Machine Intelligence:: Deep Learning
Week 2

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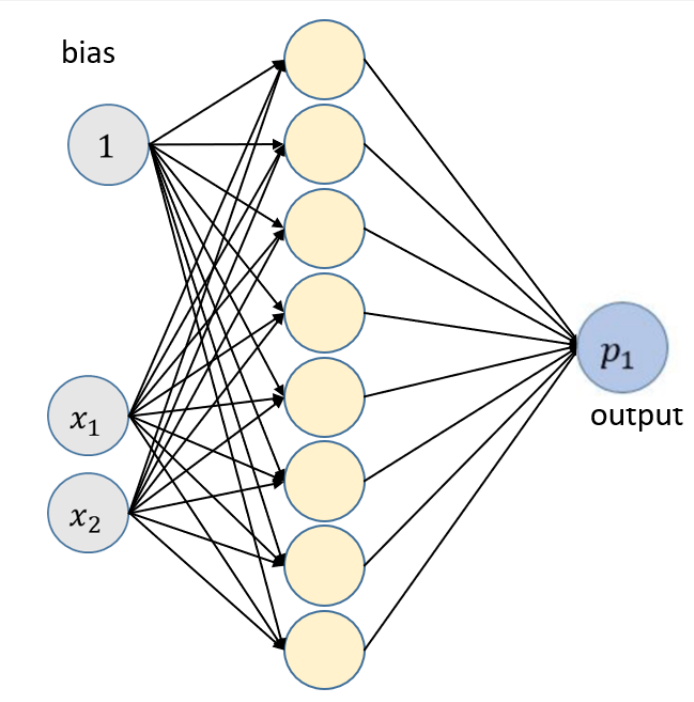
Topics of today

- A second look on fully connected Neural Networks (fcNN)
  - Classification loss if more then one class
  - ReLU
  - Training Testset

- Convolutional Neural Networks (CNN) for images
  - Motivation for switching from fcNN to CNNs
  - Introduction of convolution
  - ReLu and Maxpooling Layer
  - Biological inspiration of CNNs
  - Building CNNs

Besprechung



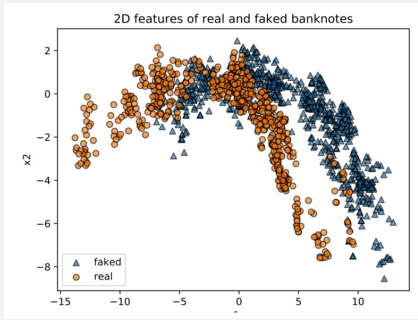
input hidden

Open NB 01_simple_forward_pass.ipynb and do the Keras part

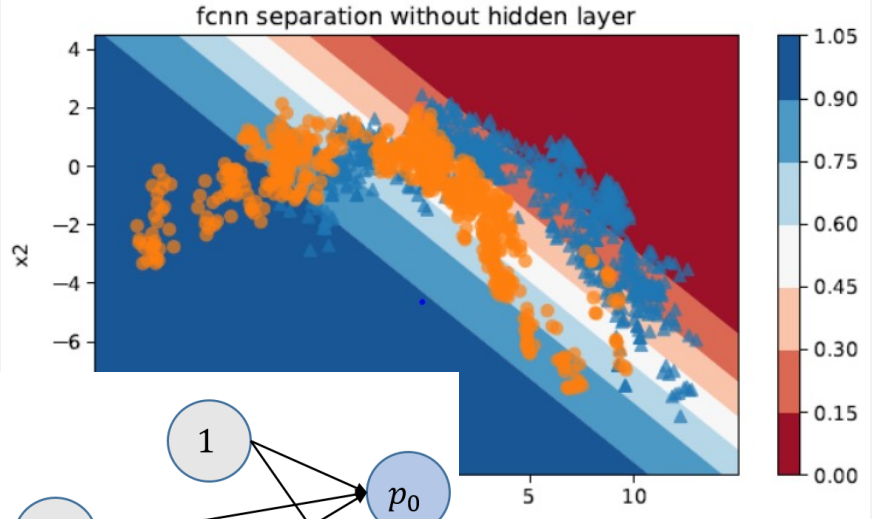
Additional Homework

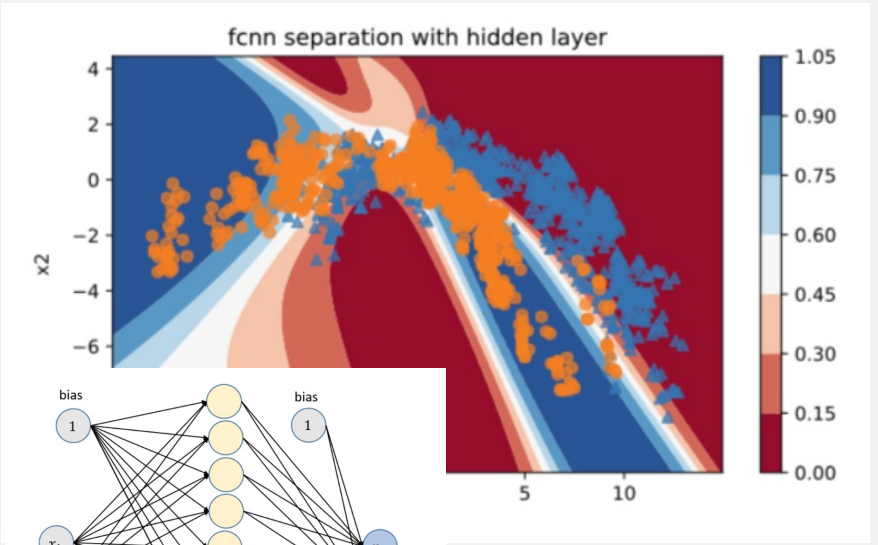
Do exercise NB 02:

Use Keras for modeling the banknotes data with binary outcome and 2 continuous input features (x1,x2)



Fit the a fcNN w/o and with hidden layer to discriminate fake bank notes from real bank notes: NB02



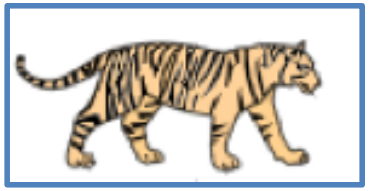


Recap Training

Input $x^{(i)}$

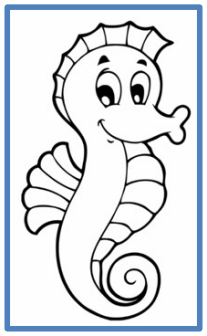
True class $y^{(i)}$

Suggested class
(Show is most likely class)



Tiger

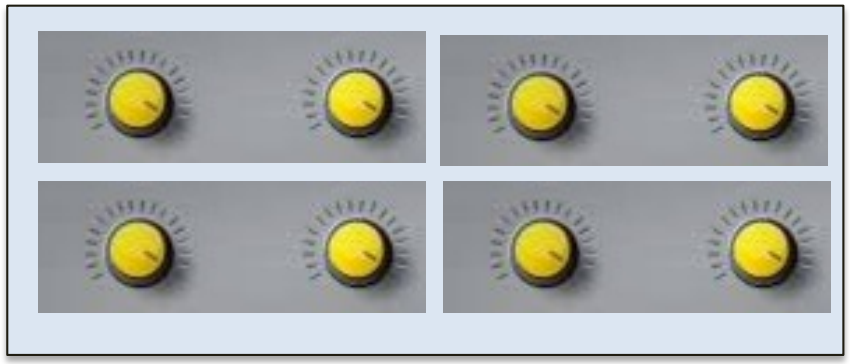
Tiger



Seeh
orse

...

Neural network with many weights *W*



→ Seal 👎

→ Tiger 👍

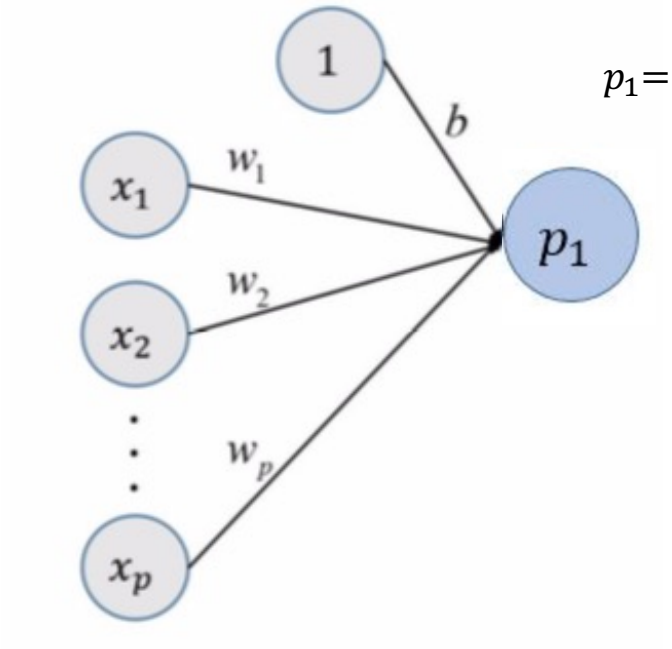
→ Seehorse 👍

Typical 1 Mio. Trainingsdaten

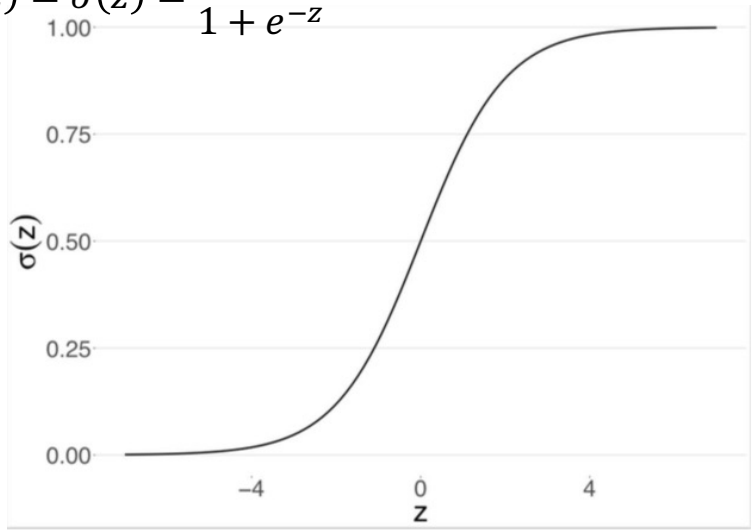
Trainingsprinciple:
Weights are tuned so a loss functions gets minimized.

$$loss = loss(\{y^{(i)}, x^{(i)}\}, W)$$

Recap Loss for Single Output



$$p_1 = P(Y = 1|z) = \sigma(z) = \frac{1}{1 + e^{-z}}$$



Loss

$p_1 = P(Y = 1|x)$ if the observed class is $y_i = 1$
$p_0 = P(Y = 0|x)$ if observed is $y_i = 0$

$$\text{LogLikelihood} = \sum_{i=1}^{n} [y_i \log(p_{1i}) + (1 - y_i) \log(1 - p_{1i})]$$

Classification

- Predict class
- Usually in DL the model predicts a probability for each possible class
- Example:
  - Banknote from exercise – classes: “real” or “fake”
  - Typical example Number from hand-written digit – classes: 0, 1, …, 9

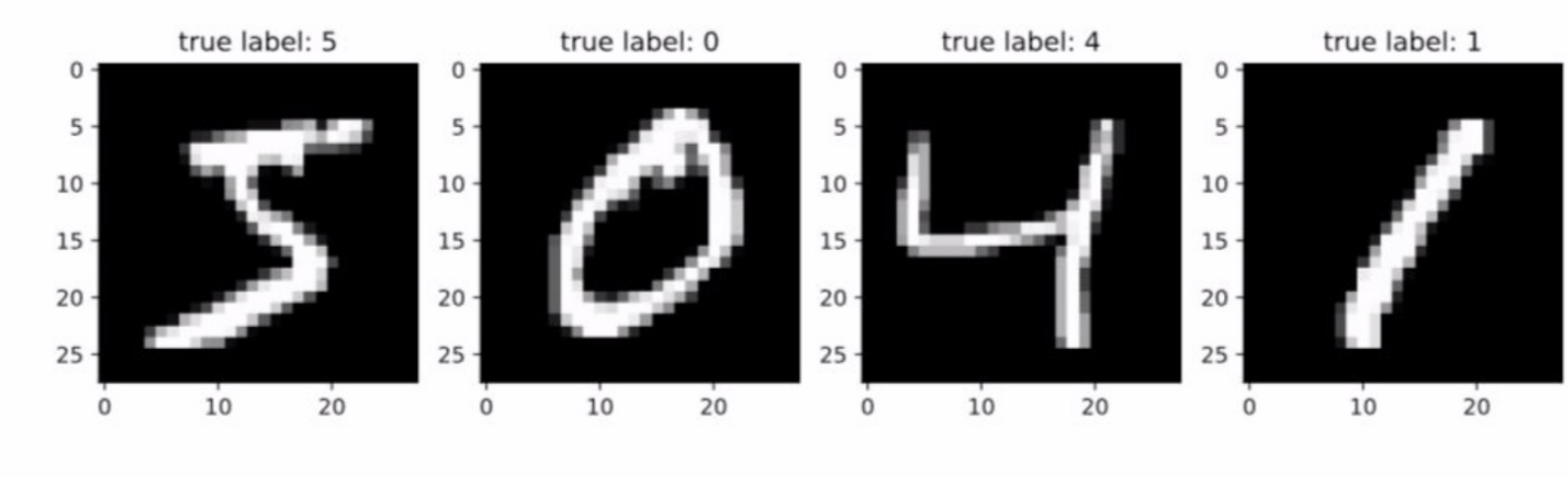
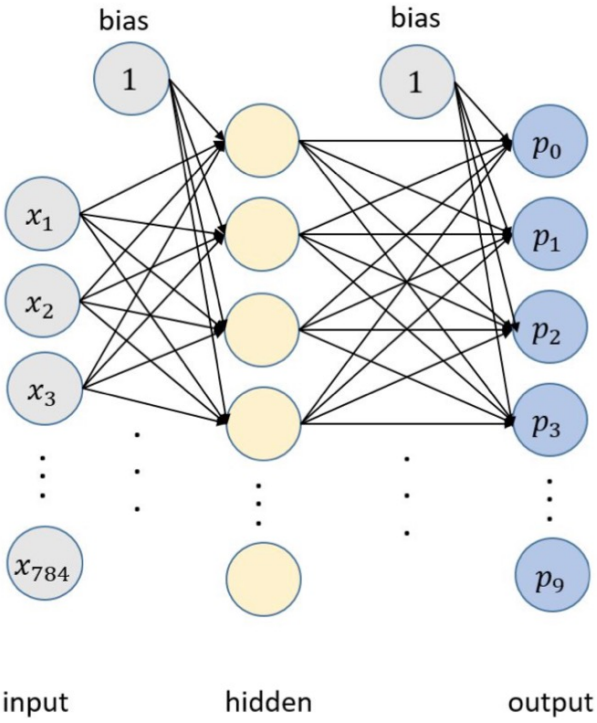


Figure 2.11 The first four digits of the MNIST data set—the standard data set used for benchmarking NN for images classification

Classification: Softmax Activation



$p_o, p_1 \ldots p_9$ are probabilities for the classes 0 to 9.

Activation of last layer z_i incomming

$$p_i = \frac{e^{z_i}}{\sum_{j=0}^{9} e^{z_j}}$$

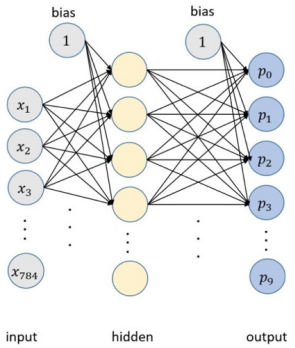
Makes outcome positive

Ensures that pi's sum up to one

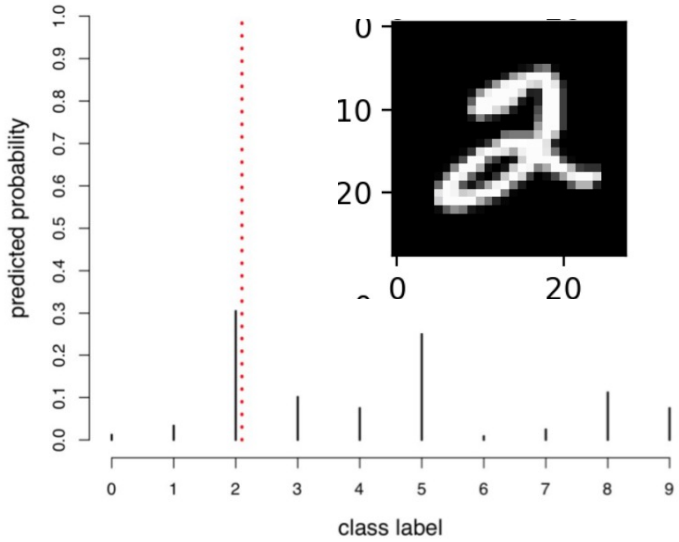
This activation is called softmax

Figure 2.12: A fully connected NN with 2 hidden layers. For the MNIST example, the input layer has 784 values for the 28 x 28 pixels and the output layer out of 10 nodes for the 10 classes.

Loss for classification ('categorical cross-entropy')



$p_0, p_1 \ldots p_9$ are probabilities for the classes 0 to 9.



Definition (Negative Log-likelihood NLL / cat. crossentropy):
The loss l_i of a single training example $\mathrm{x}^{(i)}$ with true label $y^{(i)}$ is

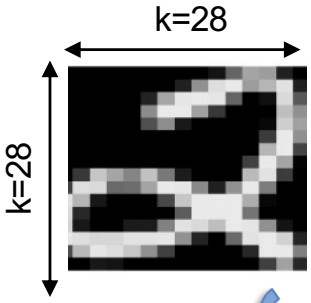
$$l_i = -\log\left(p_{model}\left(y^{(i)}\middle|x^{(i)}\right)\right)$$

Notation: if true label is 2 then $p_{model}\left(y^{(i)}\middle|x^{(i)}\right) = p_2$

- Perfect, i.e. predicts class of training example $y^{(i)}$ with probability 1 $\Rightarrow\ l_i = 0$
- Worst, i.e. predicts class $y^{(i)}$ with probability 0 $\Rightarrow\ l_i = \infty$

For more all examples, just average $\mathrm{loss} = \frac{1}{N}\sum l_i$

What is going on in a 1 layer fully connected NN?



Flatten to vector with k^2 elements

input $\mathbf{x}^t$

24.0
−5.1
12.2
89.9
:
3.2

$$\mathbf{x}_{(1,k^2)} \cdot \mathbf{W}_{(k^2,10)} + \mathbf{b}_{(1,10)} = \mathbf{z}_{(1,10)}$$

Score or logit $\mathbf{z}^t$

-3.89
-3.18
-0.80
-2.20
-2.44
-1.05
-4.60
-3.48
-2.09
-2.44

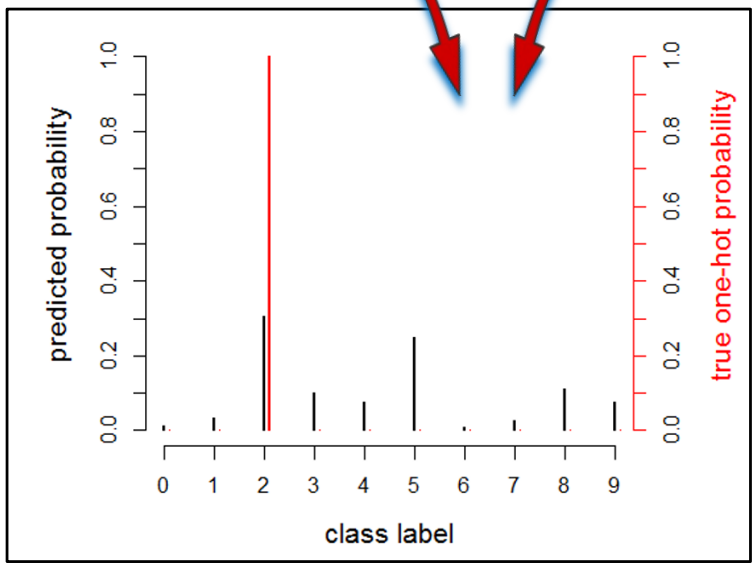
$$\hat{p}_k = \frac{e^{z_k}}{\sum_j e^{z_j}}$$

Softmax or probability $\mathbf{p}=S(\mathbf{z})$

0.02
0.04
0.31
0.10
0.08
0.26
0.01
0.03
0.11
0.08

1-hot labels ${}^{obs}y$

0
0
1
0
0
0
0
0
0
0



Cost C or Loss = cross-entropy averaged over all images in mini-batch

$$C = \frac{1}{N}\sum_i D(\mathbf{p}_i, \mathbf{y}_i)$$

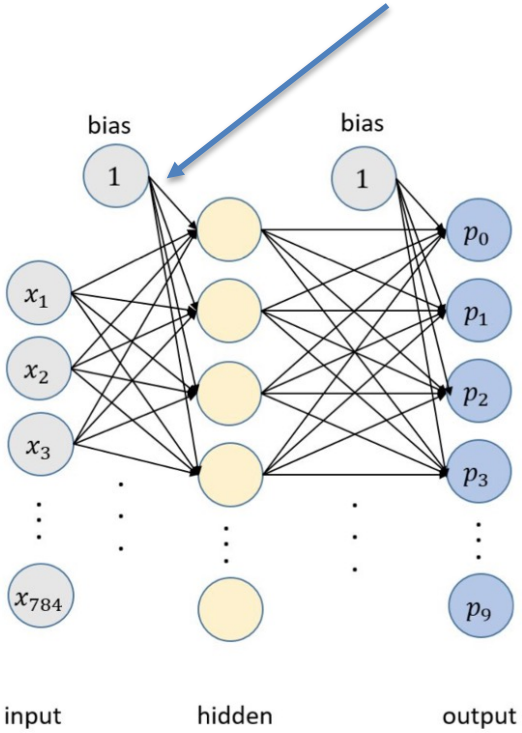
Cross-Entropy

$$D(\mathbf{p}, \mathbf{y}) = -\sum_{k=1}^{10} {}^{obs}y_k \cdot \log(p_k)$$

Optimization in DL

- DL many parameters
  - Optimization loss by simple gradient descent
- Algorithm: Stochastic Gradient Descent (SGD)*
  - Take a random batch of training examples $\{y^{(i)}, x^{(i)}\}_{i=1,\cdots,B}$
  - Calculate the loss of that batch $loss(\{y^{(i)}, x^{(i)}\}, W)$
  - Tune the weights so that loss gets minimized a bit (gradient descent)
  - Repeat

Parameters of the network are the weights.



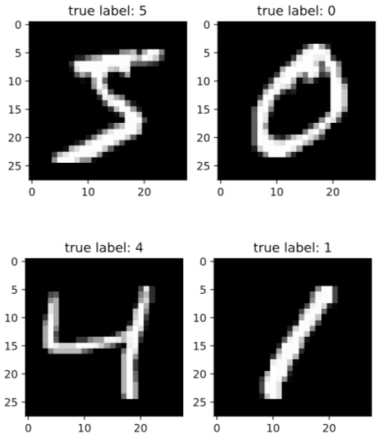
Modern Networks have Billions (10^9) of weights.

Record 2020: $175 \cdot 10^9$ (GPT-3)

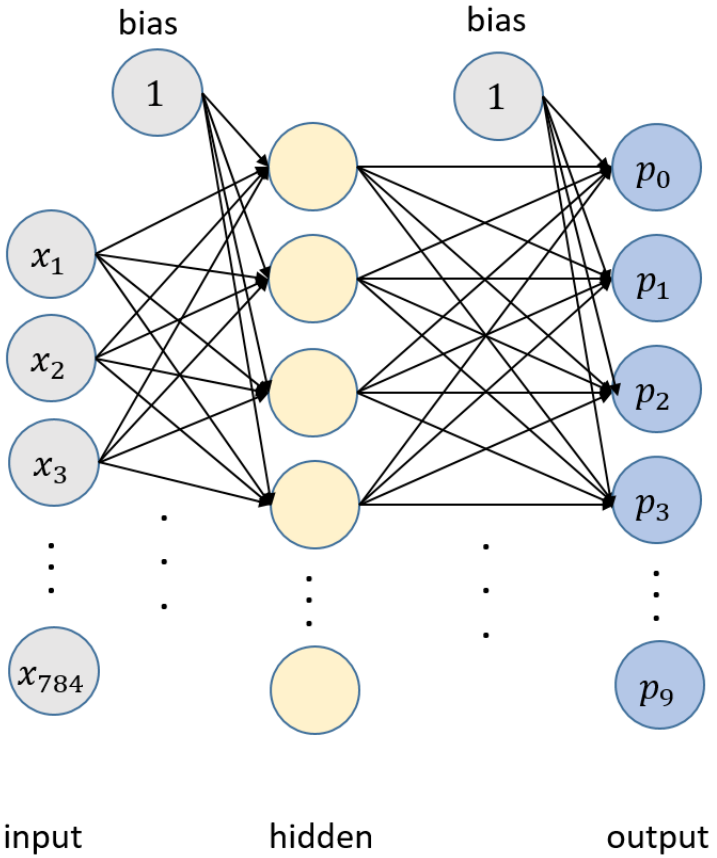
*aka minibatch gradient descent.

Fully connected NN for image data
Good Idea?

A fcNN for MNIST data



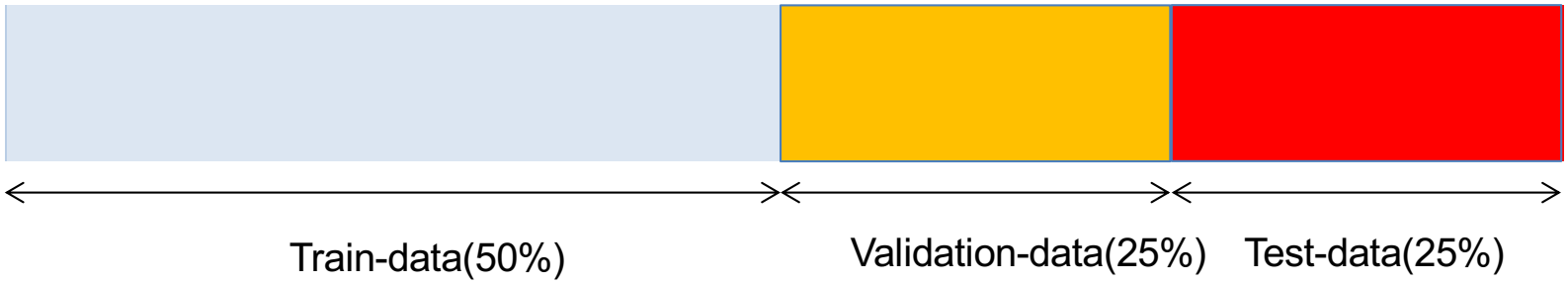
The first four digits of the MNIST data set - each image consisting of 28x28=784 pixels



A fully connected NN with 2 hidden layers.

For the MNIST example, the input layer has 784 values for the 28 x 28 pixels and the output layer has 10 nodes for the 10 classes.

Best practice: Split in Train, Validation, and Test Set

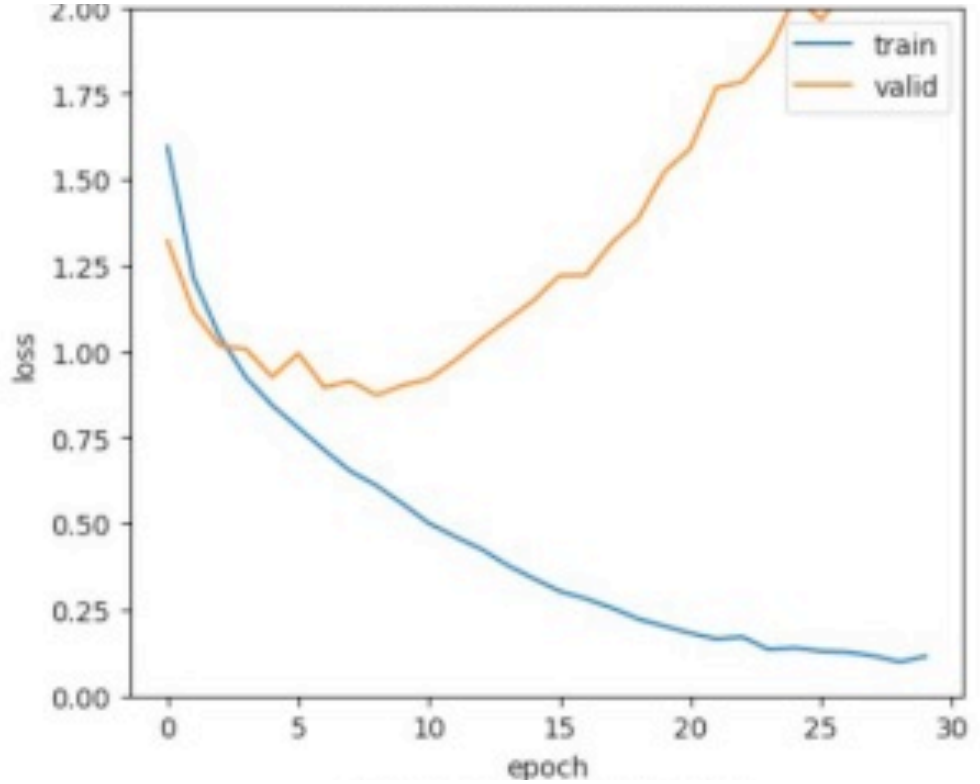


Best practice: Lock an extra test data set away, and use it only at the very end, to evaluate the chosen model, that performed best on your validation set.
Reason: **When trying many models, you probably overfit on the validation set**.

Determine performance metrics, such as MSE, to evaluate the predictions **on new validation or test data**

What can loss curves tell us?

Very common check: Plot loss in train and validation data vs epoch of training.



- If training loss does not go down to zero: model is not flexible enough
- In case of overfitting (validation loss >> train loss): regularize model

Typical Training Curve / ReLU

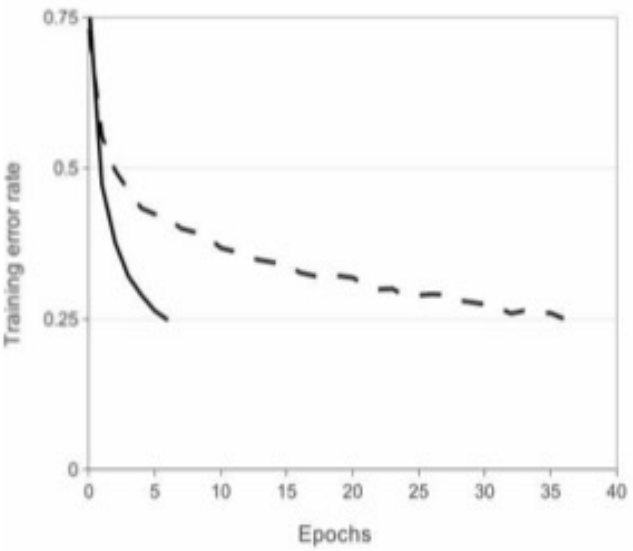
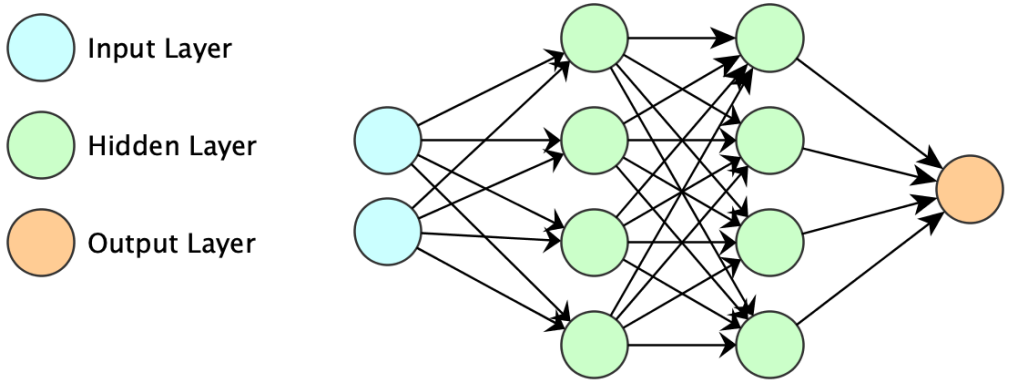
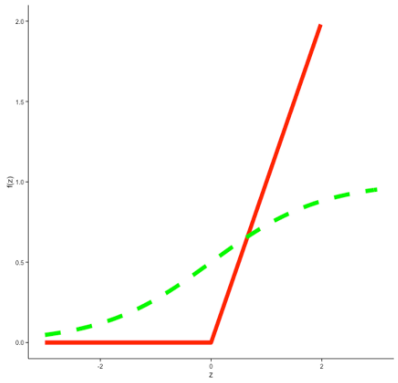


Figure 1: A four-layer convolutional neural network with ReLUs **(solid line)** reaches a 25% training error rate on CIFAR-10 six times faster than an equivalent network with tanh neurons

Source:
Alexnet
Krizhevsky et al 2012

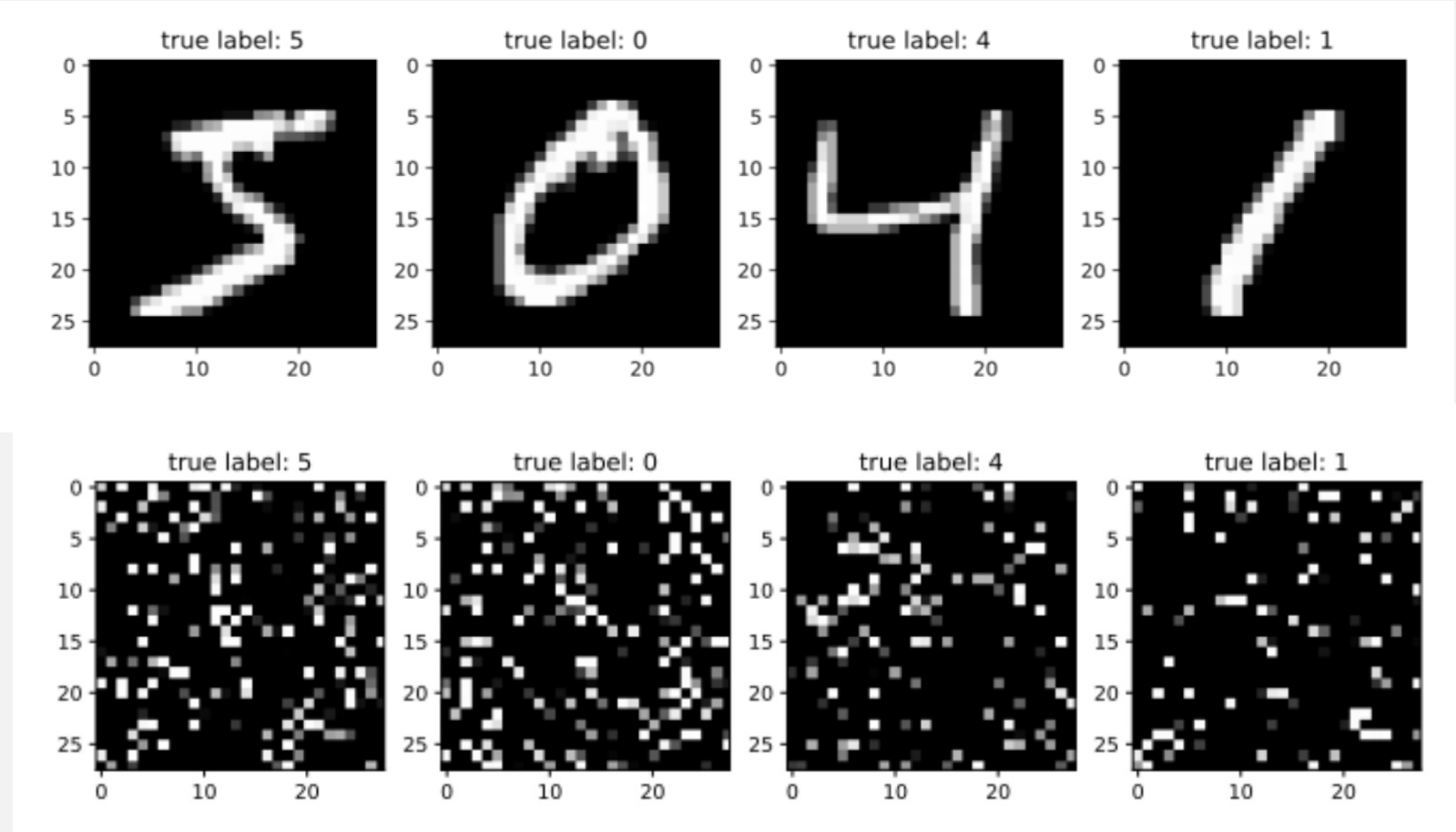




Motivation:
Green:
sigmoid.
Red:
ReLU faster
convergence

Epochs: ”each training examples is used once”

Exercise: Does shuffling disturb a fcNN?

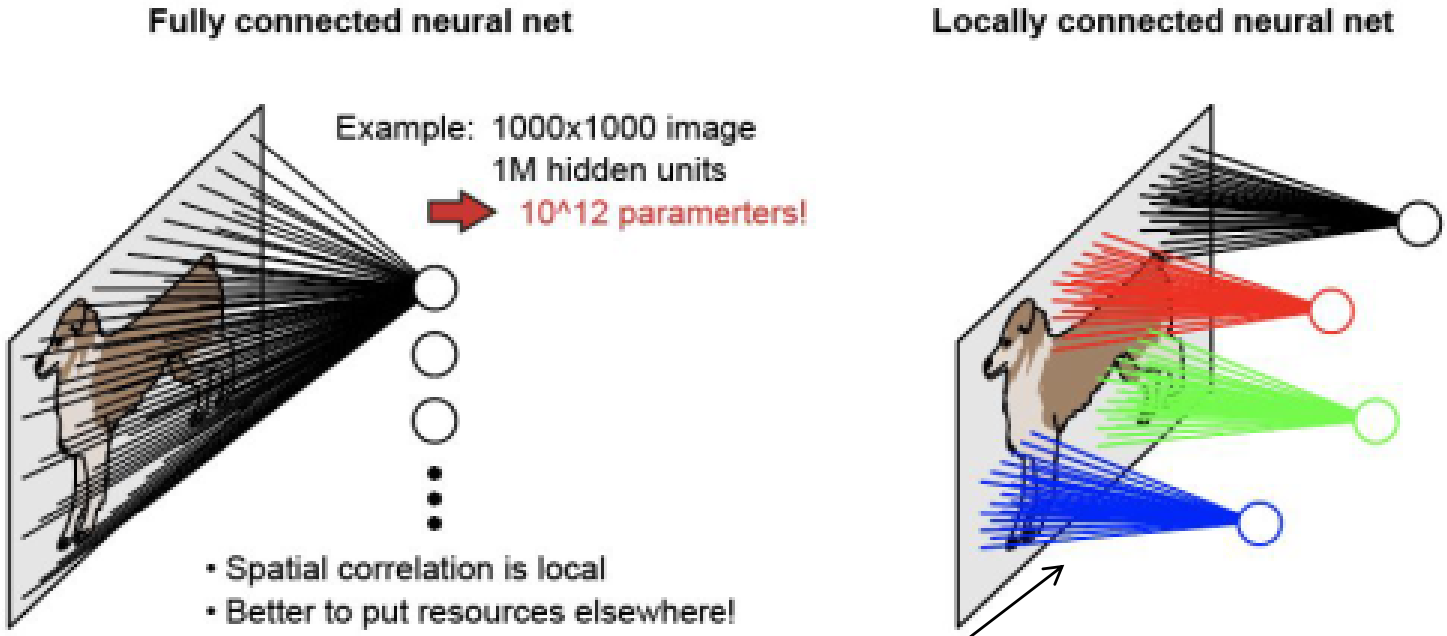


Use fcNN for MNIST:
03_fcnn_mnist.ipynb

If time
04_fcnn_mnist_shuffled.ipynb

Convolutional Neural Networks
SOTA for image data

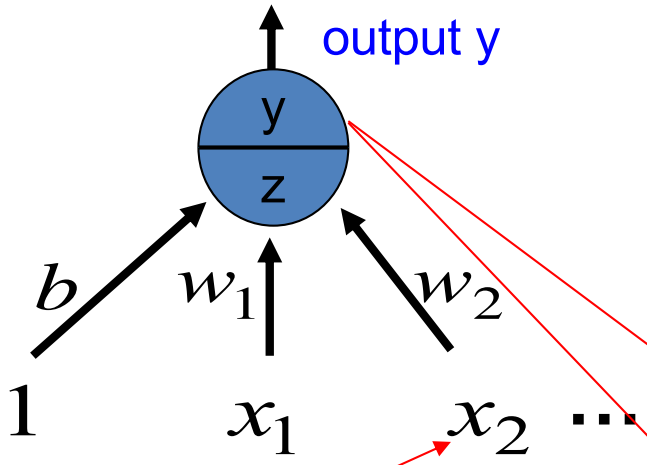
Convolution extracts local information using few weights



Shared weights:

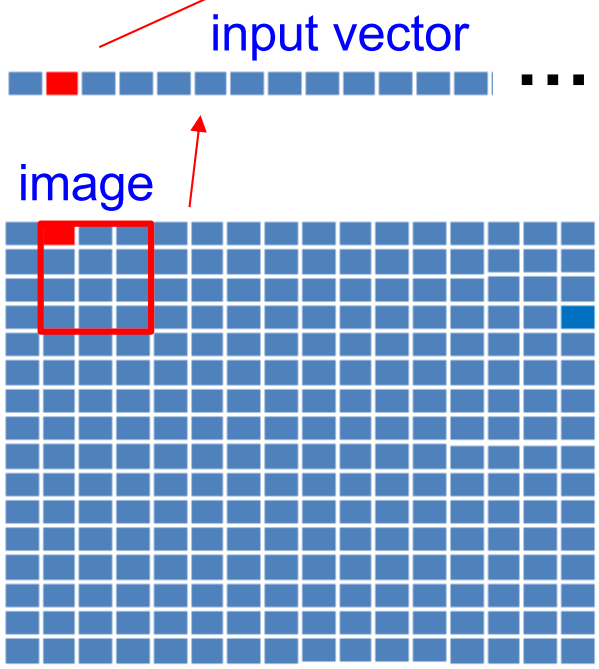
by using the same weights for each patch of the image we need much less parameters than in the fully connected NN and get from each patch the same kind of local feature information such as the presence of a edge.

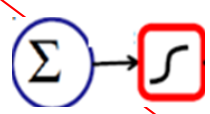
An artificial neuron

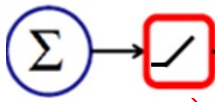


bias weights

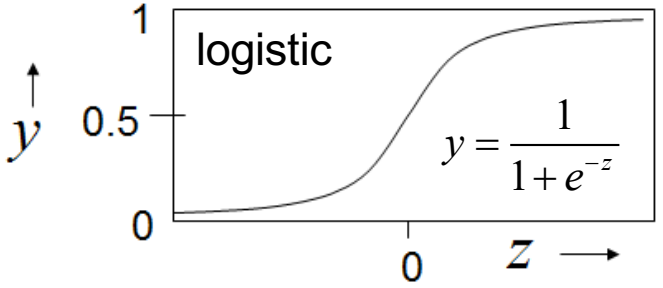
$$z = b + \sum_i x_i w_i$$

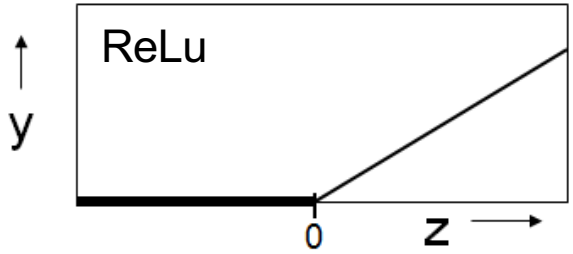






Different non-linear transformations are used to get from z to output y



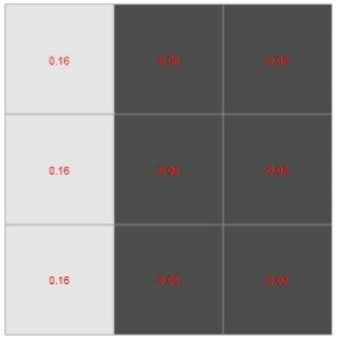


Convolutional networks use neighborhood information and replicated local feature extraction

In a locally connected network the calculation rule

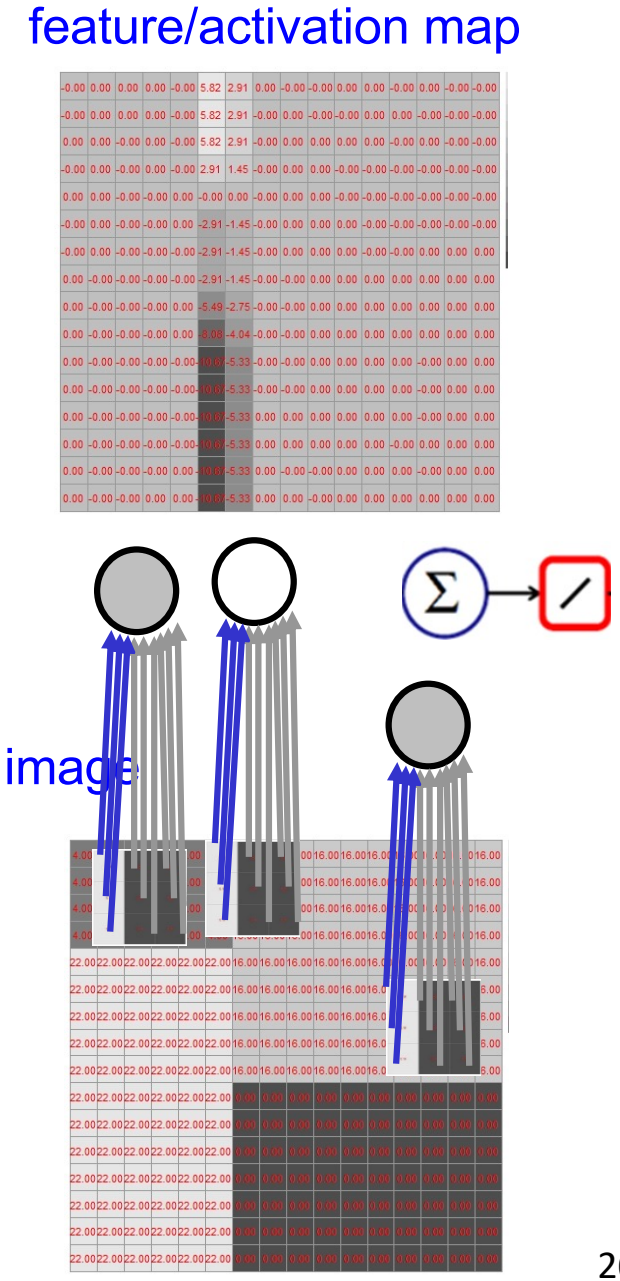
$$z = b + \sum_i x_i w_i$$

Pixel values in a small image patch are element-wise multiplied with weights of a small filter/kernel:



The filter is applied at each position of the image and it can be shown that the result is maximal if the image pattern corresponds to the weight pattern.

The results form again an image called feature map (=activation map) which shows at which position the feature is present.



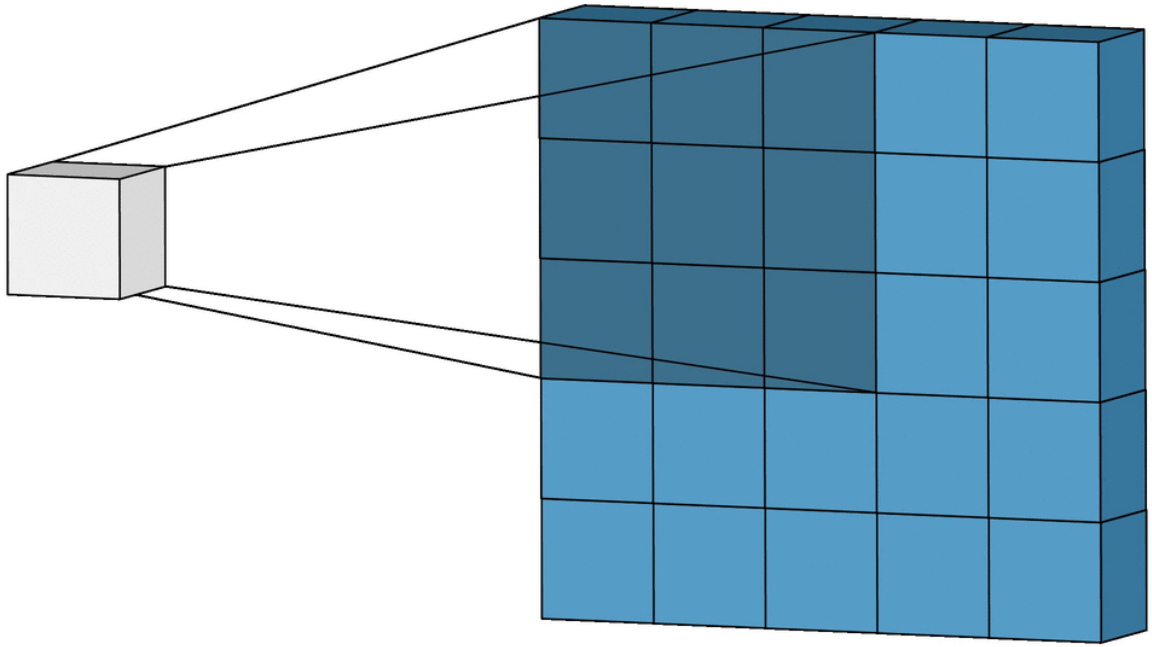
Exercise: Do one convolution step by hand

The kernel is 3x3 and is applied at each valid positon
– how large is the resulting activation map?

The small numbers in the shaded region are the kernel weights.
Determine the position and the value within the resulting activation map.

3	3	2	1	0
0_0	0_1	1_2	3	1
3_2	1_2	2_0	2	3
2_0	0_1	0_2	2	2
2	0	0	0	1

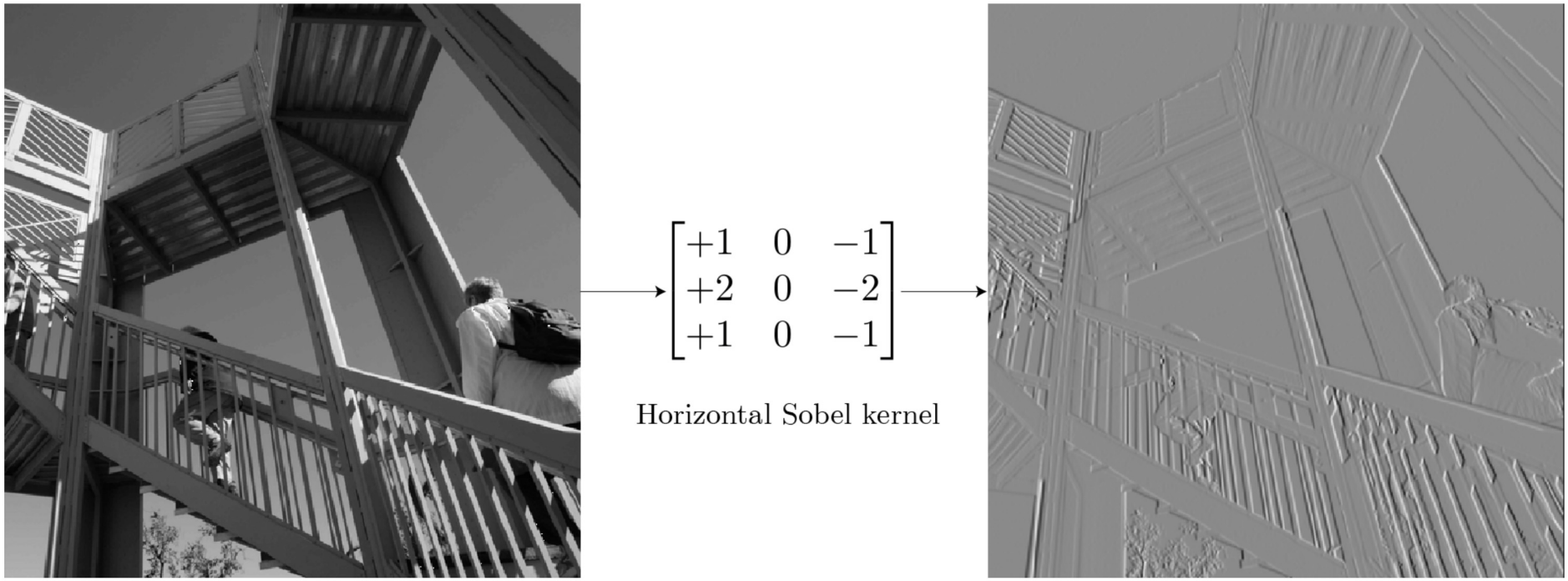
Applying the same 3x3 kernel at each image position



Applying the 3x3 kernel on a certain position of the image yields one pixel within the activation map where the position corresponds to the center of the image patch on which the kernel is applied.

Taken from the great website on convolution: https://towardsdatascience.com/intuitively-understanding-convolutions-for-deep-learning-1f6f42faee1

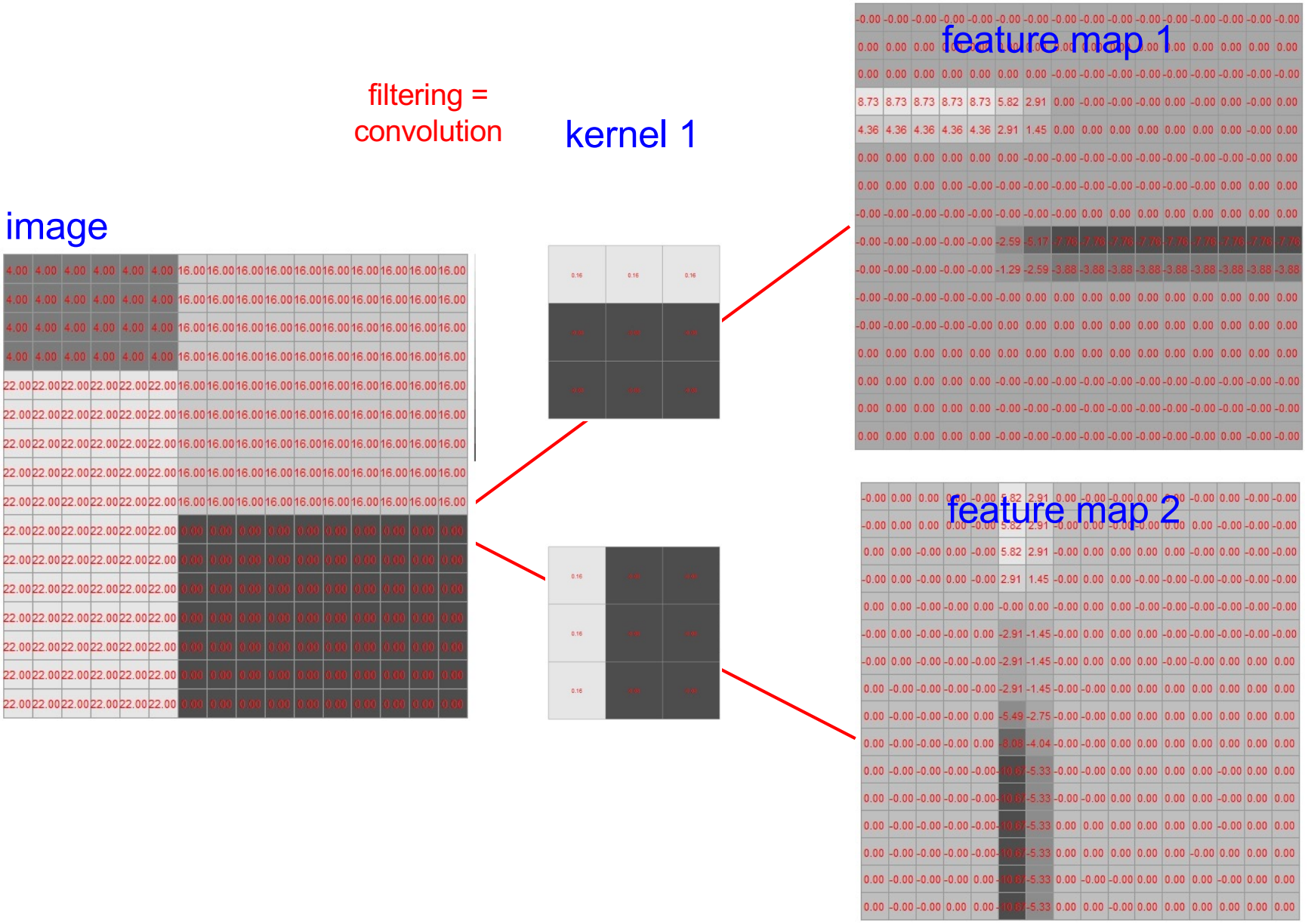
Example of designed Kernel / Filter



Applying a vertical edge detector kernel

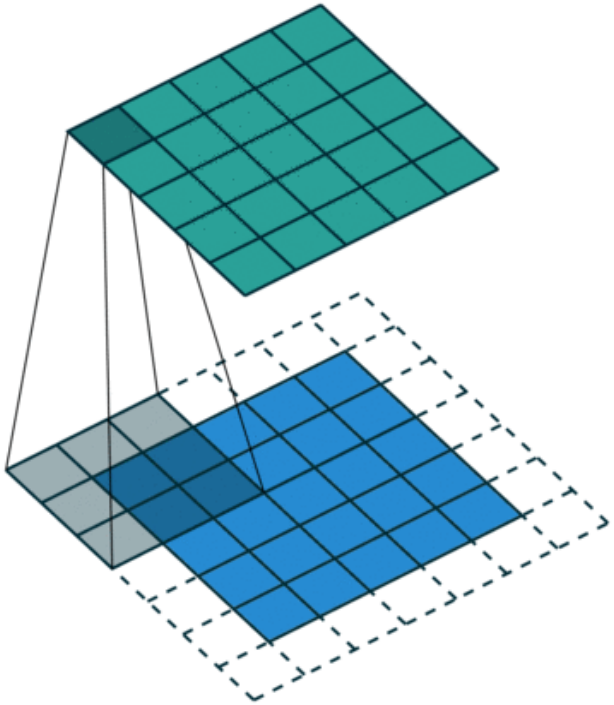
Taken from the great website on convolution: https://towardsdatascience.com/intuitively-understanding-convolutions-for-deep-learning-1f6f42faee1

Convolutional networks use neighborhood information and replicated local feature extraction

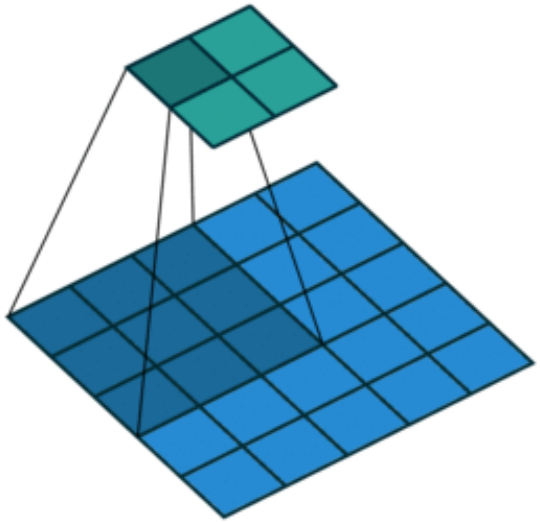


The weights of each filter are randomly initiated and then adapted during the training.

CNN Ingredient I: Convolution



Zero-padding to achieve
same size of feature and input

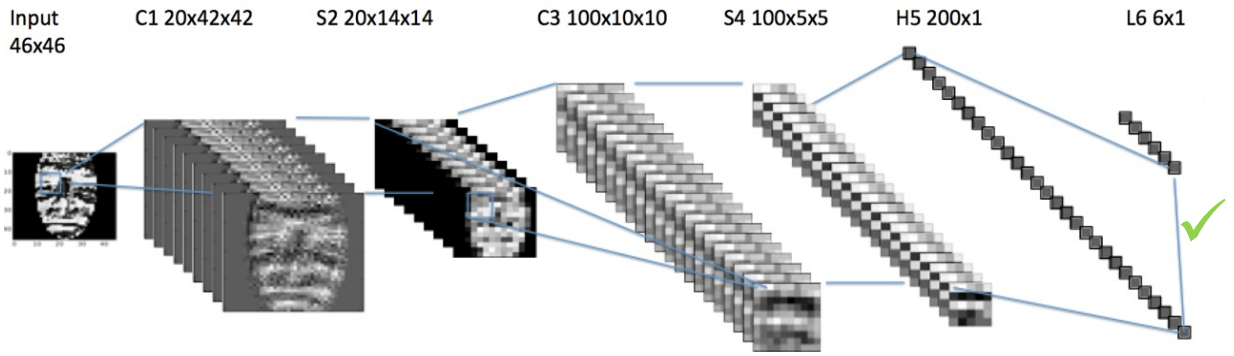


no padding to only use
valid input information

The *same* weights are used at each position of the input image.

Taken from the great website on convolution: https://towardsdatascience.com/intuitively-understanding-convolutions-for-deep-learning-1f6f42faee1

CNN ingredient II: Maxpooling Building Blocks reduce size



conv1 maxpool conv2 maxpool flatten dense

4x4

12	20	30	0
8	12	2	0
34	70	37	4
112	100	25	12

→

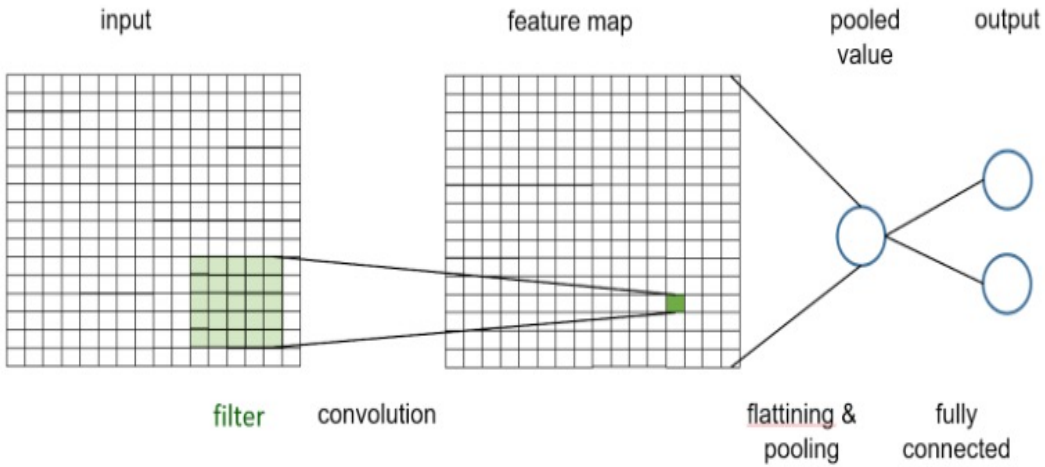
2x2

20	30
112	37

Simply join e.g. 2x2 adjacent pixels in one by taking the max.
→ less weights in model
→ Less train data needed
→ increased performance

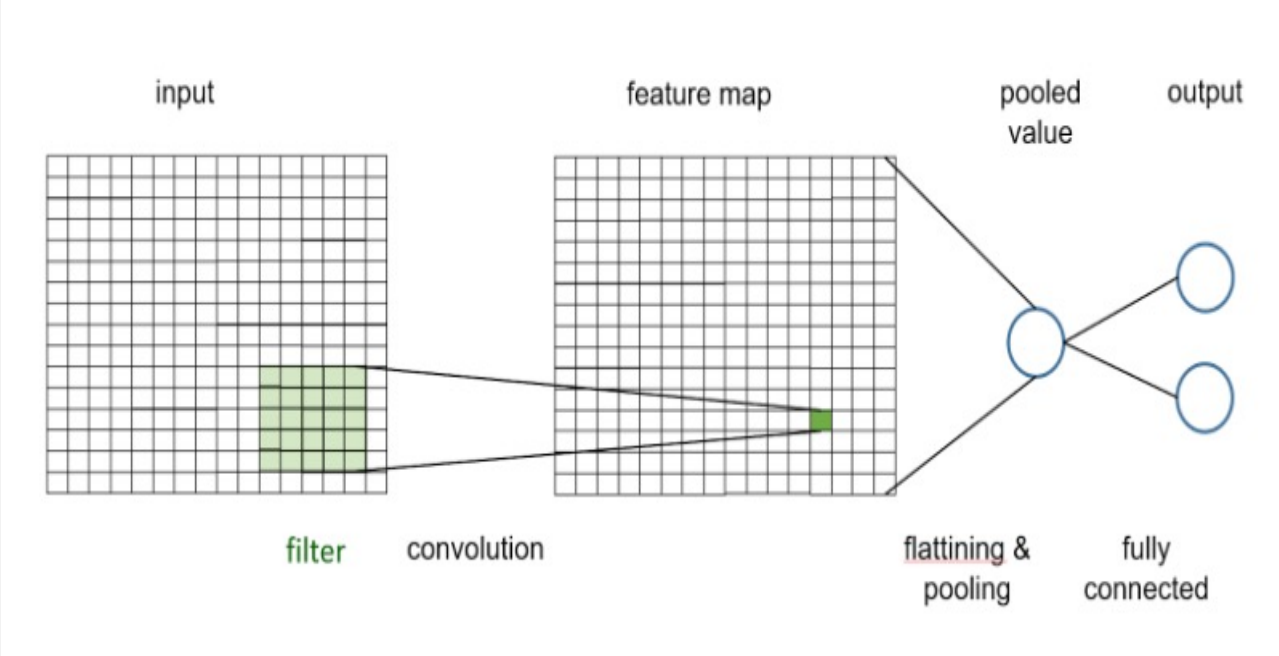
Hinton: „The pooling operation used in convolutional neural networks is a big mistake and the fact that it works so well is a disaster“

Building a very simple CNN with keras



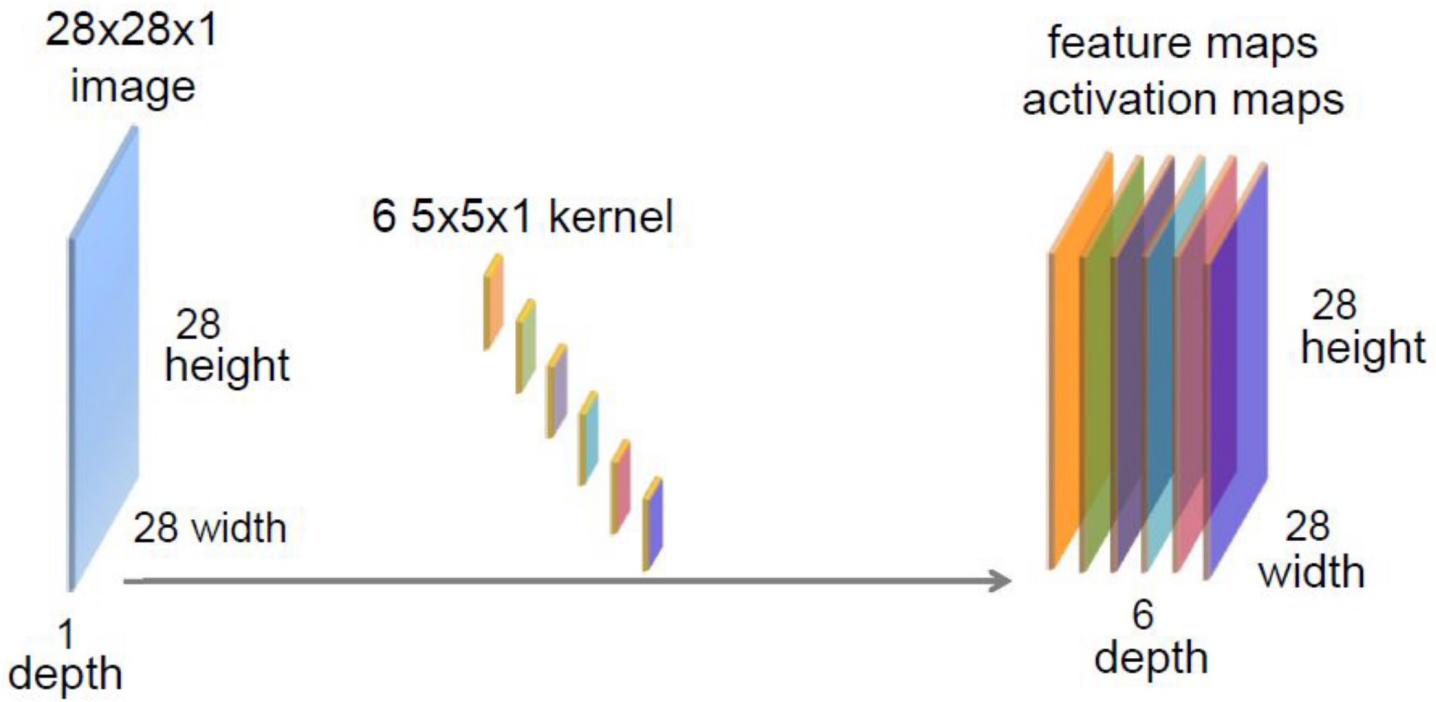

```
model = Sequential()
model.add(Convolution2D(1,(5,5), # one 5x5 kernel
        padding='same',          # zero-padding to preserve size
        input_shape=(pixel,pixel,1)))
model.add(Activation('linear'))
# take the max over all values in the activation map
model.add(MaxPooling2D(pool_size=(pixel,pixel)))
model.add(Flatten())
model.add(Dense(2))
model.add(Activation('softmax'))
```

Exercise: Artstyle Lover



Open NB in: https://github.com/tensorchiefs/dl_course_2024/blob/master/notebooks/05_cnn_edge_lover.ipynb

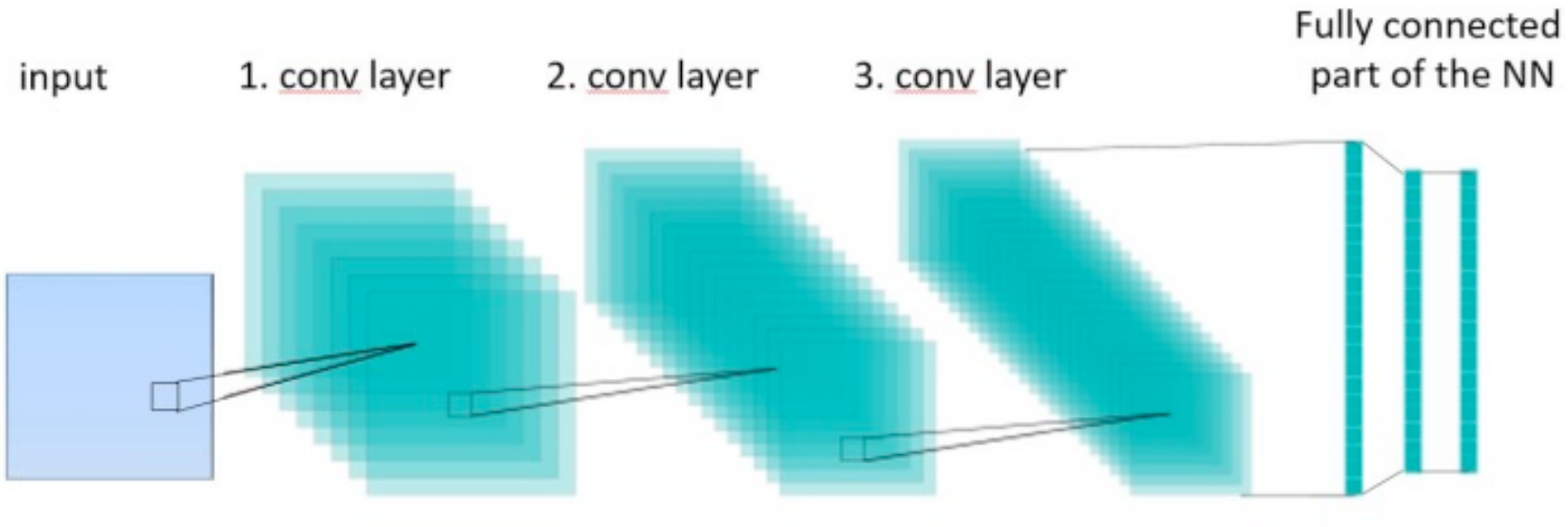
Convolution layer with a 1-chanel input and 6 kernels



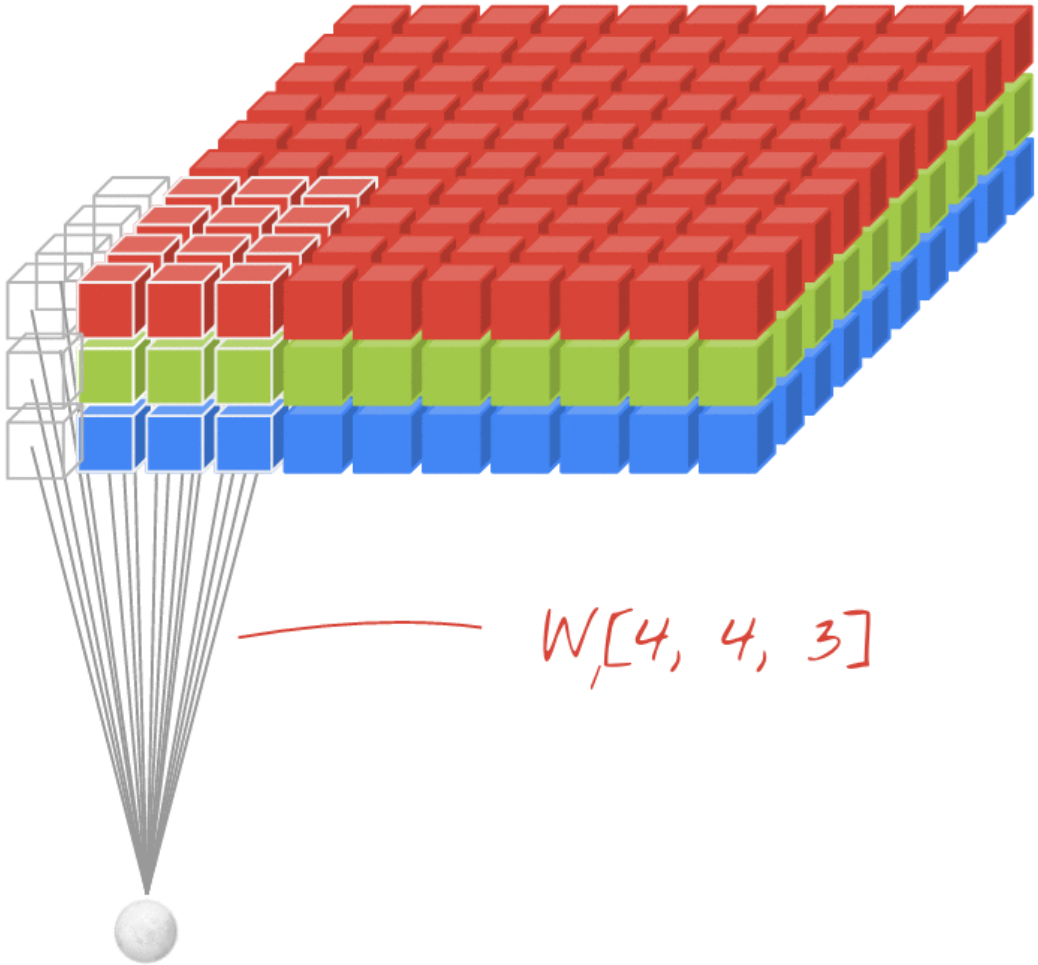
Convolution of the input image with 6 different kernels results in 6 activation maps.

If the input image has only one channel, then each kernel has also only one channel.

A CNN with 3 convolution layers



Animated convolution with 3 input channels



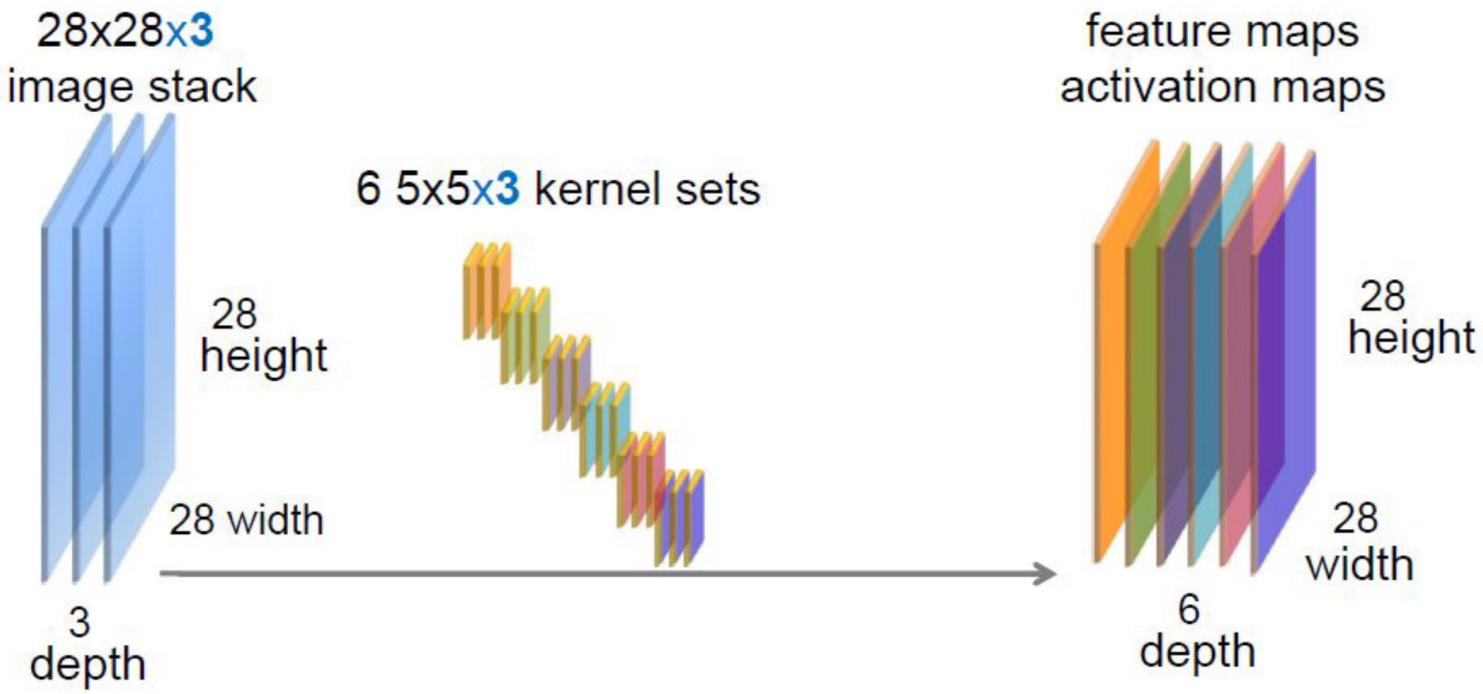
3 color channel input image

The value of neuron j in the k-th featuremap are computed from the weights in the k-th filter w_{ki} and the input values x_{ji} at the position j:

$$y_{jF_k} = f(z_{jF_k}) = f(b_k + \sum x_{ji} \cdot w_{ki})$$

Animation credits: M.Gorner, https://codelabs.developers.google.com/codelabs/cloud-tensorflow-mnist/#10

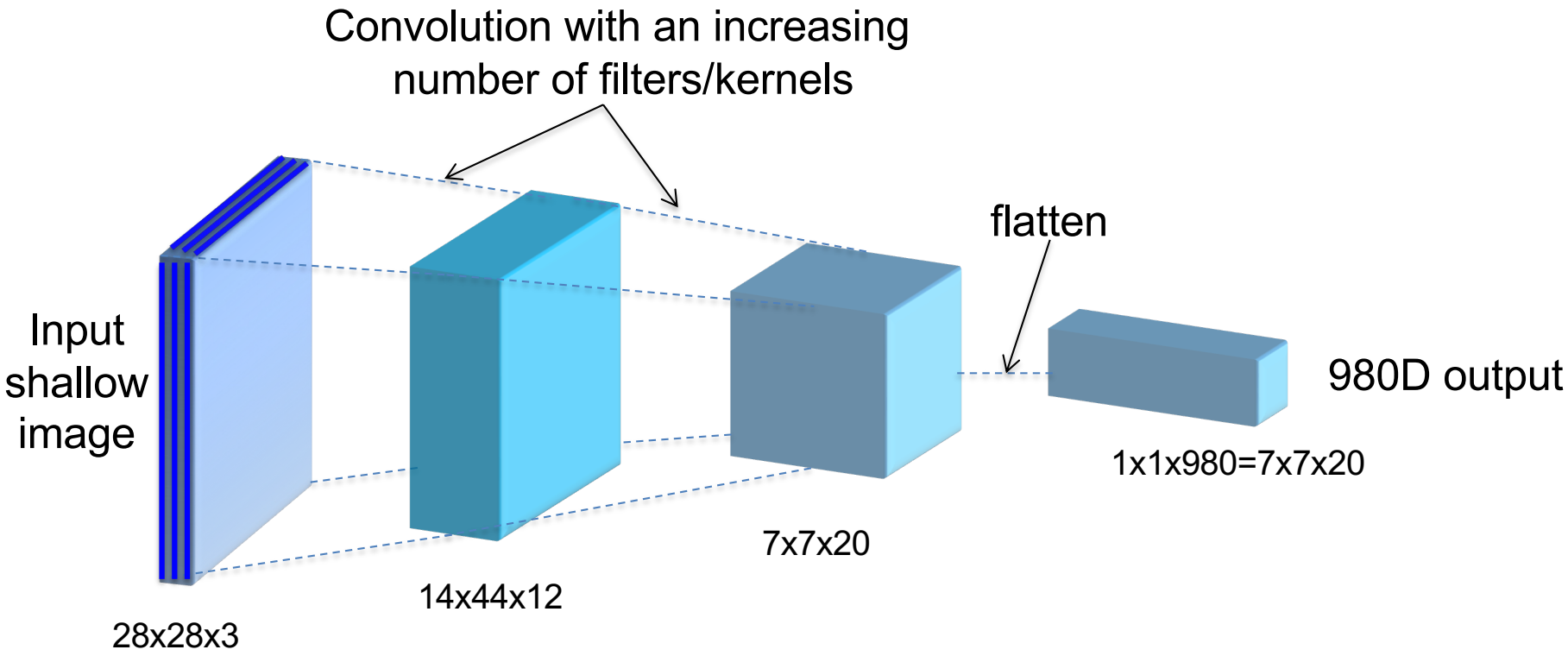
Convolution layer with a 3-chanel input and 6 kernels



Convolution of the input image with 6 different kernels results in 6 activation maps.

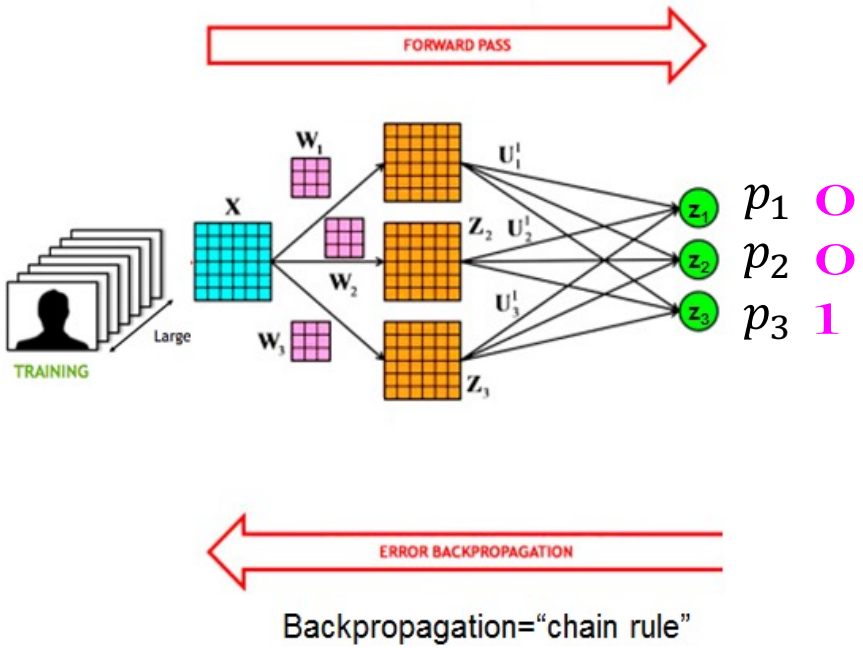
If the input image has 3 channels, then each filter has also 3 channels.

Typical shape of a classical CNN



Spatial resolution is decreased e.g. via max-pooling while more abstract image features are detected in deeper layers.

Training of a CNN is based on gradient backpropagation



p_1 O
p_2 O
p_3 1

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)**)**

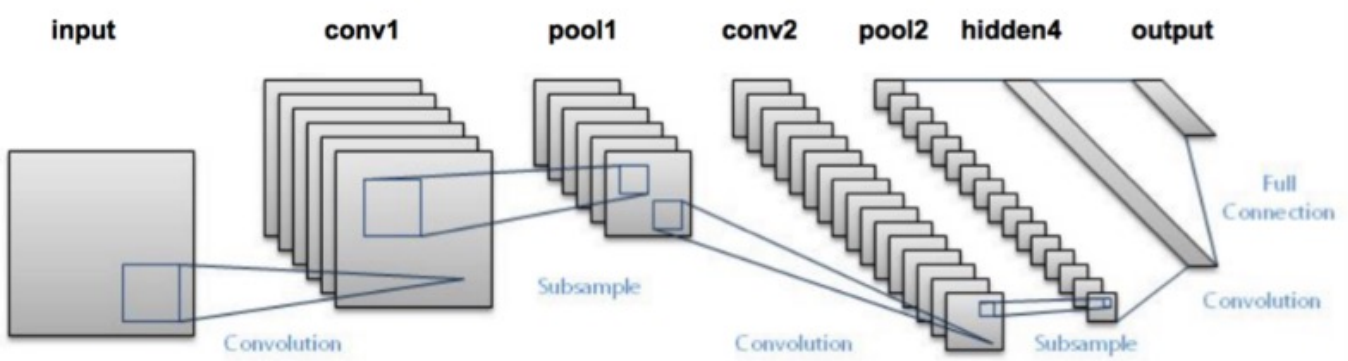
Learning is done by weight updating:

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

learning rate

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

CNN for MNIST



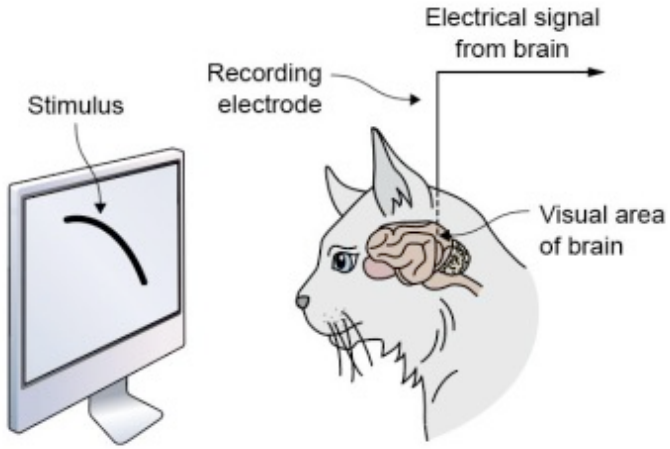

```
num_classes = 10              # 10 classes: 0, 1,…,9
input_shape = (28, 28, 1)   # 28x28 pixels, 1 channel (grey value)

model = Sequential()
model.add(Convolution2D(32, (3, 3), #32 filters of size 3x3
                  activation='relu',
                  input_shape=input_shape))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Convolution2D(64, (3, 3), activation='relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Flatten())
model.add(Dense(40, activation='relu'))
model.add(Dense(num_classes, activation='softmax'))
```

fcNN versus CNNs – some aspects

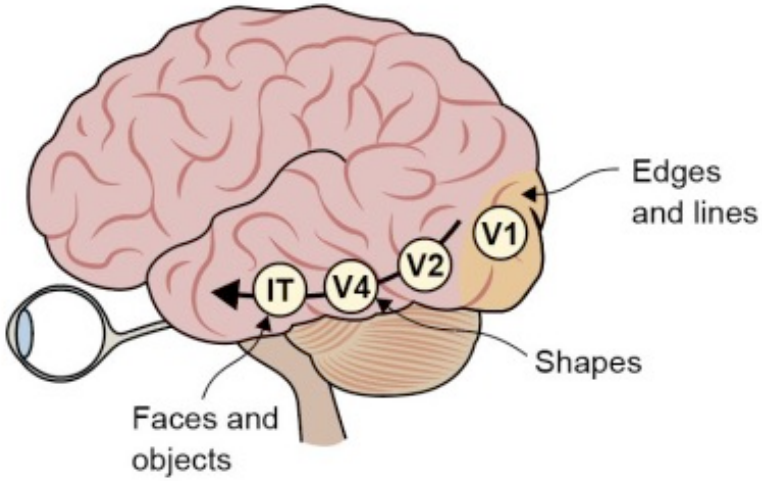
- A fcNN is good for tabular data, CNNs are good for 2D data (eg images).
- In a fcNN the order of the input does not matter, in CNN shuffling matters.
- A fcNN has no model (inductive) bias, a CNN has the model bias that neighborhood matters.
- A node in one layer of a fcNN corresponds to one feature map in a convolution layer:
- In each layer of a fcNN connecting p to q nodes, we learn q linear combinations of the incoming p signals, in each layer of a CNN connecting p channels with q channels we learn q filters (each having p channels) yielding q feature maps

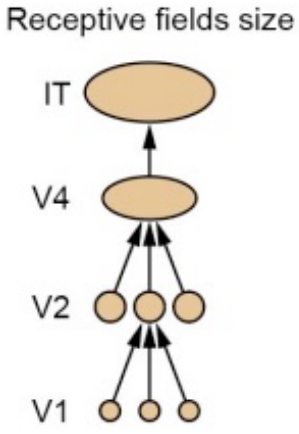
Biological Inspiration of CNNs

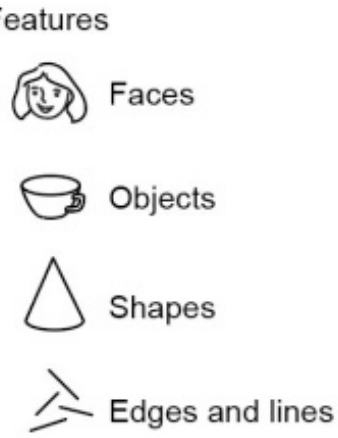
How does the brain respond to visually recieved stimuli?



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.

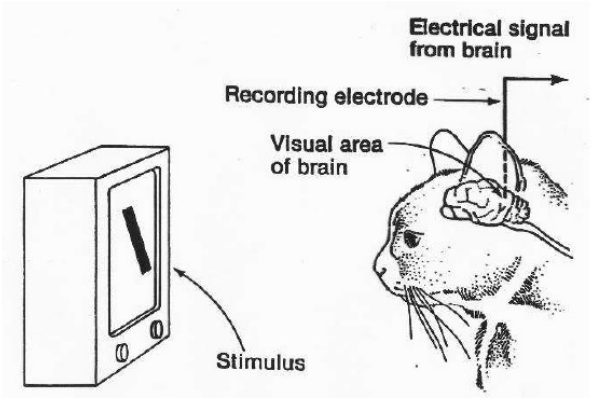


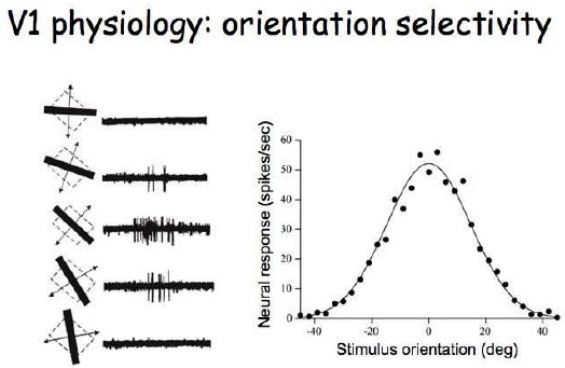


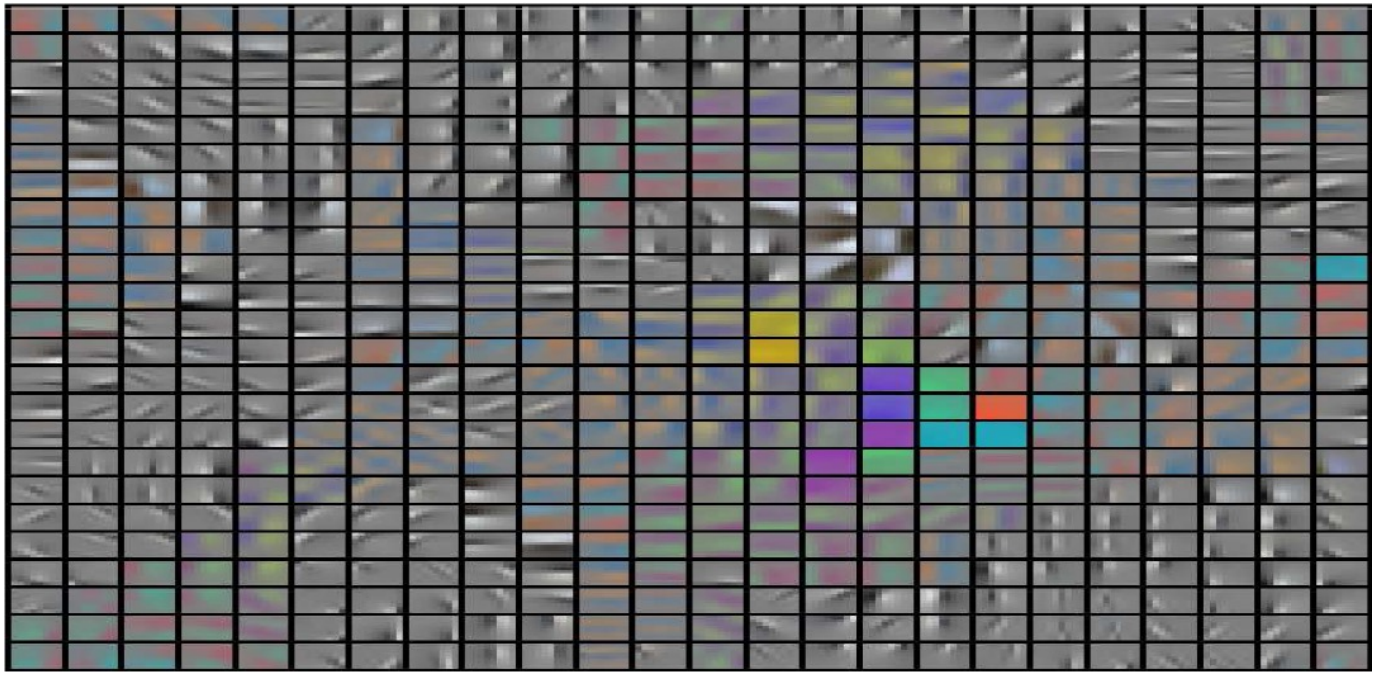


Organization of the visual cortex in a brain, where neurons in different regions respond to more and more complex stimuli

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





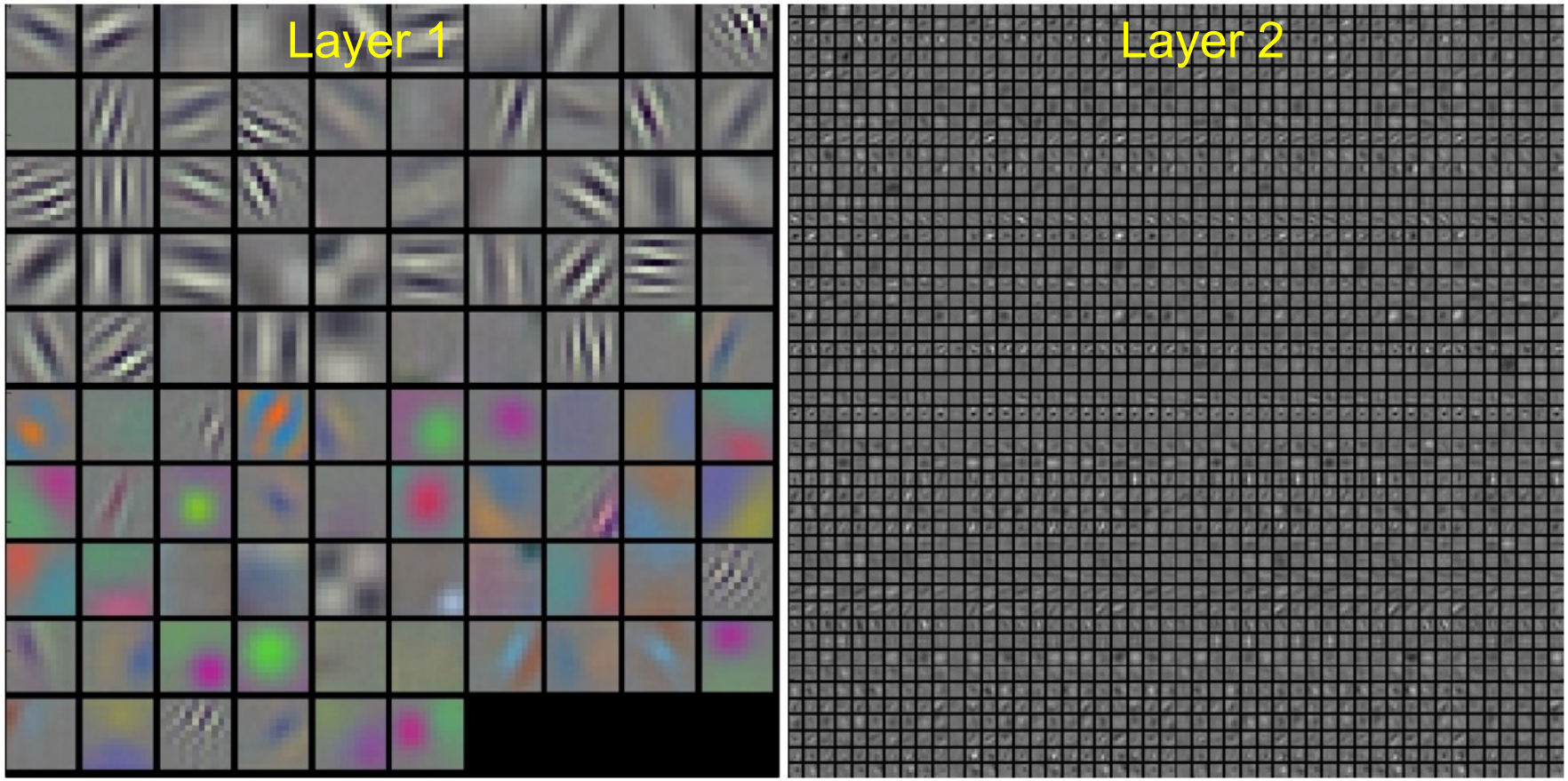


Neurons in brain region V1 and neurons in 1. layer of a CNN respond to similar patterns

Slide (modified) credits: Nando de Freitas

Visualize the weights used in filters

Filter weights from a trained Alex Net



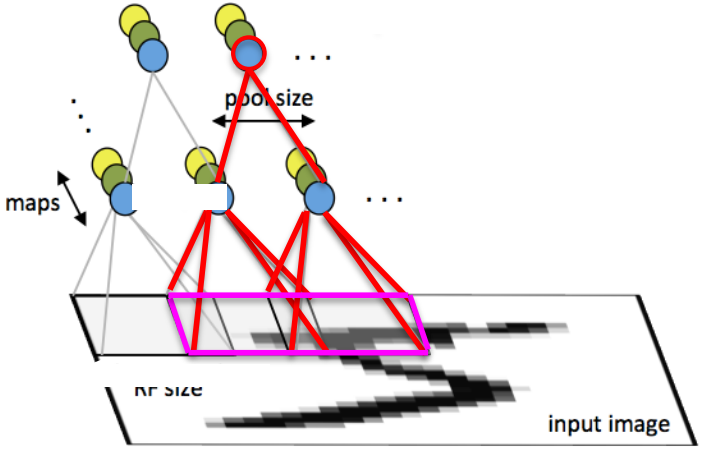
Only in layer 1 the filter pattern correspond to extracted patterns in the image.

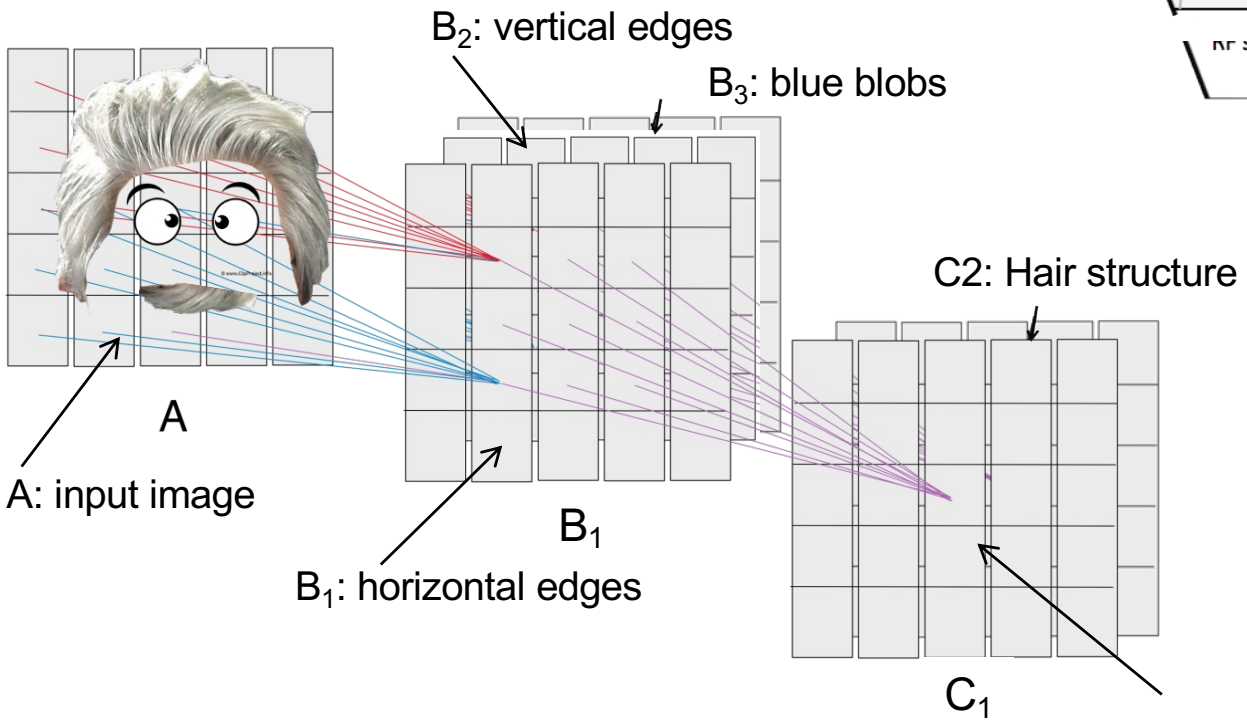
In higher layers we can only check if patterns look noisy, which would indicate that the network that hasn't been trained for long enough, or possibly with a too low regularization strength that may have led to overfitting.

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

The receptive field

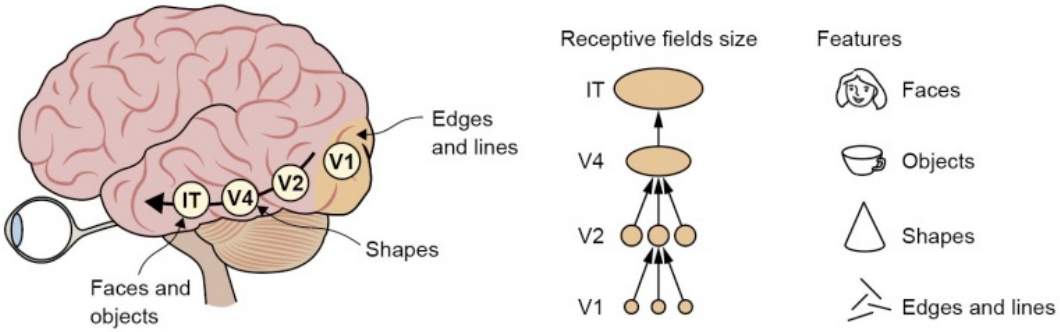
For each pixel of a feature map we can determine the connected area in the input image – this area in the input image is called receptive field.

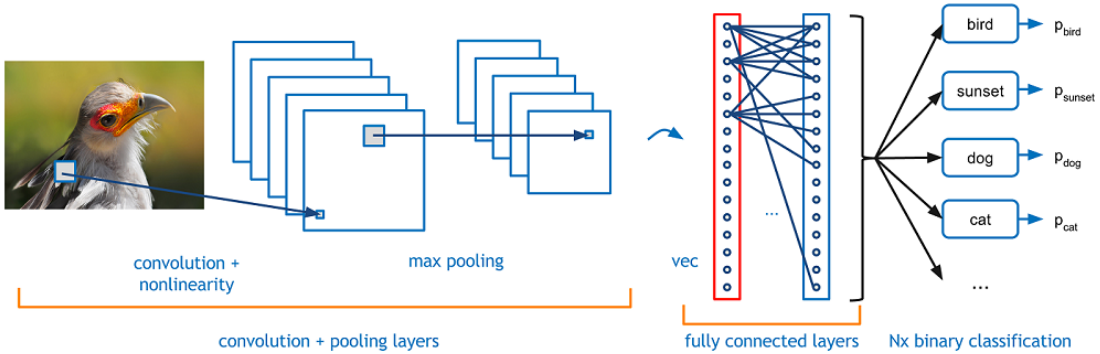


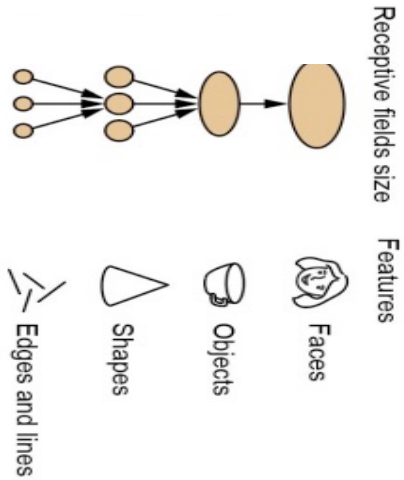


A feature map gets activated by a certain structure of the feature maps one layer below, which by itself depends on the input of a preceding layer etc and finally on the input image. Activation maps close to the input image are activated by simple structures in the image, higher maps by more complex image structures.

Weak analogies between brain and CNNs architecture



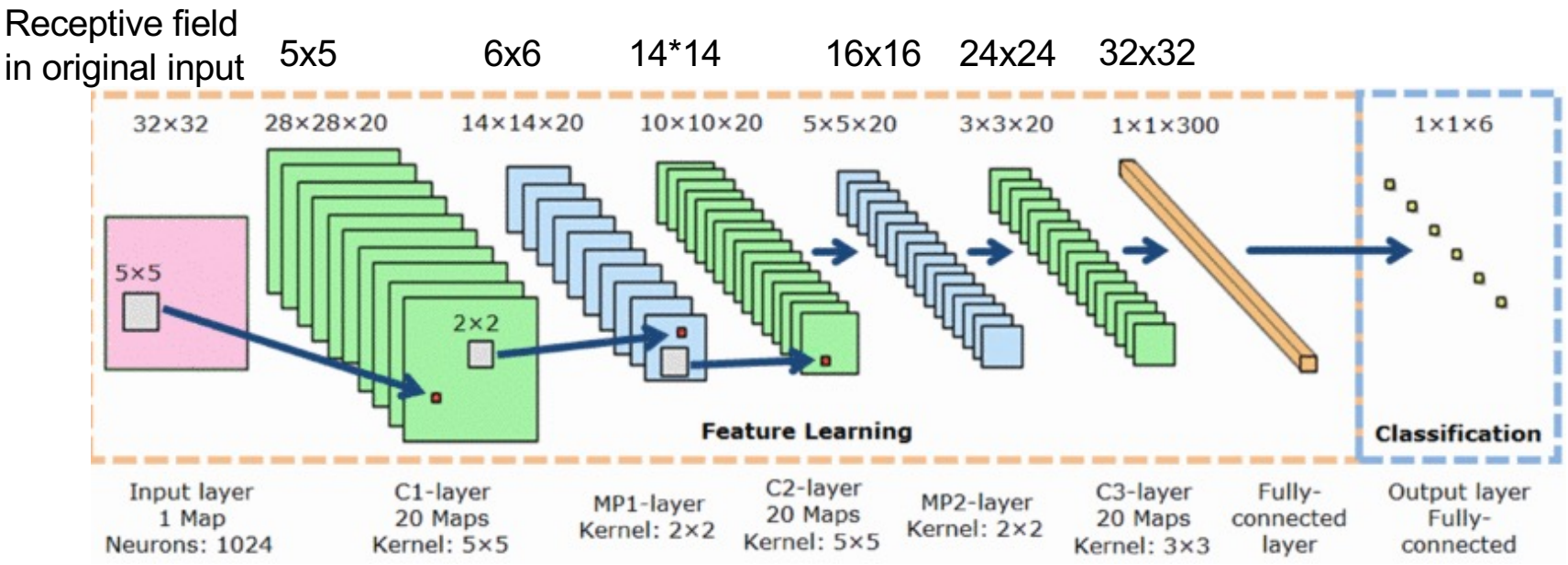




What input does activate a feature map in the CNN part or a neuron in the last layer?

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”.

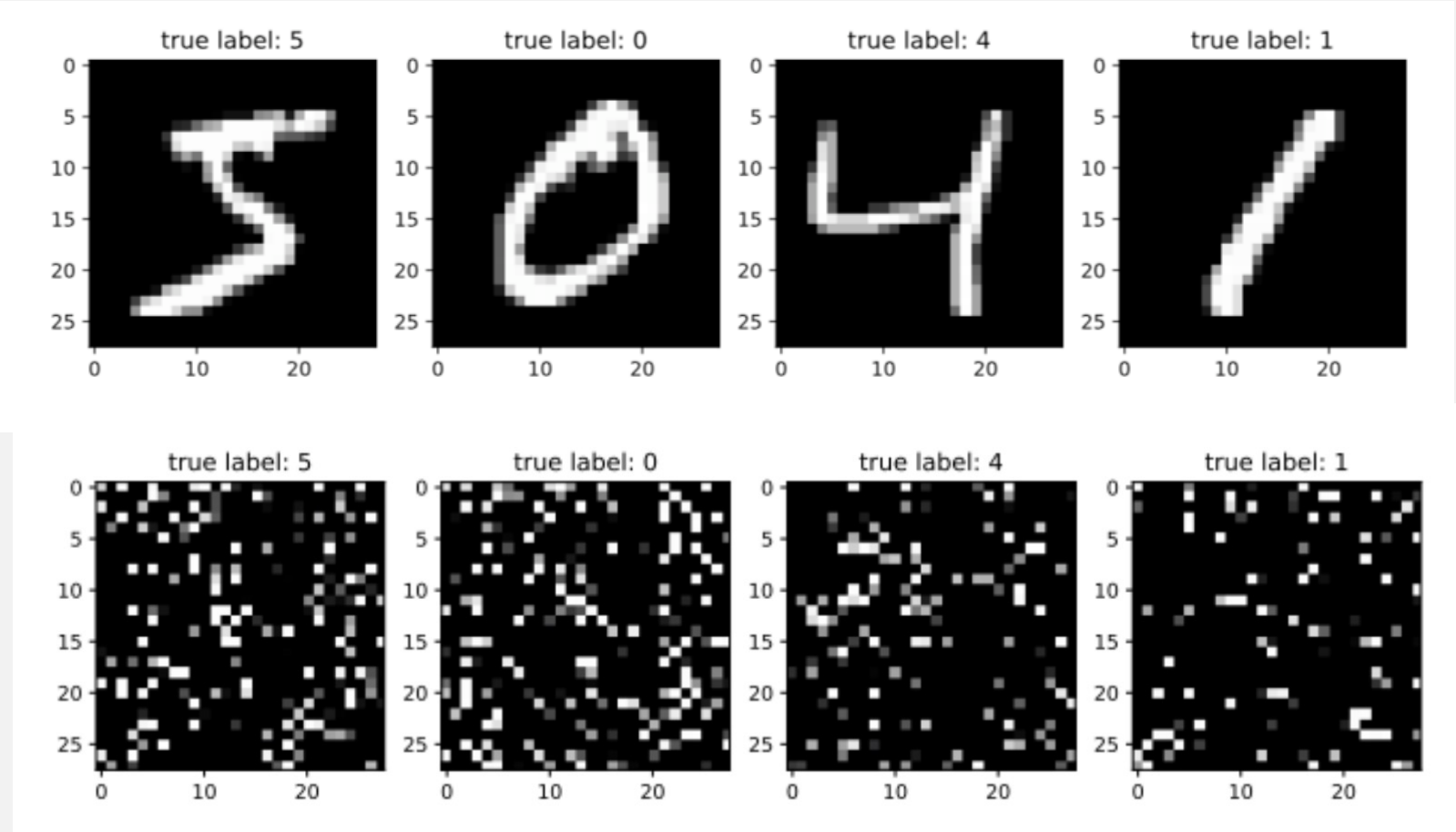


Neurons from feature maps in higher layers have a larger receptive field than neurons sitting in feature maps closer to the input.

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

Figure credits: http://pubs.sciepub.com/ajme/2/7/9/figs

Ufzgi: Does shuffling disturb a fcNN or CNN?



Investigate if shuffling disturbs the fcNN for MNIST:
04_fcnn_mnist_shuffled.ipynb
Investigate if shuffling disturbs the CNN for MNIST:
06_cnn_mnist_shuffled.ipynb

Summary

- Use loss curves to detect overfitting or underfitting problems
- NNs work best when respecting the underlying structure of the data.
  - Use fully connected NN for tabular data
  - Use convolutional NN for data with local order such as images
- CNNs exploit the local structure of images by local connections and shared weight (same kernel is applied at each position of the image).
- Use the ReLu activation function for hidden layers in CNNs.
- 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