Machine Intelligence:: Deep Learning
Week 3

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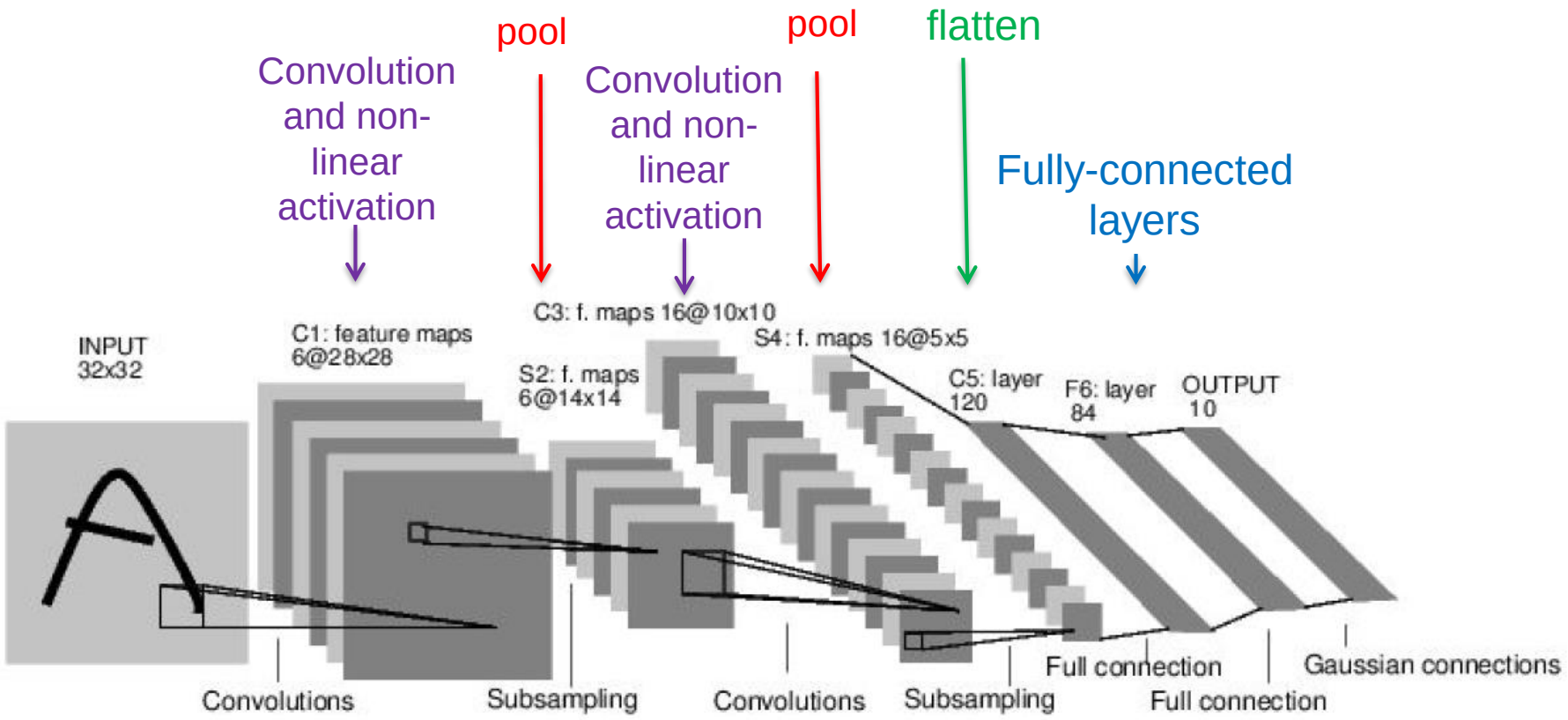
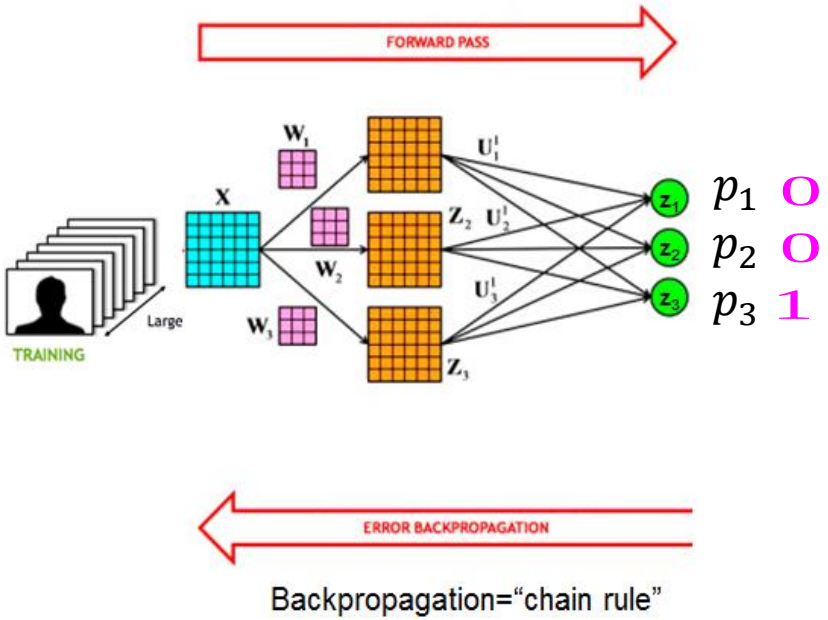
Topics of today

- Tricks of the trade to achieve good-performing CNNs
  - Standardizing / Batch-Norm
  - Dropout
- Look at challenge-winning CNN architectures
- DL with few data:
  - Augmentation
  - Using pretrained CNN for extracting “good” image features
  - Transfer learning
- Biological motivation of a CNN
- Shining light into the black-box CNN
  - Which parts of an image were important for a certain model prediction

Typical architecture of a simple CNN



Training of a CNN is based on gradient backpropagation



For the training we need the **observed label** for each image which we then compare with the **output** of the CNN.

We want to adjust the weights in a way so that difference between true label and output is minimal.

Minimize Loss-function:

L=distance(observed, output(w)**)**

Learning is done by weight updating:

$$w_i^{(t)} = w_i^{(t-1)} - l^{(t)} \left. \frac{\partial L(w)}{\partial w_i} \right|_{w_i = w_i^{(t-1)}}$$

learning rate

Image credits: Audhkhasi et al., Neural Networks 78 (2016) 15–23

Data Standardization

Batch Norm Layer

Data Standardization

- In contrast to other classifiers like trees (or Random Forest) result strongly depends on range of input data
- CNN works best if pixel values of images are in range [0,1]
- Standardization
  - Divide by range
  - Z-Transformation
- Automatic Z-transformation
  - Batch-Normalization
- Make sure to use correct standardization
  - If you “steal” an architecture
  - If you do transfer learning

Typical preprocessing of image data

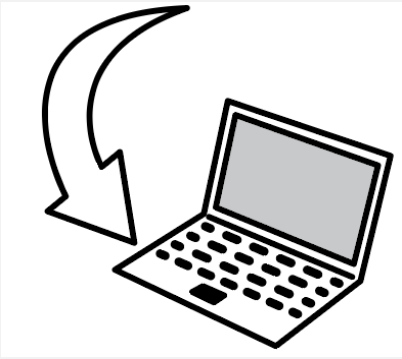
CNN works best if pixel values of images are in range [0,1] (see NB 07).

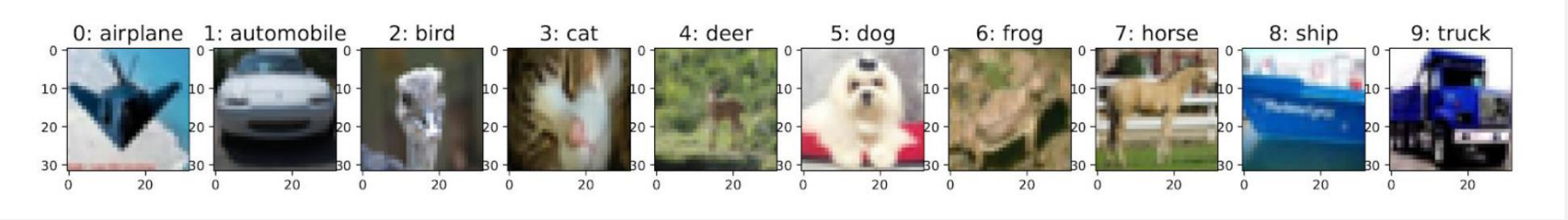
Therefore each pixel value is divided by the maximal possible pixel value:

```
# normalization
X_train_norm = X_train/255
X_val_norm = X_val/255
X_test_norm = X_test/255
```

Since also the initial weights of the NN are small values around zero, this data normalization as preprocessing is reasonable.

Exercise:





Develop a CNN to classify cifar10 images (we have 10 classes)

Investigate the impact of standardizing/normalizing the data on the performance

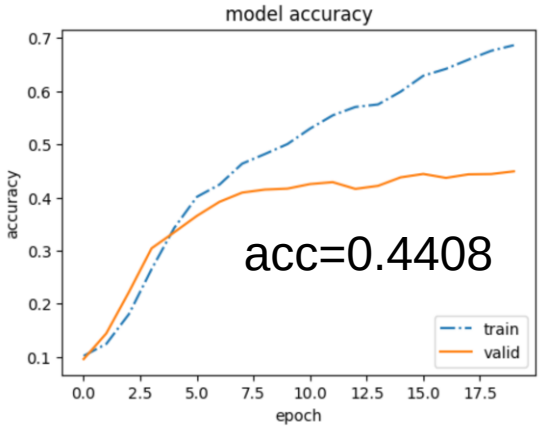
Work through the Notebook 07 and **stop before** the "dropout" section:

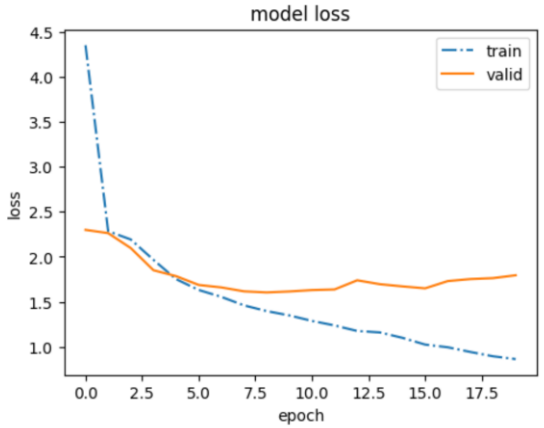
07_cifar10_tricks_sol.ipynb

Take-home messages from NB07

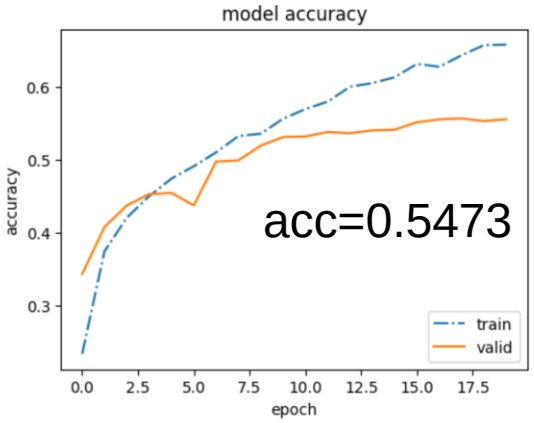
- DL does not need a lot of preprocessing, but working with standardized (small-valued) input data often helps.

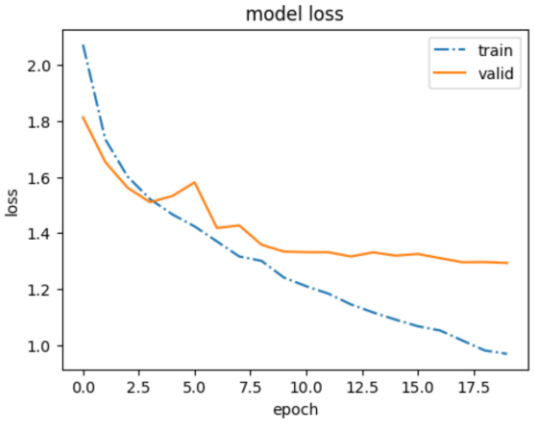
Without standardizing the input to the CNN





After standardizing the input to the CNN



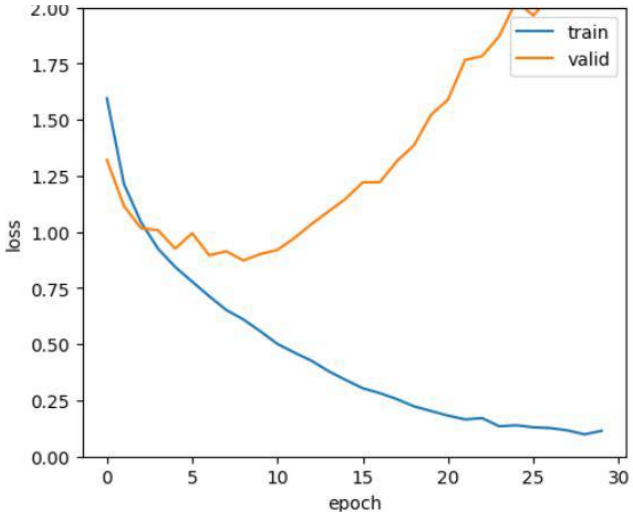


Overfitting

Early stopping and

Dropout during training

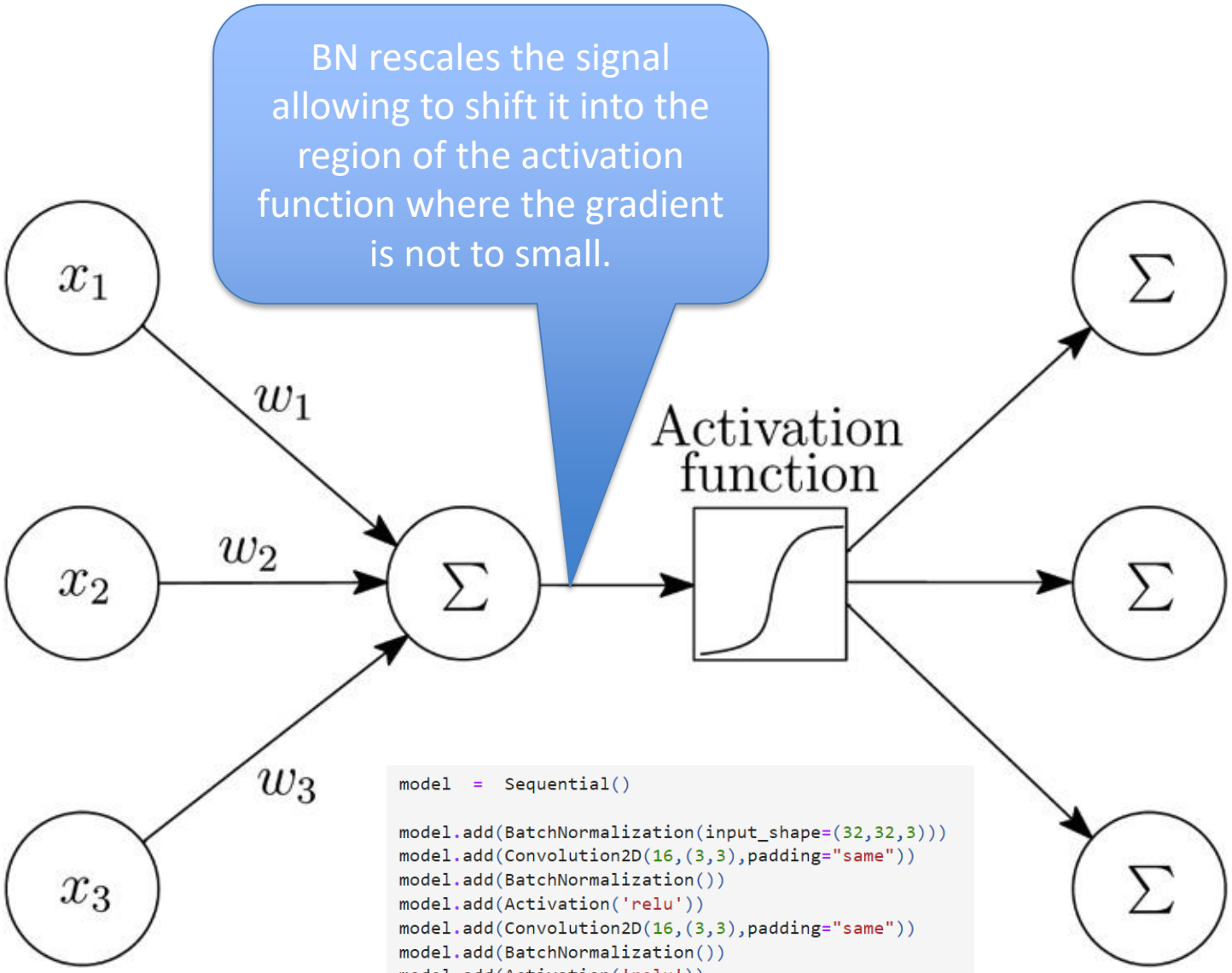
To avoid overfitting early stopping




```
>>> callback = tf.keras.callbacks.EarlyStopping(monitor='loss', patience=3)
>>> # This callback will stop the training when there is no improvement in
>>> # the loss for three consecutive epochs.
>>> model = tf.keras.models.Sequential([tf.keras.layers.Dense(10)])
>>> model.compile(tf.keras.optimizers.SGD(), loss='mse')
>>> history = model.fit(np.arange(100).reshape(5, 20), np.zeros(5),
...                     epochs=10, batch_size=1, callbacks=[callback],
...                     verbose=0)
>>> len(history.history['loss'])  # Only 4 epochs are run.
4
```

See https://keras.io/api/callbacks/early_stopping/

What is the idea of Batch-Normalization (BN)

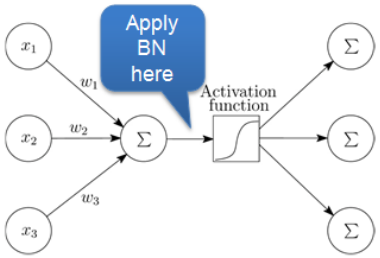



```
model = Sequential()

model.add(BatchNormalization(input_shape=(32,32,3)))
model.add(Convolution2D(16,(3,3),padding="same"))
model.add(BatchNormalization())
model.add(Activation('relu'))
model.add(Convolution2D(16,(3,3),padding="same"))
model.add(BatchNormalization())
model.add(Activation('relu'))
model.add(MaxPooling2D((2,2)))
```

⋮

Batch Normalization

- Idea: Introduce batch-norm layers between convolutions.



A BN layer performs a 2-step procedure with **α and β as learnable** parameter:

Step 1: $$\hat{x} = \frac{x - avg_{batch}(x)}{stdev_{batch}(x) + \epsilon}$$

$avg(\hat{x}) = 0$

$\text{stdev}(\hat{x}) = 1$

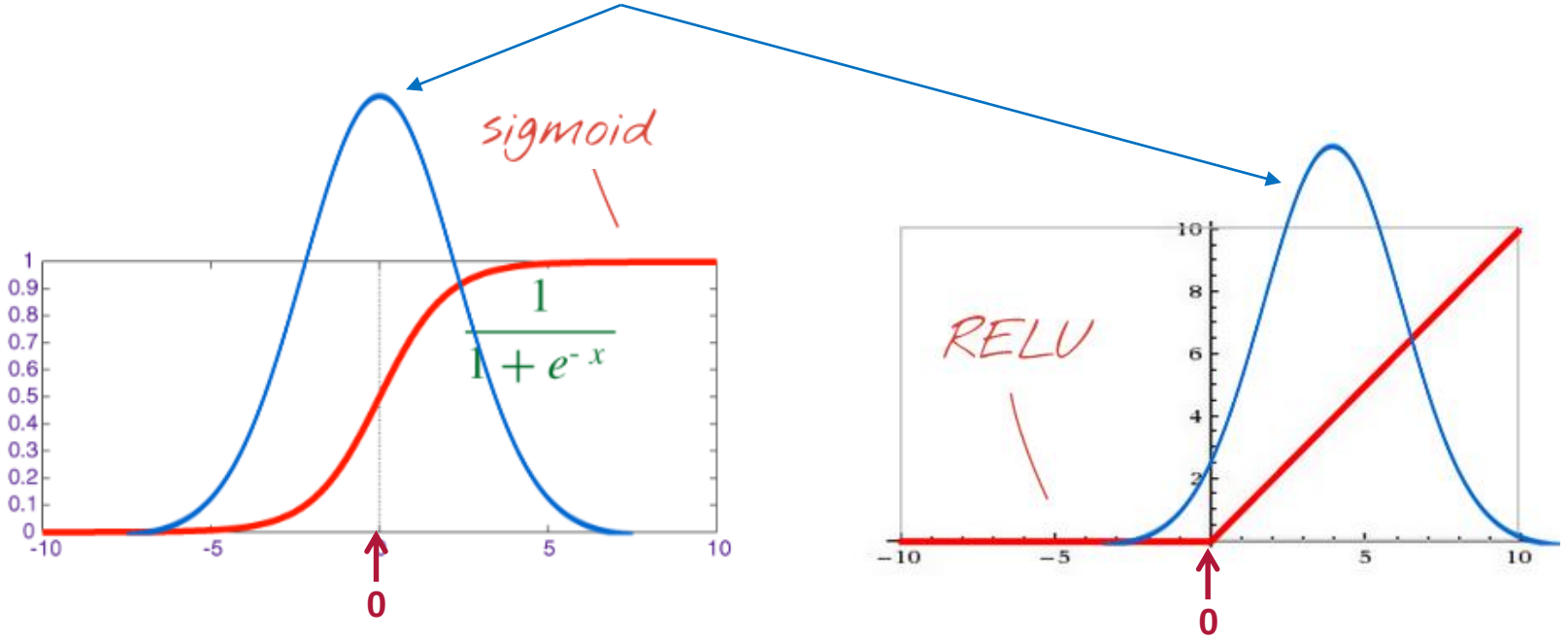
Step 2: $$BN(x) = \alpha\hat{x} + \beta$$

The learned parameters α and β determine how strictly the standardization is done. If the learned α=stdev(**x**) and the learned β=avg(**x**), then the standardization performed in step 1 is undone in step 2 and BN(**x**)=**x**.

Batch Normalization is beneficial in many NN

After BN the input to the activation function is in the sweet spot

Observed distributions of signal after BN before going into the activation layer.

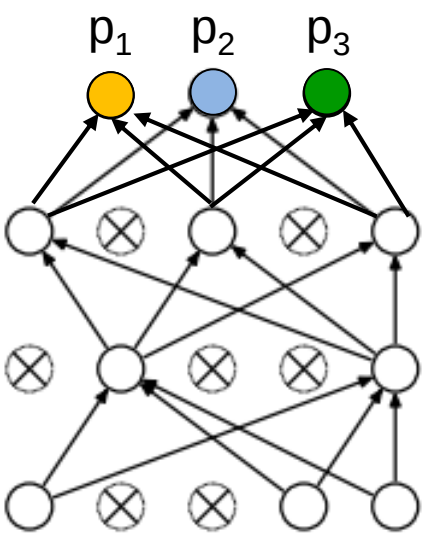


When using BN consider the following:

- Using a higher learning rate might work better
- Use less regularization, e.g. reduce dropout probability

Image credits: Martin Gorner:
https://docs.google.com/presentation/d/e/2PACX-1vRouwj_3cYsmLrNNI3Uq5gv5-hYp_QFdeoan2GlxKgIZRSejozruAbVV0IMXBoPsINB7Jw92vJo2EAM/pub?slide=id.g187d73109b_1_2921

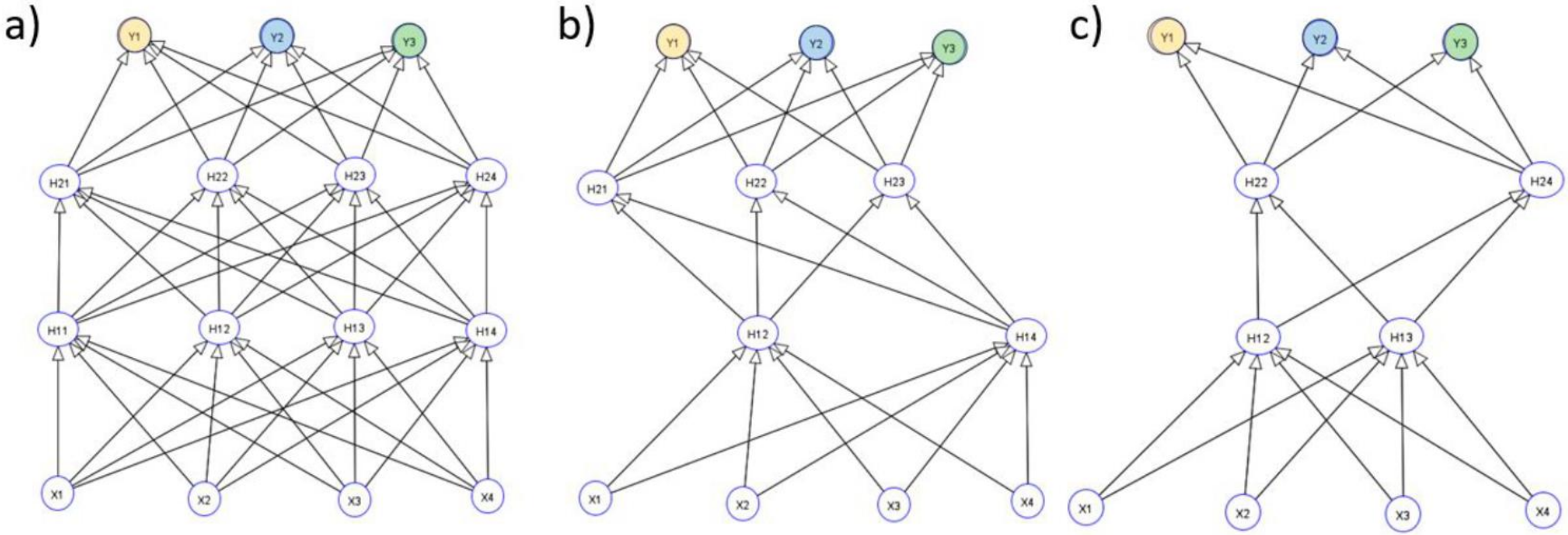
Dropout helps to fight overfitting



Using dropout during training implies:

- In each training step only weights to not-dropped units are updated → we train a sparse sub-model NN
- For predictions with the trained NN we freeze the weights corresponding to averaging over the ensemble of trained models we should be able to “reduce noise”, “overfitting”

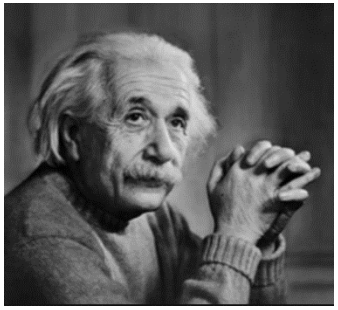
Dropout: kind of NN ensemble



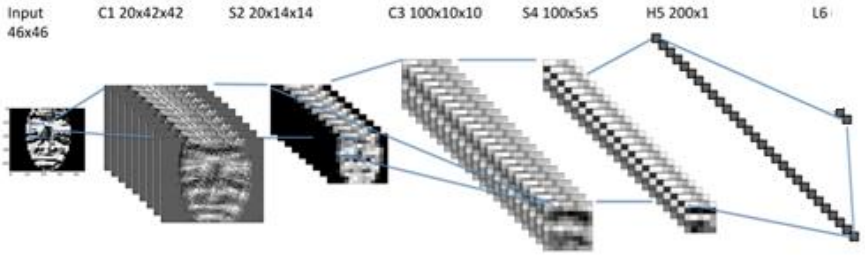
Three NNs: a) shows the full NN with all neurons, b) and c) show two versions of a thinned NN where some neurons are dropped. Dropping neurons is the same as setting all connections that start from these neurons to zero

Another intuition: Why "dropout" can be a good idea

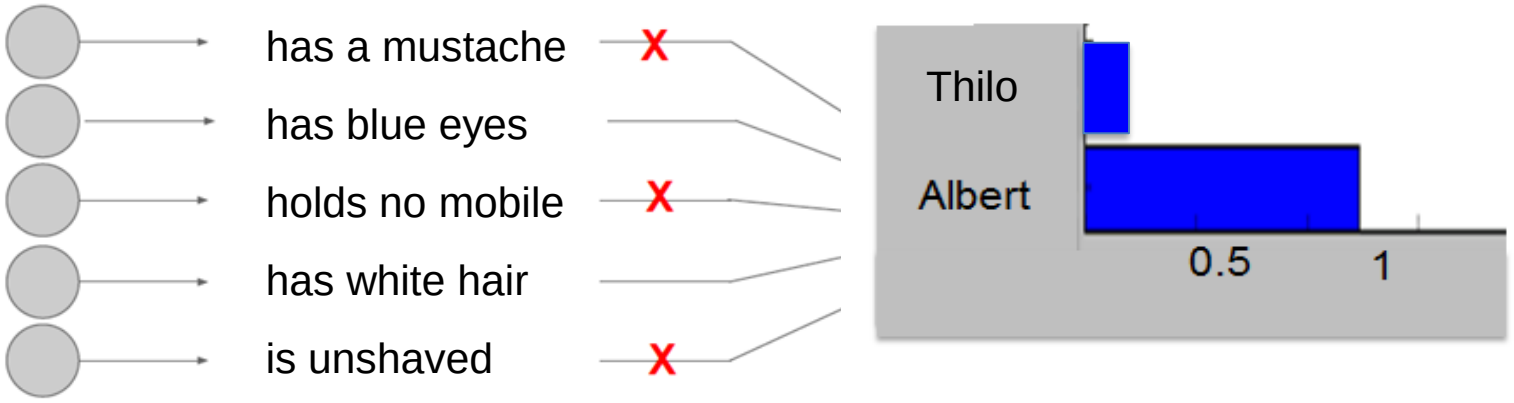
The training data consists of many different pictures of Thilo and Einstein



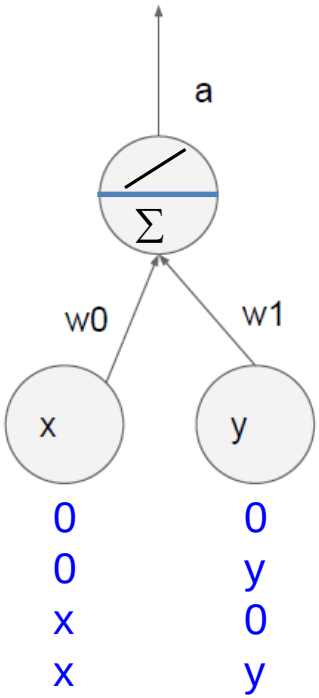
We need a huge number of neurons to extract good features which help to distinguish Thilo from Einstein



Dropout forces the network to learn redundant and independent features



Dropout-trained NN require weight adaptation



Use the trained net without dropout during test time

Q: Suppose no dropout during test time (x, y are never dropped to zero), but a dropout probability p=0.5 during training

What is the expected value for the output **a** of this neuron?

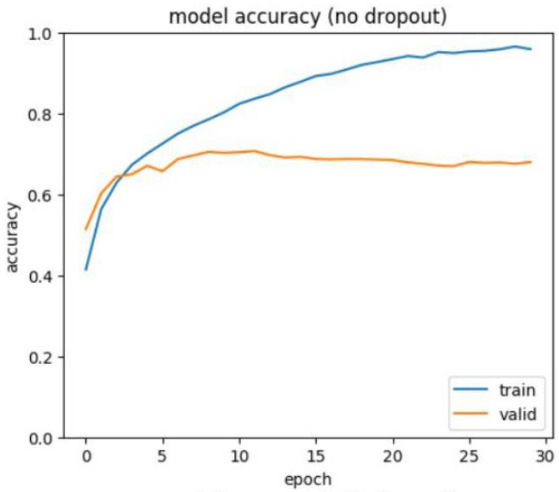
during test w/o dropout: **a = w0*x + w1*y**

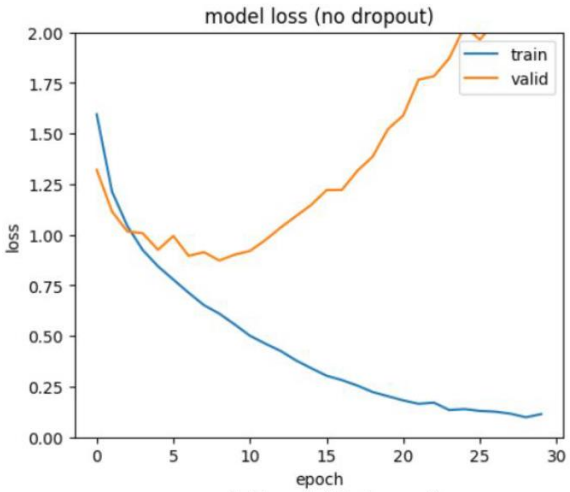
during training with dropout probability 0.5:

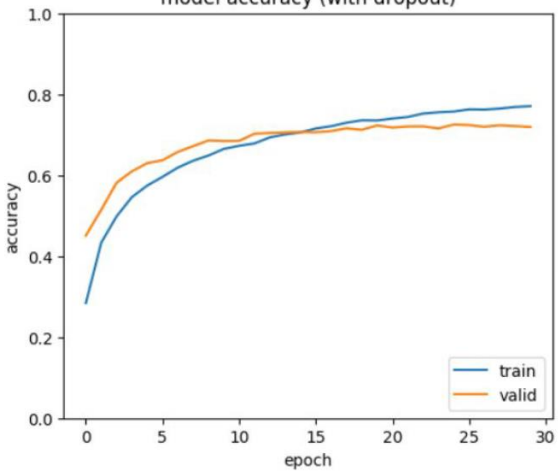
$$E[a] = \tfrac{1}{4} * (w0*0 + w1*0 + w0*0 + w1*y + w0*x + w1*0 + w0*x + w1*y)$$
$$= \tfrac{1}{4} * (2\, w0*x + 2\, w1*y)$$
$$= \tfrac{1}{2} * \mathbf{(w0*x + w1*y)}$$

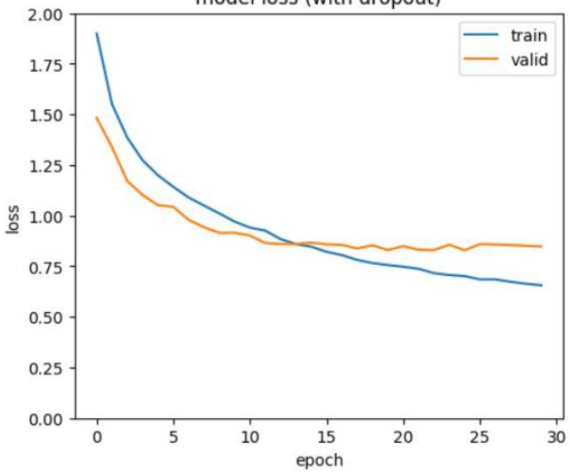
=> To get same expected output in training and test time, we reduce the weights during test time by multiplying them by the dropout probability p=0.5

Dropout fights overfitting in a CIFAR10 CNN





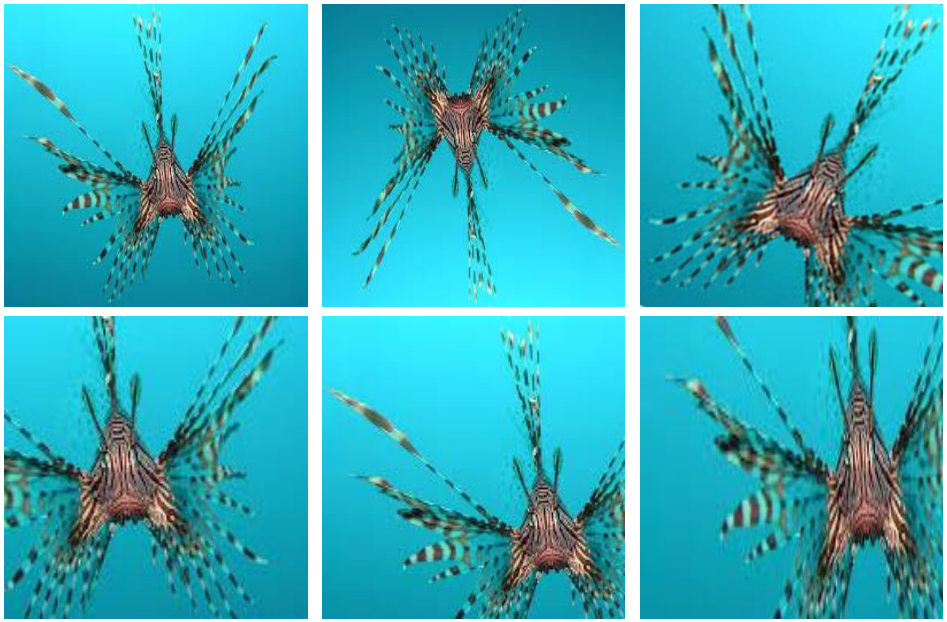





```
model  =  Sequential()

model.add(Convolution2D(16,(3,3),
           activation="relu",padding="same",
           input_shape=(32,32,3)))
model.add(Convolution2D(16,(3,3),
           activation="relu",padding="same"))
model.add(MaxPooling2D((2,2)))

model.add(Convolution2D(32,(3,3),
           activation="relu",padding="same"))
model.add(Convolution2D(32,(3,3),
           activation="relu",padding="same"))
model.add(MaxPooling2D((2,2)))

model.add(Flatten())
model.add(Dropout(0.3))
model.add(Dense(500))
model.add(Activation('relu'))
model.add(Dropout(0.3))
model.add(Dense(300))
model.add(Activation('relu'))
model.add(Dropout(0.3))
model.add(Dense(100))
model.add(Activation('relu'))

model.add(Dense(10))
model.add(Activation('softmax'))
```

Fighting overfitting by Data augmentation ("always" done): "generate more data" on the flight during fitting the model

- Rotate image within an angle range
- Flip image: left/right, up, down
- resize
- Take patches from images
- ….



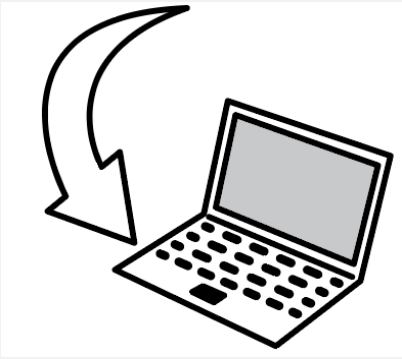
Data augmentation in Keras:

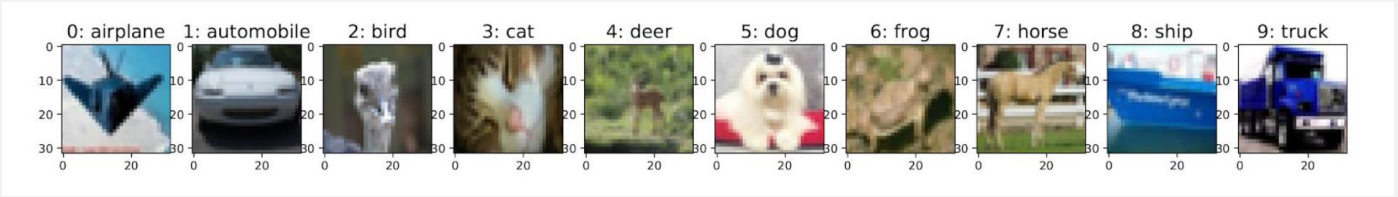
```
from keras.preprocessing.image import ImageDataGenerator

datagen = ImageDataGenerator(
    rotation_range=10,
    width_shift_range=0.1,
    height_shift_range=0.1,
    horizontal_flip=True,
    vertical_flip=True,
    #zoom_range=[0.1,0.1]
)
```

```
train_generator = datagen.flow(
          x = X_train_new,
          y = Y_train,
          batch_size = 128,
          shuffle = True)
```

```
history = model.fit_generator(
                     train_generator,
                     samples_per_epoch = X_train_new.shape[0],
                     epochs = 400,
                     validation_data = (X_valid_new, Y_valid),
                     verbose = 2,callbacks=[checkpointer]
)
```

Exercise: Tricks of the Trade: NB 07





Work through the Notebook 07 “**dropout**” section on:

[07_cifar10_tricks_sol.ipynb]

Content:

- load the original cifar10 data create a train val and test dataset
- visualize samples of cifar10 dataset
- train a random forest on the pixelvalues
- train a cnn from scratch without normalization
- train a cnn from scratch with normalization
- train a cnn from scratch with dropout
- train a cnn from scratch with batchnorm
- train a cnn from scratch with data augmentation
- compare the performances of the models

Challenge winning CNN architectures

LeNet-5 1998: first CNN for ZIP code recognition

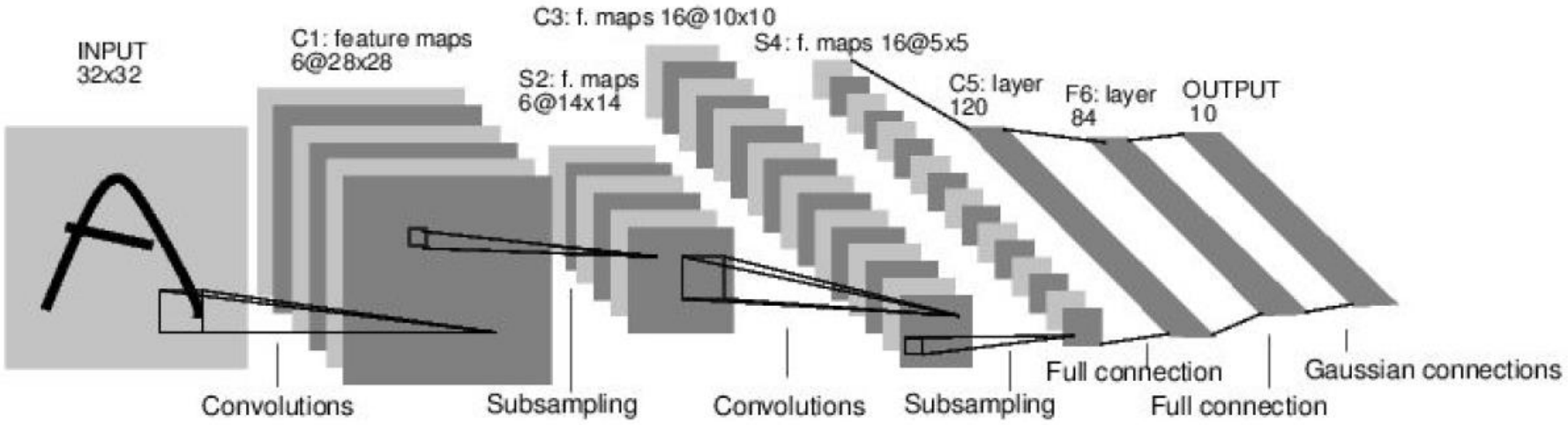


Image credits: http://yann.lecun.com/exdb/publis/pdf/lecun-98.pdf

Conv filters were 5x5, applied at stride 1
Subsampling (Pooling) layers were 2x2 applied at stride 2
i.e. architecture is [CONV-POOL-CONV-POOL-CONV-FC]

http://yann.lecun.com/exdb/lenet/index.html

The first CNN (Yan LeCun)

https://www.youtube.com/watch?v=FwFduRA_L6Q

Review of ImageNet winning CNN architectures

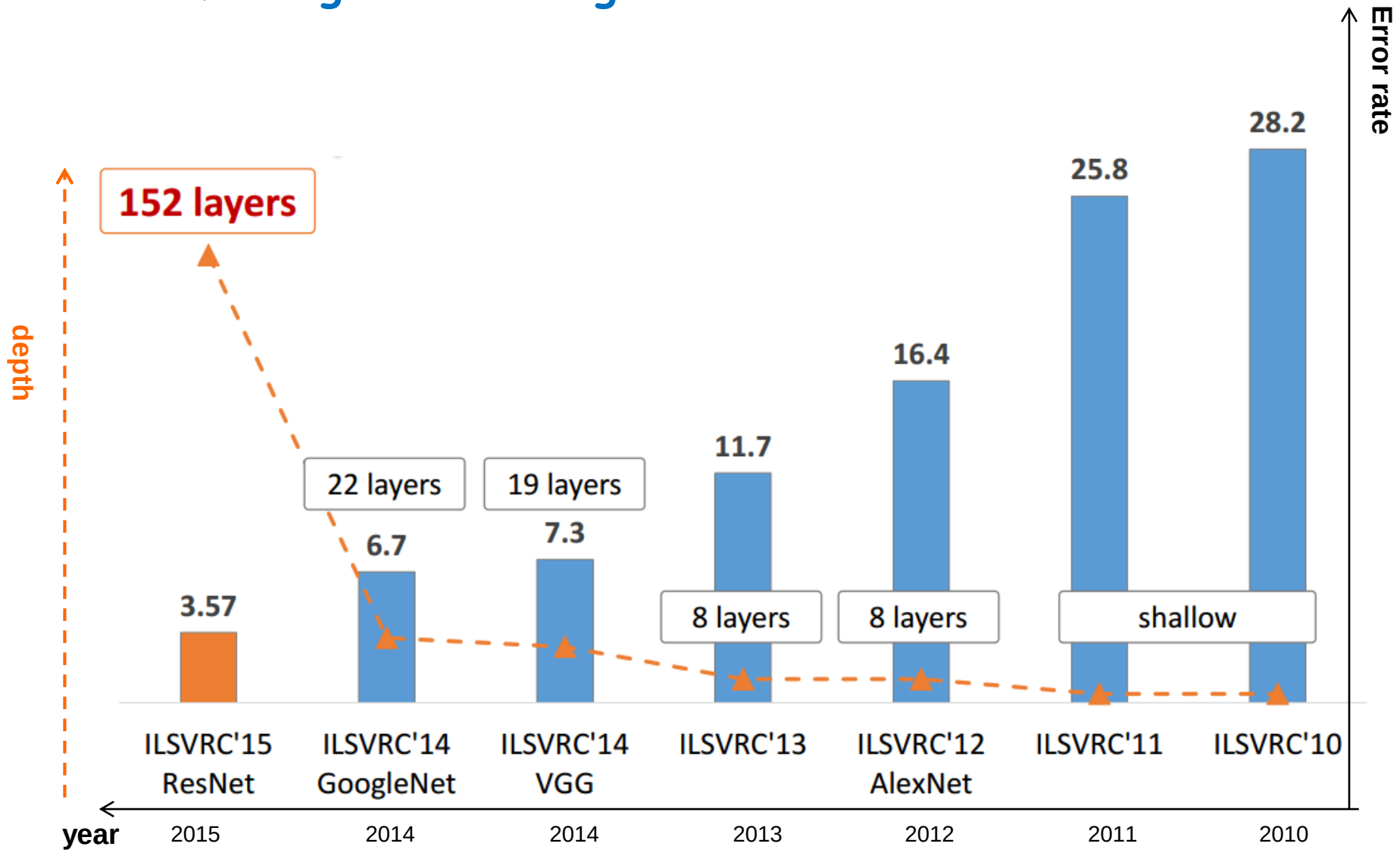


Image credits (modified): K.He, X.Zhang, S.Ren, J.Sun. “Deep Residual Learning for Image Recognition”. arXiv 2015

The trend in modern CNN architectures goes to small filters

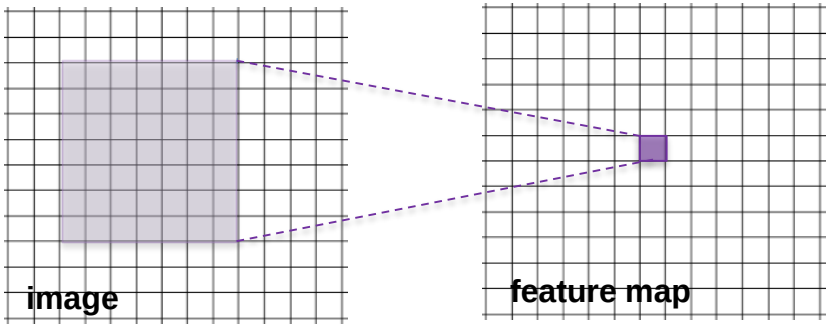
Why do modern architectures use very small filters?

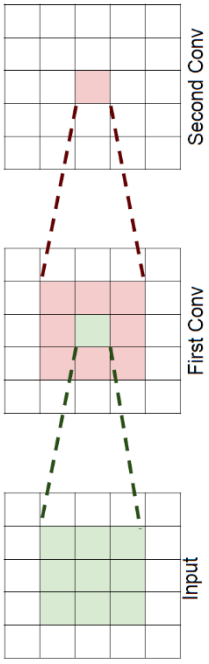
Determine the receptive field in the following situation:

1) Suppose we have **one** 7x7 conv layers (stride 1)

49 weights

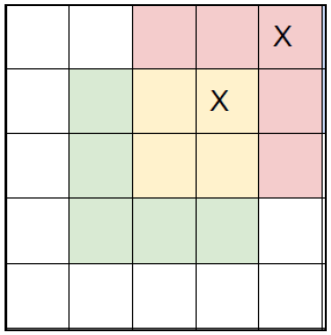
Answer1): 7x7





2) Suppose we stack **two** 3x3 conv layers (stride 1)

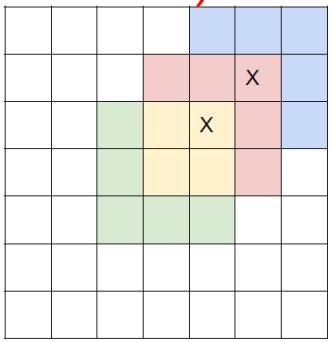
Answer 2): 5x5



3) Suppose we stack **three** 3x3 conv layers (stride 1)

3*9=27 weights

Answer 3): 7x7



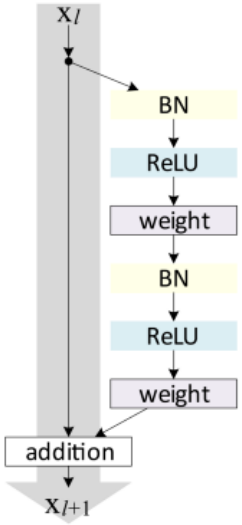
We need less weights for the same receptive field when stacking small filters!

"ResNet" from Microsoft 2015 winner of imageNet

152 layers

ResNet basic design (VGG-style)

- add shortcut connections every two
- all 3x3 conv (almost)



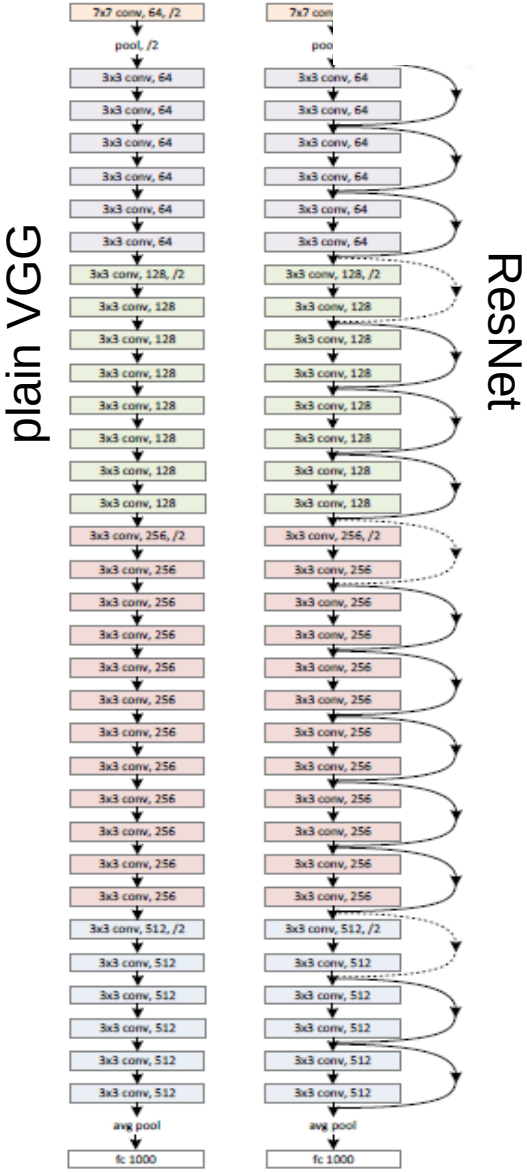
$F(x_l)$

152 layers:
Why does this train at all?

This deep architecture could still be trained, since the gradients can skip layers which diminish the gradient!

$H(x_l)=x_{l+1} = x_l + F(x_l)$

F(x) is called "residual" since it only learns the "delta" which is needed to add to x to get H(x)



credits: https://chatbotslife.com/resnets-highwaynets-and-densenets-oh-my-9bb15918ee32

"Oxford Net" or "VGG Net" 2014 2nd place

- 2nd place in the imageNet challenge
- More traditional, easier to train
- More weights than GoogLeNet
- Small pooling
- Stacked 3x3 convolutions before maxpooling

  -> large receptive field
- no strides (stride 1)
- ReLU after conv. and FC (batchnorm was not used)
- Pre-trainined model is available

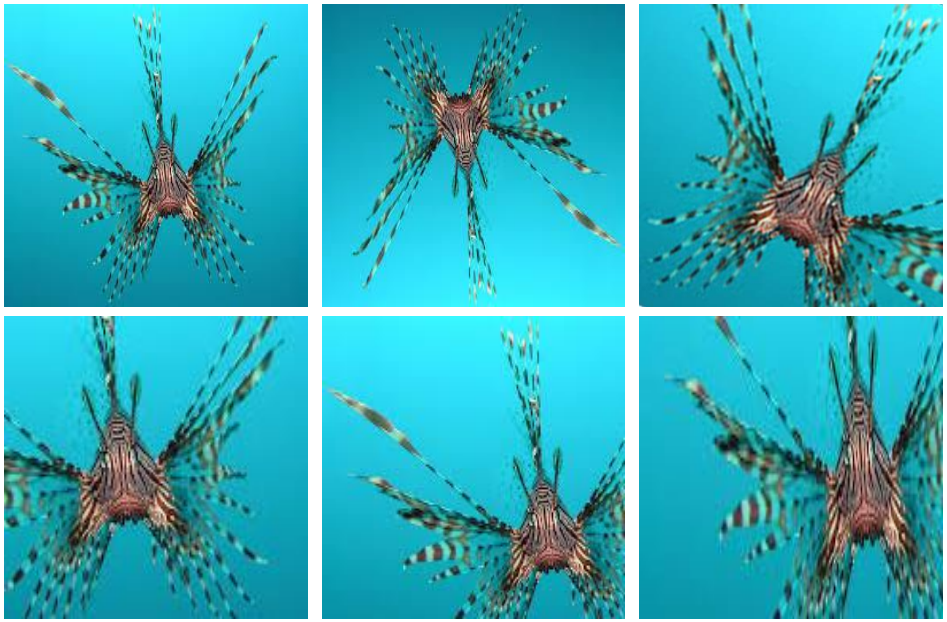
http://arxiv.org/abs/1409.1556

What to do in case of limited data?

- Do augmentation during training of a CNN
- Use shallow learner (e.g. RF) based on image features extracted via pretrained CNNs
- Fine-tune a pretrained CNN on few data (transfer learning)

Recall: Augmentation

- Generate “more data from the available data” by augmentation



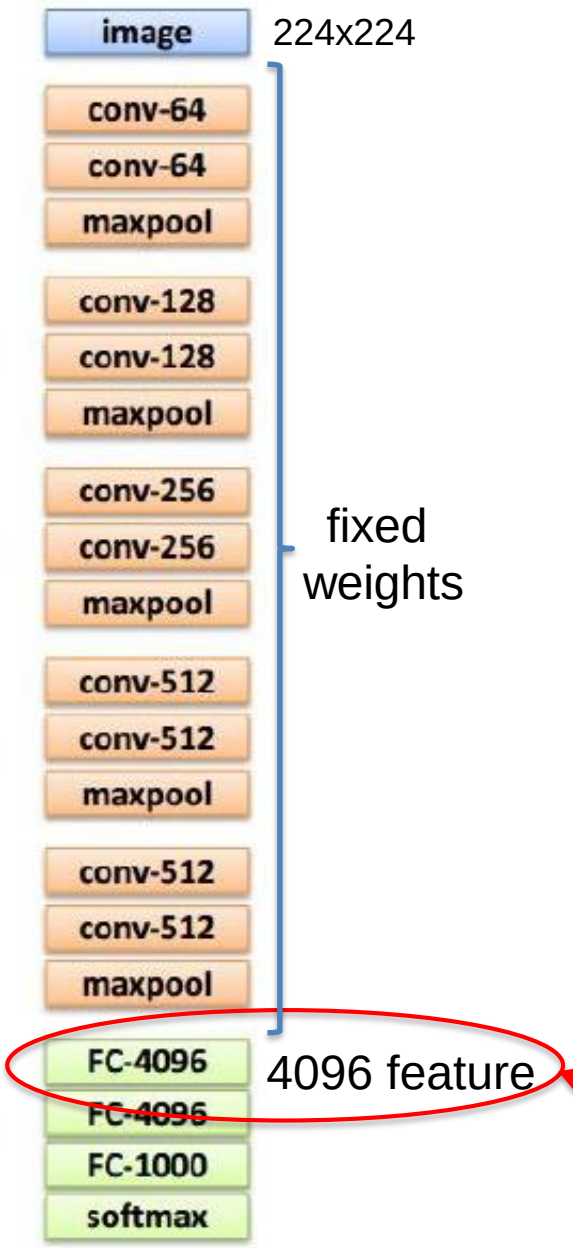
Data augmentation in Keras:

```
from keras.preprocessing.image import ImageDataGenerator

datagen = ImageDataGenerator(
    rotation_range=10,
    width_shift_range=0.1,
    height_shift_range=0.1,
    horizontal_flip=True,
    vertical_flip=True,
    #zoom_range=[0.1,0.1]
)
```

```
train_generator = datagen.flow(
          x = X_train_new,
          y = Y_train,
          batch_size = 128,
          shuffle = True)
```

```
history = model.fit_generator(
                    train_generator,
                    samples_per_epoch = X_train_new.shape[0],
                    epochs = 400,
                    validation_data = (X_valid_new, Y_valid),
                    verbose = 2,callbacks=[checkpointer]
)
```

Use pre-trained CNNs for feature extraction



- Load a pre-trained CNN – e.g. VGG16
- Resize image to required size (224x224 for VGG16)
- Rescaling of the pixel values to “VGG range”
- Do a forward pass and fetched features that are used as CNN representations, dump these features into a file on disk
- Use these CNN features as input to a simple classifier – e.g. fc NN, RF, SVM …
  (here it is easily possible to adapt to the new number of class labels)

Are VGG features useful?

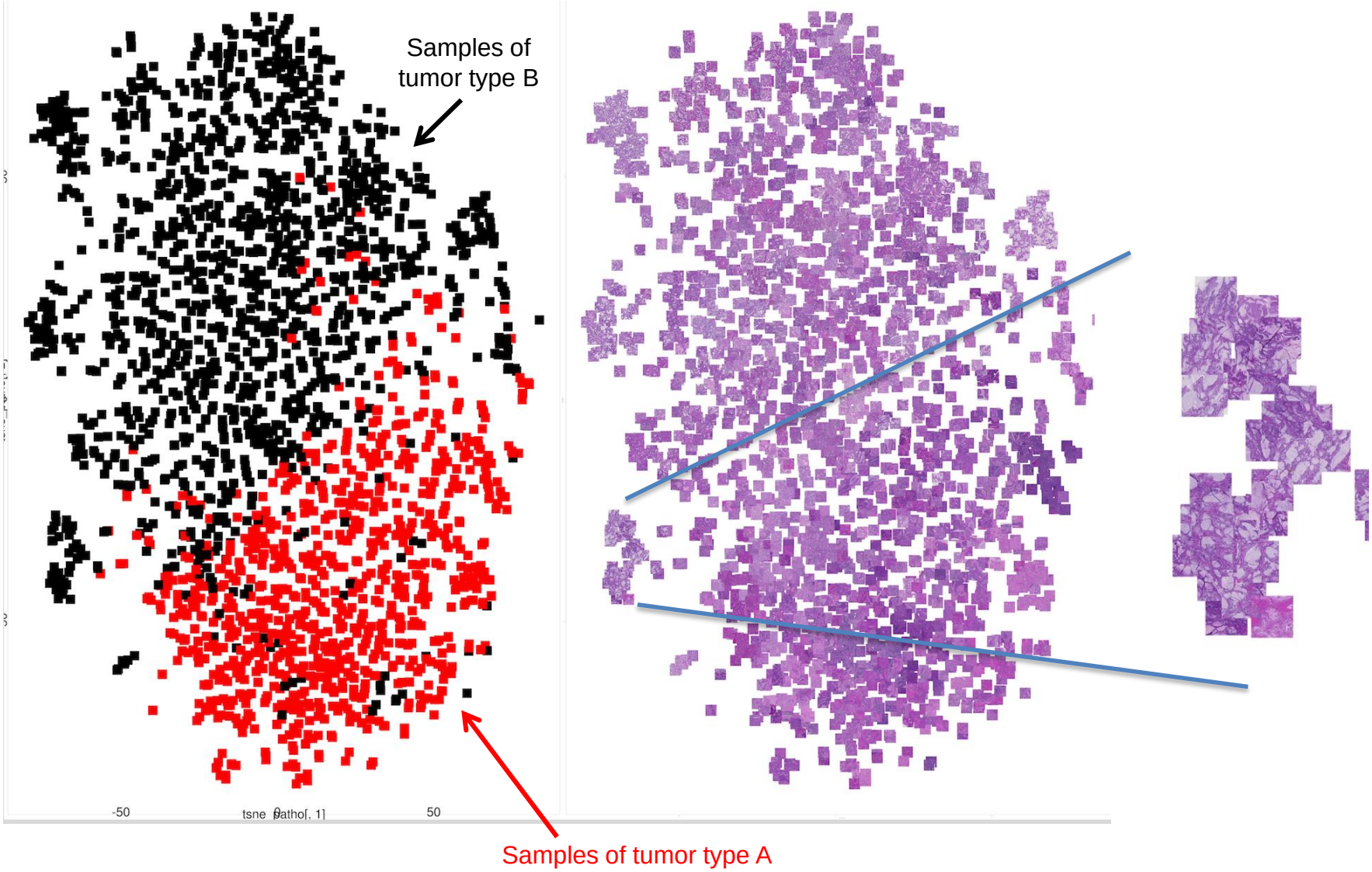
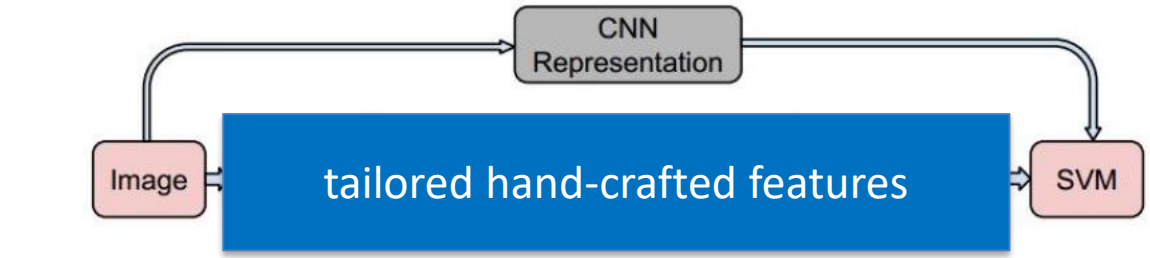
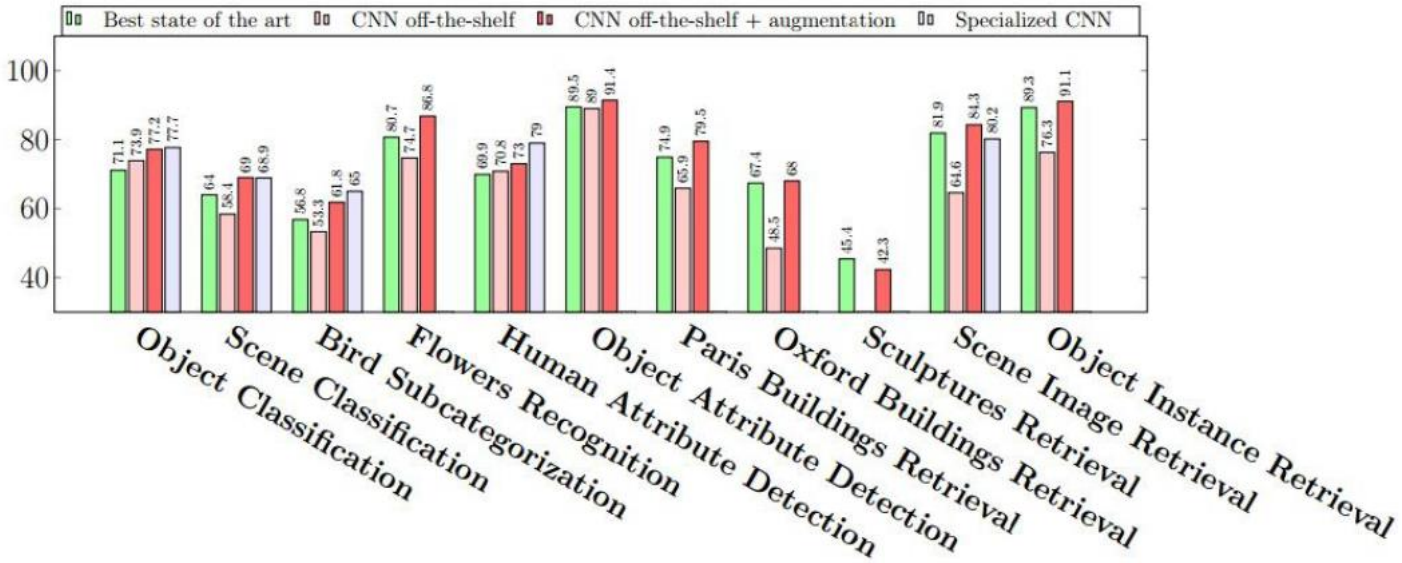


image credit: Elvis Murina

Performance of off-the-shelf CNN features when compared to tailored hand-crafted features



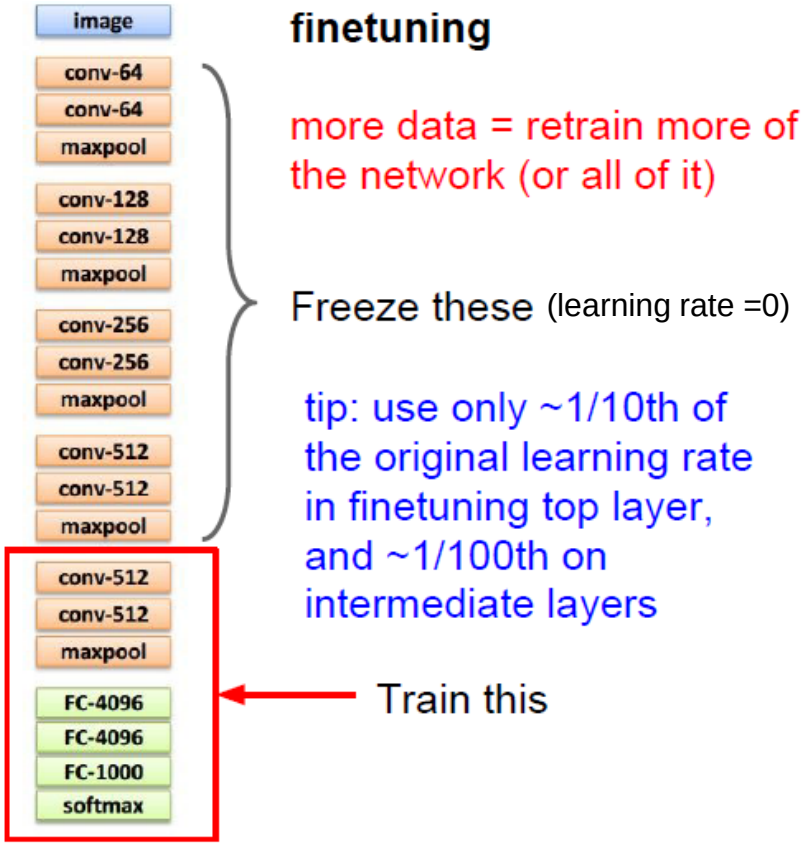


"Astonishingly, we report consistent superior results compared to the highly tuned state-of-the-art systems in all the visual classification tasks on various datasets."

CNN Features off-the-shelf: an Astounding Baseline for Recognition [Razavian et al, 2014]

Transfer learning beyond using off-shelf CNN feature

e.g. medium data set (<1M images)



The strategy for fine-tuning depends on the size of the data set and the type of images:

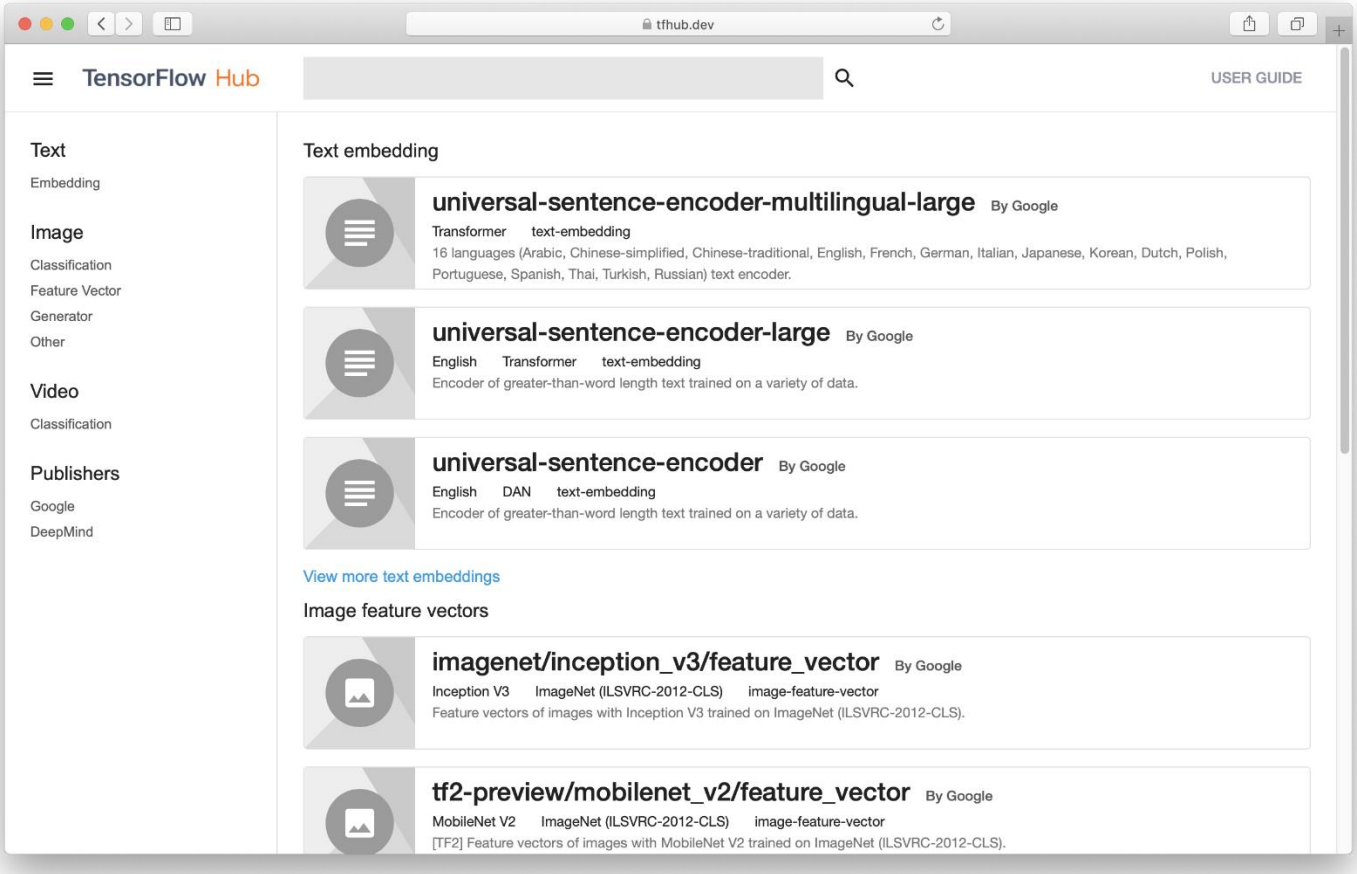
	Similar task (to imageNet challenge)	**Very different task** (to imageNet challenge)
little data	Extract CNN representation of one top fc layer and use these features to train an external classifier	You are in trouble - try to extract CNN representations from different stages and use them as input to new classifier
lots of data	Fine-tune a few layers including few convolutional layers	Fine-tune a large number of layers

Hint: first retrain only fully connected layer, only then add convolutional layers for fine-tuning.

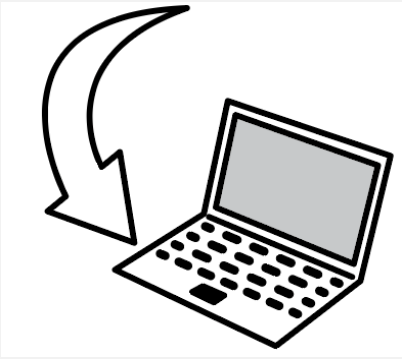
Slide credits (modified): cs231n

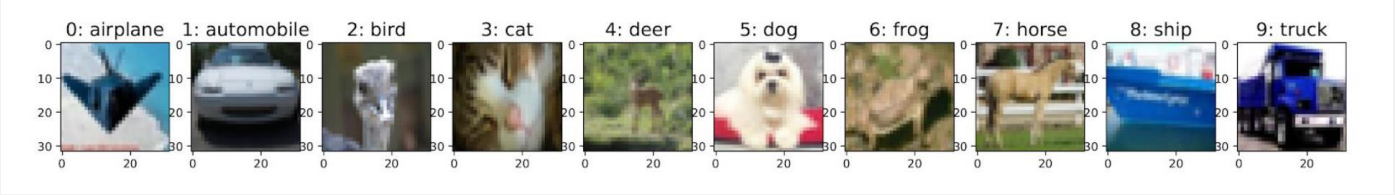
Where to find pretrained networks

- https://tfhub.dev/



Exercise:
08_classification_transfer_learning_few_labels





Notebook: [08_classification_transfer_learning_few_labels.ipynb]

Learning with few data

In case of few data you can work with features that you extract from a pretrained cnn. Data augmentation inceases the training data and usually help to improve the performace.

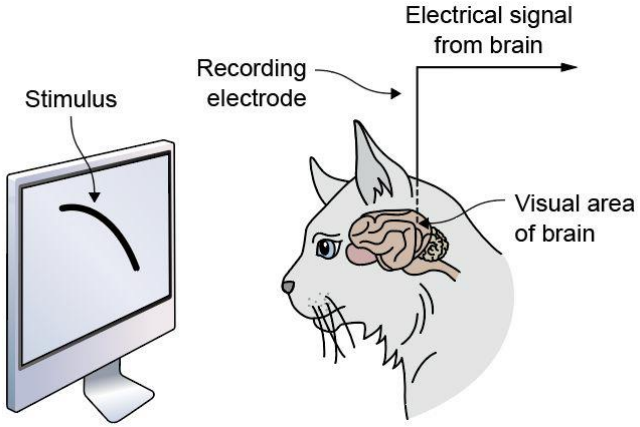
Learning with few data

Baseline model: RF on VGG features

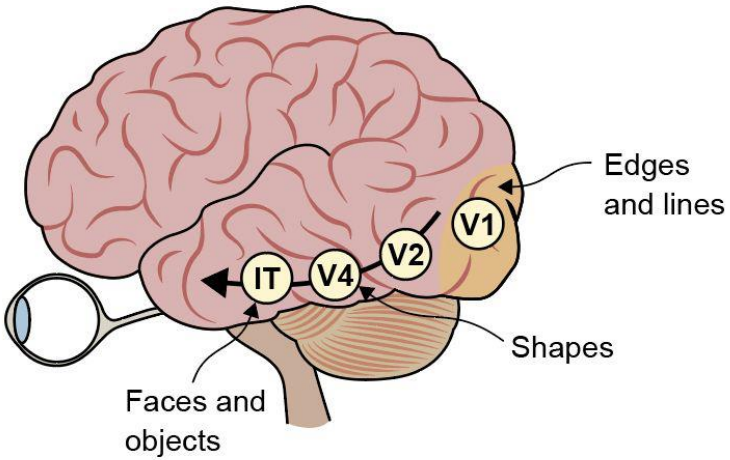
Transfer learning

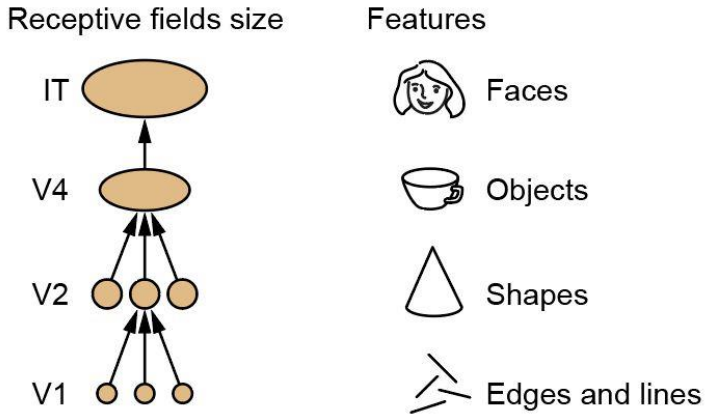
Biological Inspiration of CNNs

How does the brain respond to visually recieved stimuli?



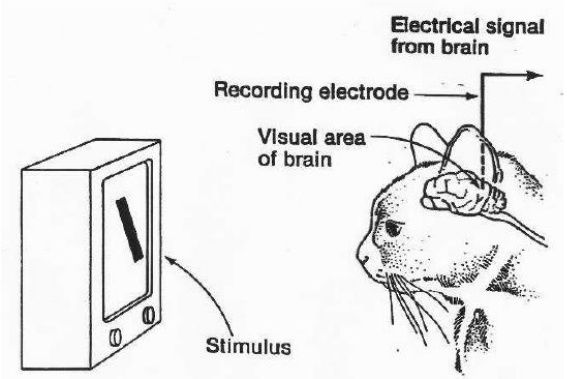
Setup of the experiment of Hubel and Wiesel in late 1950s in which they discovered neurons in the visual cortex that responded when moving **edges** were shown to the cat.

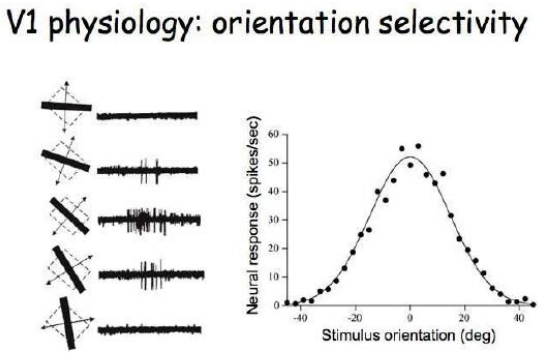


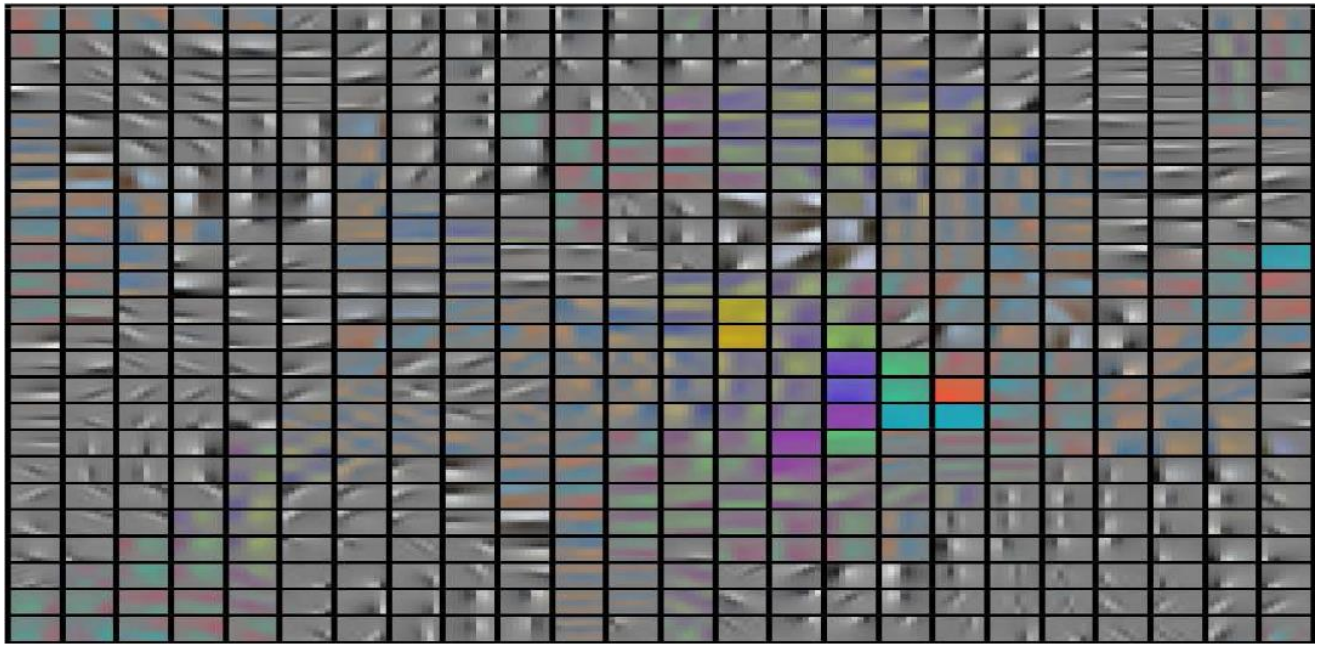


Organization of the visual cortex in a brain, where neurons in different regions respond to more and more complex stimuli

Compare neurons in brain region V1 in first layer of a CNN





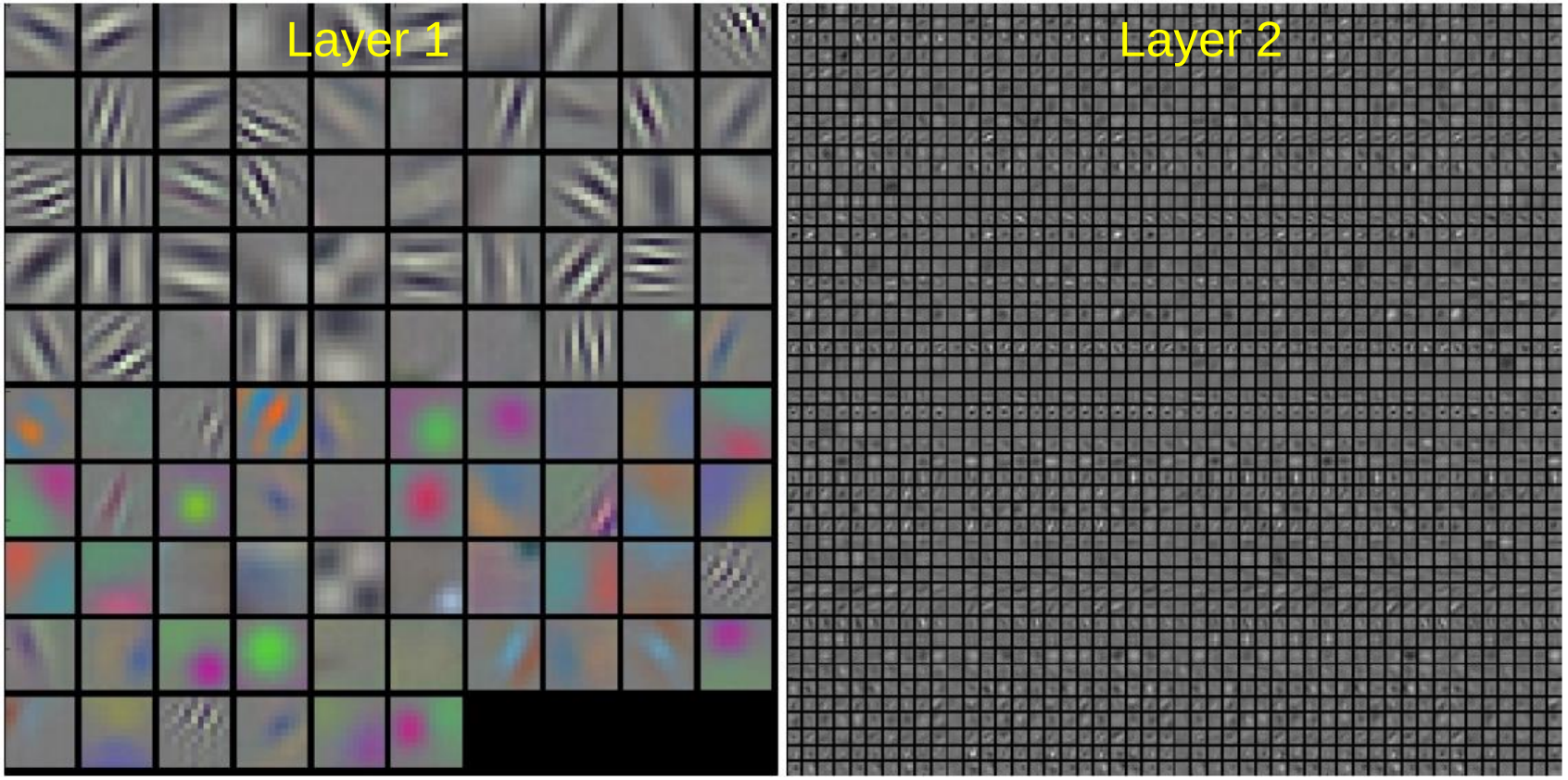


Neurons in brain region V1 and neurons in 1. layer of a CNN respond to similar patterns

Slide (modified) credits: Nando de Freitas

Visualize the weights used in filters

Filter weights from a trained Alex Net

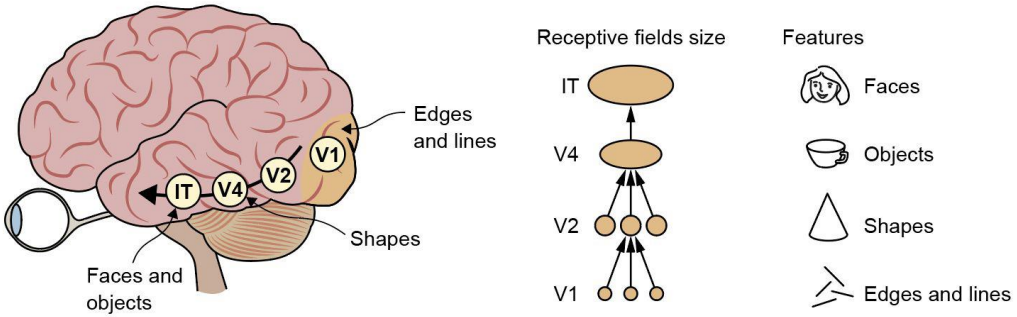


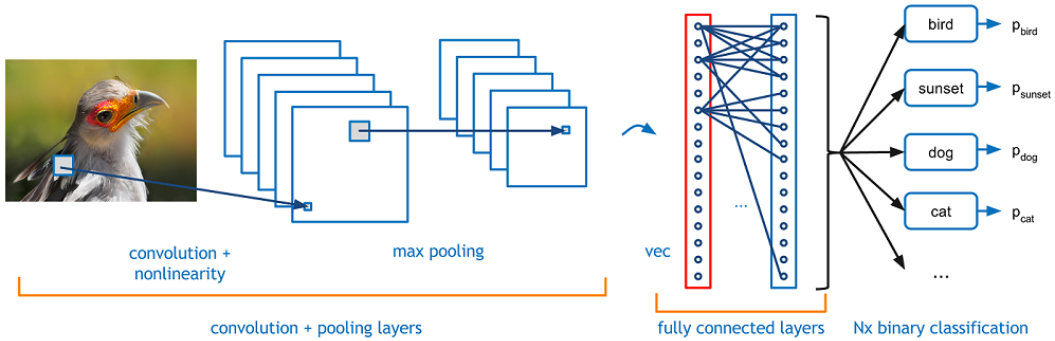
Only in layer 1 the filter pattern correspond to extracted patterns in the image.

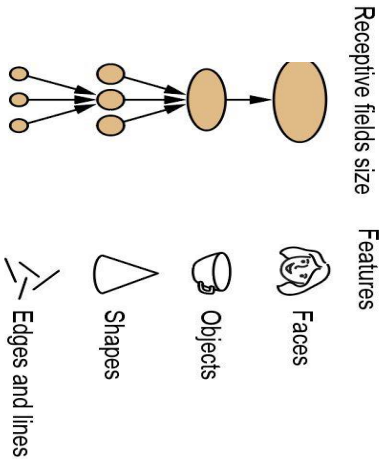
In higher layers we can only check if patterns look noisy, which would indicate that the network that hasn't been trained for long enough, or possibly with a too low regularization strength that may have led to overfitting.

Image credits: http://cs231n.github.io/understanding-cnn/

Weak analogies between brain and CNNs architecture







Where does a CNN look at?

Visualize patches yielding high values in activation maps

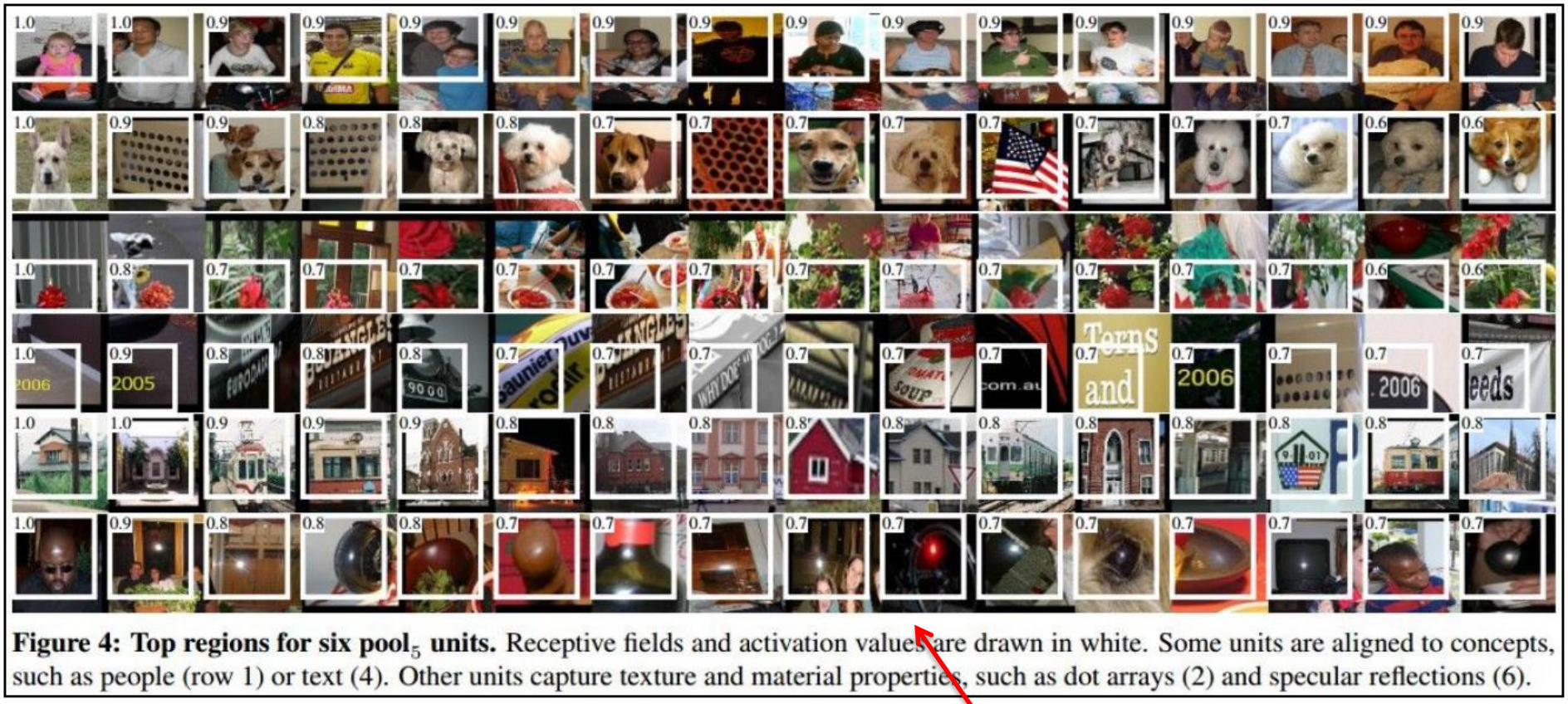
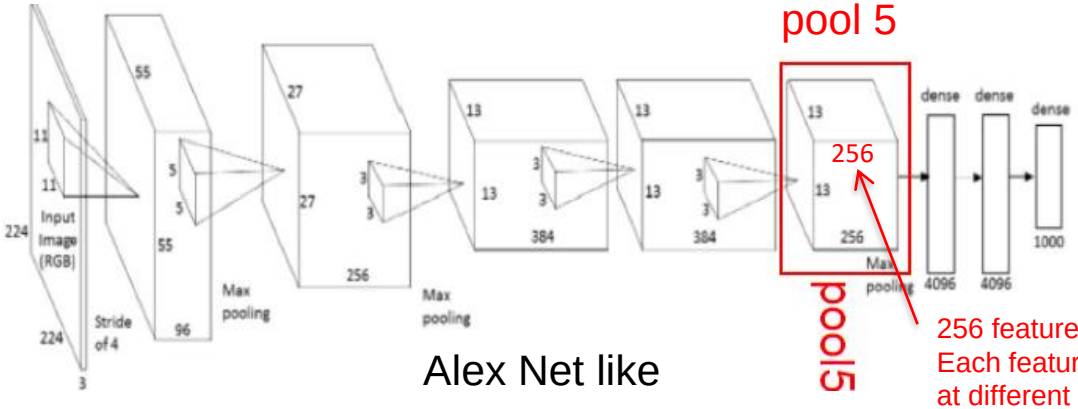


Figure 4: Top regions for six pool$_5$ units. Receptive fields and activation values are drawn in white. Some units are aligned to concepts, such as people (row 1) or text (4). Other units capture texture and material properties, such as dot arrays (2) and specular reflections (6).



Alex Net like

http://cs231n.github.io/understanding-cnn/

Here we show image patches that activate maps in layer 5 most.

256 feature maps generated by 256 different 3x3 filters. Each feature map consists of equivalent neurons looking at different positions of the input volume.

What kind of image (patches) excites a certain neuron corresponding to a large activation in a feature map?

10 images from data set leading to high signals 6 feature maps of **conv6**

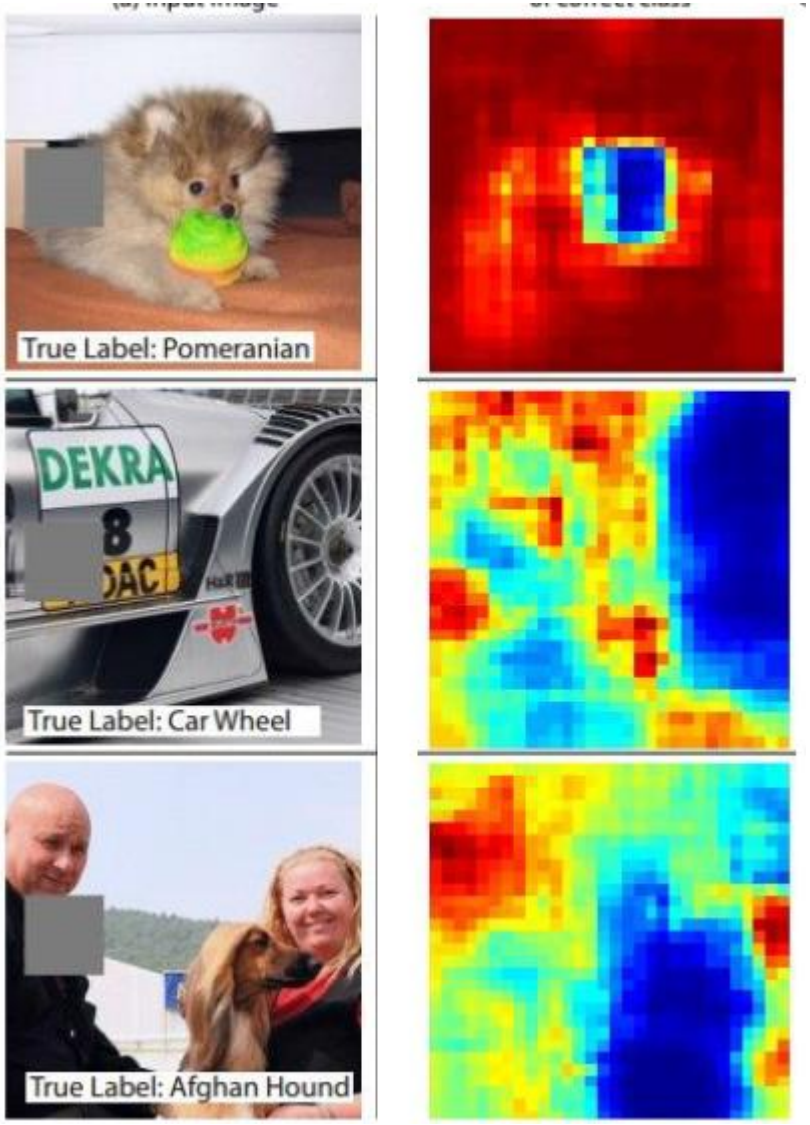
10 images from data set leading to high signals 6 feature maps of **conv9**

image credit: cs231n

Which pixels are important for the classification?
Occlusion experiments

Occlude part of the image with a mask
and check for each position of the mask how strongly the score for the correct class is changing.

Warning:
Usefulness depends on application…



Occlusion experiments [Zeiler & Fergus 2013]

image credit: cs231n

Which pixels are important for the classification?
LIME: Local Interpretable Model-agnostic Explanations

Idea:

1) perturb interpretable features of the instance – e.g. randomly delete super-pixels in an image and track as perturbation vector such as (0,1,1,0,…,1)=x.
2) Classify perturbed instance by your model, here a CNN, and track the achieved classification-score=y
3) Identify for which features/super-pixels the presence in the perturbed input version are important to get a high classification score (use RF or lasso for y~x)

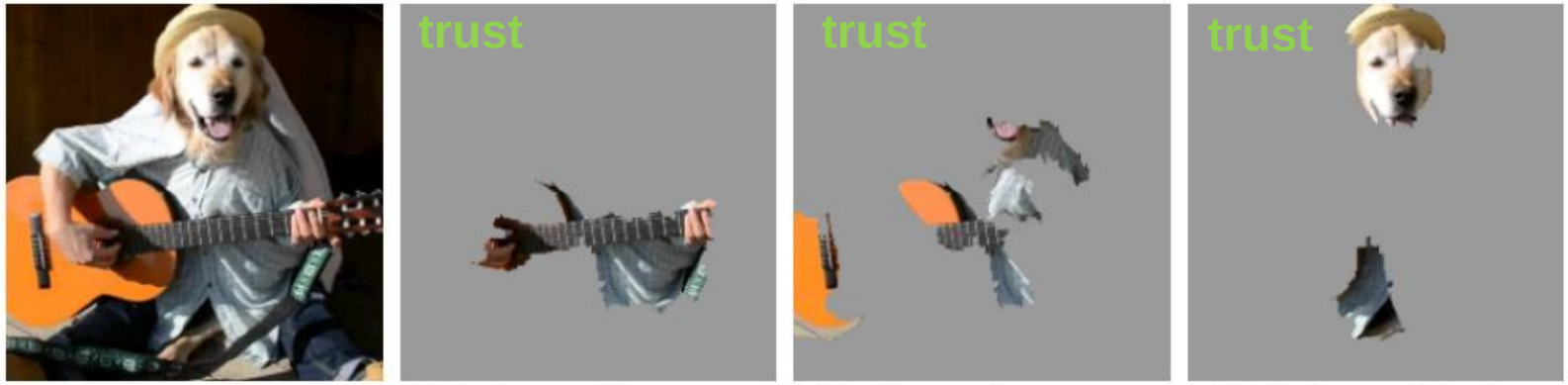
https://arxiv.org/abs/1602.04938

(a) Husky classified as wolf (b) Explanation

-> presence of snow was used to distinguish wolf and husky

-> Explain the CNN classification by showing instance-specific important features

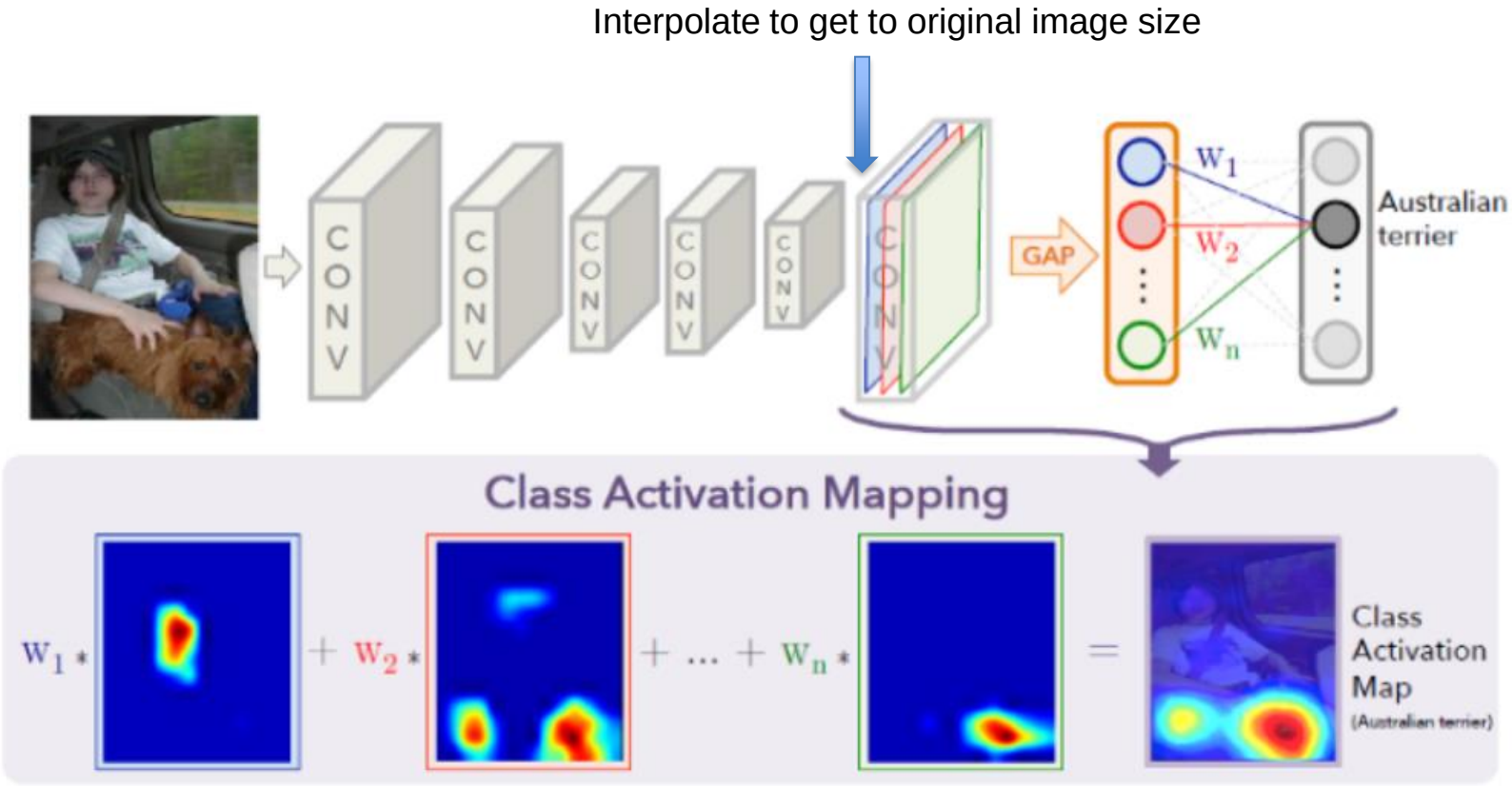
visualize important feature allows to judge the individual classification



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

Tf, python code: https://github.com/marcotcr/lime -> image tutorial
https://github.com/marcotcr/lime/blob/master/doc/notebooks/Tutorial%20-%20Image%20Classification%20Keras.ipynb

Class Activation Mapping (CAM)

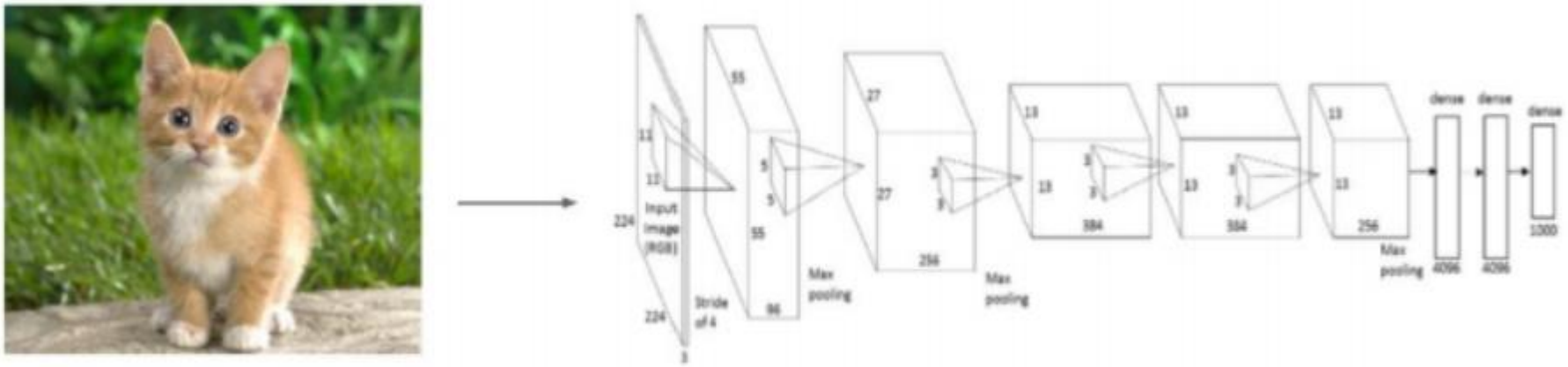


We compute the CAM by multiplying each feature map of the final convolution layer with the corresponding weight connected to the neuron of the winning class.

https://arxiv.org/abs/1512.04150

https://towardsdatascience.com/class-activation-mapping-using-transfer-learning-of-resnet50-e8ca7cfd657e

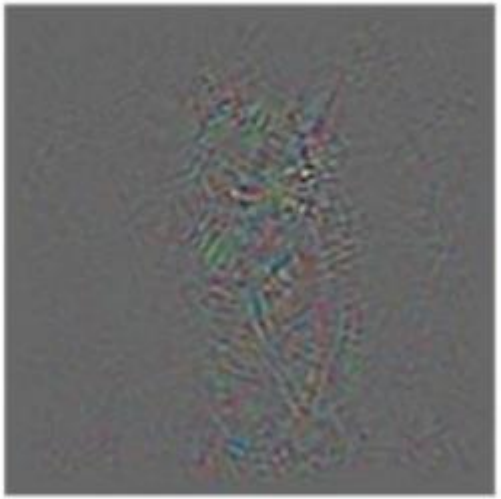
Gradient Backpropagation



1) Do a forward pass with the image

2) Compute the gradient of the winning class neuron using backprop

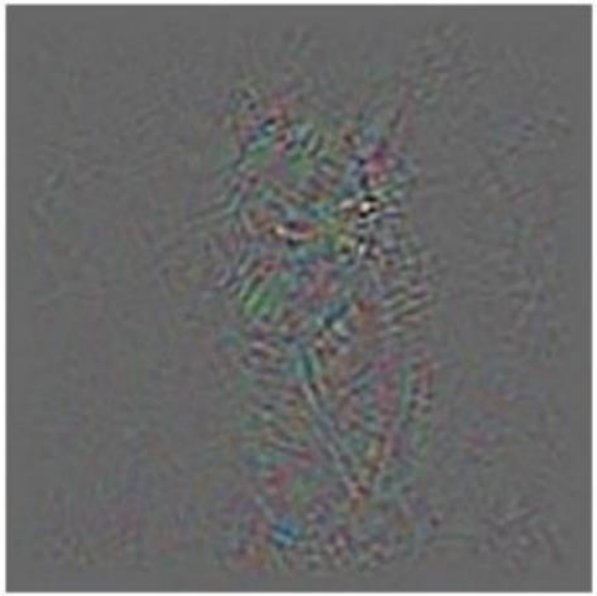
   Which pixels would make the class neuron not turn on if they had been different?
   In other words, for which inputs is $\partial(\text{class} - \text{neuron})/\partial xi$ large?



https://www.cs.toronto.edu/~guerzhoy/321/lec/W07/HowConvNetsSee.pdf

Guided Gradient Backpropagation

- We are only interested to see which image features the neuron detects, not in what kind of stuff it doesn't detect
- So only propagating positive gradients (set all the negative gradients to 0)



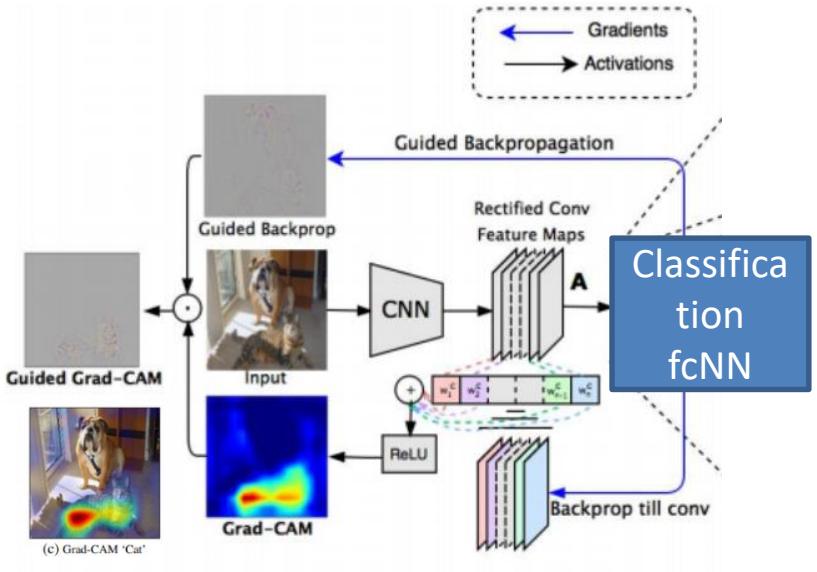
Backprop

Guided Backprop

https://www.cs.toronto.edu/~guerzhoy/321/lec/W07/HowConvNetsSee.pdf
Code: see iNNvestigate colab NB https://github.com/avciidp/explainable_ai/blob/master/iNNvestigate_fashion_light.ipynb
paper: https://arxiv.org/abs/1808.04260

Grad-Cam: Gradient based Class Activation maps

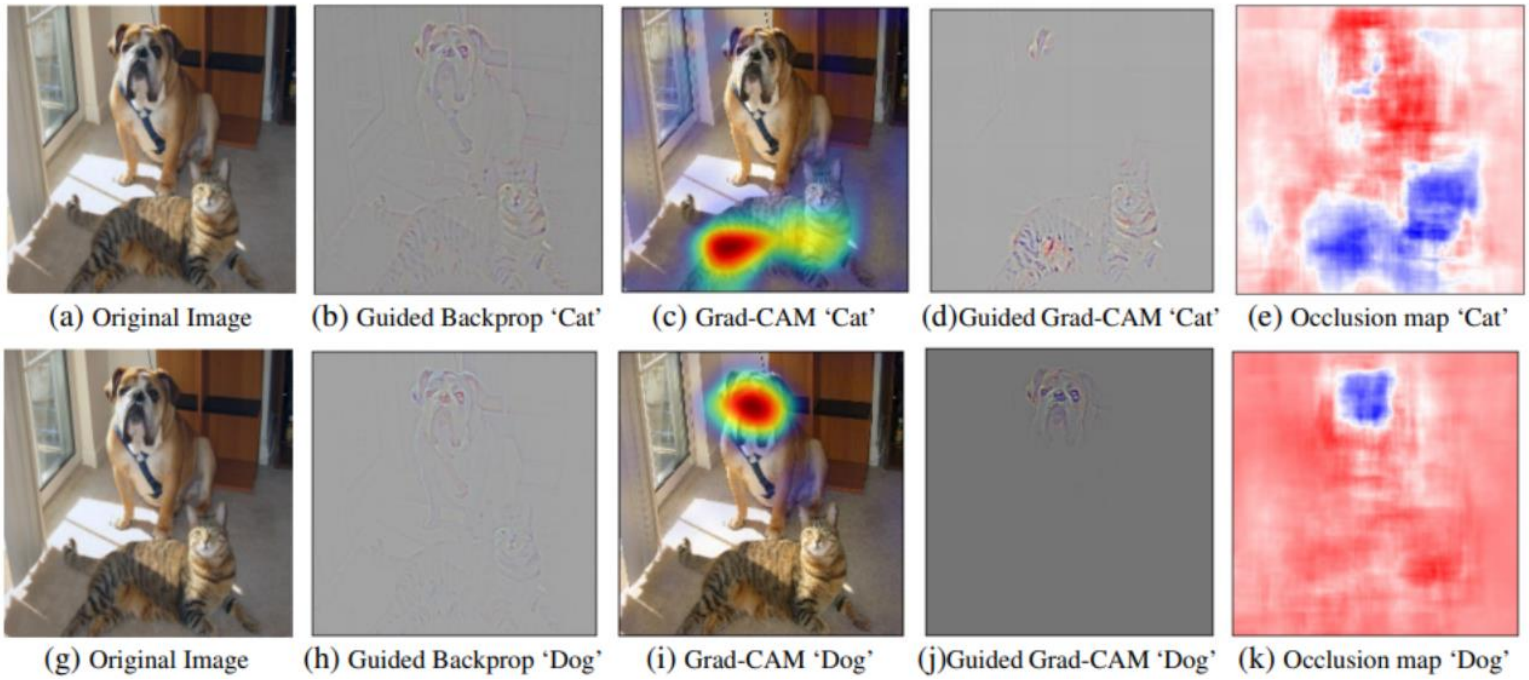
Grad-Cam: Use Guided Backprop to scale contributions in CAMs



- Set gradient to zero for all classes expect the predicted class
- Backpropagate this gradient to the last conv-layer
  -> get coarse grad-CAM localization
- Multiply coarse grad-CAM with the guided back-prop signal

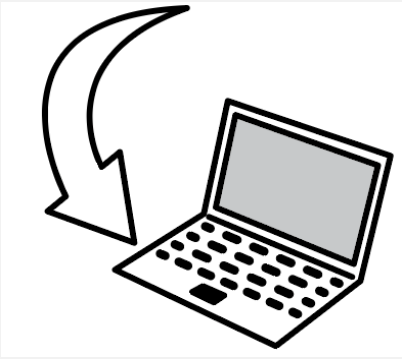
https://arxiv.org/abs/1610.02391
Code: https://keras.io/examples/vision/grad_cam/
https://www.pyimagesearch.com/2020/03/09/grad-cam-visualize-class-activation-maps-with-keras-tensorflow-and-deep-learning/

What in the image was important for the prediction?

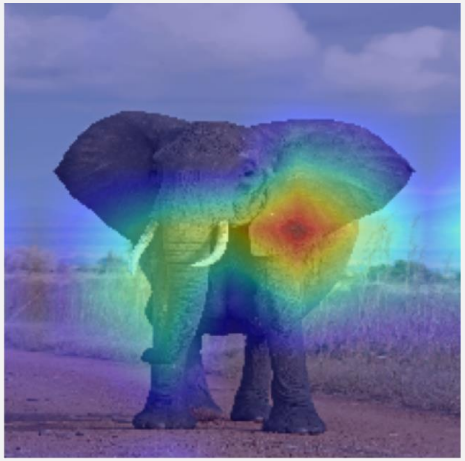


Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization https://arxiv.org/abs/1610.02391

Exercise:



Which part of the image was important for the prediction «African elephant»?
Does the prediction change when a part of the image is occluded?



Work through the NB [08_gradcam_and_occlusion.ipynb]

Summary

- **Use tricks of the trade when building a CNN**
  - Normalization of input data
  - Batchnorm
  - Dropout
  - Augmentation
  - Use challenge winning architectures
- **In case of few data**
  - Do augmentation during training of a CNN
  - Use shallow learner (e.g. RF) based on image features extracted via pretrained CNNs
  - Fine-tune a pretrained CNN on few data (transfer learning)
- **NNs are loosely inspired by the structure of the brain.**
  - When going deep the receptive field increases (~layer 5 sees whole input)
  - Deeper layer respond to more complex feature in the input
- **Shine light into the black-box (xAI) by**
  - Occlusion
  - gradCam
  - Lime