MY474: Applied Machine Learning for Social Science

Lecture 10: Introduction to Neural Networks

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Weeks 9 - 11

1. Bagging, random forests, and boosting
2. Unsupervised learning
3. **Neural networks**

Outline

1. Introduction
2. Fundamental architectures
3. Training
4. In practise
5. Variants
6. Guided coding

1. Introduction

This lecture

- Tries to give a high level overview of many topics around neural networks and deep learning
- Due to the short amount of time, concepts can only be mentioned briefly
- In addition to giving an overview, the approach hopefully allows students to identify topics that can be of interest for further study

Some history

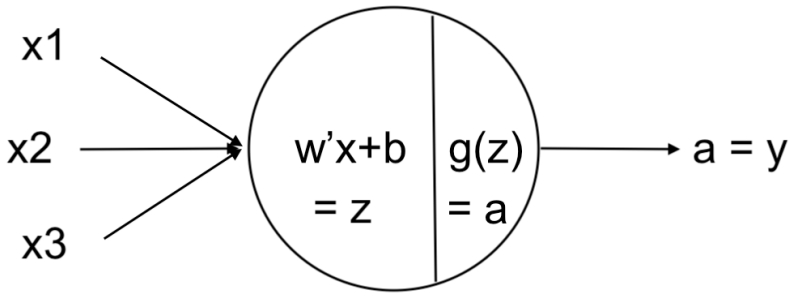
- McCulloch and Pitts (1943) created a computational model for neural networks
- Research on the topic continued throughout the 20th century, however, at times as a niche field
- In the early 21st century the models began to outperform others at a large scale
- For example AlexNet, a convolutional neural network, won the ImageNet (an image classification) competition in 2012 by a very high margin (for many researchers at the time that was unexpected)
- The paper has been cited almost 80,000 times since then

Why have neural networks become so important in recent years

- Data: Much more (labeled) data available
- Hardware: Faster computation; extensive use of GPUs
- Software: Improved architectures, libraries, optimisation algorithms, etc.

2. Fundamental architectures

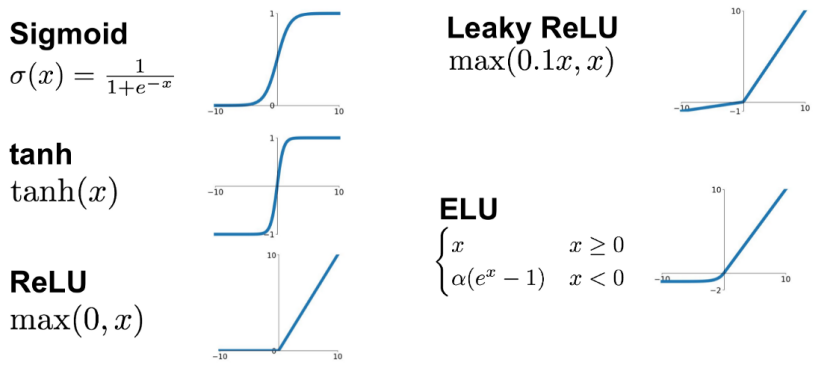
Single layer perceptron



- $z = x'w + b$ with $w = (w_1, w_2, w_3)$
- $a = g(z)$
- $g(z)$ is called an "activation function"
- Neurons (nodes) in these commonly shown figures actually depict both z and a

Activation functions

- Activation functions introduce non-linearities
- Stacking only linear layers would just create a linear model
- Today, the benchmark activation/nonlinearity is often ReLU (rectified linear unit) which has advantages for learning due to its constant positive gradient for positive inputs
- Sigmoid had been used earlier, but often suffers from close to zero gradients and can imply very slow learning



Some common activation functions. Image from Jadon (2018)

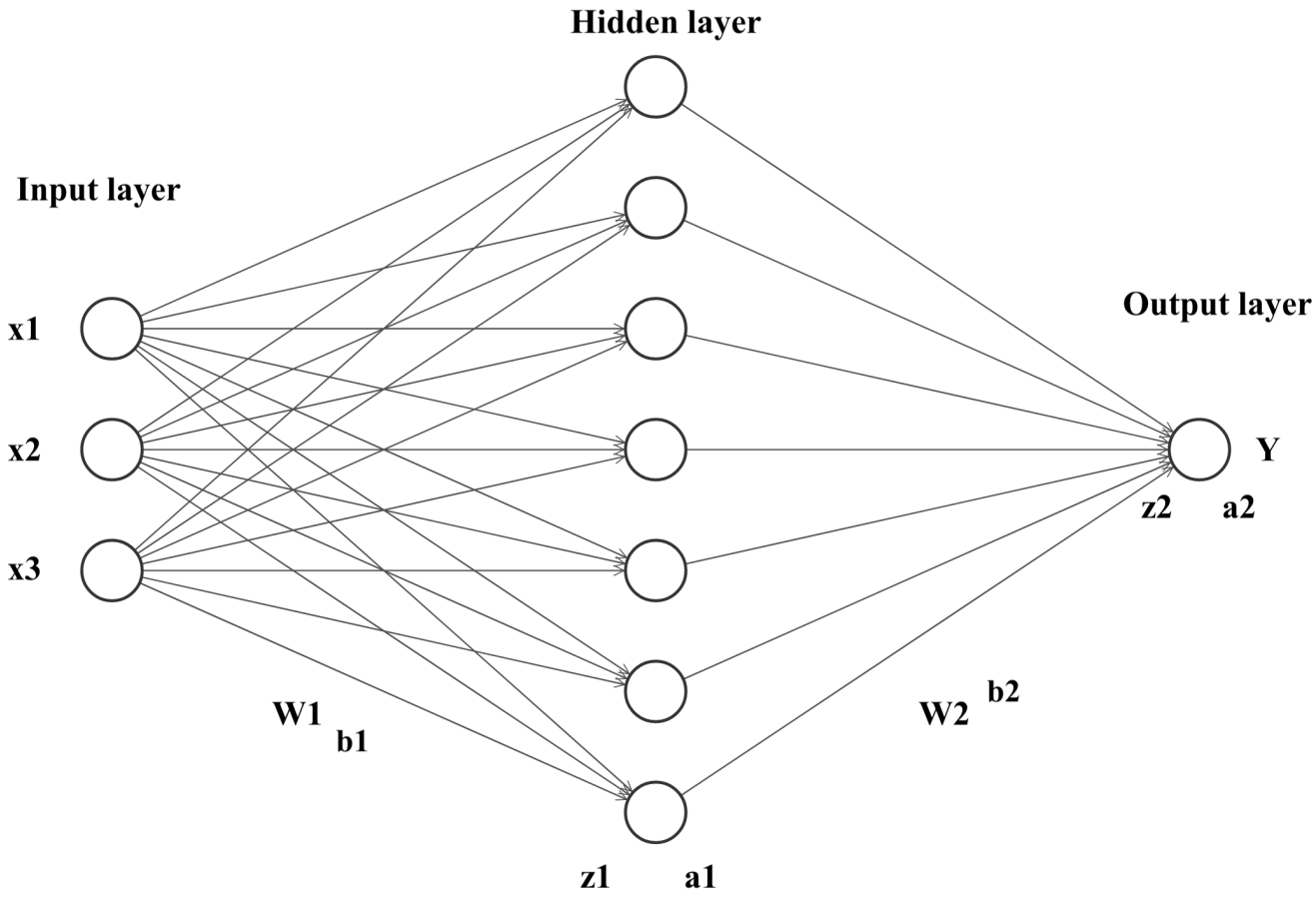
Limitations

- A single layer perceptron can already perform well in some classification tasks
- Yet, it can only correctly classify observations that are linearly separable
- Good website for building intuition
  https://playground.tensorflow.org/

Multi layer perceptron

- We generally count hidden and output layers, so a network with one hidden and one output later is already a multi layer perceptron (MLP)
- Cells are called neurons, layers with many neurons are called *wide* and with few neurons are called *narrow*
- Network with few hidden layers are called *shallow*
- Networks with many hidden layers are called *deep*

MLP with one hidden layer

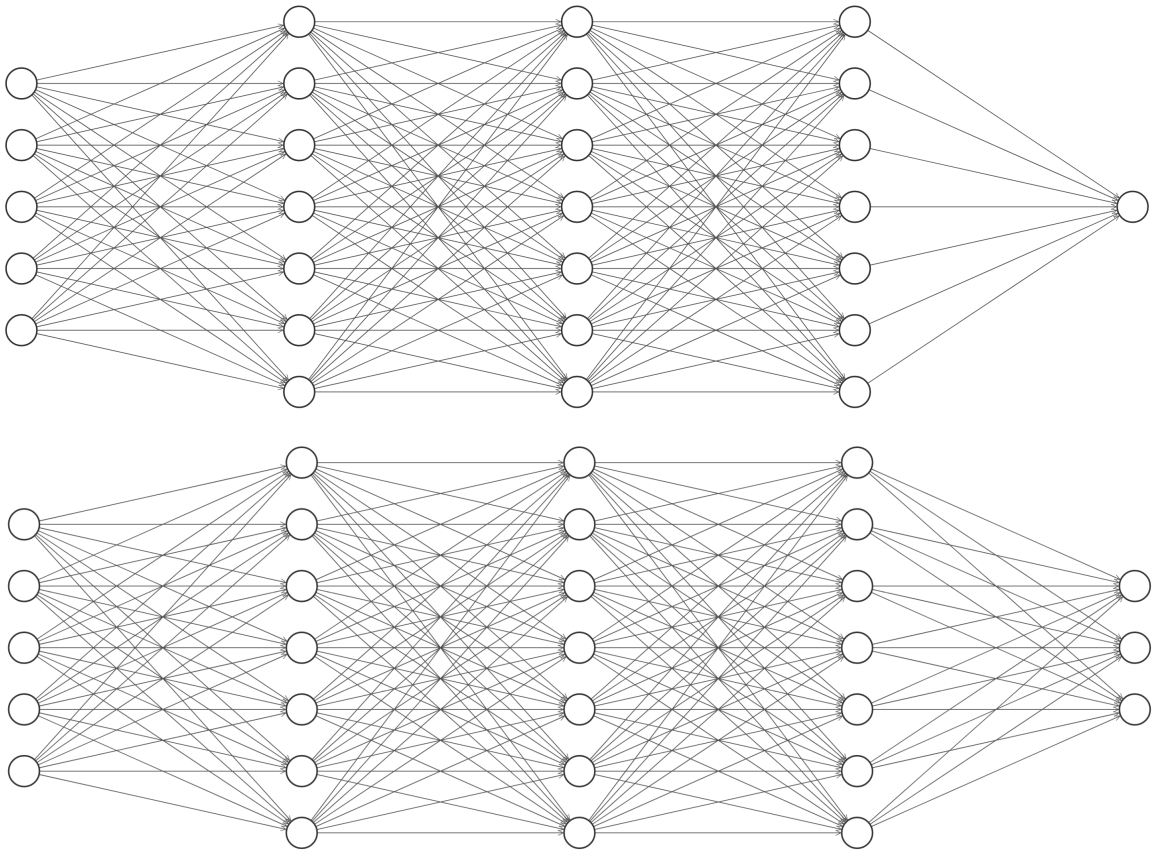


Drawn with http://alexlenail.me/NN-SVG/index.html and annotated

MLP with one hidden layer

- Input layer: $\underbrace{x}_{3\times 1}$
- Hidden layer z: $\underbrace{W^{(1)}}_{7\times 3}\underbrace{x}_{3\times 1}+\underbrace{b^{(1)}}_{7\times 1}=\underbrace{z^{(1)}}_{7\times 1}$
- Hidden layer activation: $\underbrace{a^{(1)}}_{7\times 1}=\underbrace{g(z^{(1)})}_{7\times 1}$ (applied element-wise)
- Output layer z: $\underbrace{W^{(2)}}_{1\times 7}\underbrace{a^{(1)}}_{7\times 1}+\underbrace{b^{(2)}}_{1\times 1}=\underbrace{z^{(2)}}_{1\times 1}$
- Output layer activation: $\underbrace{g(z^{(2)})}_{1\times 1}=\underbrace{a^{(2)}}_{1\times 1}=\underbrace{\hat{y}}_{1\times 1}$
- Expressed in one piece:
  $x \underbrace{\rightarrow}_{W^{(1)},b^{(1)}} z^{(1)} \underbrace{\rightarrow}_{g(\cdot)} a^{(1)} \underbrace{\rightarrow}_{W^{(2)},b^{(2)}} z^{(2)} \underbrace{\rightarrow}_{g(\cdot)} a^{(2)}=\hat{y}$

MLP with three hidden layers



Drawn with http://alexlenail.me/NN-SVG/index.html

Regression and classification

- Neural networks are used for both regression and classification
- Most commonly for regression, the activation function of the last layer is linear, i.e. $g(z) = z$
- For two class classification, it is usually sigmoid, i.e. $g(z) = \frac{1}{1+e^{-z}}$
- For multi class classification its generalisation is used, the softmax: $g(z_i) = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$

Universal approximation theorem

- In fact, an important theorem states that, under some regularity conditions, already a single hidden layer neural network can approximate continuous functions, that map from $[0, 1]^K$ to the real number line, arbitrarily closely (see Cybenko, 1989, and Hornik, 1991)
- Note that this said nothing about the how we can practically find the optimal weights of such a network, just that it exists

Deep vs shallow networks

- Why do researchers then generally prefer deep networks over very wide one hidden layer networks?
- Because they have been found to outperform shallow networks empirically
- Montúfar et al., 2014 also provide theoretical evidence why the ability to separate observations in features space can react more quickly to adding depth than width

3. Training

Loss

- To train the neural network, we first need to define a loss function
- Typical loss for observation i in regression: Squared error $L(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$
- Typical loss for observation i classification: Cross entropy $L(y_i, \hat{y}_i) = -\sum_{k=1}^{K} y_{i,k} log(\hat{y}_{i,k})$

Cost

- One convention in the field is to name the loss aggregated over training observations the *cost function*
- Summarise all weights, $W^{(1)}, W^{(2)}, \ldots$ and biases $b^{(1)}, b^{(2)}, \ldots$ in one vector θ for convenience
- $J(\theta) = \frac{1}{n} \sum_{i=1}^{n} L(y_i, f(x_i, \theta))$

Backpropagation

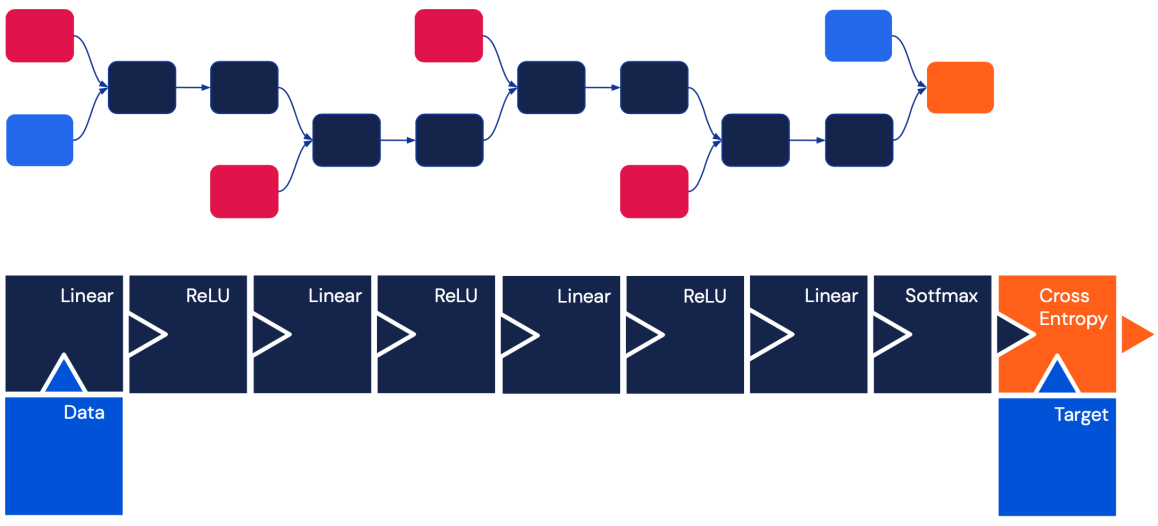
- Next we need to derive the gradient vector of the cost function
- This is done with the backpropagation algorithm
- Recall as an example the structure of a shallow neural network with one hidden layer:
- $x \underbrace{\rightarrow}_{W^{(1)},b^{(1)}} z^{(1)} \underbrace{\rightarrow}_{g(\cdot)} a^{(1)} \underbrace{\rightarrow}_{W^{(2)},b^{(2)}} z^{(2)} \underbrace{\rightarrow}_{g(\cdot)} a^{(2)} = \hat{y}$
- Furthermore, recall the chain rule: If $f(g(x))$, then $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial x}$

Backpropagation

- Carried over from the last slide. Forward pass:
  $x \underbrace{\rightarrow}_{W^{(1)},b^{(1)}} z^{(1)} \underbrace{\rightarrow}_{g(\cdot)} a^{(1)} \underbrace{\rightarrow}_{W^{(2)},b^{(2)}} z^{(2)} \underbrace{\rightarrow}_{g(\cdot)} a^{(2)} = \hat{y}$ Backward:
  $x \underbrace{\leftarrow}_{W^{(1)},b^{(1)}} z^{(1)} \underbrace{\leftarrow}_{g(\cdot)} a^{(1)} \underbrace{\leftarrow}_{W^{(2)},b^{(2)}} z^{(2)} \underbrace{\leftarrow}_{g(\cdot)} a^{(2)} = \hat{y}$
- Thus, we get:
- $\frac{\partial J(\theta)}{\partial W^{(2)}} = \frac{\partial J(\theta)}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial W^{(2)}}$
- $\frac{\partial J(\theta)}{\partial b^{(2)}} = \frac{\partial J(\theta)}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial b^{(2)}}$
- $\frac{\partial J(\theta)}{\partial W^{(1)}} = \frac{\partial J(\theta)}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial W^{(1)}}$
- $\frac{\partial J(\theta)}{\partial b^{(1)}} = \frac{\partial J(\theta)}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial b^{(1)}}$
- Combine to get $\frac{\partial J(\theta)}{\partial \theta}$ or $\nabla_\theta J(\theta)$

Computation graphs

- Modern libraries such as Tensorflow depict networks as computation graphs
- The gradients they compute flow through the individual elements of that graph
- This modular structure allows to easily process gradients in much more complex architecture than the one shown below



From Czarnecki (2020)

Gradient descent

- Computing the gradient for the entire dataset (full batch gradient descent) is usually computationally infeasible
- Instead, we approximate the gradient of the full training data with either the gradient of a single observations (stochastic gradient descent) or with the gradient over a small batch of data (mini batch gradient descent)
- Importantly, note that as loss functions for neural networks are mostly non convex, these algorithms converge to local optima, but not global ones

Stochastic gradient descent (SGD)

- Randomly initialise weights and choose learning rate α
- Repeate the following for E epochs or until approximate convergence:
  - Shuffle all observations in the training dataset
  - For observation i $= 1,2, \ldots,$n:
    - Update $\theta \leftarrow \theta - \alpha \nabla_\theta L(y_i, f(x_i, \theta))$

Mini batch gradient descent

- Randomly initialise weights and choose learning rate α
- Repeat the following for E epochs or until approximate convergence:
  - Shuffle all observations in the training dataset
  - For each batch with $B << n$ observations:
    - Update $\theta \leftarrow \theta - \alpha \nabla_\theta \frac{1}{B} \sum_{i=1}^{B} L(y_i, f(x_i, \theta))$

Most popular optimisers

- SGD is too noisy, mini batch optimisation is the most common choice
- There are some particularly popular optimisers which have proven robust and applicable to a wide range of tasks and models, e.g. Adam or RMSprop which include moving average based momentum of gradients
- A good starting point is usually Adam

4. In practise

Regularisation

- With their very high numbers of parameters, neural networks can memorise large amounts of data and relatively easy over-fit
- Possible approaches to counter over-fitting are:
- Add norms of weights to objective function
- Dropout: Randomly set a fraction of p neurons in a layer to zero during training and thereby force a wider set of neurons to learn patterns
- Early stopping: Stop the gradient descent once the loss on some validation set increases
- Add noise to activities during training

Further approaches that can be helpful

- Batch normalisation: Batch specific normalisation of inputs or activations; can speed up training and make model more robust to changes in learning rates
- Often helpful to first fit the model to a very small sample of the data and see whether it can perfectly fit it. If not, then there are probably some issues
- Weights are randomly initialised, but initialisation matters
- Heuristics such as e.g. the "He" or "Xavier" initialisations

Hyper-parameter search

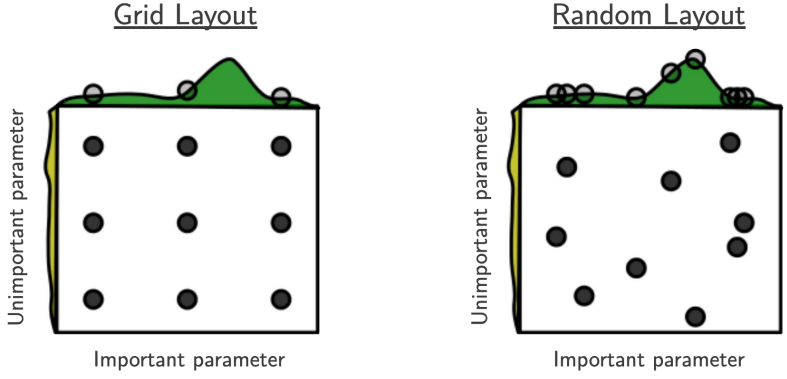
- In addition to their weights/parameters, neural networks have many so called hyper-parameters
- The amount of hidden layers, neurons per hidden layer, the learning rate, dropout percentages, degree of regularisation with norms, etc.
- Imagine you have 10 hyper-parameters and for each of them 10 possible values in mind, then you would have to search trough a grid with 10^10 possible combinations and train a model for each of them (curse of dimensionalty)

Random hyper-parameter search

- Two takeaways:

  1) Because of the curse of dimensionality, a good first approach is to search randomly and then narrow down on parts of the space that seem promising

  2) Evenly spaced out grids with pre-specified values are not usually a good idea (see figure below from Bergstra and Bengio, 2012)



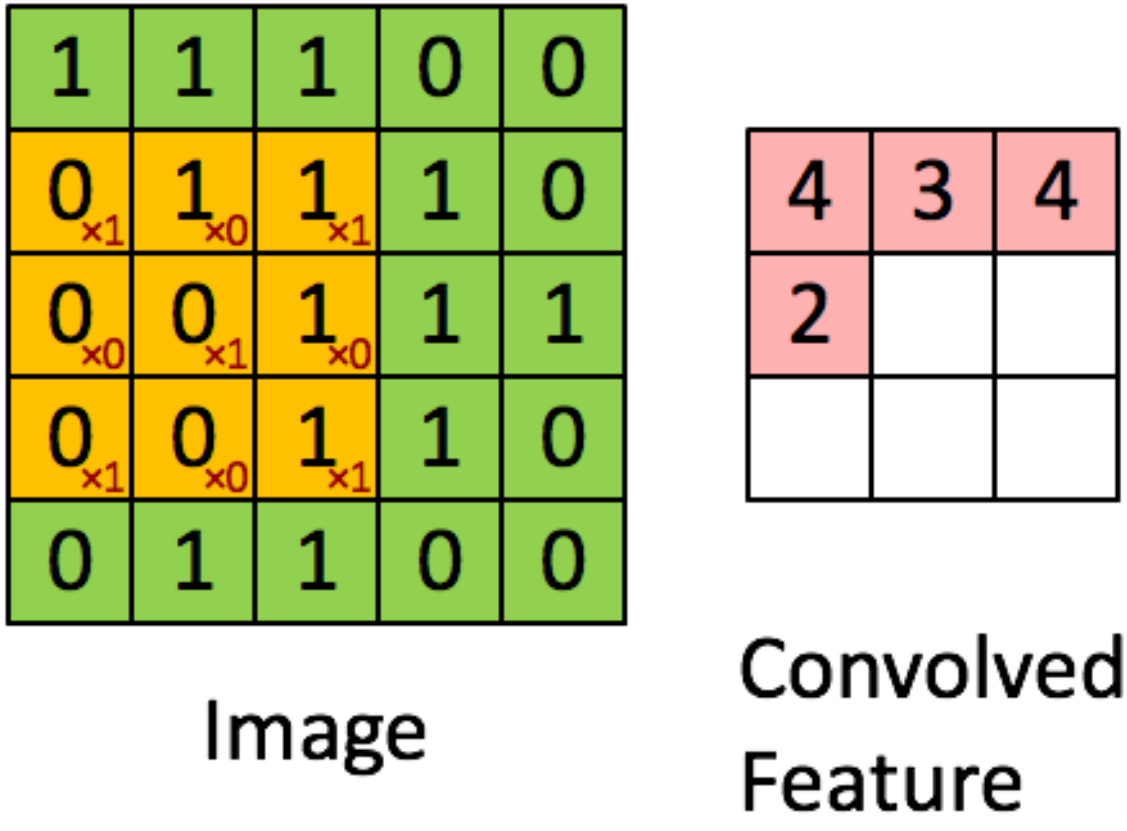
Bergstra and Bengio (2012)

5. Variants

Convolutional neural networks

- Convolutional neural networks are mainly used for computer vision
- They learn filters and combine operations such as convolutions and pooling

Convolutions with filters



From: Stanford UFLDL wiki

Filter examples

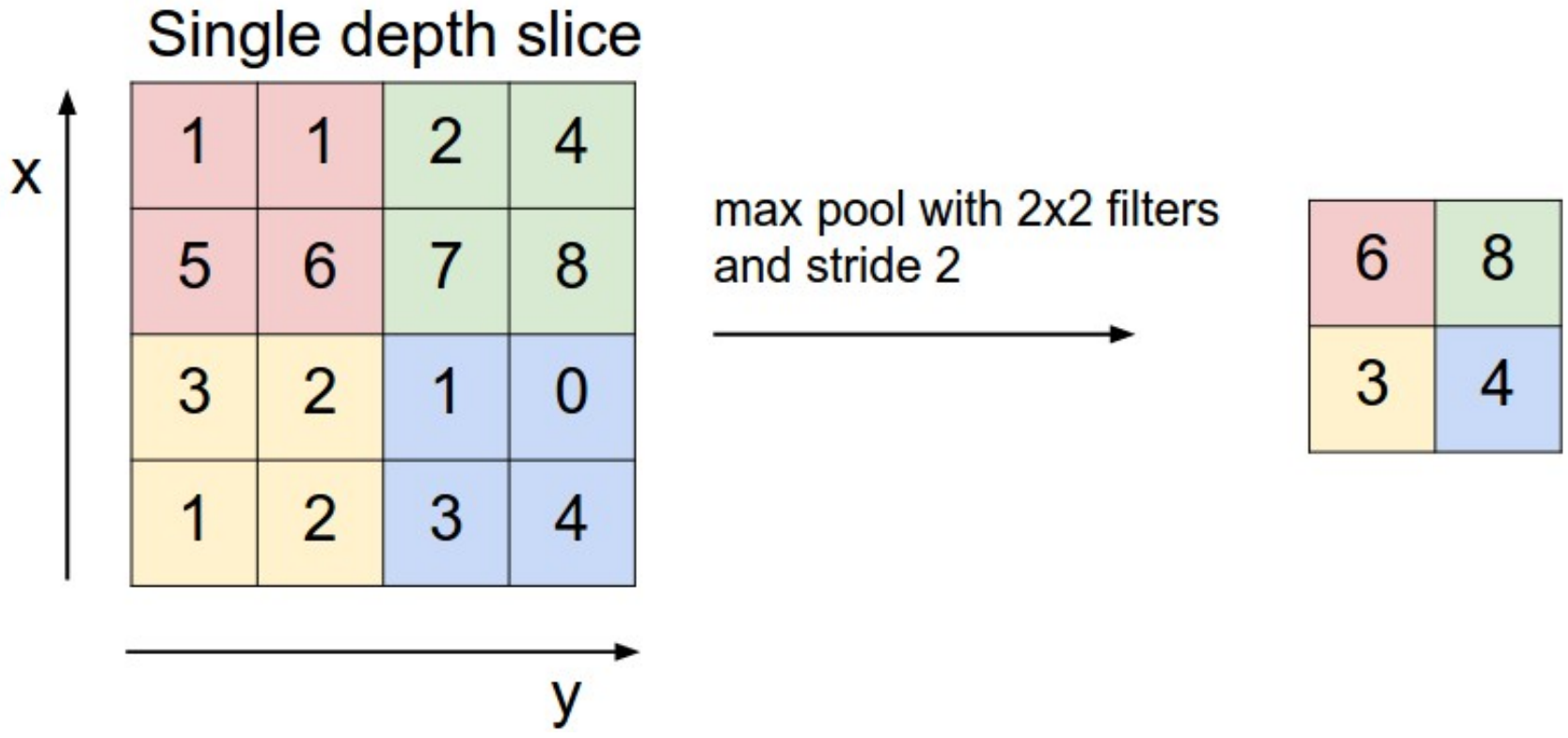
0	0	0	0	0
0	1	1	1	0
0	1	1	1	0
0	1	1	1	0
0	0	0	0	0

	0	1	0	
	1	-4	1	
	0	1	0	

From: Gimp documentation

- The first filter makes the image blury, the second one detects edges
- CNNs learn these filters through training, minimising e.g. the classification loss

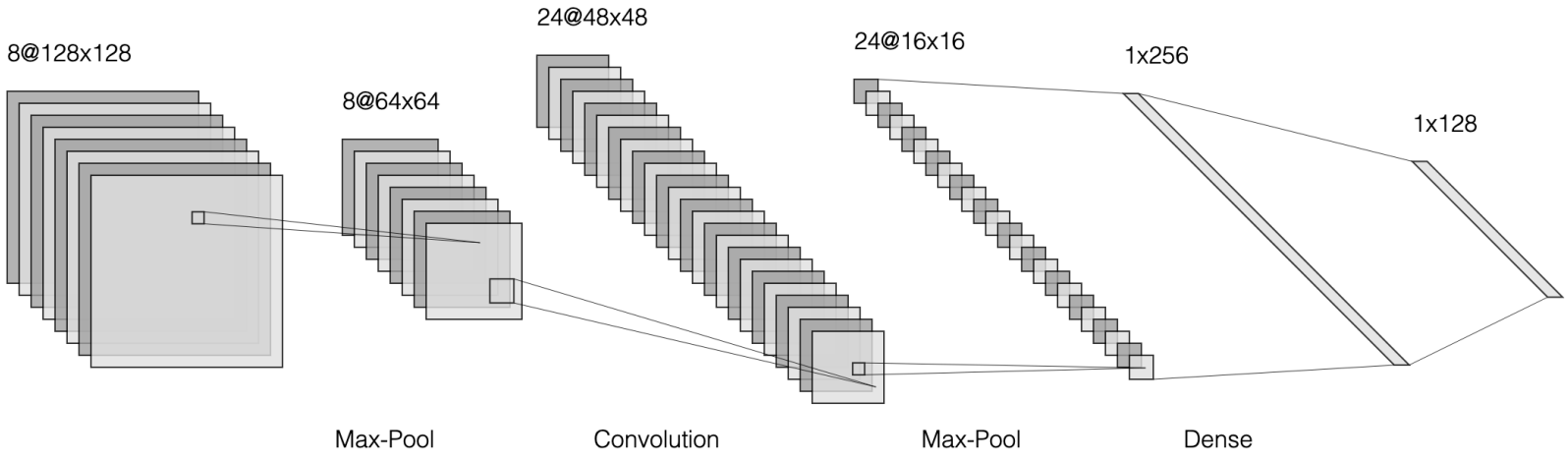
Max pooling



From: https://cs231n.github.io/convolutional-networks/

- Another option is e.g. average pooling

Exemplary CNN architecture

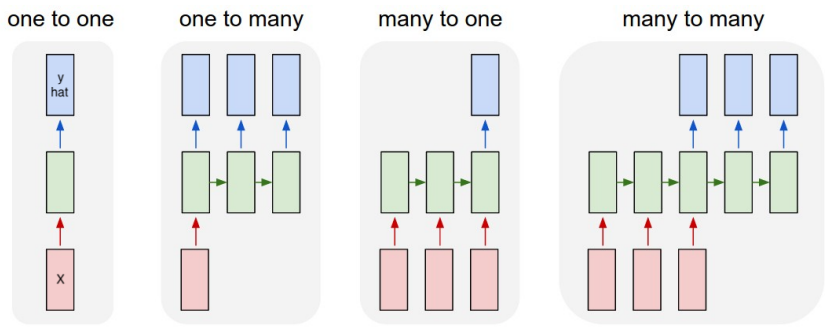


Drawn with http://alexlenail.me/NN-SVG/index.html

Recurrent neural networks

- Recurrent neural networks (RNNs) can process sequences of inputs and predict sequences of outputs
- RNNs are e.g. used in machine translation, sentence completion, sentiment analysis, image captioning, etc.
- Common types of RNNs such as Long Short-Term Memory (LSTM) or Gated Recurrent Unit (GRU) are based on cells which improve the model's ability to remember long term dependencies

Recurrent neural networks



From Andrej Karpathy's blog; slightly edited

- Arrows are functions/transformations, rectangles are vectors, green rectangles hold states
- One to one: Standard feed forward neural network/MLP
- One to many: RNN that e.g. takes an image as input and then outputs a sentence describing it
- Many to one: RNN that e.g. inputs a sequence of words and outputs a sentiment label
- Many to many: RNN that e.g. inputs a sentence in one language and outputs it in another language

Generative adversarial networks (GANs)

- Consist of a pair of neural networks, a generator and a discriminator
- The generator generates samples (e.g. images, music, artwork etc.) and the discriminator has to distinguish these fake samples from a set of true samples
- Through training, the samples produced by the generator can become very realistic
- https://thispersondoesnotexist.com/ by Wang (2019)

6. Guided coding

Neural network libraries in R

- More libraries in Python for neural networks, but increasing support also for R:
- 1. **TensorFlow** and **Keras**: https://tensorflow.rstudio.com/tutorials/ and https://keras.rstudio.com/
- 2. **PyTorch**: https://torch.mlverse.org/start/
- Excellent repo with many baseline models in Keras for R (also used in coding examples): https://github.com/rstudio/keras/tree/master/vignettes/examples

R files

- 01-mlp.Rmd
- 02-cnn.Rmd

References

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