Machine Intelligence: Deep Learning Week 5



CNNs part II

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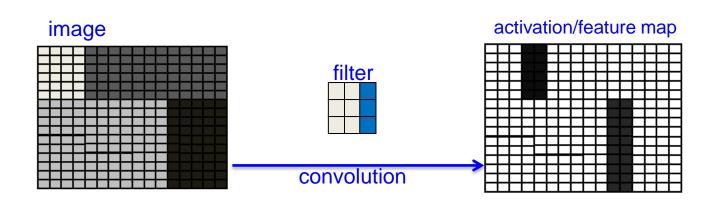
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Topics

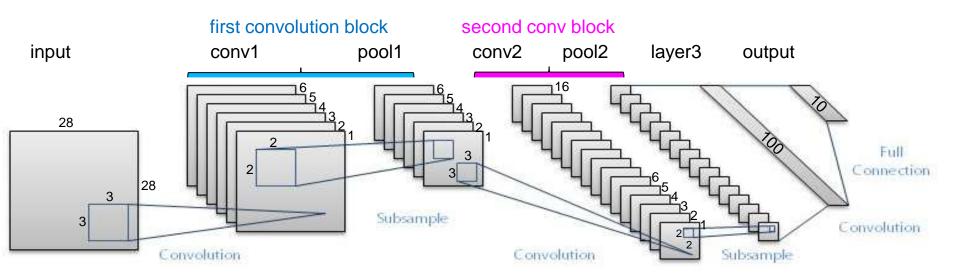
- Recap basics of CNNs
- Important ingredients to get a well performing (simple) CNN
 - Weight initialization, choice of activation function, rescaling input (recap)
 - Dropout, batch-normalization, choice of optimizer
- What to do in case of limited data?
 - Data augmentation
 - Transfer learning: use pre-trained CNNs and fine tune only last couple of layers
- Understand what a CNN has learned
 - Visualize the image patches that give rise for high activations of intermediate neurons
 - visualize image parts that are important for the assignment to a certain class
- Famous CNN architectures and tricks they make use of
 - LeNet, AlexNet, GoogleNet, VGG, Microsoft ResNet

Recap: Why do we want to use convolutional layer?

- We want not to rely on rigid templates (like in fully connected NN)
- We want to exploit the information that is contained in the neighborhood structure of pixels in a image.
- We want to learn hierarchical and semantic features
- We want to capture relative positions of the features in the image and not depend on absolute positions of the objects in the image
- We share weights for one filter extracting the activation of the same feature at each positions of the input volume.

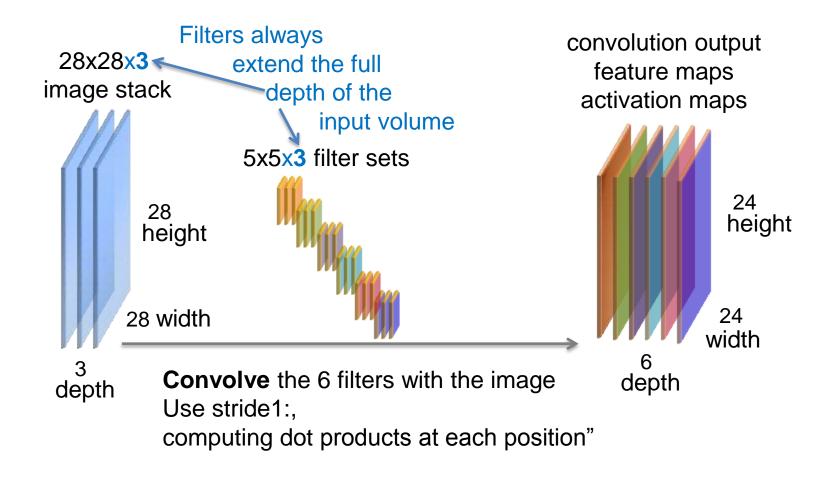


Architecture of a Convolutional Neural Network



```
from keras import layers
from keras import models
model = models.Sequential()
model.add(layers.Conv2D(6, (3, 3), activation='relu', input_shape=(28, 28, 1)))
model.add(layers.MaxPooling2D((2, 2)))
model.add(layers.Conv2D(16, (3, 3), activation='relu'))
model.add(layers.MaxPooling2D((2, 2)))
model.add(layers.Flatten())
model.add(layers.Dense(100, activation='relu'))
model.add(layers.Dense(100, activation='softmax'))
```

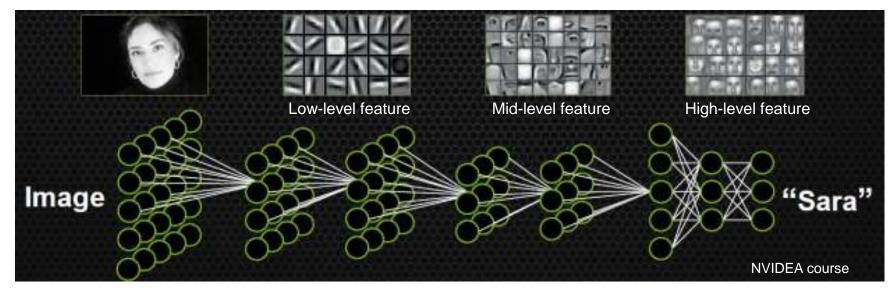
A convolution block (recap)

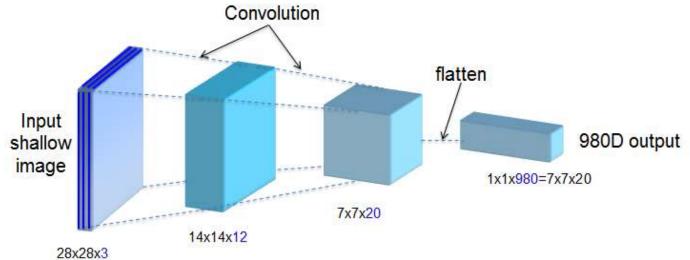


In Keras we do not need to specify the depth of the filter (since Keras can deduce it):

```
model = Sequential()
model.add(Convolution2D(6, (5, 5), input_shape=(28, 28, 3)))
```

Goal of a CNN: learn hierarchical abstract feature





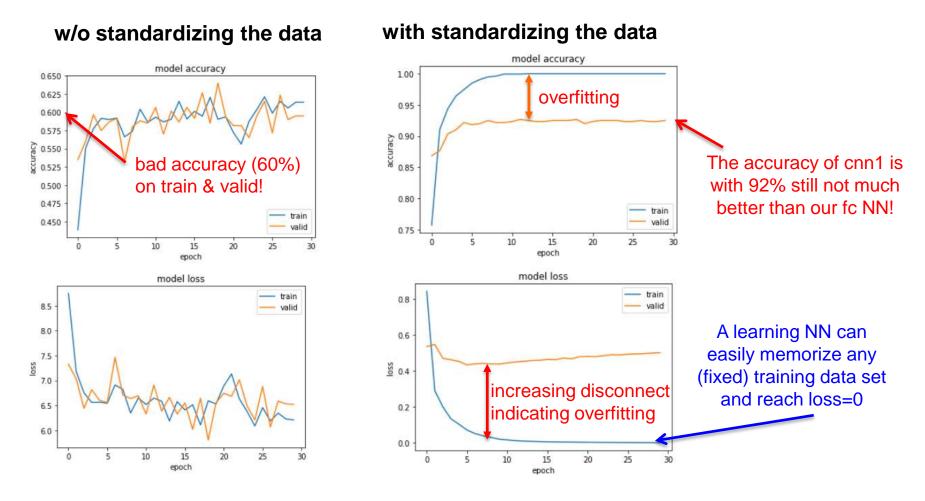
How to get a well performing CNN?

- What to do that the network can learn good weights?
 - How to initialize the weights: small, random numbers are preferred
 - How to let the gradients flow: activation functions (ReLu), preprocessing, batch-norm...
 - How to update weights: learning rate, choice of optimizer ...
- What kind of image data do we need?
 - Only limited data preprocessing is needed: scaling and resizing images
 - How to detect and fight overfitting: learning curves, data augmentation, dropout...
 - What to do if data is limited: transfer learning and fine-tuning pre-trained nets
- What does a CNN learn?
 - What a CNN looks at: receptive field, image pattern that activate neurons, lime...
- Architecture matters
 - Learn from winning architectures

Why scaling the input?

Is preprocessing required? Lessons learned from 07_cnn1

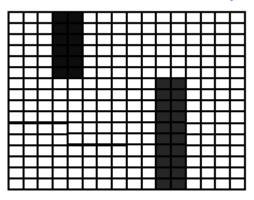
Results on MNIST subset using cnn1 with only 1 conv block 32 filter



Only after standardizing the input data the CNN could be trained properly!

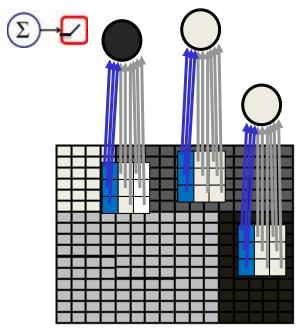
Why can standardizing get important for CNNs?

feature/activation map



Since we share weights in CNNs — only one filter is used per feature map - each patch of the input image should be appropriate for the filter weights, i.e. yielding inputs to the activation function that are party in their sweet spot.

→ standardize the input pixel-wise



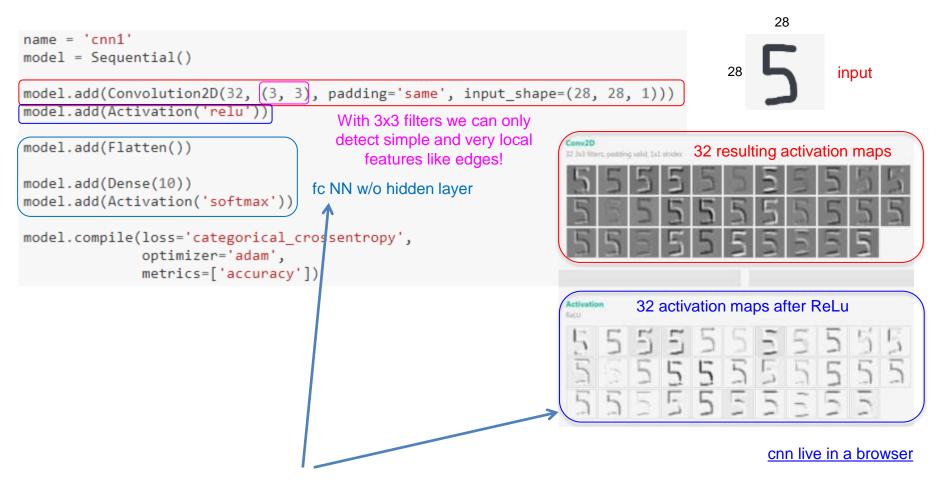
```
print(X_train.shape)
print(X_val.shape)

(4000, 28, 28, 1)

# here we center and standardize the data per pixel
# calculate mean, std over all training images at each pixel position
X_mean = np.mean( X_train, axis = 0)
X_std = np.std( X_train, axis = 0)

X_train = (X_train - X_mean ) / (X_std + 0.0001)
X_val = (X_val - X_mean ) / (X_std + 0.0001)
```

Why is our small cnn1 not outperforming a fc NN?



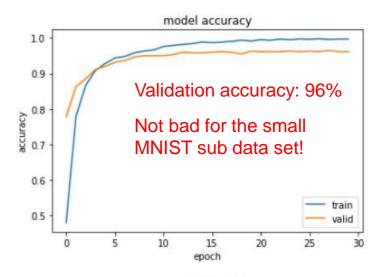
The first convolution block turns the 1-channel image into a 32 block of activation maps (still 5-looking with emphasized edges of different orientations). The following fc NN part has to find 10 rigid templates for the 32 channel image representation for the possible outputs 0,1,...9 → little improvement vs a fc NN. However: MNIST pattern can be quite good detected using rigid patterns;-)

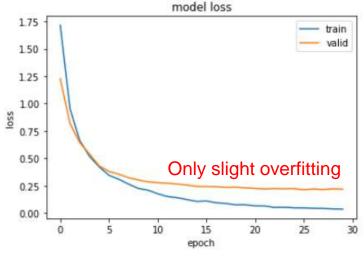
For better features we need to go deeper



```
name = 'cnn2'
                               08 cnn2
model = Sequential()
model.add(Convolution2D(8,kernel_size,padding='same',input_shape=input_shape))
model.add(BatchNormalization())
model.add(Activation('relu'))
model.add(Convolution2D(8, kernel size,padding='same'))
model.add(BatchNormalization())
model.add(Activation('relu'))
model.add(MaxPooling2D(pool size=pool size))
model.add(Convolution2D(16, kernel_size,padding='same'))
model.add(BatchNormalization())
model.add(Activation('relu'))
# here is your code comming:
model.add(Convolution2D(16,kernel size,padding='same'))
model.add(BatchNormalization())
model.add(Activation('relu'))
model.add(MaxPooling2D(pool size=pool size))
# end of your code
model.add(Flatten())#macht einen vektor aus dem output
model.add(Dense(40))
model.add(BatchNormalization())
model.add(Dropout(0.3))
model.add(Activation('relu'))
model.add(Dense(nb classes))
model.add(Activation('softmax'))
model.compile(loss='categorical crossentropy',
              optimizer='adam',
              metrics=['accuracy'])
```

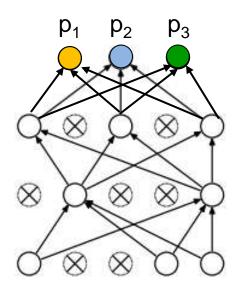
This cnn2 allows to construct more complex hierarchical features, but has less parameters (~36k) than cnn1 (~251k weights) since the parameter-consuming fc layer in the end is smaller.





Why dropout?

Dropout helps to fight overfitting

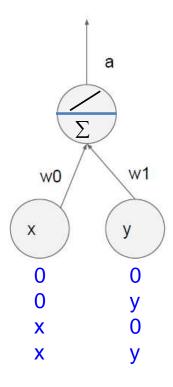


Using dropout during training implies:

- 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-trained NN are kind of NN ensemble averages

during test



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?

w/o dropout:

$$a = w0*x + w1*y$$
during training with dropout probability 0.5:

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

$$= \frac{1}{4} * (2 w0*x + 2 w1*y)$$

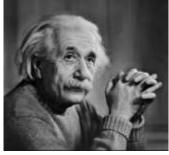
$$= \frac{1}{2} * (w0*x + w1*y)$$

=> 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

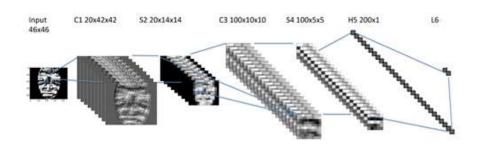
Another intution: Why "dropout" can be a good idea

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

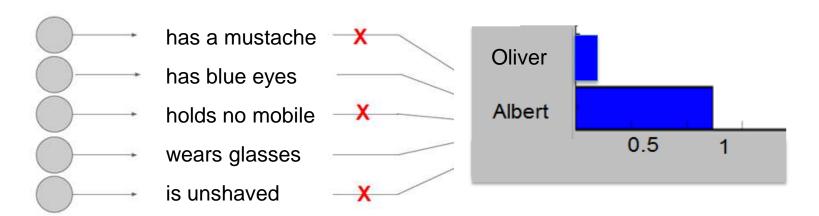




We need a huge number of neurons to extract good features which help to distinguish Oliver from Einstein

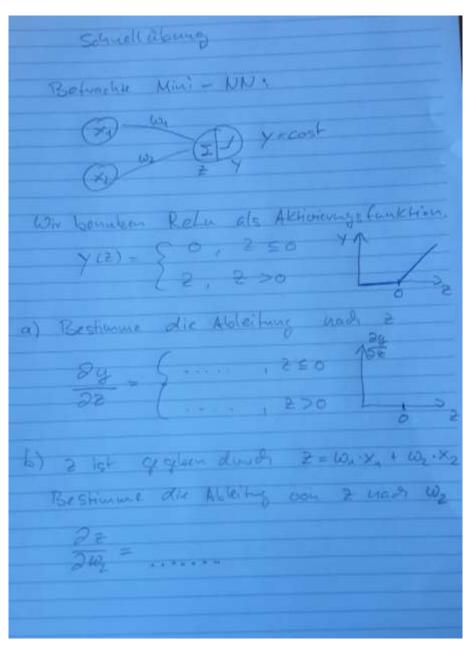


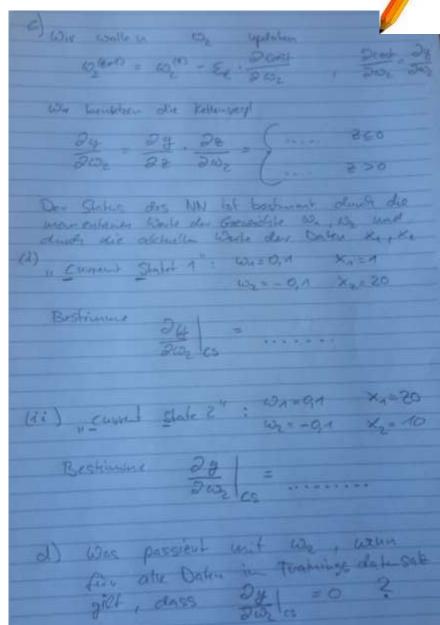
Dropout forces the network to learn redundant and independent features



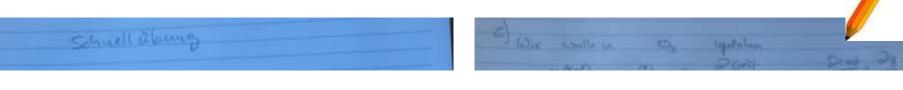
Why batchnorm?

Gradient propagation when using ReLu



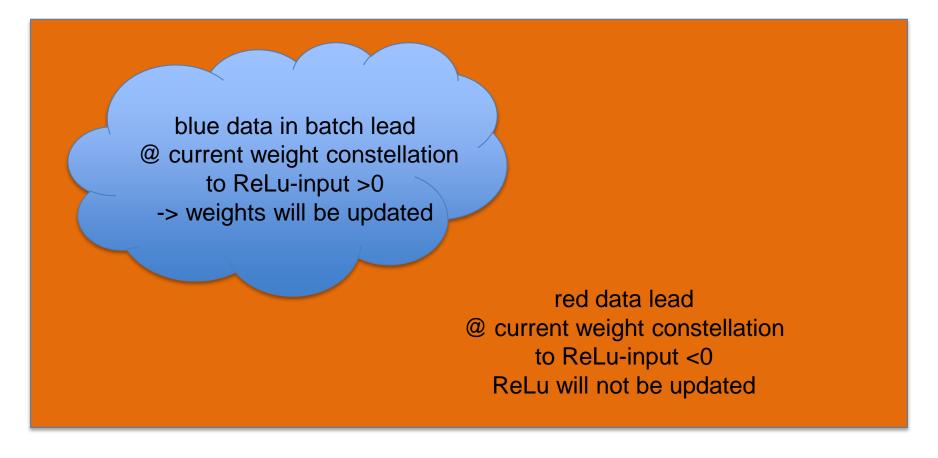


Gradient propagation when using ReLu



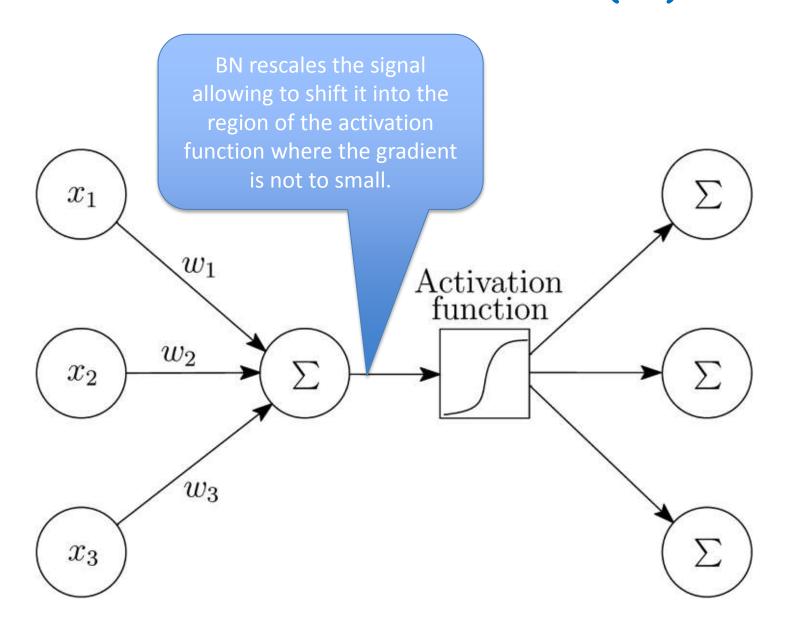
Why do we need batch-normalization?

We have seen (Schnellübung) that there is no way to train=update-weights when the data and weight constellation is such that for **all** data the input to the ReLu is <0! Then we have a dead ReLu and the NN to left (direction input) is not trainable.



Depending on the data values, it can happen that there is no blue cloud and the NN is not trainable. This risk can be reduced when working with BN (or without BN with good initialization and small learning rates).

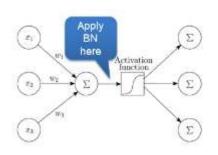
What is the idea of Batch-Normalization (BN)



Batch Normalization

 Idea: Allow before each activation (non-linear transformation) to standardize the ingoing signal, but also allow to learn redo (partly) the standardization if it is not beneficial.

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



Step 1:
$$\widehat{x} = rac{x - avg_{batch}(x)}{stdev_{batch}(x) + \epsilon}$$
 $avg(\widehat{x}) = 0$ $stdev(\widehat{x}) = 1$

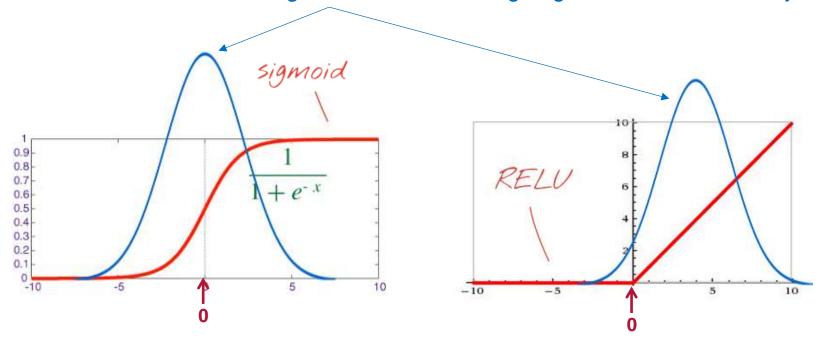
Step 2:
$$BN(x) = \alpha \widehat{x} + eta$$
 $rac{lpha}{eta}$ learned $rac{eta}{eta}$ learned

The learned parameters α and β determine how strictly the standardization is done. If the learned α =stdev(\mathbf{x}) and the learned β =avg(\mathbf{x}), then the standardization performed in step 1 is undone (for $\varepsilon \approx 0$) in step 2 and BN(\mathbf{x})= \mathbf{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:

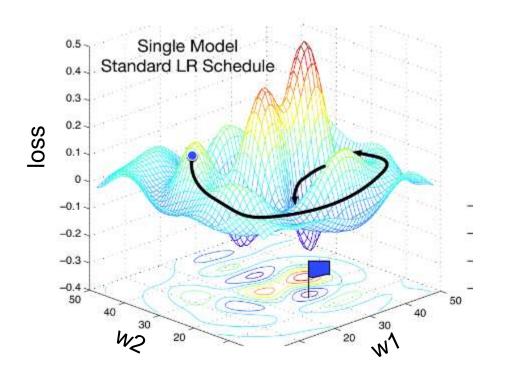
- Using a higher learning rate might work better
- Use less regularization, e.g. reduce dropout probability
- In the linear transformation the biases can be dropped (step 2 takes care of the shift)
- In case of ReLu only the shift β in steps 2 need to be learned (α can be dropped)



Which optimizer?

Choice of optimizers: How to find the weight constellation of the minimum cost

For an overview of optimizers check out <u>keras documentation</u> and the nice blog of Sebastian Ruder <u>http://ruder.io/deep-learning-optimization-2017/</u>



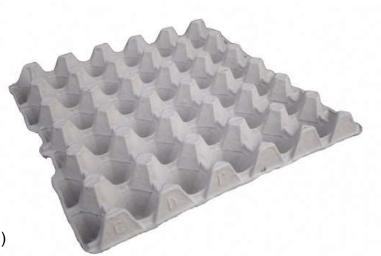
- Gradient descent variants
 - Batch gradient descent
 - Stochastic gradient descent
 - Mini-batch gradient descent
- Challenges
- Gradient descent optimization algorithms
 - Momentum
 - Nesterov accelerated gradient
 - Adagrad
 - Adadelta
 - RMSprop
 - Adam
- Most often used! All three are doing very similar things
- AdaMax
- Nadam
- AMSGrad

Valuati 1922 12 12 15 15 25 1

Good news: In DL all minima are good!

Things observed but not well understood:

- All minima are "similar" good
- DL models generalize well despite p>>n
- Also sharp minima are good in DL with ReLu
- loss landscape depends on parametrization (e.g. BN)



Bengio 2017 paper on loss landscape, flat and sharp minima, and generalization

One standing hypothesis that is ... that the flatness of minima of the loss function found by stochastic gradient based methods results in good generalization. This paper argues that most notions of flatness are problematic for deep models and can not be directly applied to explain generalization. Specifically, when focusing on deep networks with rectifier units, we can ... build equivalent models corresponding to arbitrarily sharper minima... without affecting its generalization properties.

Gradient Descent (GD) and stochastic GD (SGD) method: Getting the learning rate right is most important!

Take step in direction of descent gradient

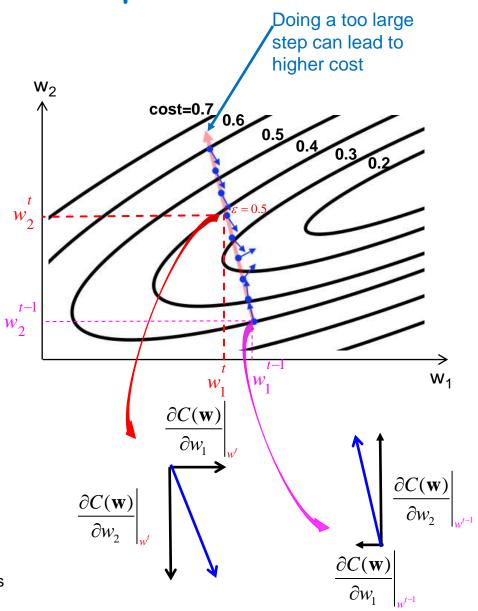
$$w_i^{(t)} = w_i^{(t-1)} - \varepsilon^{(t)} \frac{\partial C(\mathbf{w})}{\partial w_i} \bigg|_{w_i = w_i^{(t-1)}}$$
step

From GD to SGD:

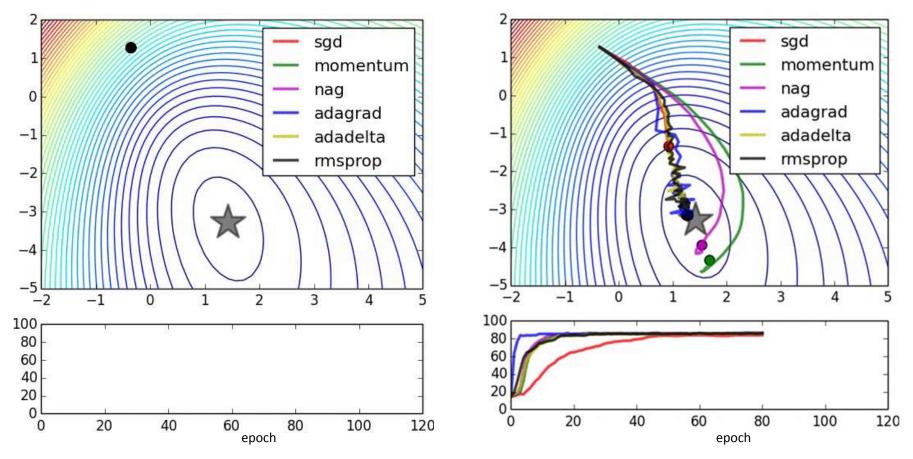
Instead of using all data to determine the cost at one weight constellation we use a "random" mini batch of the data.

Remark:

GD is guaranteed to find the optimum of a convex loss functions if learning rate is adapted (shrinked) in the course of training.



What is wrong with good old gradient descent?



http://ruder.io/optimizing-gradient-descent/index.html#fn:6

Comparison of a few optimization methods (animation by <u>Alec Radford</u>). The star denotes the global minimum on the error surface.

Notice that stochastic gradient descent (SGD) is the slowest method to converge!

RMSprop: decreases step sizes in oscillating directions

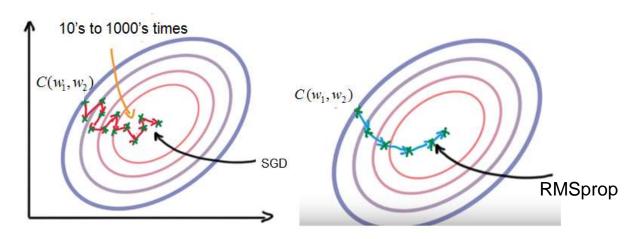
SGD:
$$w_i^{(t)} = w_i^{(t-1)} - \varepsilon^{(t)} \cdot g_i^{(t)}$$

with gradient $g_i^{(t)} = \frac{\partial C(\mathbf{w})}{\partial w_i} \bigg|_{w_i = w_i^{(t-1)}}$

RMSprop adapts the learning rates $\varepsilon^{(t)}$ for each weight w_i based on the past couple of gradients that have been computed for this weight w_i .

RMSprop:
$$w_i^{(t)} = w_i^{(t-1)} - \frac{\varepsilon^{(t)}}{\mu_i^{(t)}} \cdot g_i^{(t)}$$

 μ_i^t gets large if either the current gradient of this weight is large or the exponentially decaying average of past squared gradients of this weight were large.



RMSprop is almost identical to AdaDelta and was indepently proposed by Geoff Hinton in <u>Lecture 6e of his Coursera Class</u> Hinton suggests to be set the weight of past squared gradients to 0.9 and use for the learning rate 0.001 as default.

rmsprop: Keep a moving average of the squared gradient for each weight $Mean Square(w,t) = 0.9 \ Mean Square(w,t-1) + 0.1 \left(\frac{\partial E}{\partial w}(t)\right)^2$ Dividing the gradient by $\sqrt{Mean Square(w,t)}$ makes the learning work much better (Tijmen Tieleman, unpublished).

AdaDelta: decreases step sizes in oscillating directions

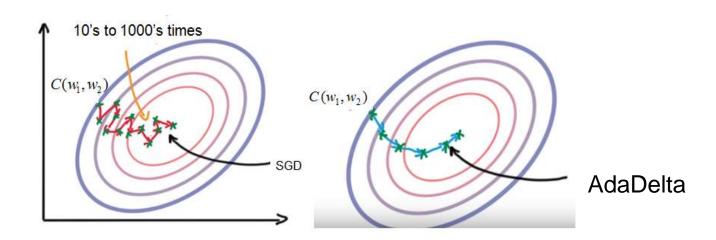
SGD:
$$w_i^{(t)} = w_i^{(t-1)} - \varepsilon^{(t)} \cdot g_i^{(t)}$$

with gradient $g_i^{(t)} = \frac{\partial C(\mathbf{w})}{\partial w_i} \bigg|_{w_i = w_i^{(t-1)}}$

AdaDelta also adapts the learning rates $\varepsilon^{(t)}$ for each weight w_i based on the past couple of gradients that have been computed for this weight w_i .

AdaDelta:
$$w_i^{(t)} = w_i^{(t-1)} - \frac{\varepsilon^{(t)}}{\mu_i^{(t)}} \cdot g_i^{(t)}$$

 μ_i^t gets large if either the current gradient of this weight is large or the exponentially decaying average of past squared gradients (oscillation) of this weight were large.



Adam: Adaptive Gradients using momentum principle

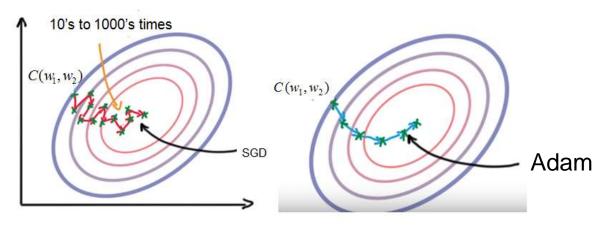
SGD:
$$w_i^{(t)} = w_i^{(t-1)} - \varepsilon^{(t)} \cdot g_i^{(t)}$$

with gradient $g_i^{(t)} = \frac{\partial C(\mathbf{w})}{\partial w_i} \bigg|_{w_i = w_i^{(t-1)}}$

Adam (like RMSprop or AdaDelta) adapts the learning rates $\varepsilon^{(t)}$ for each weight w_i based on the past couple of gradients that have been computed for this weight w_i .

Adam:
$$w_i^{(t)} = w_i^{(t-1)} - \frac{\varepsilon^{(t)}}{\mu_i^{(t)}} \cdot g_i^{(t)}$$

 μ_i^t in Adam depends not only on the decaying average of past squared gradients but also on the exponentially decaying average of past gradients.



Adam Adaptive Moment Estimation, where the first moment (mean velocity) is given by average of past gradients and the second moment (uncentered variance, acceleration, oscillation) is given by average of past squared gradients

Kingma, D. P., & Ba, J. L. (2015). Adam: a Method for Stochastic Optimization. International Conference on Learning Representations, 1–13 https://arxiv.org/abs/1412.6980

Challenge: Who got the best CNN and which architecture and tricks were used?

Now you get the test set:

For a given image from the internet, decide which out of 8 celebrities is on the image.

Example images:

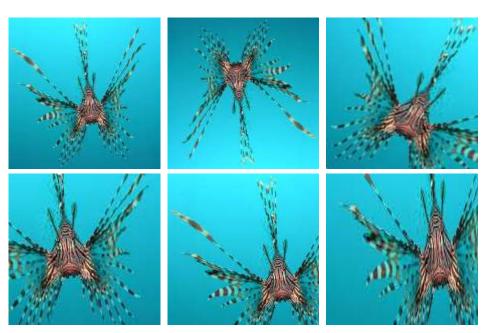




What to do in case of limited data?

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
-

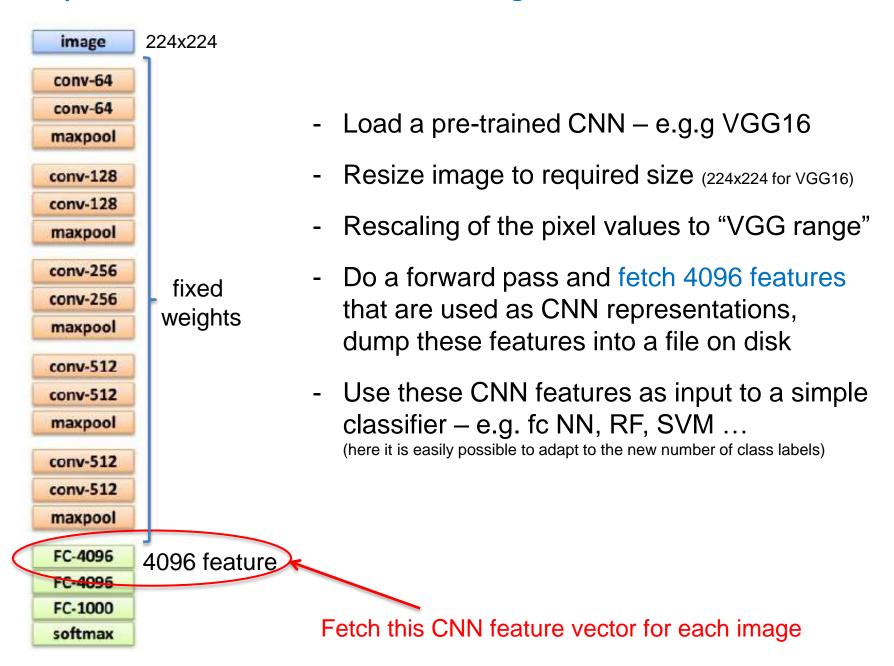


Data augmentation in Keras:

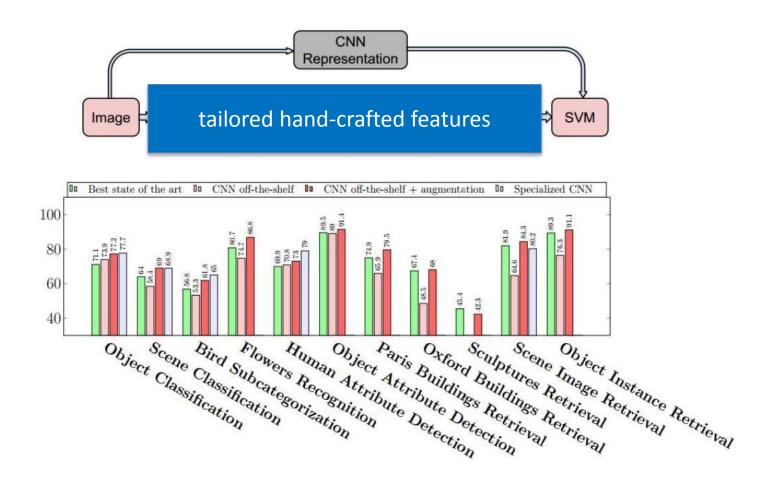
```
from keras.preprocessing.image import ImageDataGenerator
datagen = ImageDataGenerator(
    rotation_range=10,
    width_shift_range=0.1,
    height_shift_range=0.1,
    horizontal_flip=True,
    vertical_flip=True,
    #zoom_range=[0.1,0.1]
train_generator = datagen.flow(
          x = X_train_new
          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]

Use pre-trained CNNs for feature generation



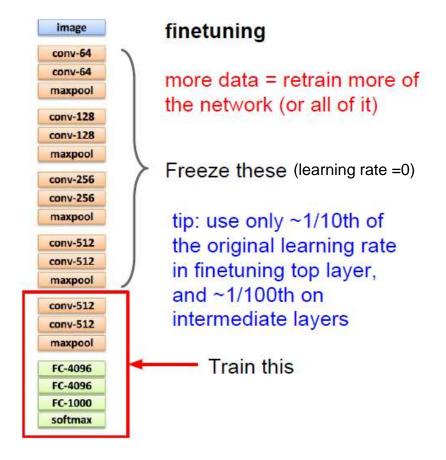
Performance of off-the-shelf CNN features when compared to tailored hand-crafted features



"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."

Transfer learning beyond using off-shelf CNN feature

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



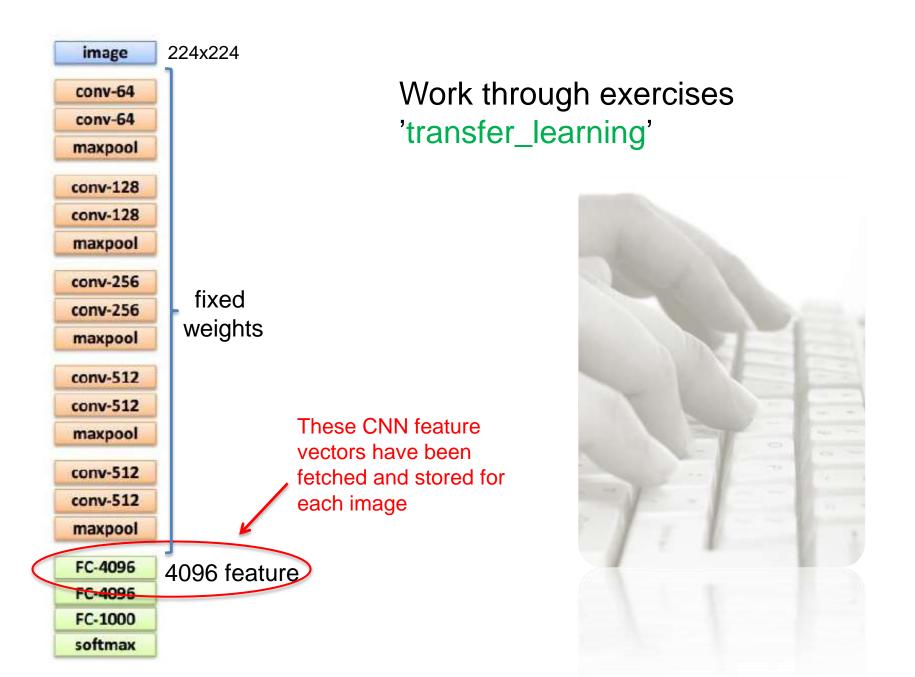
The strategy for fine-tuning depends on the size of the data set and the type of images:

	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

Exercise: Use CNN features for classification of 8 celebs





What does the CNN look at?

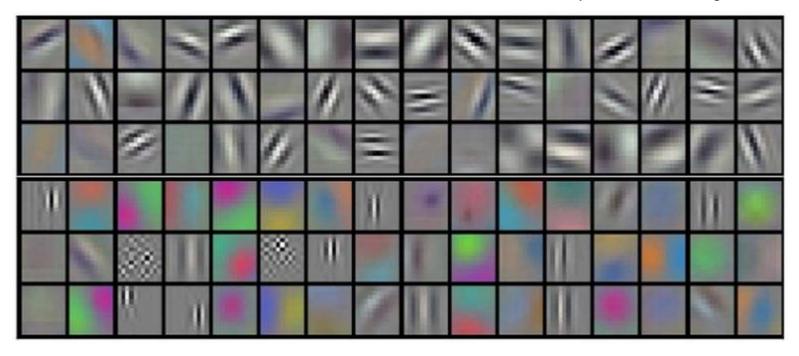
How to understand a CNN model?

- Visualize filter weights (mainly useful in first layer)
- Visualize activation patterns that correspond to a specific input image in different layers and activation maps
- Receptive field
- Show images or image patches that lead to maximal activations in a certain activation map
- Synthesize images that lead to maximal activations in a certain activation map
- Occlusion Experiments, Saliency Maps, LIME

Example of learned filters

96 filters in first layer

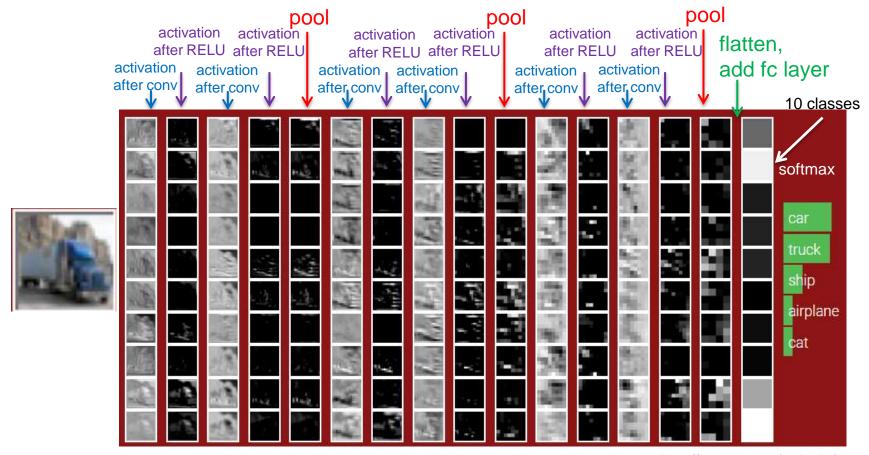
Here the input had 3 channels and the used filters had the dimension $11 \times 11 \times 3$ which nowadays is unusual large.



Examples of 96 11x11x3 filters learned (taken from Krizhevsky et al. 2012). Looks pretty much like old fashioned handcrafted filters to detect edges and simple patterns.

The filters show the detected patterns in the input which is for the first layer the original image. For all other layers the filter pattern do not directly correspond to patterns in the input image to the CNN.

Appearance of activation/feature maps in different layers



http://cs231n.stanford.edu/

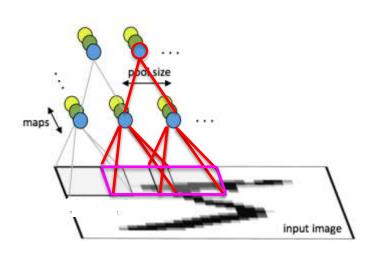
Activation maps can be seen as a transformed version of the input image. A CNN aims to learn such new data representations (features) that help for the classification (only the activation maps in the first hidden layer correspond directly to features of the input image).

How can a CNN model be visualized?

- Visualize filter weights (mainly useful in first layer)
- Visualize activation patterns that correspond to a specific input image in different layers and activation maps
- Receptive field
- Show images or image patches that lead to maximal activations in a certain activation map
- Synthesize images that lead to maximal activations in a certain activation map
- Occlusion Experiments, Saliency Maps, LIME

The receptive field

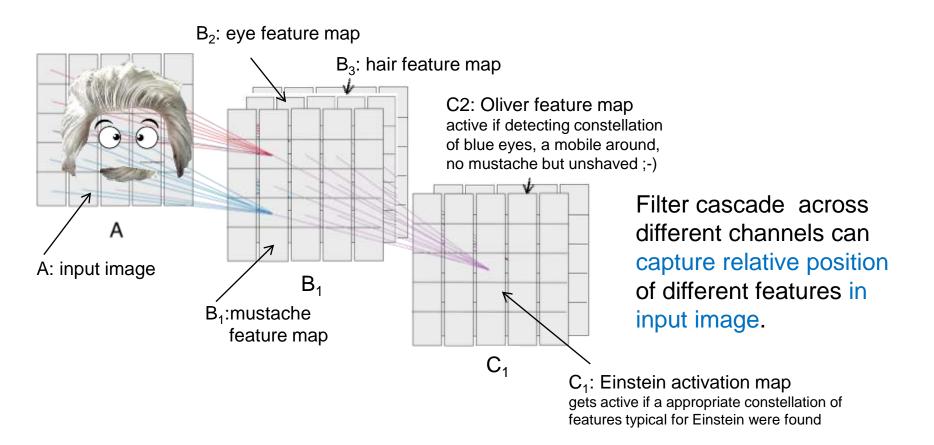
Receptive field of a neuron refers either to the area of the ingoing activation maps from the previous layer to which that neuron is connected or to the area in the original input image of the CNN that impacts the value of this neuron.



A neuron in the pooled layer has a larger receptive field of the original image than a neuron before pooling.

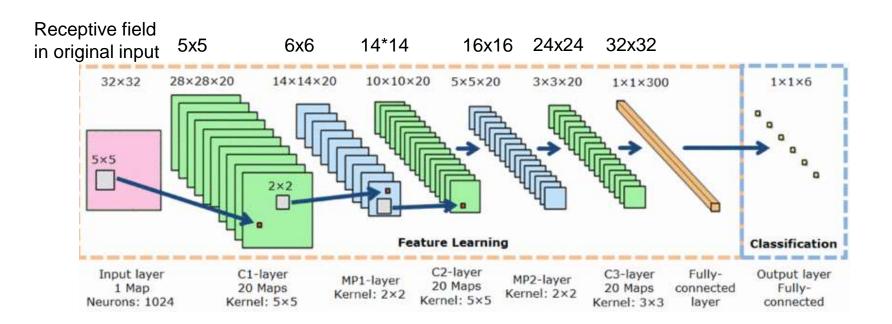
For each neuron we can determine the connected area in the input from the previous layer(s). This area in the input image is called receptive field.

A simplified view: hierarchy of features



The receptive field is growing from layer to layer

The receptive field of a neuron is the area in the original input image that impact the value of this neuron – "that can be seen by this neuron".



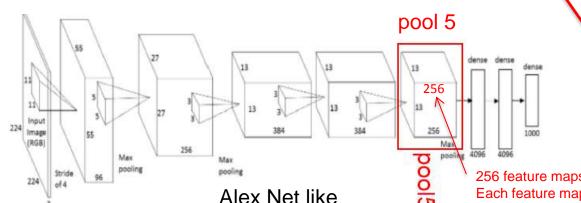
Neurons from feature maps in higher layers have a larger receptive field than neurons sitting in feature maps of lower layers.

Code to determine size of receptive field: http://stackoverflow.com/questions/35582521/how-to-calculate-receptive-field-size

Visualize patches that maximally activate neurons



Figure 4: Top regions for six pool₅ 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).



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

Here we show image patches that activate neurons 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 exciting the 6 first neurons/filters in **conv6** most



10 images from data set exciting the 6 first neurons/filters in **conv9** most



Alternative approach: Construct a synthetic image giving rise to an high mean activation in a selected neuron-type/feature-map of a selected layer of the CNN.

image credit: cs231n

Optimize image for a high activation of a selected neuron type

Use a trained CNN with fixed weights.

Which content should the image have to get a high activation in this feature map?

We want to optimize the pixel values!

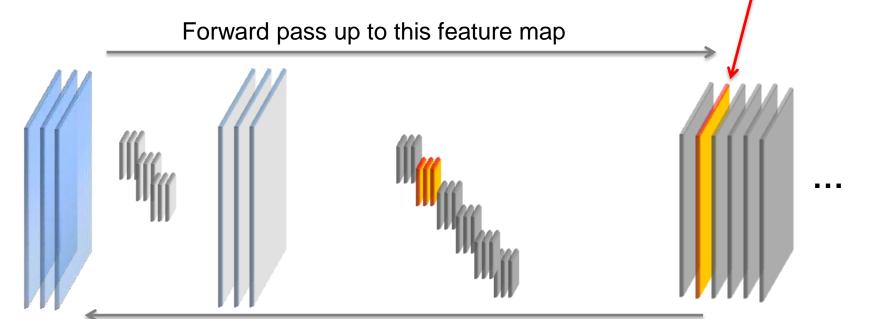


image initialize with random values

Gradient of mean activation A in the selected feature map with respect to the pixel values in the image.

pixel update

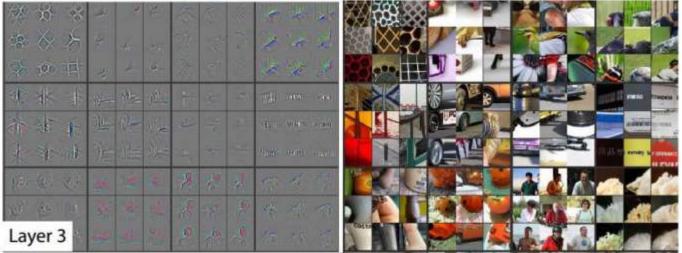
$$p_i^{(t)} = p_i^{(t-1)} + \varepsilon^{(t)} \frac{\partial \mathbf{A}(\mathbf{p})}{\partial p_i} \bigg|_{p_i = p_i^{(t-1)}}$$

Set the gradient of neurons in this feature map to 1 and gradients of all other maps to zero. Since all neurons in one feature map use the same filter, they will fire for the same image pattern.

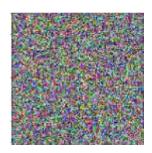
What kind of image (patches) excites a certain neuron corresponding to a large activation in a feature map?

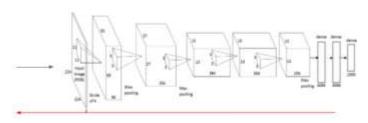
9 synthetic images, optimized for the 12 first neurons

9 images from data set exciting the 12 first neurons/filters most



Layer 3





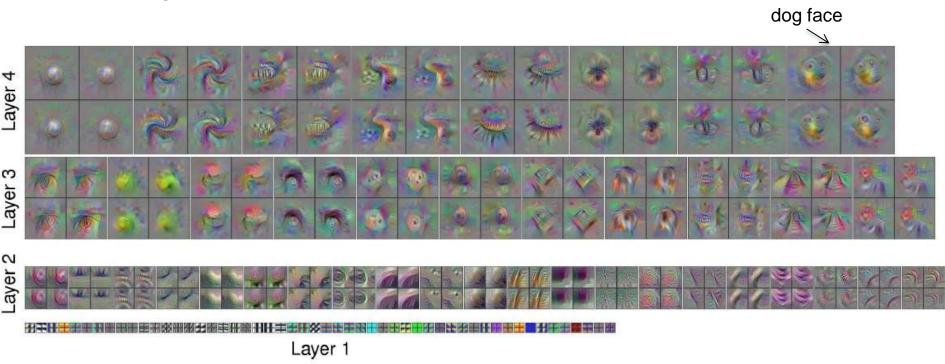
- 1) Initialize image with random grey values
- 2) Set the gradient to this neuron =1 all others=0
- 3) Do a small "image update" (constrained to be smooth)
- 4) Forward the image through net go back to 2)

Use keras to synthesize image patch that activates a certain feature map

image credit: cs231n

What kind of synthesized image (patch) excites the neurons in layer1, layer2, layer3, layer4?

Kernels from higher layers have a larger receptive field and are excited by more complex image content.



It is more instructive to visualize image-parts of input images that excite certain filter at deeper layers of a CNN instead of the filter pattern or observed activation maps.

Optimize image for a high class probability

Use a trained CNN with fixed weights.

Which content should the image have to get a high probability for class k? We want to optimize the pixel values!

Forward pass up to this feature map

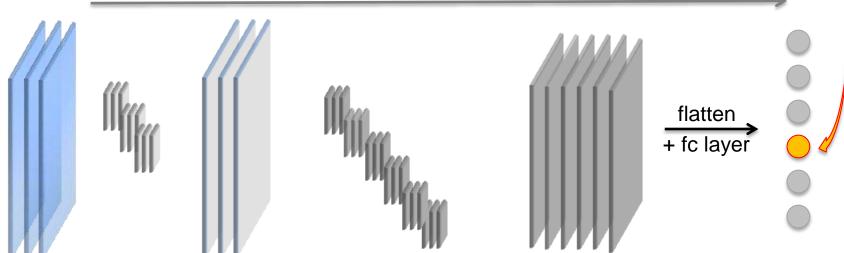


image initialize with random values Gradient of activation A in the selected softmax neuron with respect to the pixel values in the image.

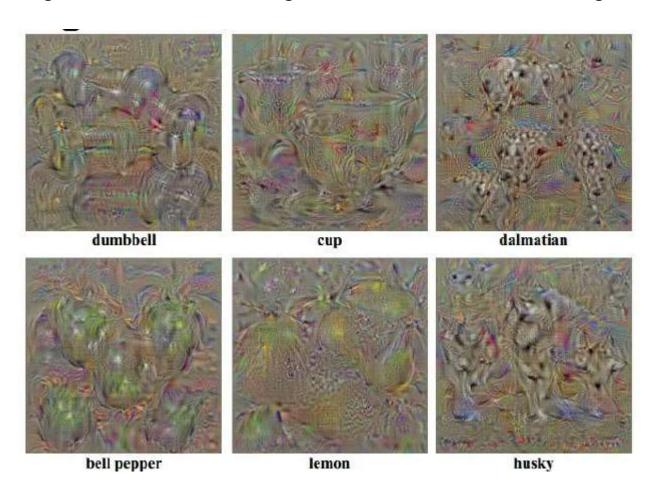
pixel update

$$p_i^{(t)} = p_i^{(t-1)} + \varepsilon^{(t)} \frac{\partial \mathbf{A}(\mathbf{p})}{\partial p_i} \bigg|_{p_i = p_i^{(t-1)}}$$

Set the gradient of neuron for class k to one and all other gradients to zero.

Optimize image for a high class probability

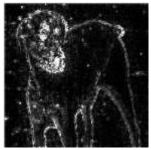
Synthetic images that maximize the probability for a selected class label when using a CNN with fixed weights that were trained on imageNet data.



Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps Karen Simonyan, Andrea Vedaldi, Andrew Zisserman, 2014

Which pixels are important for the classification? Saliency Maps





Determine the strength of the pixels influence on the correct class score:

Forward image through trained CNN.

Start from softmax neuron of correct class and set its gradient to 1. Back-propagate the gradient through the CNN.

Visualize the gradient that arrives at the image as 2D heatmap (each pixel intensity corresponds to the absolute value of the gradients at this position maximized over the channels).

Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps, Karen Simonyan, Andrea Vedaldi, Andrew Zisserman, 2014

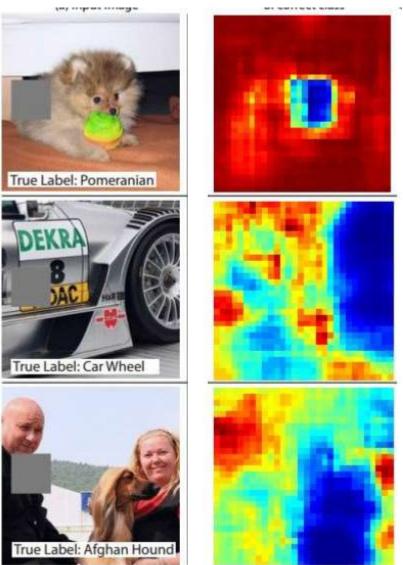
Example how to compute <u>saliency with keras</u>

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.
- 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)





(a) Husky classified as wolf

(b) Explanation

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

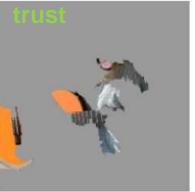
-> Explain the CNN classification by showing instance-specific important features visualize important feature allows to judge the individual classification



(a) Original Image



(b) Explaining Electric quitar (c) Explaining Acoustic quitar





(d) Explaining Labrador