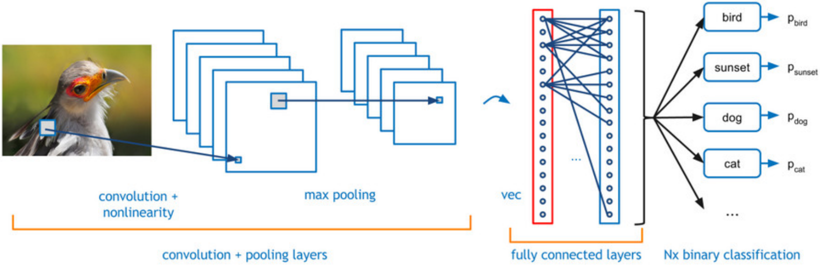
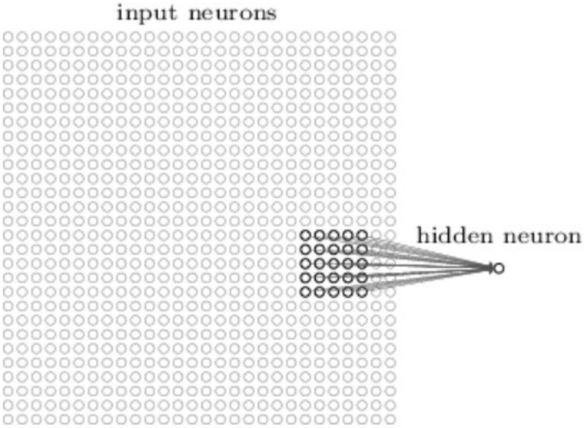
Convolutional networks – theory

Convolutional network



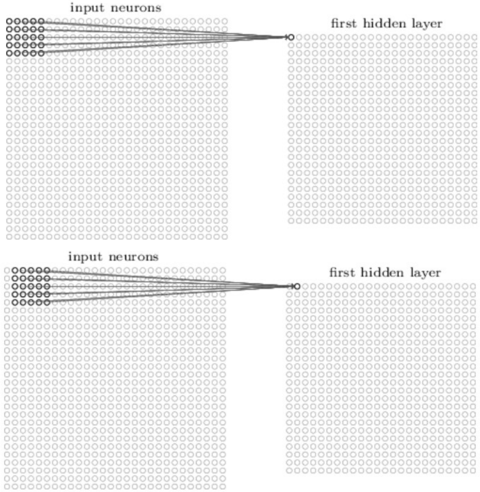
Convolutional layers



Every neuron is connected with a (typically small) *receptive field* of neurons in the lower layer.

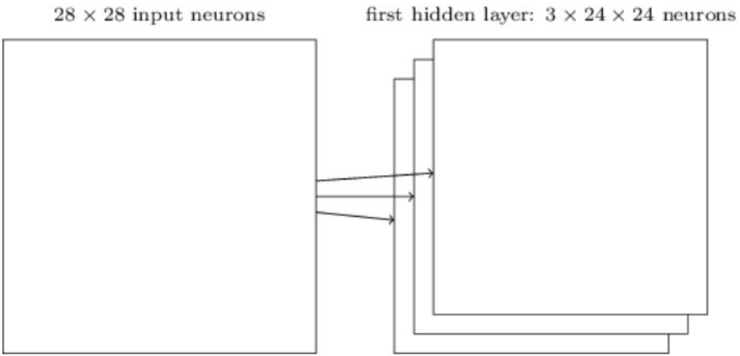
Neuron is "standard": Computes a weighted sum of its inputs, applies an activation function.

Convolutional layers



Neurons grouped into *feature maps* sharing weights.

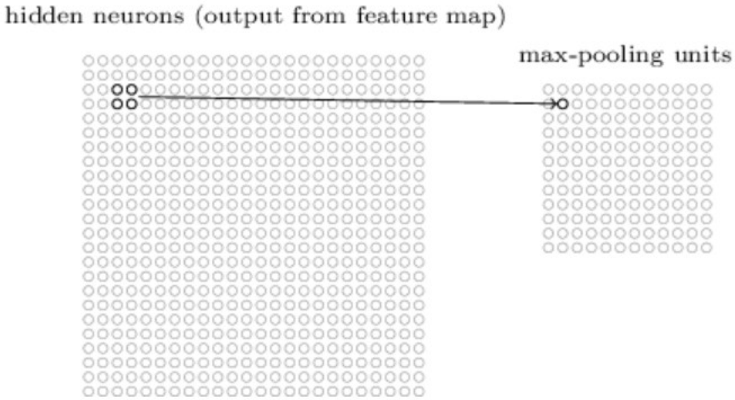
Convolutional layers



Each feature map represents a property of the input that is supposed to be spatially invariant.

Typically, we consider several feature maps in a single layer.

Pooling layers



Neurons in the pooling layer compute simple functions of their receptive fields (the fields are typically disjoint):

- **Max-pooling** : maximum of inputs
- **L2-pooling** : square root of the sum of squres
- **Average-pooling** : mean
- ...

Convolutional networks – architecture

Neurons organized in layers, $L_0, L_1, \ldots, L_n$, connections (typically) only from L_m to L_{m+1}.

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- **convolutional** layer L_m: Neurons organized into disjoint **feature maps**, all neurons of a given feature map *share weights* (but have different inputs)
- **pooling** layer: "Neurons" organized into **pooling maps**, all neurons
  - compute a simple aggregate function (such as max),
  - have *disjoint inputs*.

Pooling after convolution is applied to each feature map separately.

I.e. a single pooling map after each feature map.

Convolutional networks – architecture

- Denote
  - X a set of *input* neurons
  - Y a set of *output* neurons
  - Z a set of *all* neurons ($X, Y \subseteq Z$)
- individual neurons denoted by indices i, j etc.
  - ξ_j is the inner potential of the neuron j *after the computation stops*
  - y_j is the output of the neuron j *after the computation stops*

  (define $y_0 = 1$ is the value of the formal unit input)
- w_{ji} is the weight of the connection **from** i **to** j

  (in particular, w_{j0} is the weight of the connection from the formal unit input, i.e. $w_{j0} = -b_j$ where b_j is the bias of the neuron j)
- $j_{\leftarrow}$ is a set of all i such that j is adjacent from i
  (i.e. there is an arc **to** j from i)
- $j^{\rightarrow}$ is a set of all i such that j is adjacent to i
  (i.e. there is an arc **from** j to i)
- $[ji]$ is a set of all connections (i.e. pairs of neurons) sharing the weight w_{ji}.

Convolutional networks – activity

- neurons of dense and convolutional layers:
  - inner potential of neuron j:

$$\xi_j = \sum_{i \in j_{\leftarrow}} w_{ji} y_i$$

  - activation function σ_j for neuron j (arbitrary differentiable):

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- Neurons of pooling layers: Apply the "pooling" function:
  - max-pooling:

$$y_j = \max_{i \in j_{\leftarrow}} y_i$$

  - avg-pooling:

$$y_j = \frac{\sum_{i \in j_{\leftarrow}} y_i}{|j_{\leftarrow}|}$$

A convolutional network is evaluated layer-wise (as MLP), for each $j \in Y$ we have that $y_j(\vec{w}, \vec{x})$ is the value of the output neuron j after evaluating the network with weights $\vec{w}$ and input $\vec{x}$.

Convolutional networks – learning

Learning:

- Given a **training set** $\mathcal{T}$ of the form

$$\left\{ \left(\vec{x}_k, \vec{d}_k\right) \quad \middle| \quad k = 1, \ldots, p \right\}$$

Here, every $\vec{x}_k \in \mathbb{R}^{|X|}$ is an *input vector* end every $\vec{d}_k \in \mathbb{R}^{|Y|}$ is the desired network output. For every $j \in Y$, denote by d_{kj} the desired output of the neuron j for a given network input $\vec{x}_k$ (the vector $\vec{d}_k$ can be written as $\left(d_{kj}\right)_{j \in Y}$).

- **Error function – mean squared error (for example):**

$$E(\vec{w}) = \frac{1}{p} \sum_{k=1}^{p} E_k(\vec{w})$$

where

$$E_k(\vec{w}) = \frac{1}{2} \sum_{j \in Y} \left(y_j(\vec{w}, \vec{x}_k) - d_{kj}\right)^2$$

Convolutional networks – SGD

The algorithm computes a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2\ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:
  - Choose (randomly) a set of training examples $T \subseteq \{1, \ldots, p\}$
  - Compute

    $$\vec{w}^{(t+1)} = \vec{w}^{(t)} + \Delta\vec{w}^{(t)}$$

    where

    $$\Delta\vec{w}^{(t)} = -\varepsilon(t) \cdot \frac{1}{|T|} \sum_{k \in T} \nabla E_k(\vec{w}^{(t)})$$

Here T is a *minibatch* (of a fixed size),

- $0 < \varepsilon(t) \leq 1$ is a *learning rate* in step $t+1$
- $\nabla E_k(\vec{w}^{(t)})$ is the gradient of the error of the example k

Note that the random choice of the minibatch is typically implemented by randomly shuffling all data and then choosing minibatches sequentially. **Epoch** consists of one round through all data.

Backprop

Recall that $\nabla E_k(\vec{w}^{(t)})$ is a vector of all partial derivatives of the form $\frac{\partial E_k}{\partial w_{ji}}$.

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- Now for every w_{ji} where j is in a convolutional layer:

$$\frac{\partial E_k}{\partial w_{ji}} = \sum_{r\ell \in [ji]} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot y_\ell$$

- Neurons of pooling layers do not have weights.

Backprop

Now compute derivatives w.r.t. y_j:

- for every $j \in Y$:

$$\frac{\partial E_k}{\partial y_j} = y_j - d_{kj}$$

  This holds for the squared error, for other error functions the derivative w.r.t. outputs will be different.

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- for every $j \in Z \setminus Y$ such that $j^{\rightarrow}$ is either a dense layer, or a convolutional layer:

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- for every $j \in Z \smallsetminus Y$ such that $j^{\rightarrow}$ is max-pooling: Then $j^{\rightarrow} = \{i\}$ for a single "max" neuron and we have

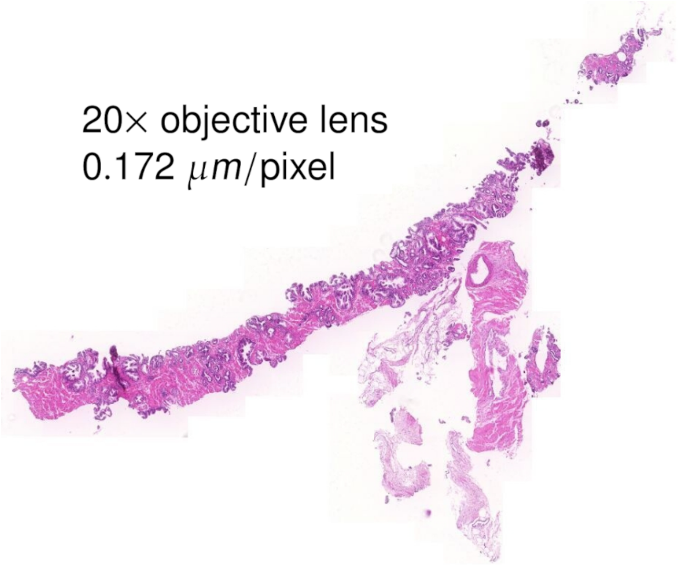
$$\frac{\partial E_k}{\partial y_j} = \begin{cases} \frac{\partial E_k}{\partial y_i} & \text{if } j = arg\ max_{r \in i_{\leftarrow}} y_r \\ 0 & \text{otherwise} \end{cases}$$

I.e. gradient can be propagated from the output layer downwards as in MLP.

Convolutional networks – summary

- Conv. nets. are nowadays the most used networks in image processing (and also in other areas where input has some local, "spatially" invariant properties)
- Typically trained using backpropagation.
- Due to the weight sharing allow (very) deep architectures.
- Typically extended with more adjustments and tricks in their topologies.

The problem of cancer detection in WSI



The problem: Detect cancer in this image.

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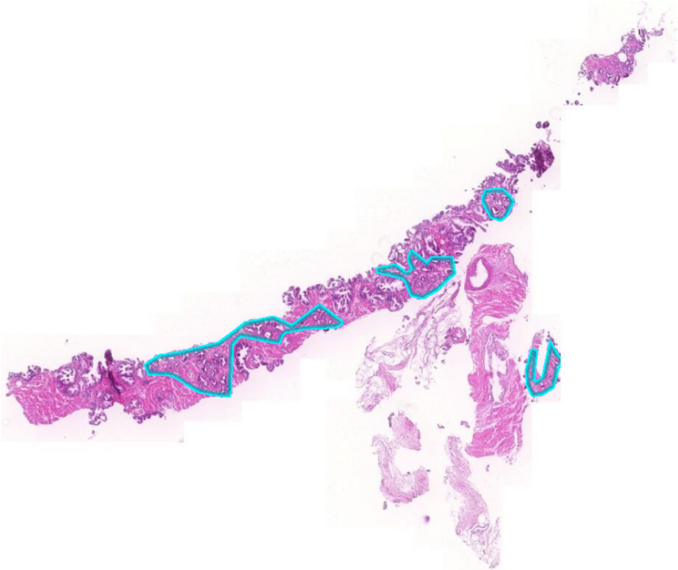
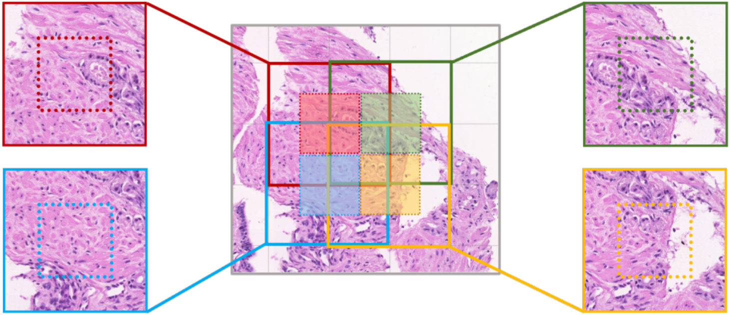


- WSI annotated by pathologists, **not** pixel level precise!

Input data

WSI too large, 105,185 px x 221,772 px

Cut into patches of size 512 px x 512 px



Patch positive **iff** the inner square intersects the annotation

Training on WSI

Our dataset from Masaryk Memorial Cancer Insitute:

- 785 WSI from 166 patients
  (698 WSI for training, 87 WSI for testing)
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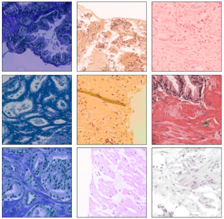

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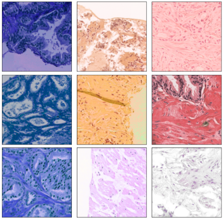

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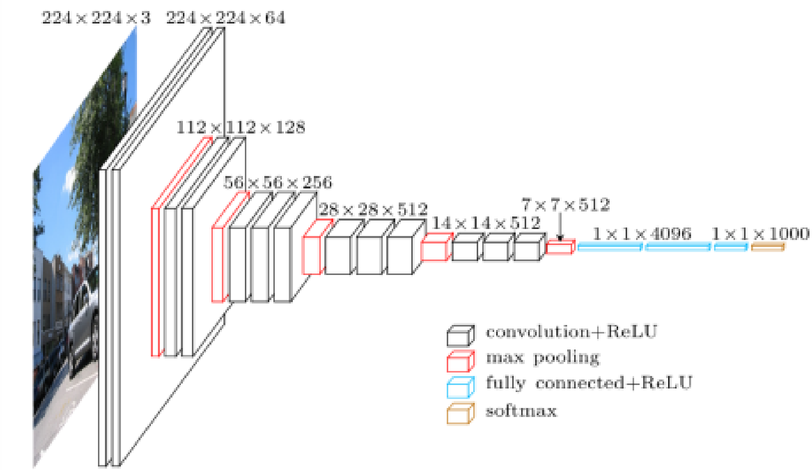
- Training data three step sampling:
  1. randomly select a label
  2. randomly select a slide containing at least a single patch with the label
  3. randomly select a patch with the label from the slide

VGG16



3×3 convolutions, stride 1, padding 1. Max pooling 2×2, stride 2.

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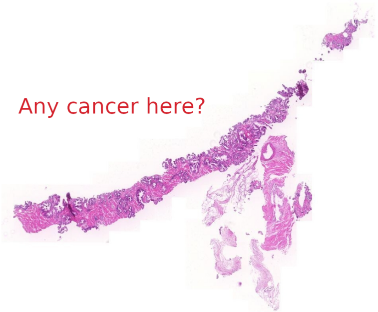
- The error *E* = cross-entropy
- Training:
  - RMSprop optimizer
  - The "forgetting" hyperparameter: $\rho = 0.9$
  - The initial learning rate 5×10^{-5}
    - If no improvement in *E* on validation data for 3 consecutive epochs $\Rightarrow$ half the learning rate
    - If no improvement in ROCAUC on validation data for 5 consecutive epochs $\Rightarrow$ terminate
  - Momentum with the weight $\alpha = 0.9$

Prediction

Model evaluation - attempt 1

Can we detect cancer somewhere in WSI?



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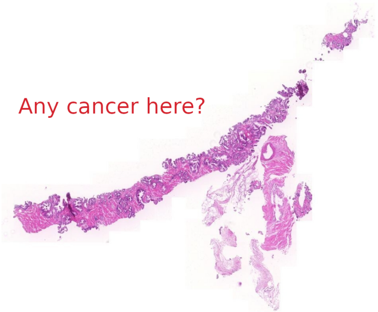

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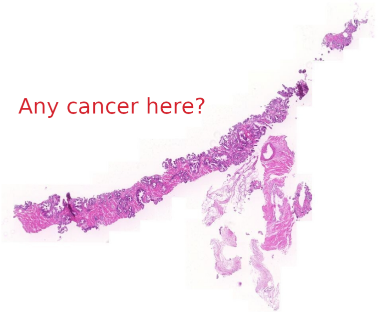

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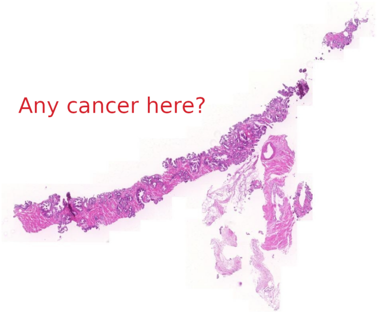

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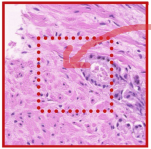
Predict WSI positive iff at least one patch I satisfies $F(I) \geq t$ for a fixed threshold $t \in [0,1]$.

Choosing t close to 1, we have achieved 100% accuracy, i.e., slide positive iff predicted positive. Problem solved ... No?

Model evaluation - attempt 2

Can we detect cancer in patches?



Any cancer here?

Predict I positive iff $F(I) \geq 0.75$

Single WSI:

		PREDICTED Pos	PREDICTED Neg
TRUE	Pos	805	18
TRUE	Neg	48	614

All WSIs:

		PREDICTED Pos	PREDICTED Neg
TRUE	Pos	24796	4340
TRUE	Neg	5345	158754

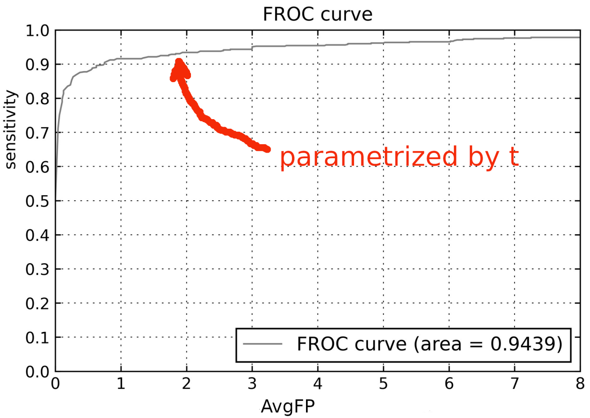
Ok, does it detect cancer?

Model evaluation – attempt 3 – FROC

Detect *particular tumors* ?

How to evaluate the quality of tumor detection?

Model evaluation – attempt 3 – FROC



sensitivity ≈ the proportion of tumors containing at least one patch I with $F(I) \geq t$ w.r.t. all tumors in all slides

AvgFP ≈ average number of patches I with $F(I) \geq t$ in *each non-cancerous slide*

Explainable methods (XAI)

XAI methods

The goal is to understand how and why the network does what it does.

We will consider classification models only.

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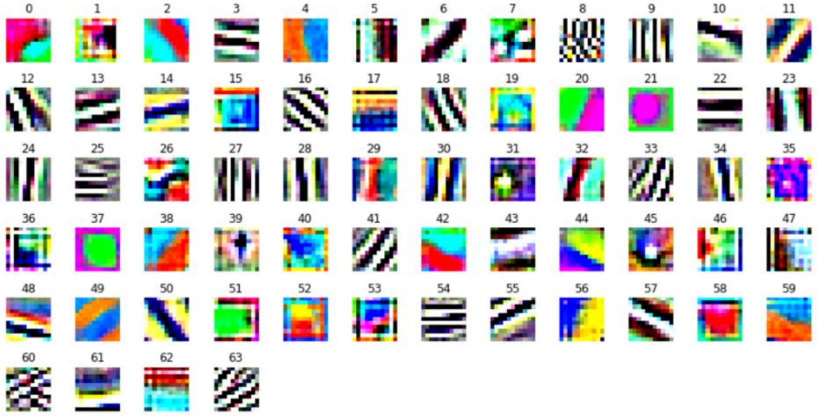
Methods based on various principles:

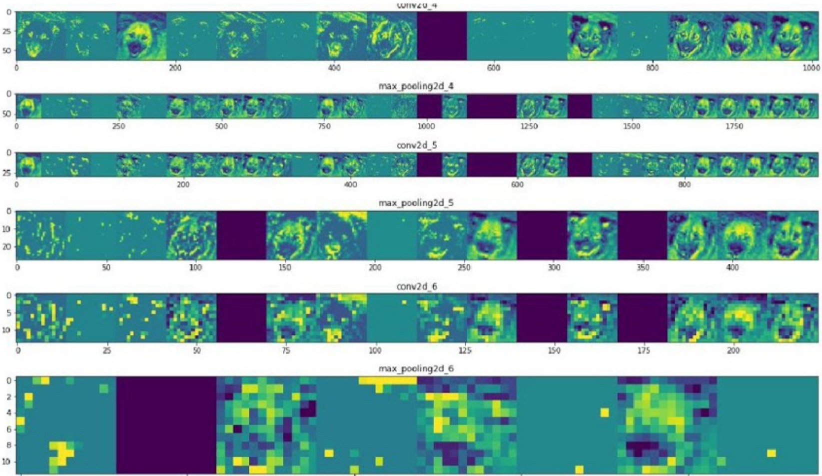
- Visualize weights and feature maps
- Visualize most important inputs for a given class
- Visualize the effect of input perturbations on the output
- Construct an intepretable surrogate model

Alex-net - filters of the first convolutional layer

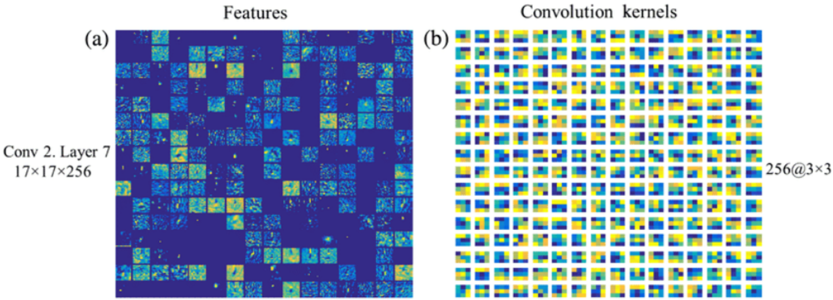


- 64 filters of depth 3 (RGB)
- Combined each filter RGB channels into one RGB image of size 11x11x3.

CNN - feature maps



CNN - feature maps - radar target classification



Synthetic-aperture radar (SAR) – used to create two-dimensional images or three-dimensional reconstructions of objects, such as landscapes.

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  over all input vectors $\vec{x}$.
- A maximizing input vector computed using the gradient descent.
- Gives the most "representative" input vector of the class represented by the neuron i.

Maximizing input - example

dumbbell cup dalmatian

Input specific saliency maps

The goal: Label features in a given input that are "most important" for the output of the network.

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Various approaches:

- gradient based
  - Gradient saliency maps
  - GradCAM
  - …
- occlusion based
  - Simple occlusion maps
  - LIME
  - …

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- Note that saliency comes from a surrogate local linear model given by the first-order Taylor approximation:

$$y_i(\vec{x}') \approx y_i(\vec{x}) + \left(\frac{\partial y_i}{\partial X}(\vec{x})\right)(\vec{x}' - \vec{x})$$

  Here $\frac{\partial y_i}{\partial X}$ is the vector of all partial derivatives $\frac{\partial y_i}{\partial y_k}$ where $k \in X$.

Saliency maps - example

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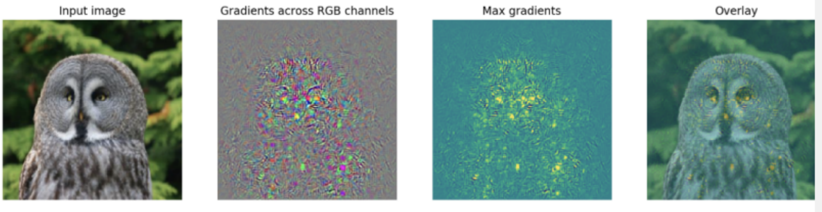
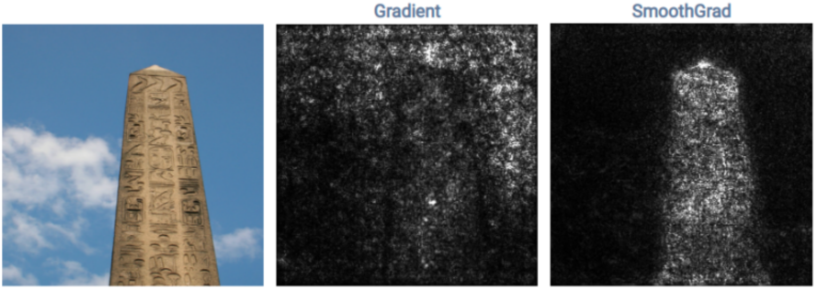


Quite noisy, the signal is spread and does not say much about the perception of the owl.

Saliency maps - example



SmoothGrad:

- Do the following several times:
  - Add noise to the input image
  - Compute a saliency map
- Average the resulting saliency maps.

GradCAM

- Consider a convolutional network and fix an input image I of the network.

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  Each F^ℓ is a set of neurons that belong to the feature map F^ℓ.

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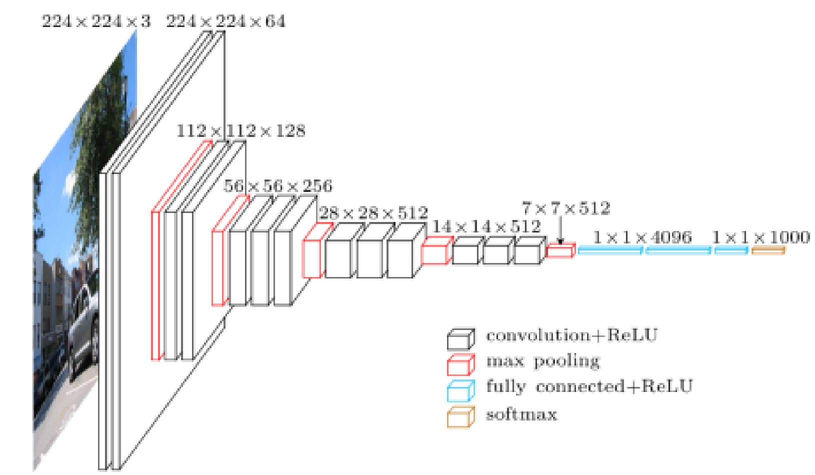
  and the final *gradCAM heat map* for L is obtained using

$$M_i^L = \mathrm{ReLU}\left(\sum_{\ell=1}^{k} \alpha_i^\ell F^\ell(I) \right)$$

GradCAM on VGG16



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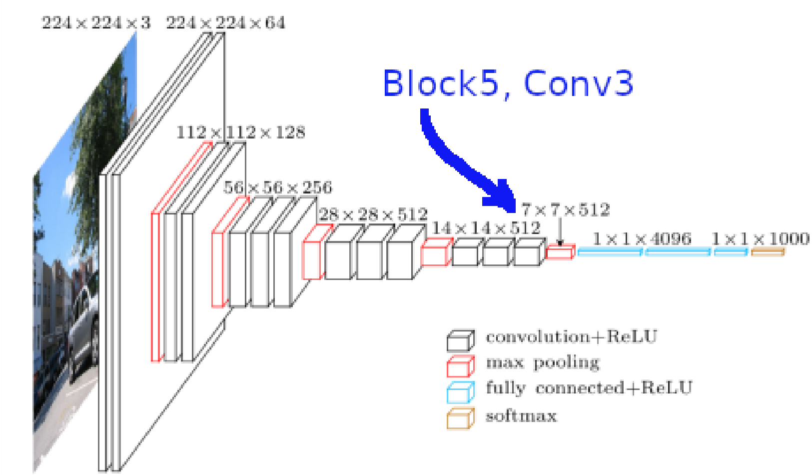
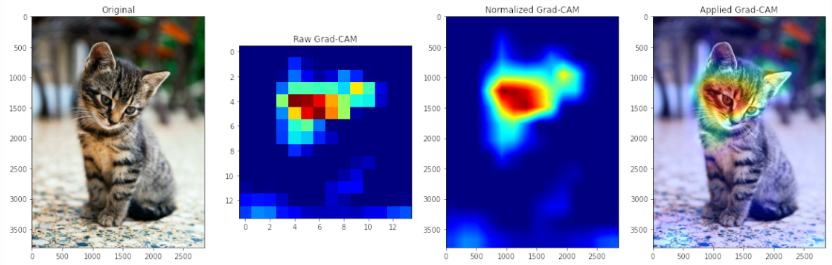


Consider the last convolutional layer of the VGG16 (Block5, Conv3)

GradCAM on VGG16



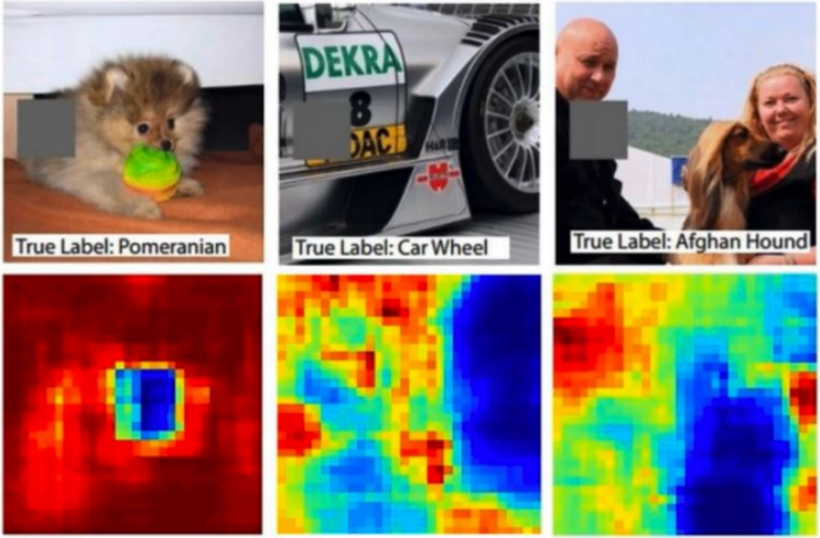
From left to right:

- An image of a cat (has to be resized to 224×224 to fit VGG16)
- The gradCAM heat map for the last convolutional layer and the class "cat"
- Rescaled and smoothed gradCAM heat map.
- The gradCAM overlay.

Occlusion

- Systematically cover parts of the input image.
- Observe the effect on the output value.
- Find regions with the largest effect.

Occlusion - example



Occlusion - example

LIME - for images

Let us fix an image I to be explained.

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Outline:

- Consider superpixels of I as interpretable components.

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Outline:

- Consider superpixels of I as interpretable components.
- Construct a linear model approximating the network aroung the image I with weights corresponding to the superpixels.
- Select the superpixels with weights of large magnitude as the important ones.

Original Image

Interpretable Components

Superpixels as interpretable components

Original Image

Interpretable Components

Denote by $P_1, \ldots, P_\ell$ all superpixels of I.

Superpixels as interpretable components

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Consider binary vectors $\vec{x} = (x_1, \ldots, x_\ell) \in \{0, 1\}^\ell$.

Superpixels as interpretable components

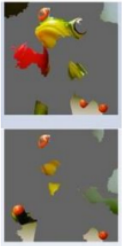
Original Image

Interpretable Components

Denote by $P_1, \ldots, P_\ell$ all superpixels of I.

Consider binary vectors $\vec{x} = (x_1, \ldots, x_\ell) \in \{0,1\}^\ell$.

Each such vector $\vec{x}$ determines a "subimage" $I[\vec{x}]$ of I obtained by removing all P_k with $x_k = 0$.



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- Given the image I to be interpreted, consider the following training set:

$$\mathcal{T} = \left\{ (\vec{x}_1, y_i(I[\vec{x}_1])), \ldots, (\vec{x}_p, y_i(I[\vec{x}_p])) \right\}$$

Here $\vec{x}_h = (x_{h1}, \ldots, x_{h\ell})$ are (some) binary vectors of $\{0, 1\}$. E.g., randomly selected.

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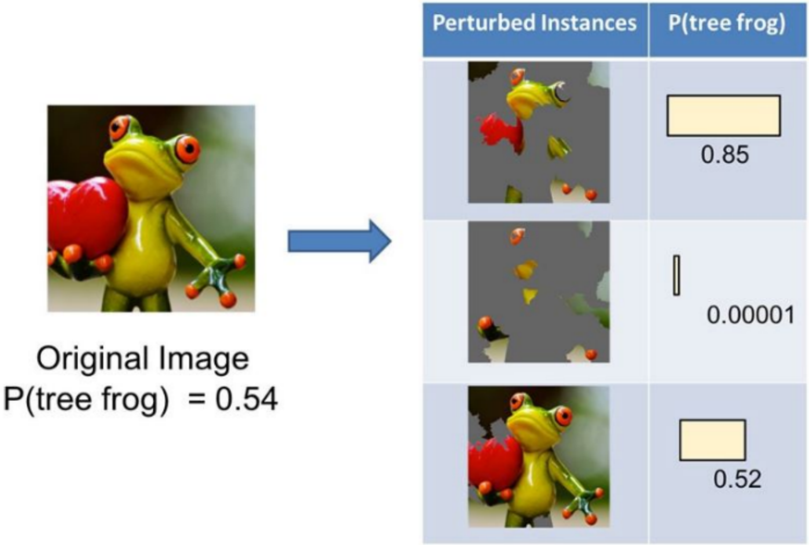
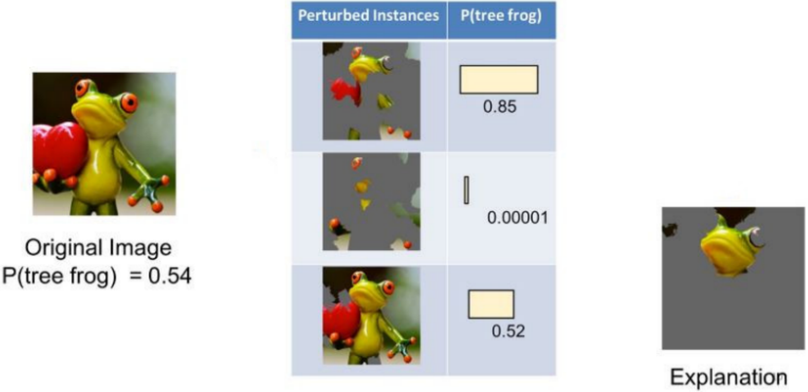
  Here $\vec{x}_h = (x_{h1}, \ldots, x_{h\ell})$ are (some) binary vectors of $\{0, 1\}$. E.g., randomly selected.
- Train a linear model (ADALINE) with weights $w_0, w_1, \ldots, w_\ell$ on $\mathcal{T}$ minimizing the mean-squared error (+ a regularization term making the number of non-zero weights as small as possible).

  Intuitively, the linear model approximates the networks on "subimages" of I obtained by removing "unimportant" superpixels.
- Inspect the weights (magnitude and sign).

LIME - example



LIME - example



LIME - example

(a) Original Image (b) Explaining *Electric guitar* (c) Explaining *Acoustic guitar* (d) Explaining *Labrador*

LIME - example

(a) Husky classified as wolf

(b) Explanation