48 kernels were learned on GPU 2 (see Section 7.1 for details).

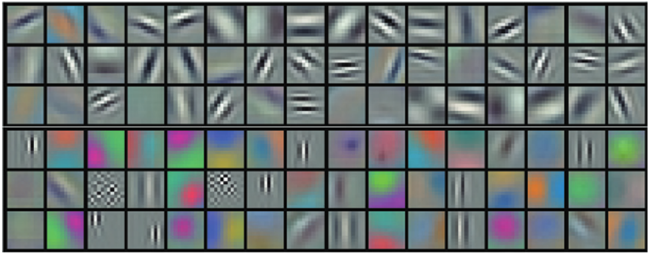


Figure: Plot from [KSH17].

Saliency Maps

[SVZ13] tell us to optimize

$$\arg\max_{\mathbf{I}} S_c(\mathbf{I}) - \lambda|\mathbf{I}|_2^2. \tag{4}$$

With S_c, the classification score for class c. $\mathbf{I}$ is the input image, and $|I|_2$ represents the 2-norm image channels. λ is a regularization parameter.

CNN-Saliency Map

Figure: Input optimization saliency maps of a deep CNN trained on imagenet as shown in [SVZ13].

Integrated-gradients

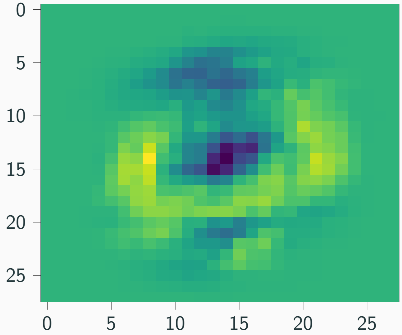
[STY17] propose to estimate individual input contributions to an output neuron via,

$$\text{IntegratedGrads}_i(x) = (x_i - x_i') \cdot \sum_{k=1}^{m} \frac{\partial F(x' + \frac{k}{m} \cdot (x - x'))}{\partial x_i}. \quad (5)$$

$\frac{\partial F}{\partial x_i}$ denotes the gradients with respect to the input color channels i. $\mathbf{x}'$ denotes a baseline black image. And $\mathbf{x}$ symbolizes an input we are interested in. Finally, m denotes the number of summation steps from the black baseline image to the interesting input.

Integrating the gradients of a multilayer CNN on MNIST

Integrated gradients for the zero neuron on the MNIST-validation set.



Images from the Wild

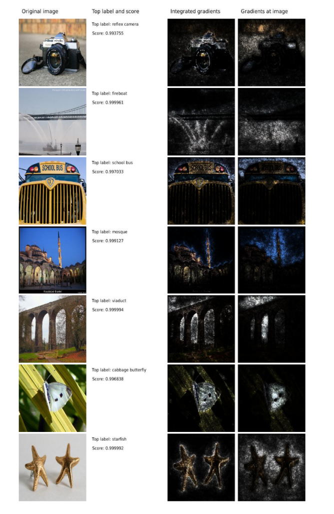


Figure: Integrated gradient visualization of input saliency for a very deep-CNN trained on Imagenet [Den+09]. Image taken from [STY17].

Conclusion

- Before you do anything else, look at the openai microscope at `https://microscope.openai.com/models`.
- We can look at features and weights and work with input optimization to understand what is going on.

Literature

References

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