WBL Deep Learning:: Lecture 1

Beate Sick, Oliver Dürr

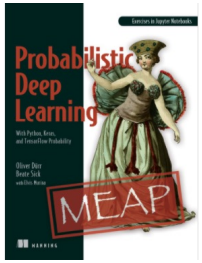
Lecture 1: Introduction and technicalities

Zürich, 9/12/2022

Literature

- Additional Course website
  - https://tensorchiefs.github.io/dl_rcourse_2022/

- Probabilistic Deep Learning (Manning in production)
  - Our probabilistic take
  - https://www.manning.com/books/probabilistic-deep-learning?a_aid=probabilistic_deep_learning&a_bid=78e55885



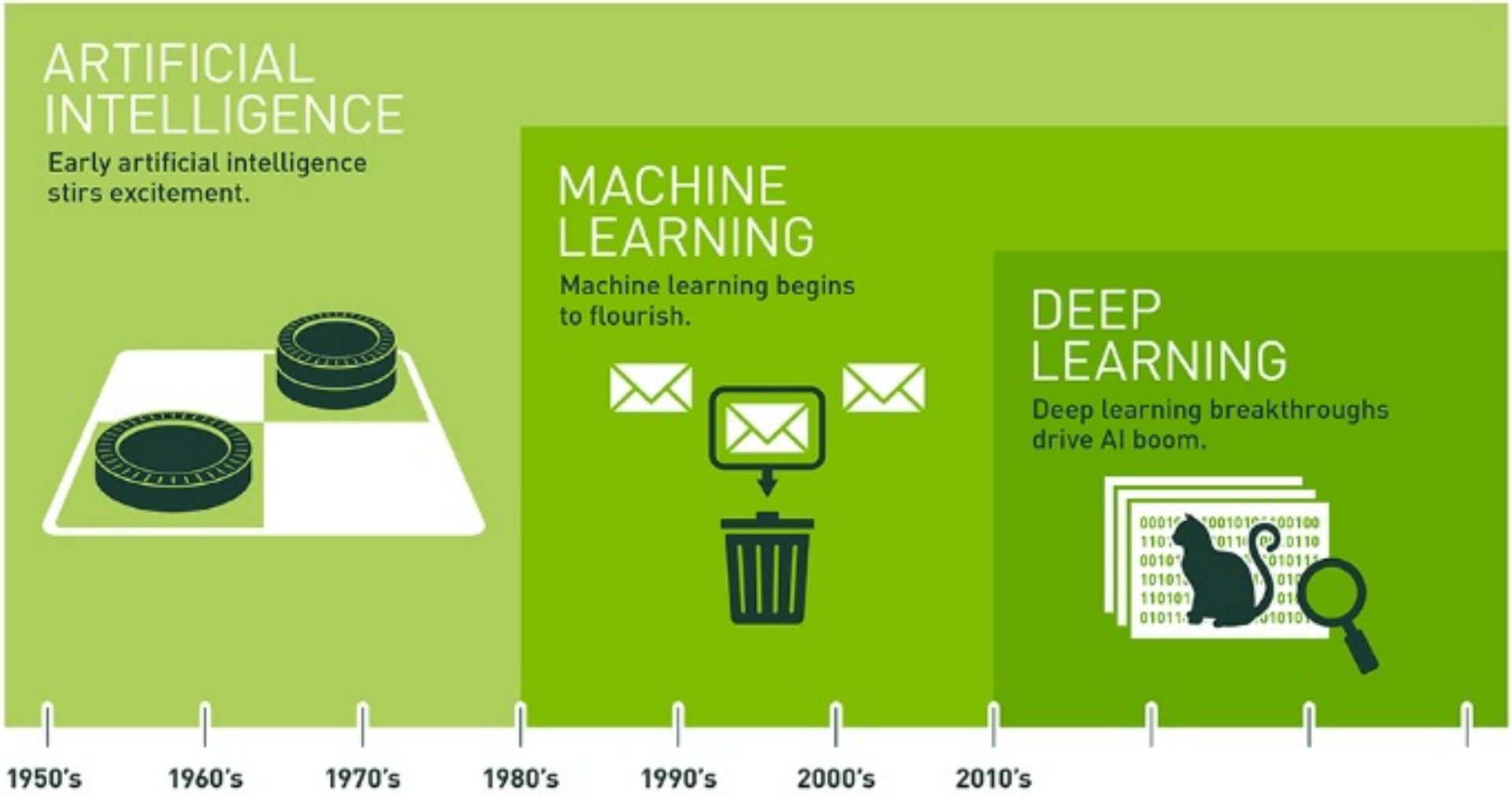
- Deep Learning Book (DL-Book) http://www.deeplearningbook.org/. This is a quite comprehensive book which goes far beyond the scope of this course.

- Courses
  - Convolutional Neural Networks for Visual Recognition http://cs231n.stanford.edu

  - Martin Görner (very practical)
    - https://cloud.google.com/blog/products/gcp/learn-tensorflow-and-deep-learning-without-a-phd

Introduction to Deep Learning --what's the hype about?

AI, Machine Learning, Deep Learning



Slide credit: https://www.datasciencecentral.com/profiles/blogs/artificial-intelligence-vs-machine-learning-vs-deep-learning

Machine Perception

- Computers have been quite bad in perceptual tasks which are easy for humans.
  - Images
  - Text
  - Sound

- A Kaggle contest 2012

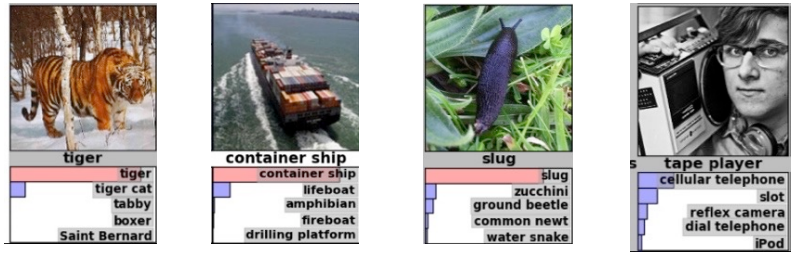
Kaggle dog vs cat competition

Deep Blue beat Kasparov at chess in 1997.
Watson beat the brightest trivia minds at Jeopardy in 2011.
Can you tell Fido from Mittens in 2013?

What happened, to solve the problem?

Deep Learning Success Story: ImageNet 2012, 2013, 2014, 2015

1000 classes
1 Mio samples



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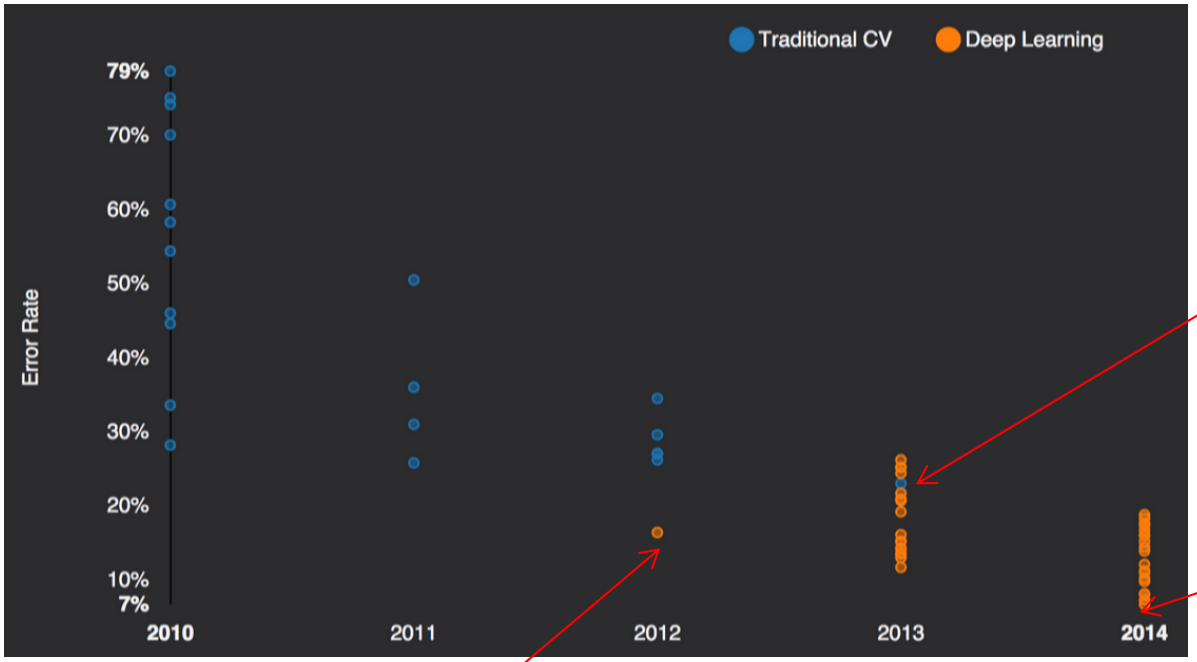


Human: 5% misclassification

Only one non-CNN approach in 2013

GoogLeNet 6.7%

A. Krizhevsky
first CNN in 2012
Und es hat zoom gemacht

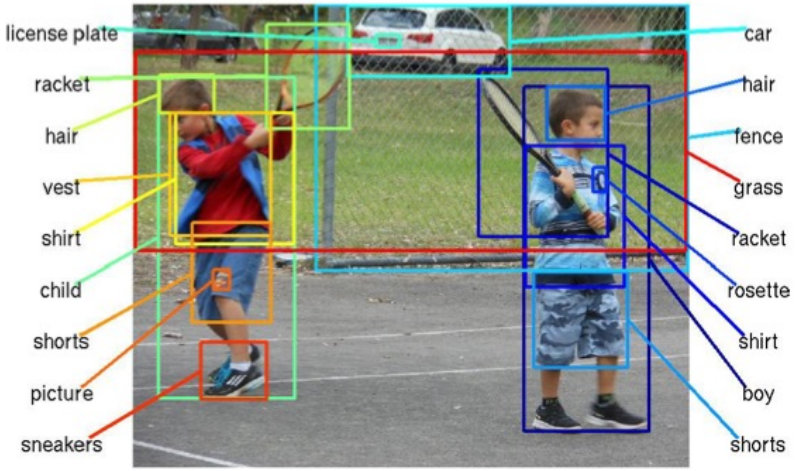
2015: It gets tougher

- 4.95% Microsoft (Feb 6 surpassing human performance 5.1%)
- 4.8% Google (Feb 11) -> further improved to 3.6 (Dec)?
- 4.58% Baidu (May 11 banned due too many submissions)
- 3.57% Microsoft (Resnet winner 2015)

Figure: https://medium.com/global-silicon-valley/machine-learning-yesterday-today-tomorrow-3d3023c7b519

Deep Learning successes

- With DL it took approx. 3 years to solve object detection and other computer vision task



"man in black shirt is playing guitar."

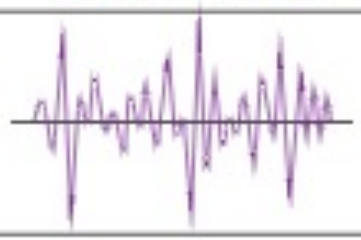
- Further examples

DeepL

...

Images form cs229n

Use cases of deep learning

Input x to DL model	Output y of DL model	Application
Images 	Label "Tiger"	Image classification
Audio 	Sequence / Text "see you tomorrow"	Voice recognition
ASCII-Sequences "Hallo, wie gehts?"	Unicode-Sequences "你好，你好吗?"	Translation
ASCII-Sequence This movie was rather good	Label (Sentiment) positive	Sentiment analysis

Deep Learning öffnet Tür zu hören, sehen und Texten. (kein Verstehen aber statistische Zusammenhänge).

Source: Oliver Dürr, Beate Sick, Elvis Murina probabilistic deep learning, Manning

Deep Learning vs. Machine Learning

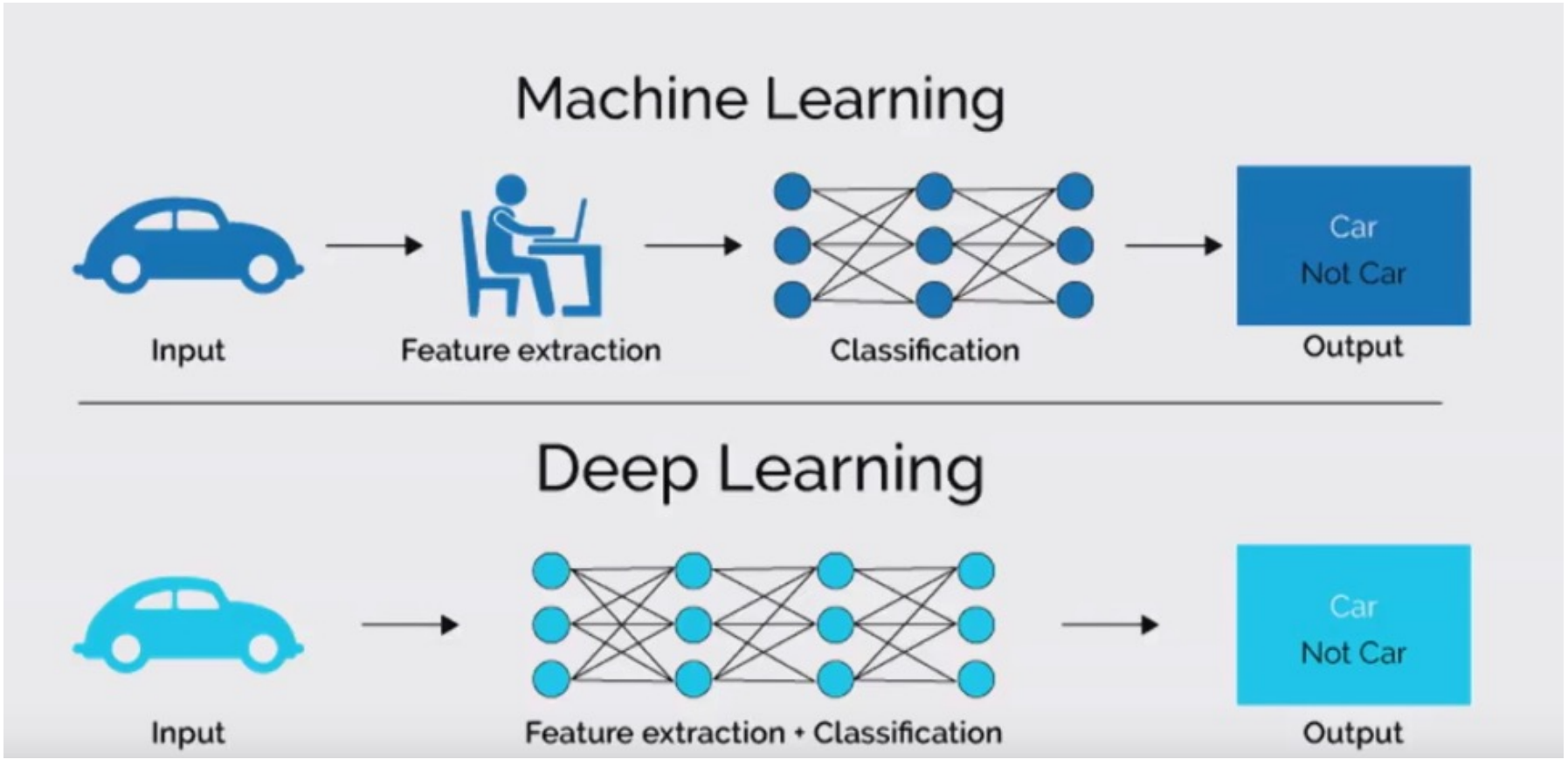
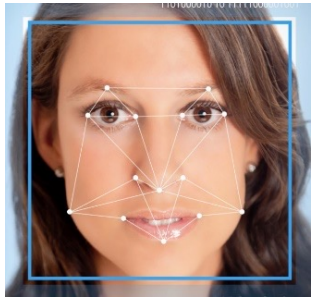


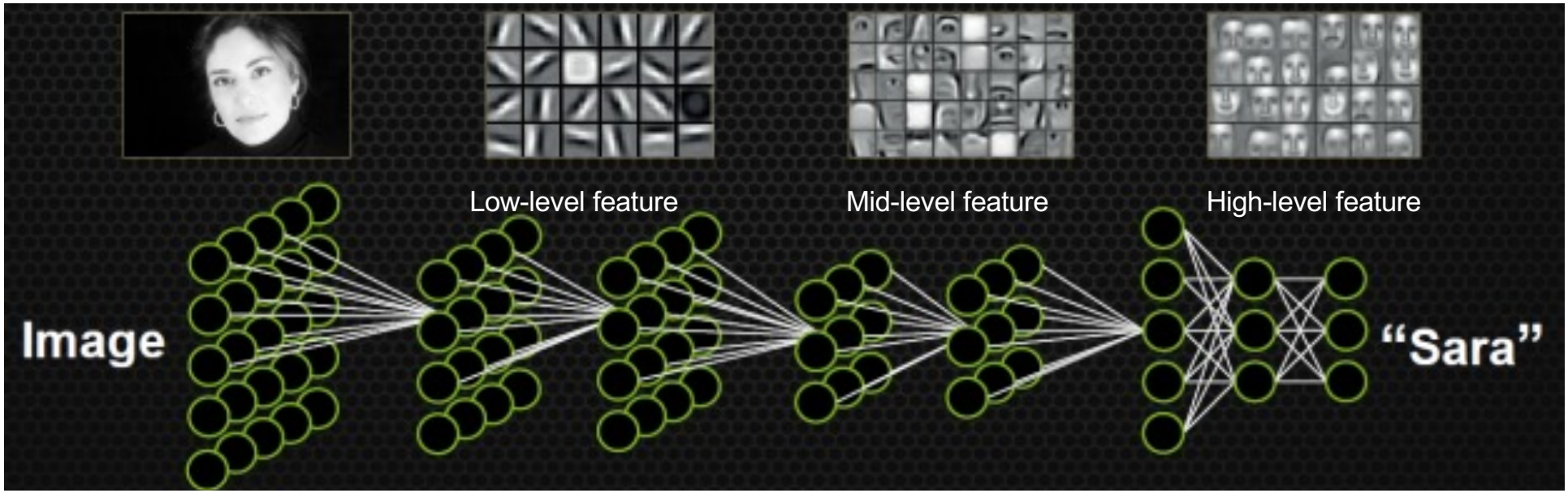
image credit: Siraj Raval

What is new in the deep learning approach?



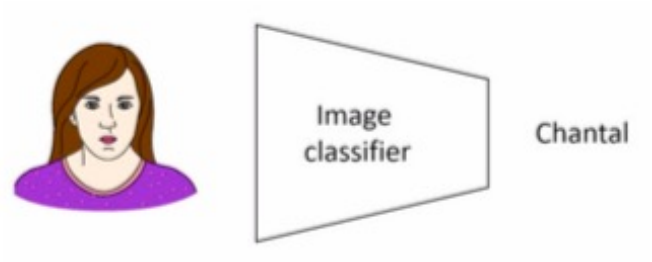
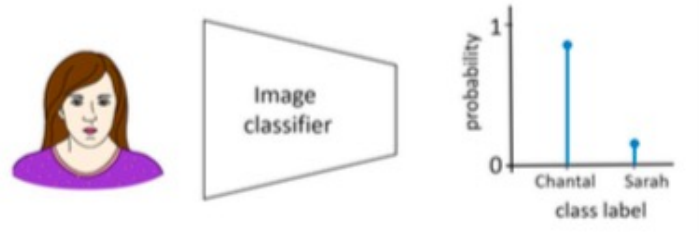
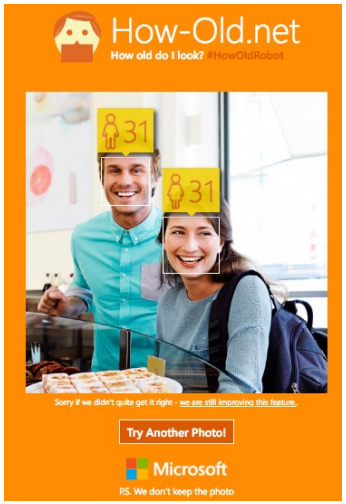
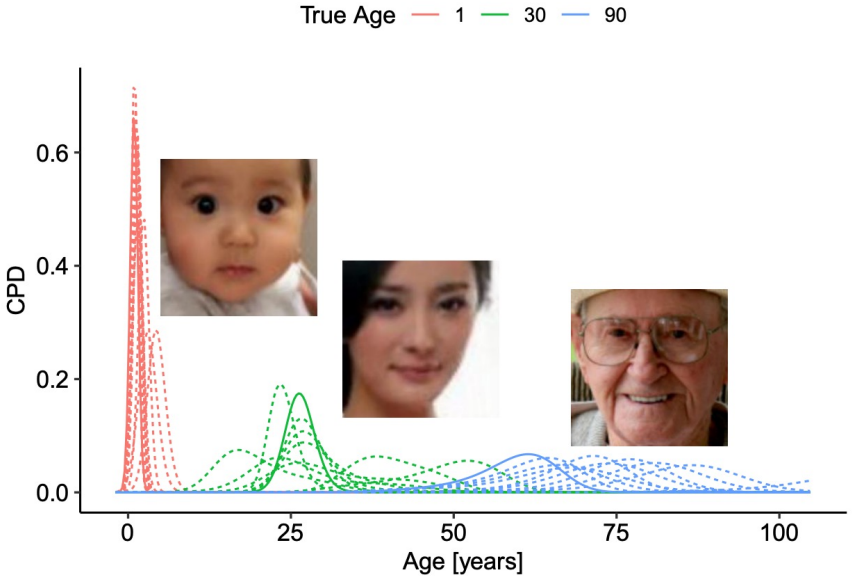
Traditional ML:
Extract handcrafted features & use these features to train / fit a model (e.g. SVM, RF) and use fitted model to perform classification/prediction.

Deep learning (end-to-end approach)
Deep neural networks start with raw data and learn during training/fitting to extract appropriate hierarchical features and to use them for classification/prediction.



Focus in this lectures: Probabilistic Viewpoint

Probabilistic vs deterministic models

	Deterministic	Probabilistic
"Classification"		
"Regression"		

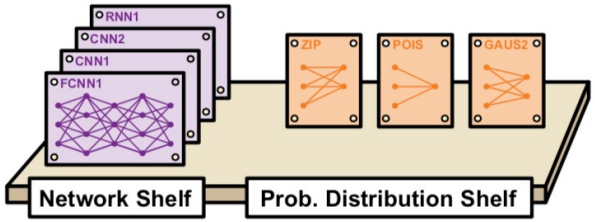
Conditional probability distribution (CPD)

$p(y|x)$

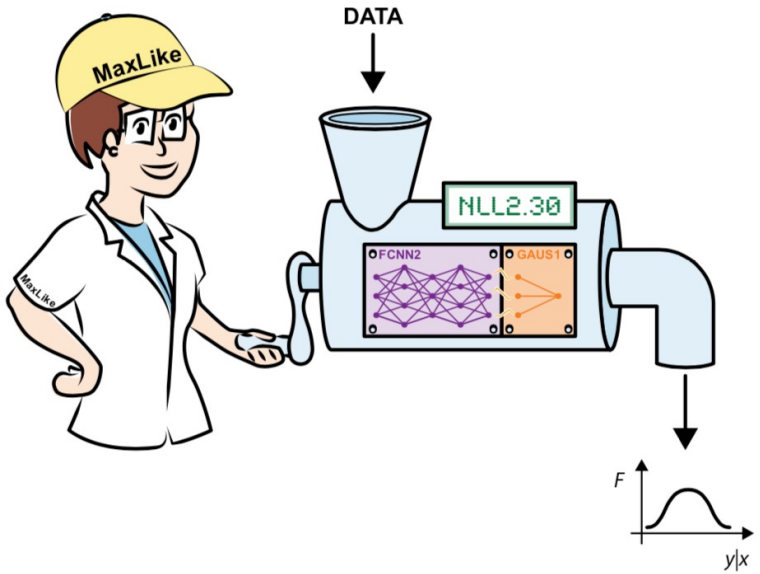
Guiding Theme of the course

- We treat DL as *probabilistic models*, as a continuation of GLMs (logistic regression, ...) for CPD $p(y|x)$
- The models are fitted to training data with maximum likelihood (or Bayes)

Special networks for x
- Vector FCNN
- Image CNN
- Text CNN/RNN



Special heads for y
- Classes
- Regression



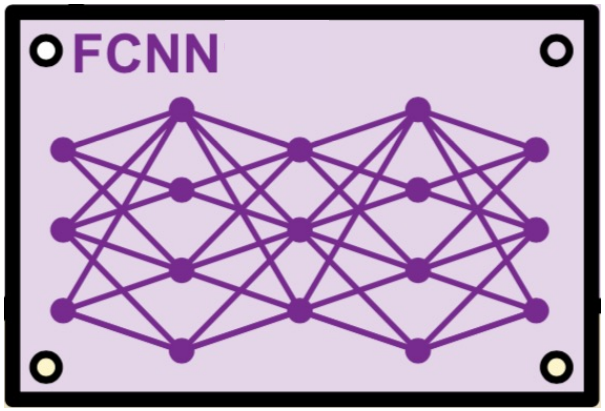
Dates

Date	Lectures
12.09.2022	L1 (10:15-12:00), L2 (14:15-16:00) and Exercises (16:15-18:00)
19.09.2022	L3 (14:15-16:00) and Exercises (16:15-18:00)
26.09.2022	L4 (14:15-16:00) and Exercises (16:15-18:00)
03.10.2022	This day is reserved to work on your projects
10.10.2022	L5 and presentatation of the projects

There will be also small exercises during the lectures

Topics

- Lecture 1
  - Introduction to DL
  - Fully connected neural Networks (fcNN)
  - Introduction to TensorFlow and Keras
- Lecture 2
  - Convolutional Neural Networks (CNN) for image data
  - Classification and Regression with fcNN and CNNs
- Lecture 3
  - Probabilistic DL
  - Extending the GLM with DL for scalar features and image data
- Lecture 4,5 (Not 100% sure yet)
  - Extending deep GLMs by deep transformation models
  - Deep interpretable ordinal regression models



Fully Connected Neural Networks
FCNN

The Single Cell: Biological Motivation

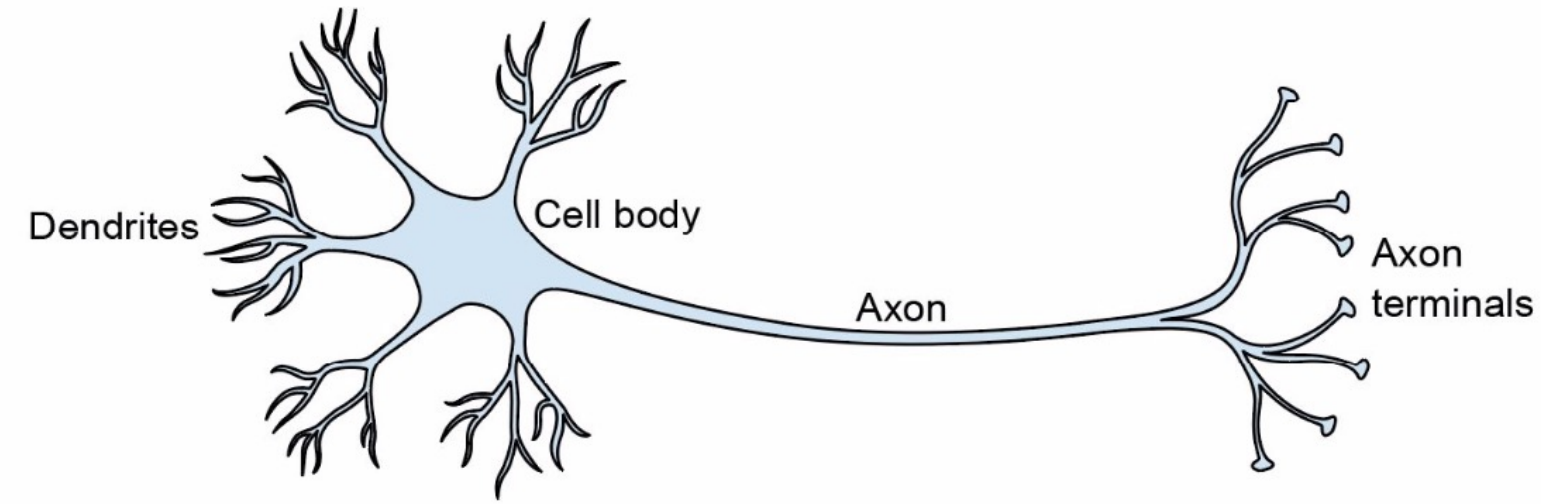
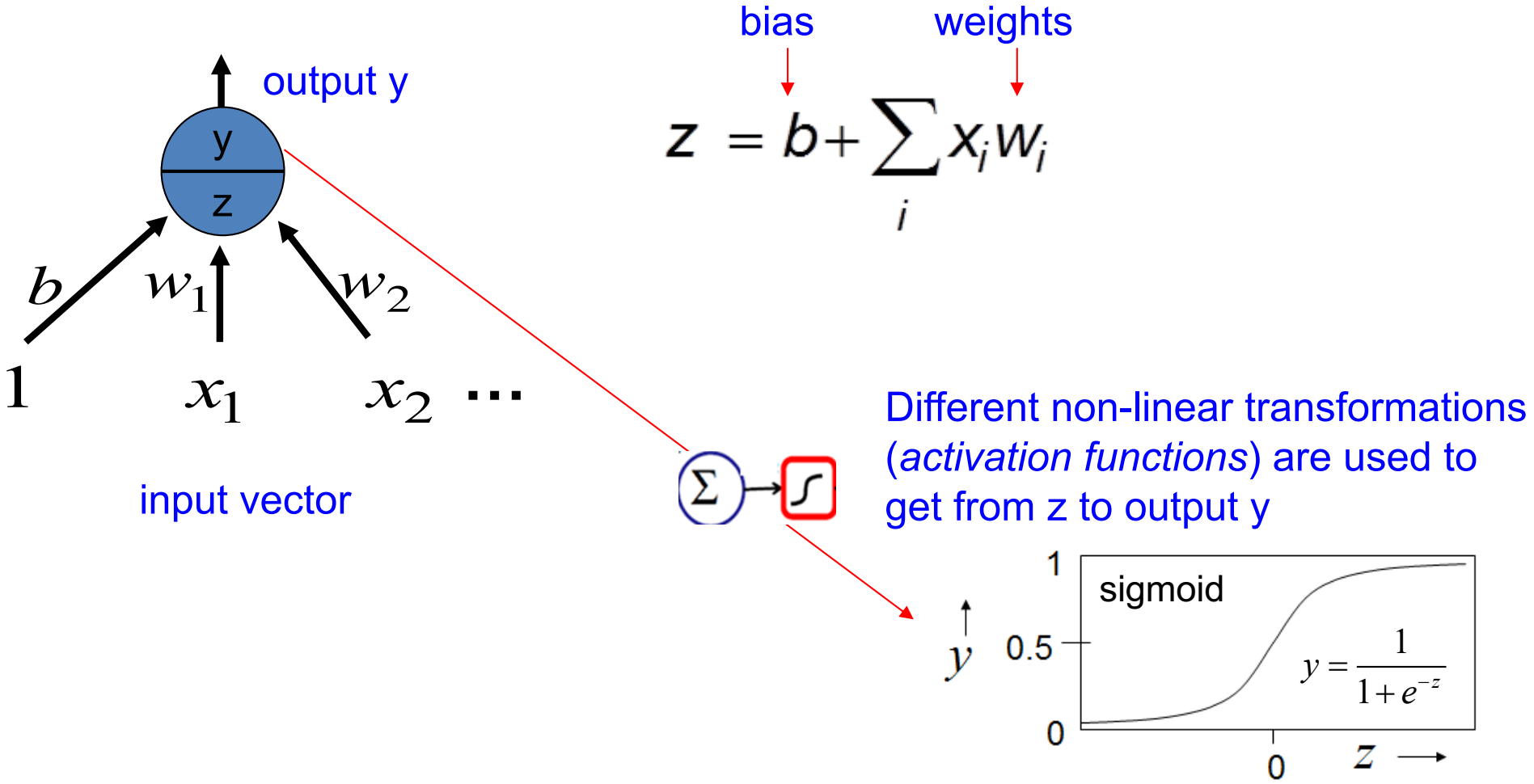


Figure 2.2 A single biological brain cell. The neuron receives the signal from other neurons via its dendrites shown on the left. If the cumulated signal exceeds a certain value, an impulse is sent via the axon to the axon terminals, which, in turn, couples to other neurons.

Neural networks are **loosely** inspired by how the brain works

An artificial neuron

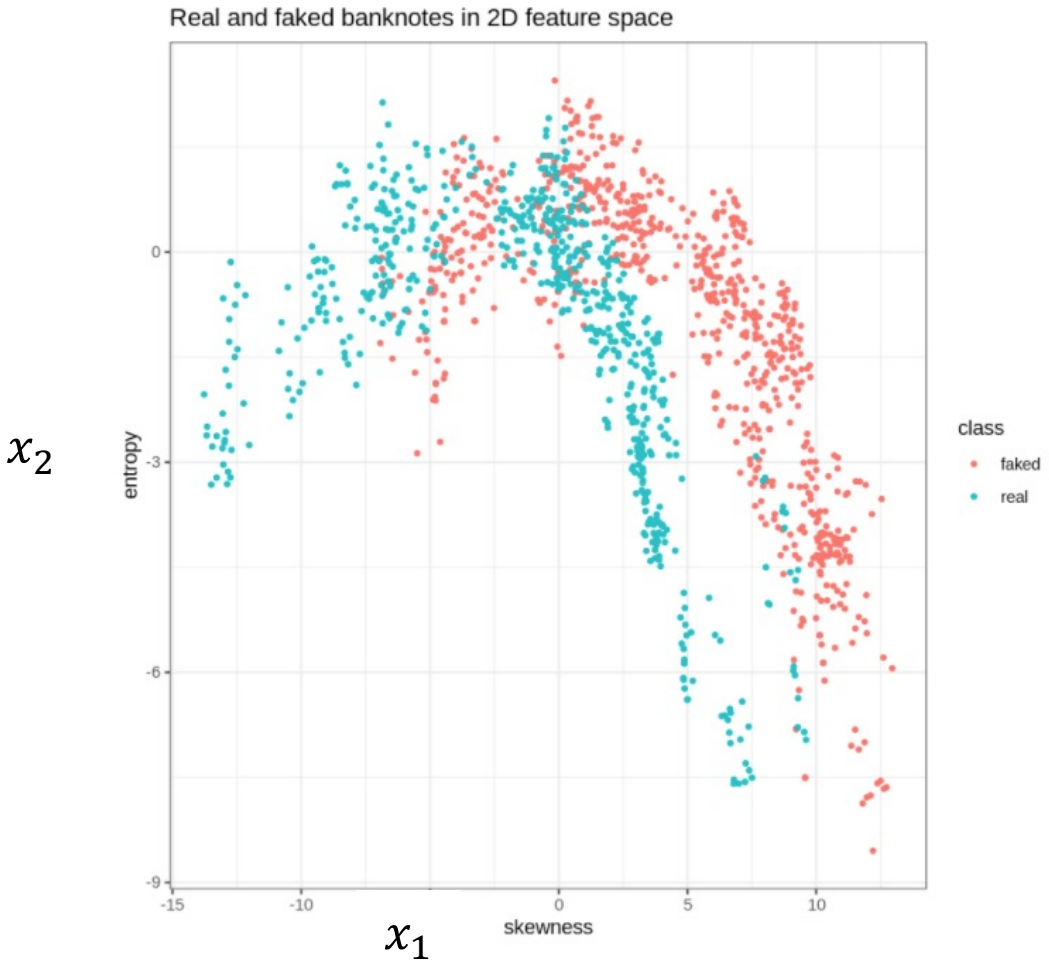


The sigmoid$(z) = \frac{1}{1+e^{-z}}$ ensures number from 0 to 1, which can be interpreted as probability.

Question: How is this model called in statistic?

Toy Task

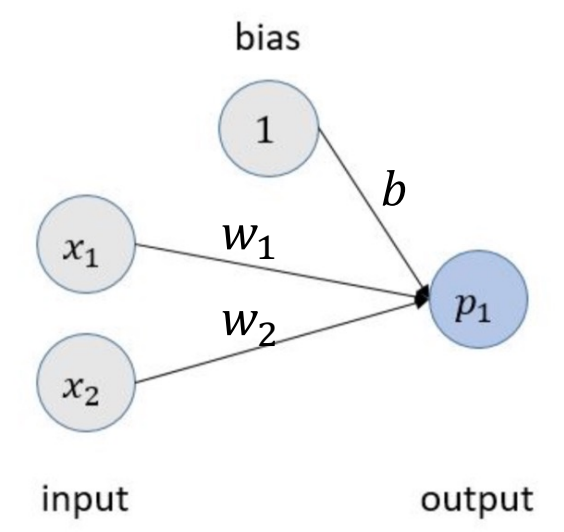
- Task tell fake from real banknotes (see exercise later 01_nb_ch02_01)
- Banknotes described by two features (x_1, x_2) extracted from image

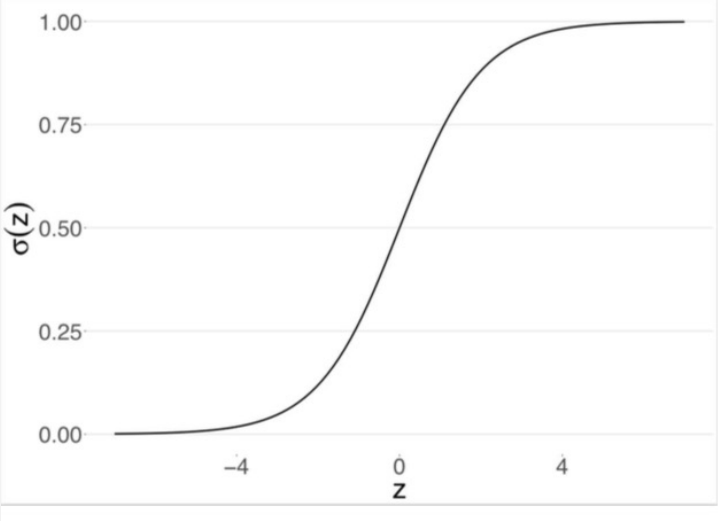


x_2

x_1

Exercise: Part 1





Model: The above network models the **probability** p_1 that a given banknote is false.

TASK

The weights (determined by a training procedure later) are given by

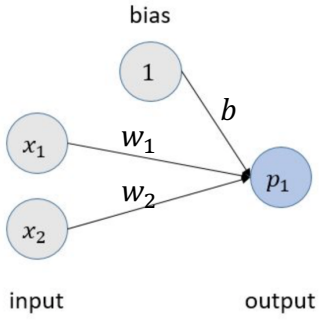
$w_1 = 0.3, w_2 = 0.1$, and $b = 1.0$

The probability can be calculated from z using the function sigmoid(z)

1. What is the probability (rough estimate) that a banknote characterized by x_1=1 and $x_2 = 2.2$ is fake?

GPUs love Vectors

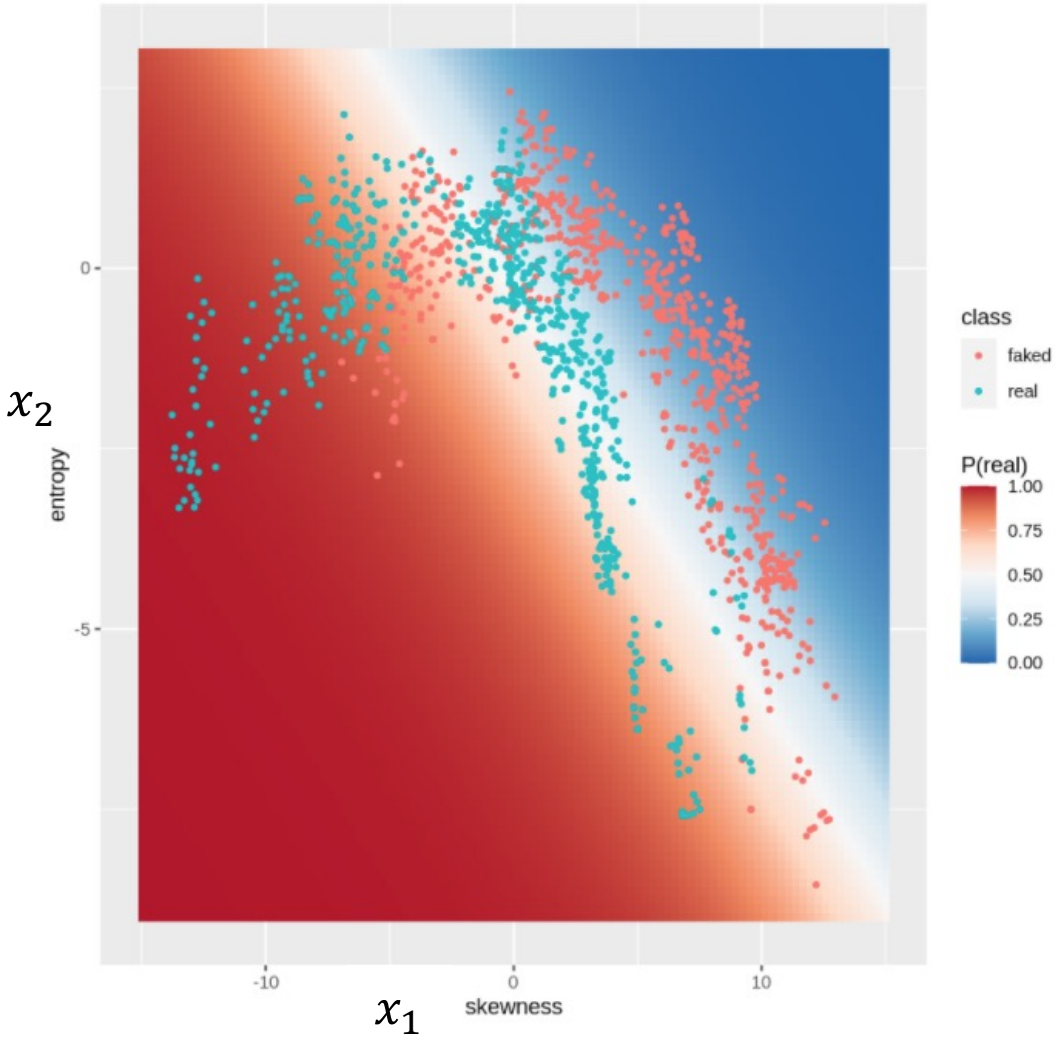
$$F^{\mu\nu}$$



$$p_1 = \text{sigmoid}\left((x_1 \quad x_2) \cdot \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} + b \right)$$

DL: better to have column vectors

Result*



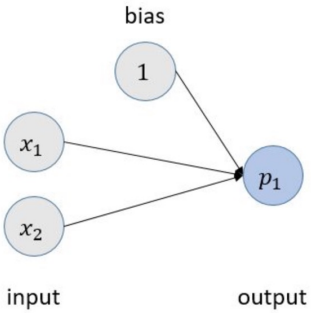
General rule: Networks without hidden layer have linear decision boundary.

*Details of training later

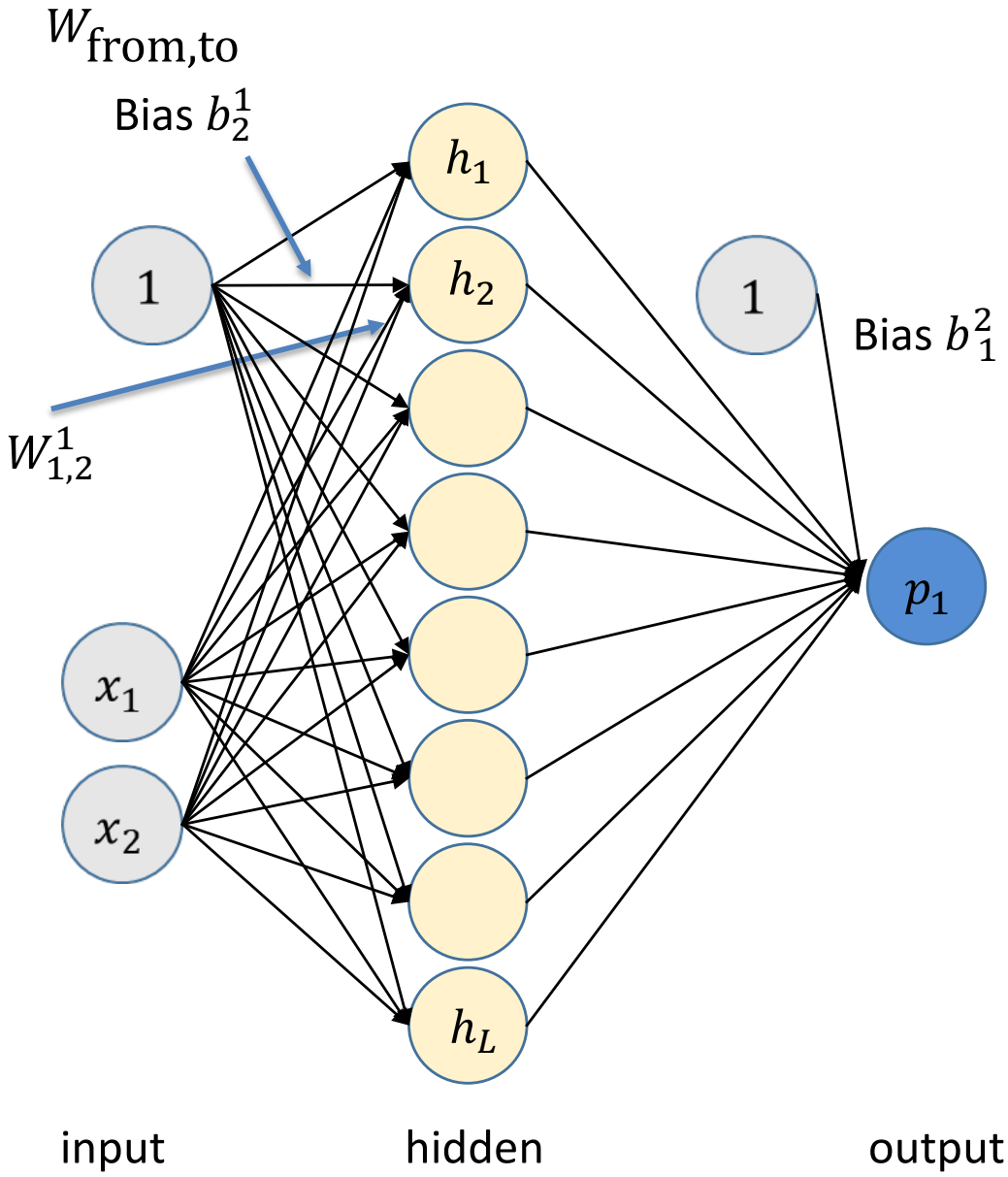

WE NEED TO GO
DEEPER
memegene

Introducing hidden layer

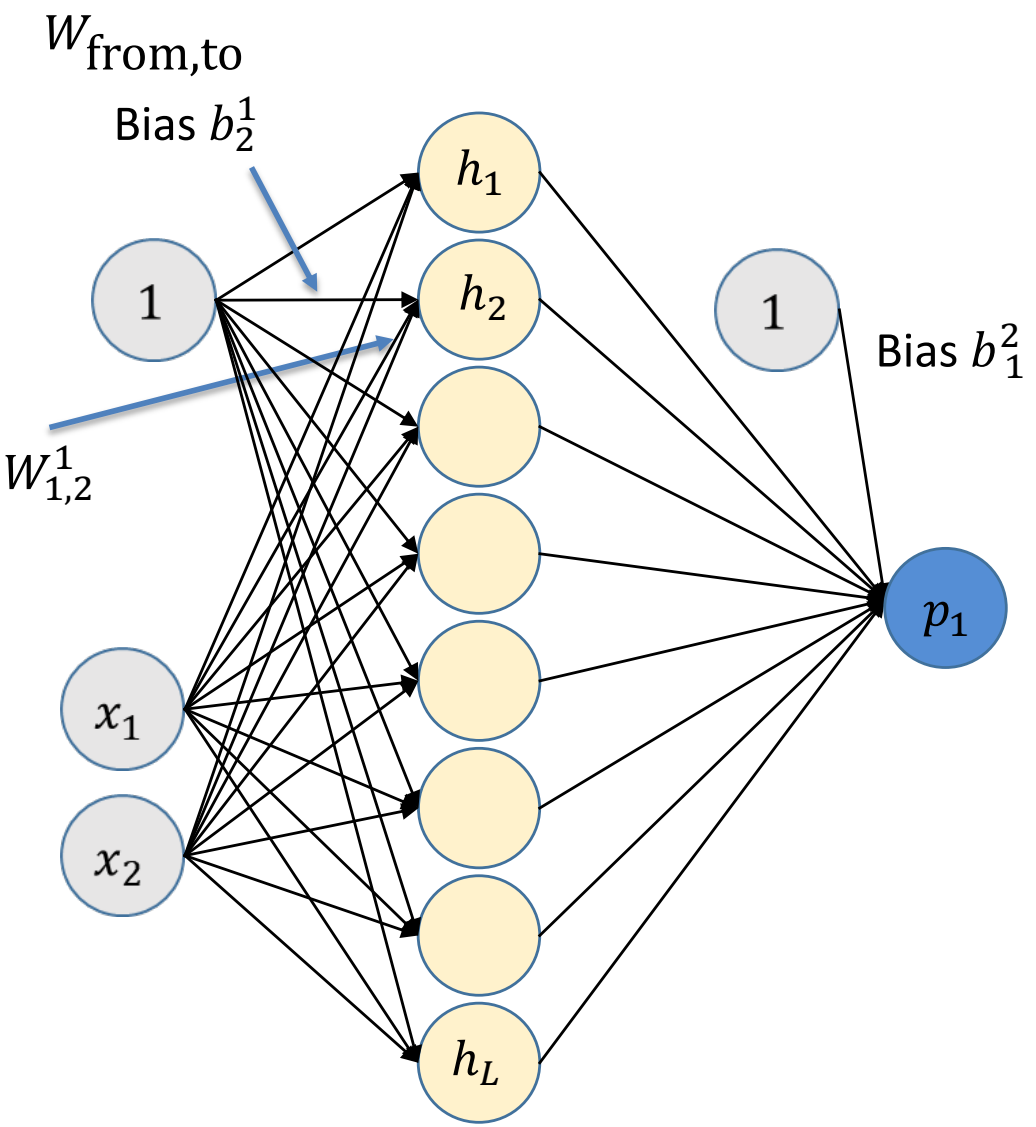
We stack single neurons in layers.
We use the output of neuron as input to the new neuron.



$$p_1 = \text{sigmoid}\left(\begin{pmatrix} x_1 & x_2 \end{pmatrix} \cdot \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} + b \right)$$



Introducing hidden layer



$$h_2 = \text{sigmoid}\left((x_1 \quad x_2) \cdot \begin{pmatrix} W_{1,2}^1 \\ W_{2,2}^1 \end{pmatrix} + b_2^1\right)$$

General

$$h_i = \text{sigmoid}\left(\sum_l x_l W_{l,i}^1 + b_i\right)$$

$$h_i = \text{sigmoid}\left((x_1 \quad x_2) \cdot \begin{pmatrix} W_{1,i}^1 \\ W_{2,i}^1 \end{pmatrix} + b_2^1\right)$$

Matrix Notation (later we drop $\vec{}$)
Note column vectors!

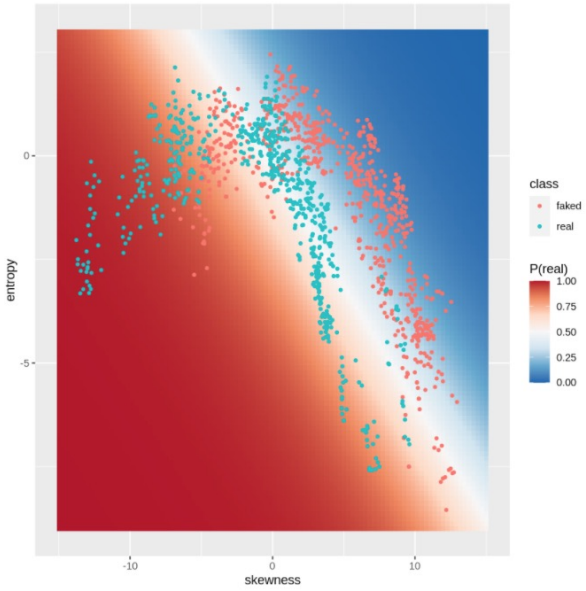
$$\vec{h} = \text{sigmoid}\left(\vec{x} \cdot \boldsymbol{W^1} + \overrightarrow{b^1}\right)$$

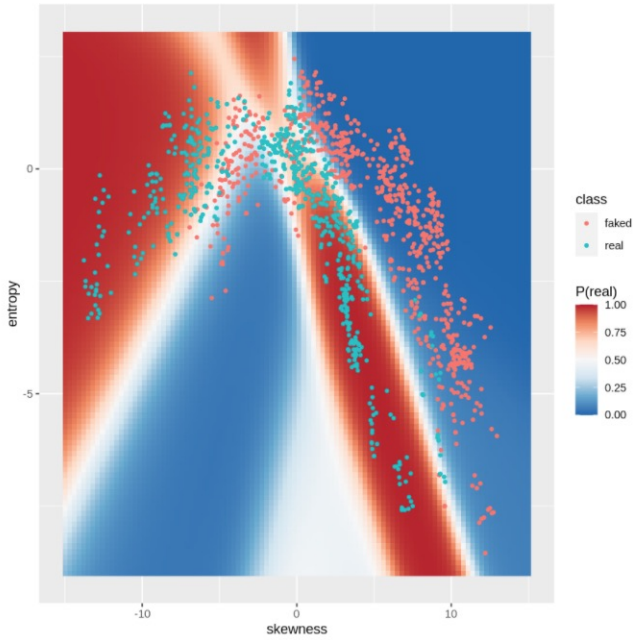
Complete Network

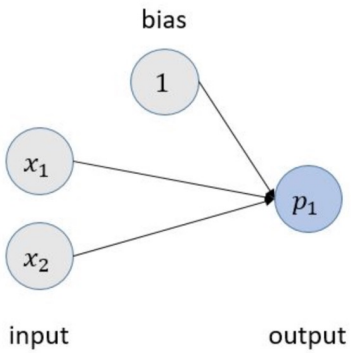
$$p_1 = \text{sigmoid}\left(\vec{h} \cdot \boldsymbol{W^2} + b_1^2\right)$$

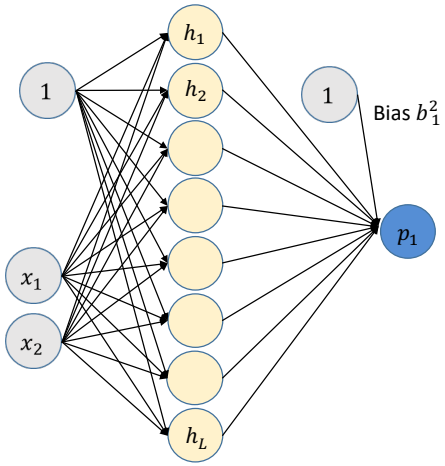
```
Code:
h =sigmoid(x %*% W1 + b1)
p1=sigmoid(h %*% W2 + b2)
```

The benefit of hidden layers

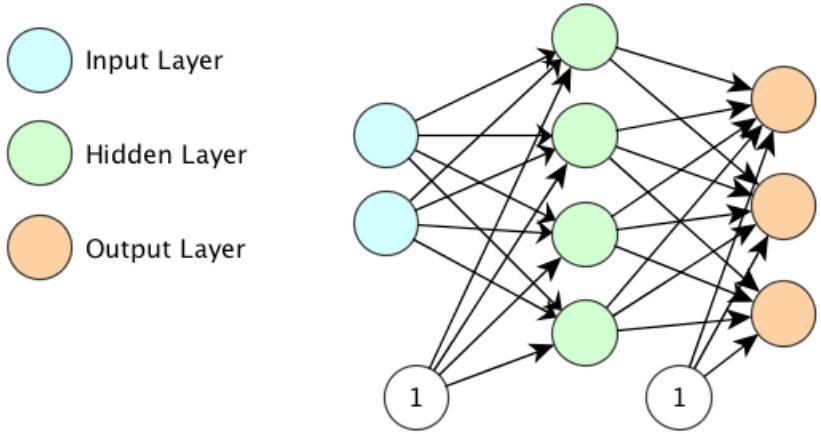




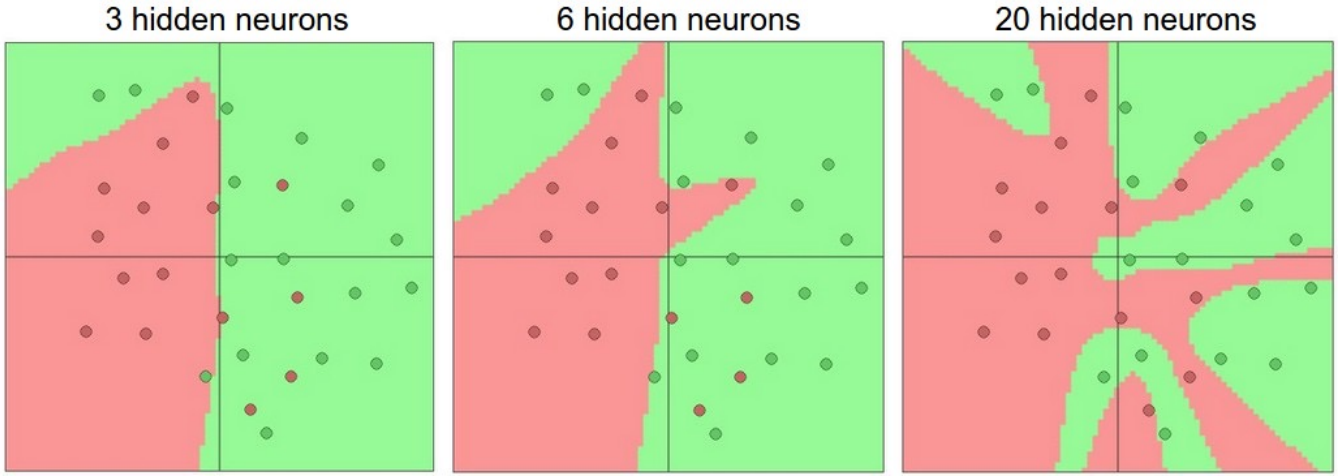




Increasing number of neurons in the hidden layer



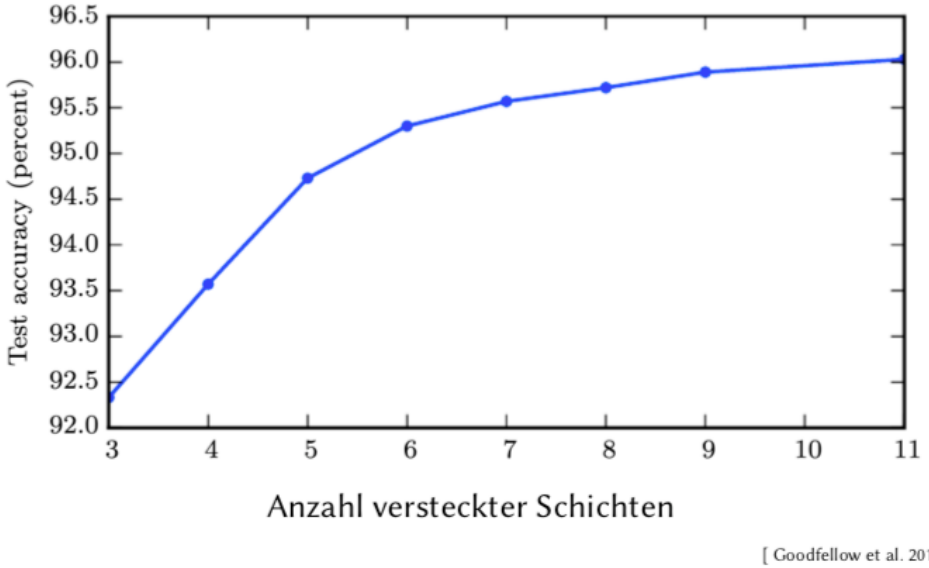
A network with one hidden layer is a universal function approximator!



http://cs231n.github.io/neural-networks-1/

DL use many hidden layers

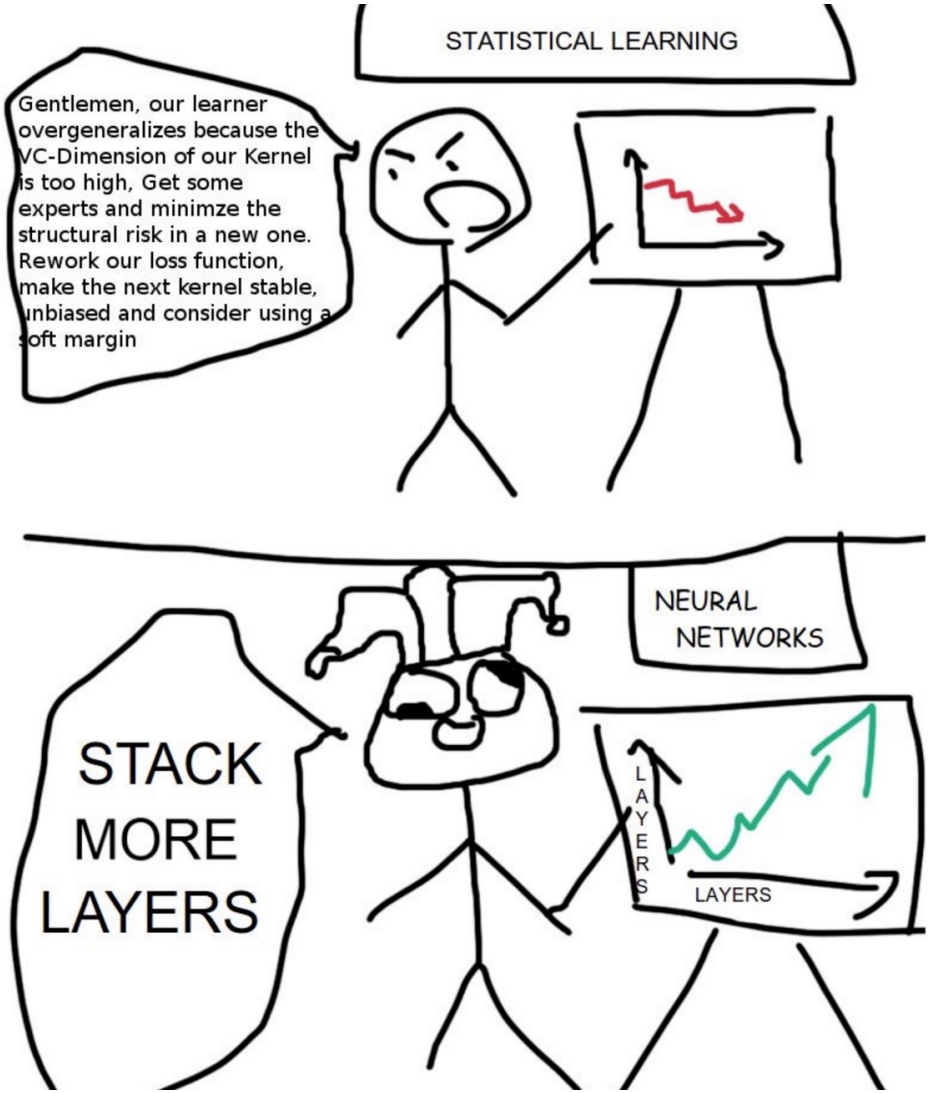
- Empirical observation that having more than one layer improves generalization (no overfitting)



[Goodfellow et al. 2014]

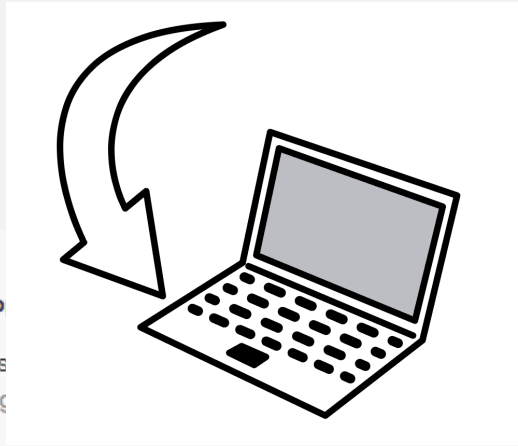
- Not completely understood why. Some intuition:
  - Multiple layers allow hierarchical features
  - With same number of weights yield more flexible networks
  - Observed in brains

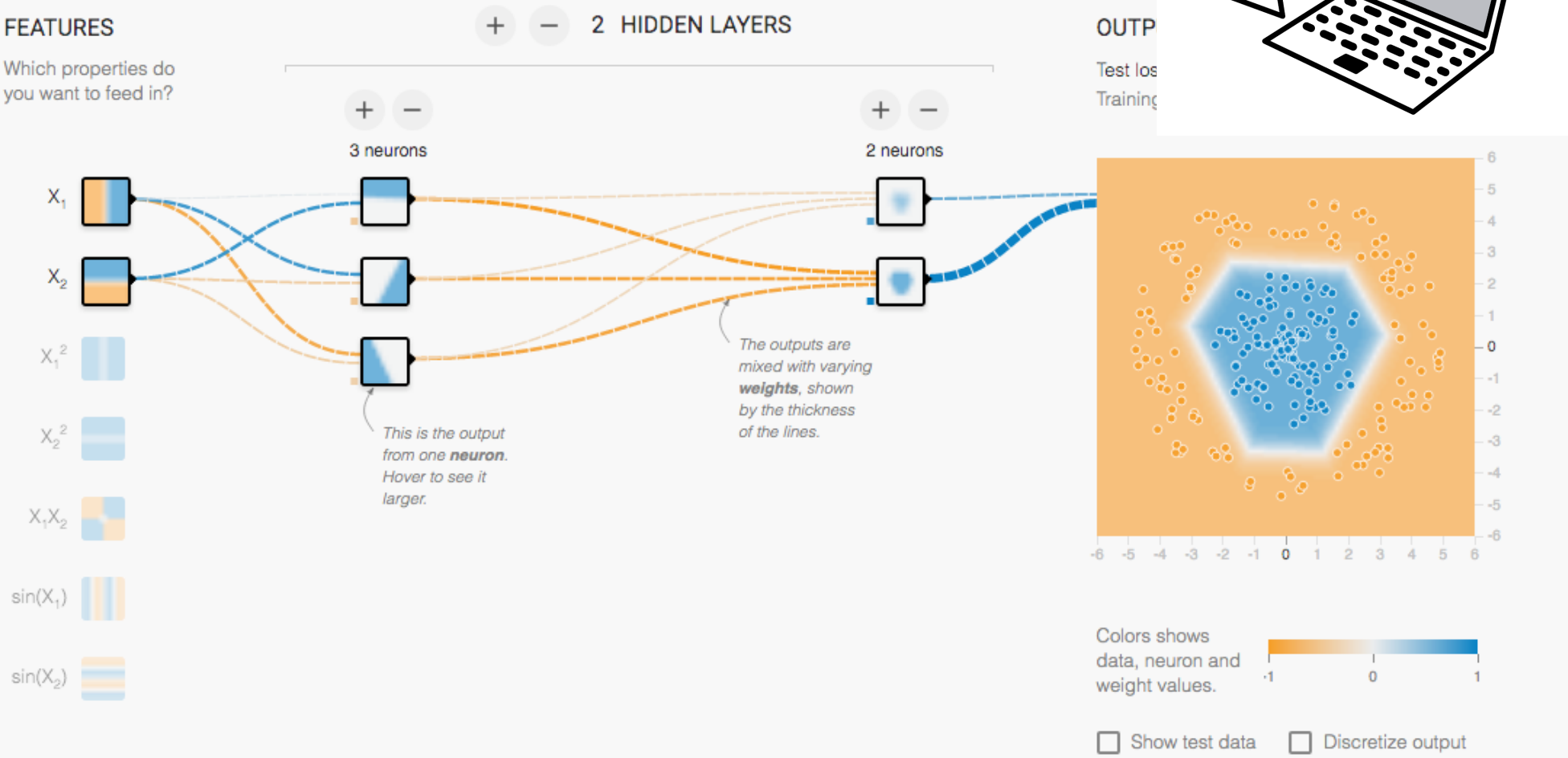
DL vs Machine Learning Meme



https://www.reddit.com/r/ProgrammerHumor/comments/8c1i45/stack_more_layers/

Experiment yourself, play at home

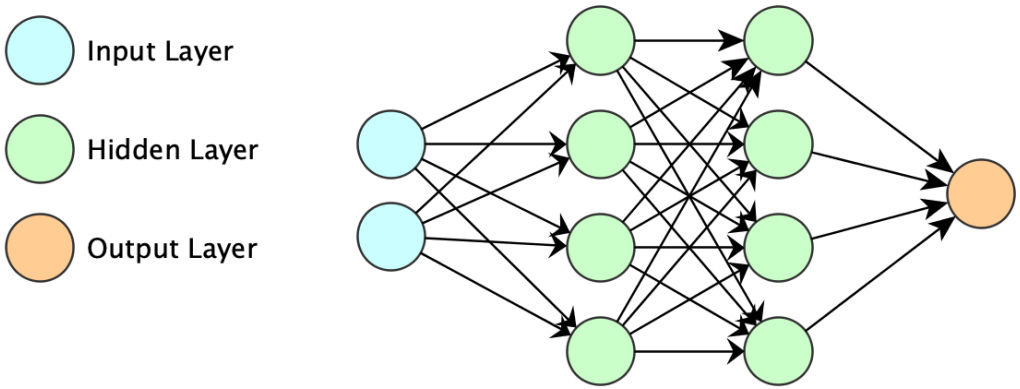




http://playground.tensorflow.org

Let's you explore the effect of hidden layers

Structure of the network



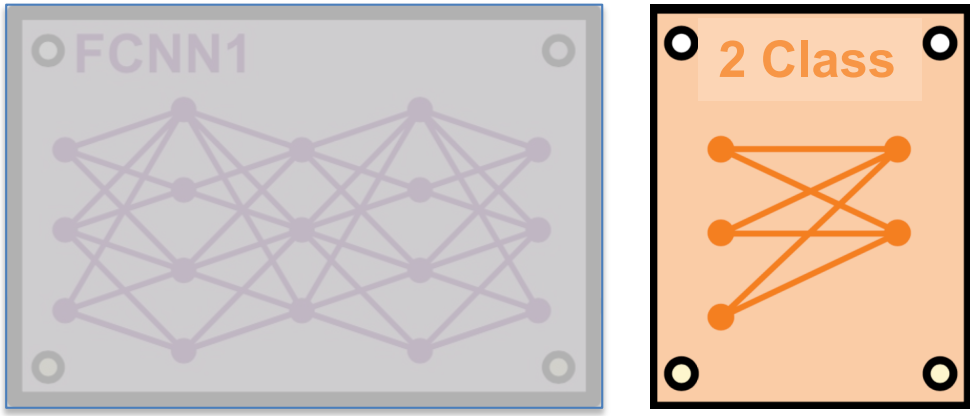
In code:

```
## Solution 2 hidden layers
hidden_1=sigmoid(X %*% W1 + b1)
hidden_2=sigmoid(hidden_1 %*% W2 + b2)
res = sigmoid(hidden_2 %*% W3 + b3)
```

In math (f = sigmoid) and b1=b2=b3=0

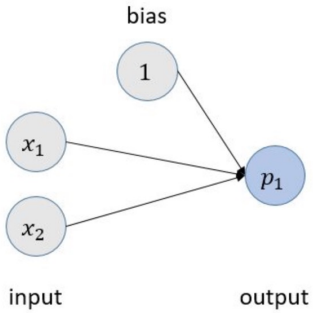
$$p = f(f(f(\mathrm{x}\,\mathrm{W}^1)\mathrm{W}^2)W^3)$$

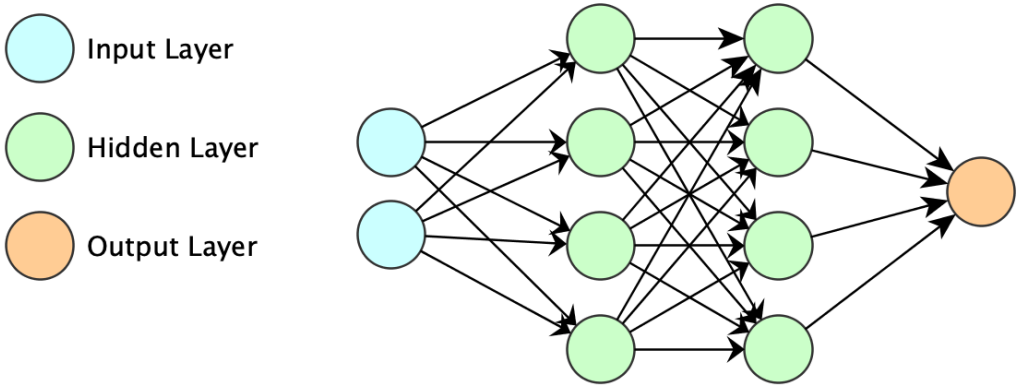
Looks a bit like onions, matryoshka (Russian Dolls) or Lego bricks



Using Networks for Classification

So far: Logistic Regression / Binary Classification





$$p_1 = \text{sigmoid}\left(\begin{pmatrix} x_1 & x_2 \end{pmatrix} \cdot \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} + b \right)$$

- Networks out the probability for one class (logistic regression / logistic regression with hidden layers).
  - In probabilistic framework: parameter of a Bernoulli $(Y|x) \sim Bern(p_1(x))$

- What to do with more than one class?

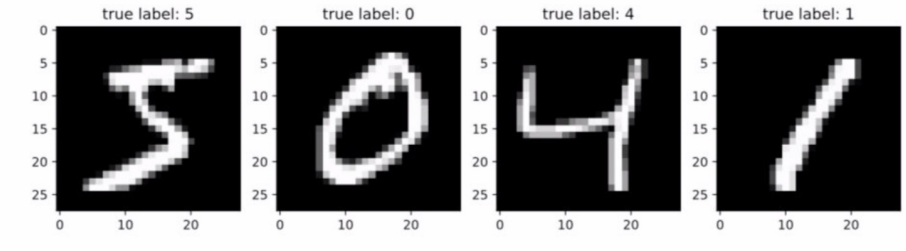
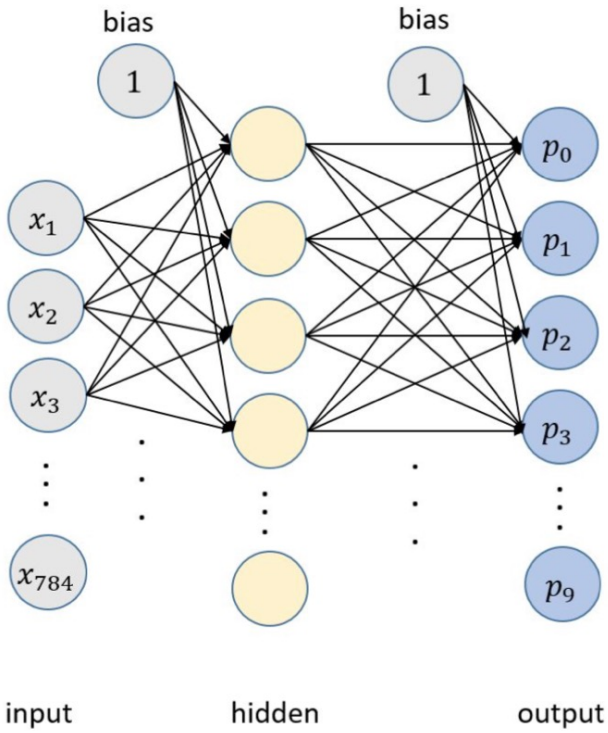


Figure 2.11 The first four digits of the MNIST data set—the standard data set used for benchmarking NN for images classification

Classification: Softmax Activation



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

Incoming to last layer z_i $i = 0 \cdots 9$

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

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.

Networks out the probabilities for the classes

In probabilistic framework (parameter vector $\vec{p}$ of a multinomial $\overrightarrow{Y|x} \sim mn(\overrightarrow{p(x)})$

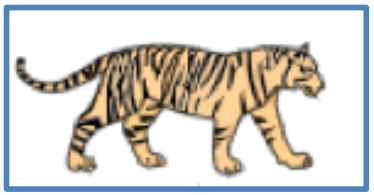
Training NN

Training

Input $x^{(i)}$

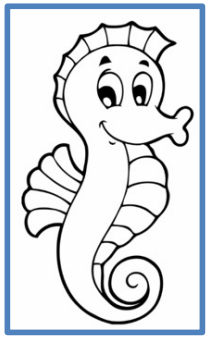
True class $y^{(i)}$

Suggesed class
(Show is most likely class)



Tiger

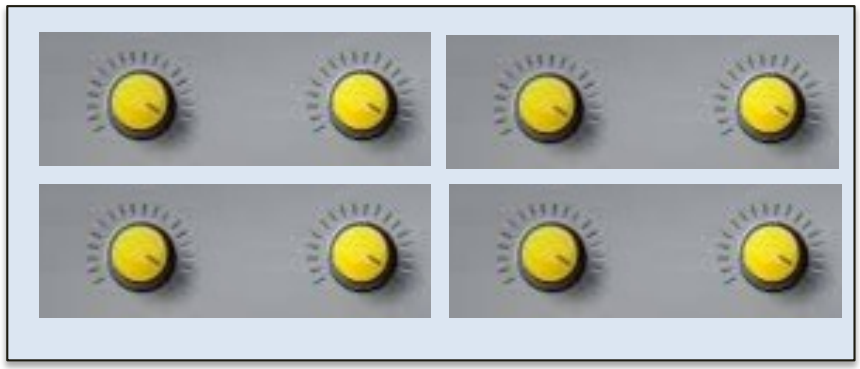
Tiger



Seeh
orse

...

Neural network with many weights *W*



→ Seal 👎

→ Tiger 👍

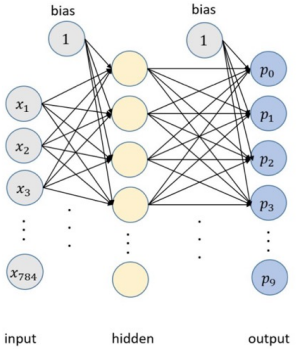
→ Seehorse 👍

Typical 1 Mio. Trainingsdaten

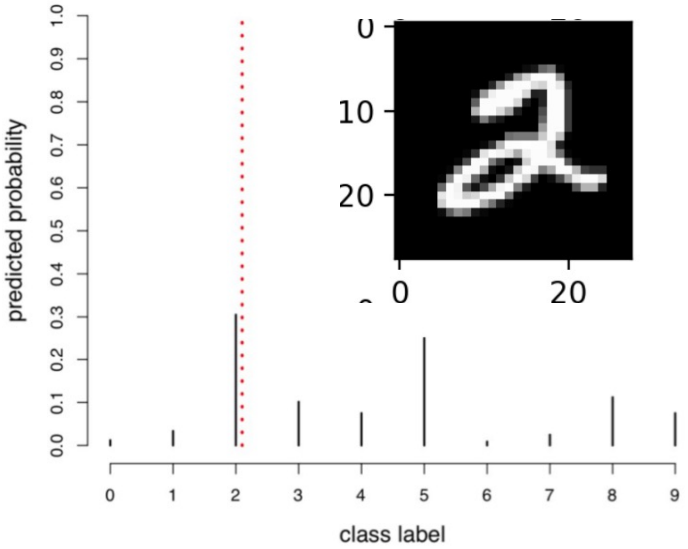
Trainingsprinciple:
Weights are tuned so a loss functions gets minimized.

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

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 $\Rightarrow\ l_i = \infty$

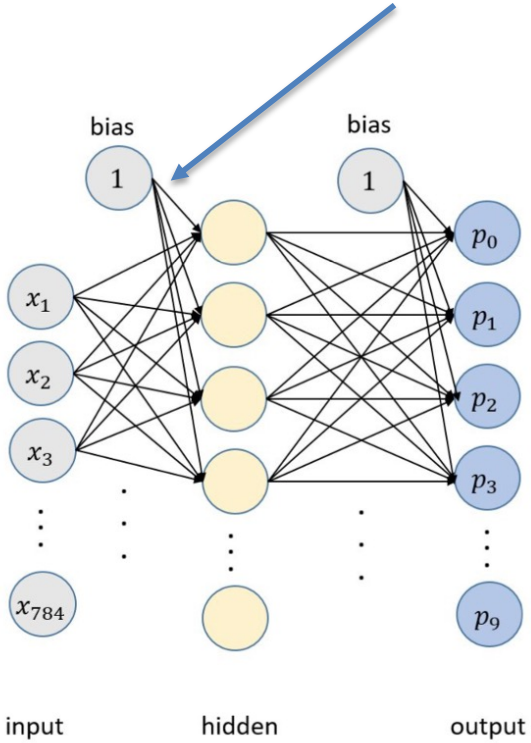
For more all examples, just average $\mathrm{loss} = \frac{1}{N}\sum l_i$

Training / Gradient Descent

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.



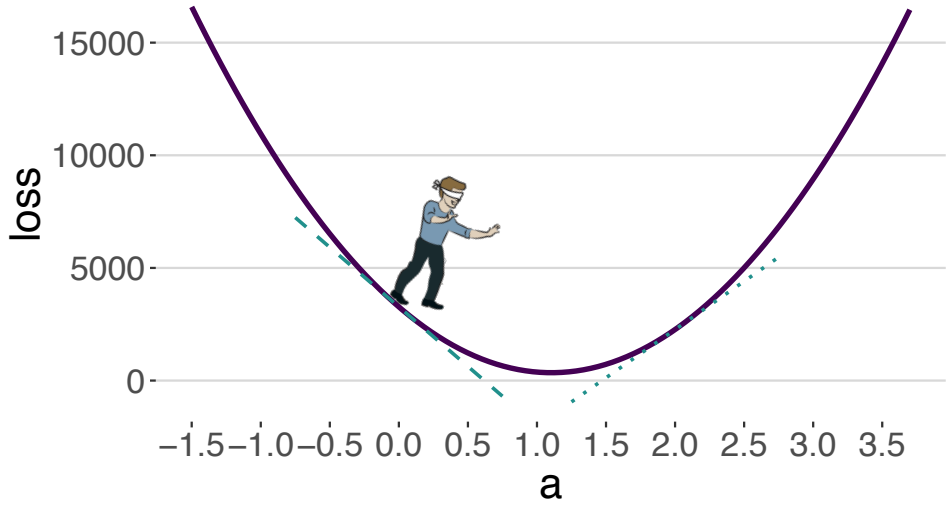
Modern Networks have Billions (10^9) of weights.

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

*aka minibatch gradient descent.

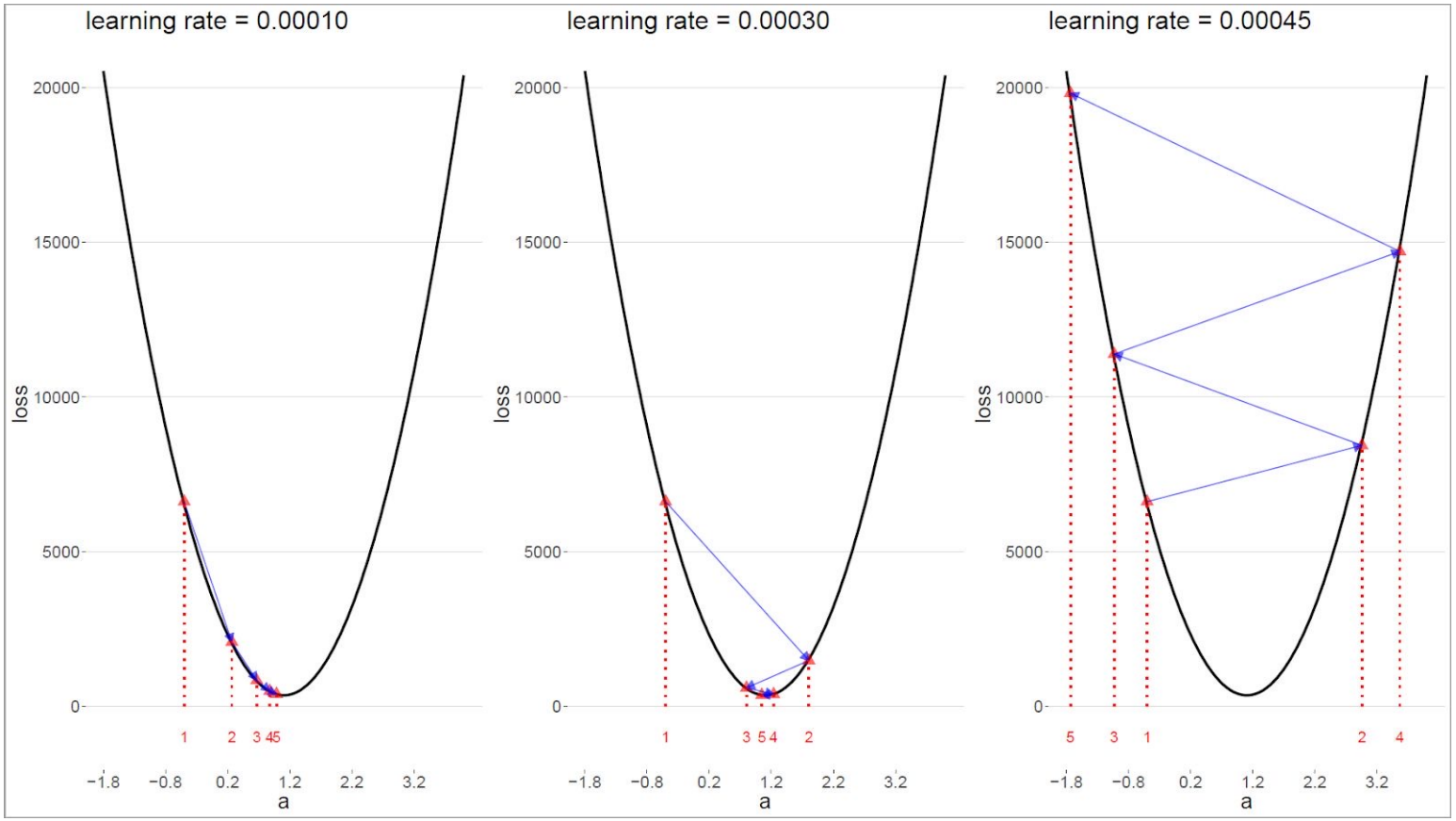
Idea of gradient descent

- Shown loss function for a single parameter *a*



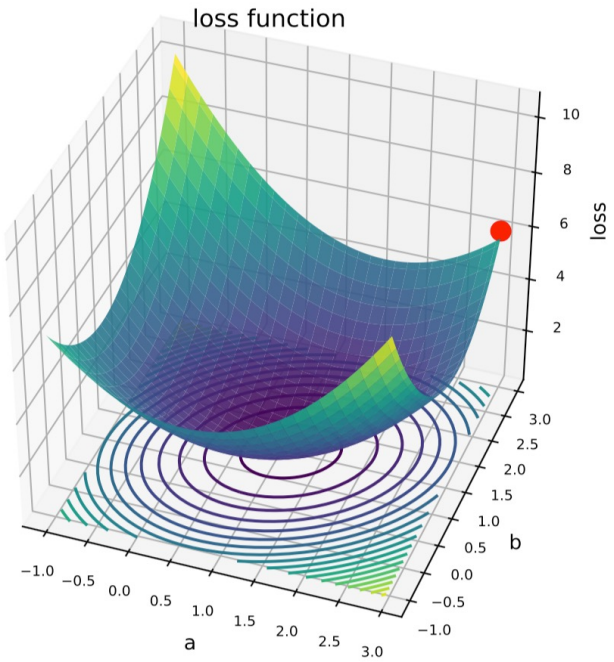
- Imagine you are the blinded wanderer and just know the loss and the slope at a position. How to reach the minimum?
  - Take a large step if slope is steep (you are away from minimum)
- Slope of loss function is given by gradient (this is a local quantity)
- Iterative update of the parameters
  - $a_{t+1} = a_t - \epsilon \; grad\_a(loss)$

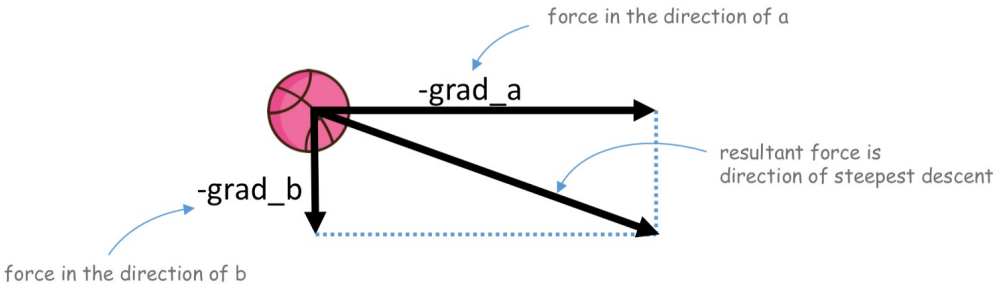
Proper learning rate (Important parameter for DL)



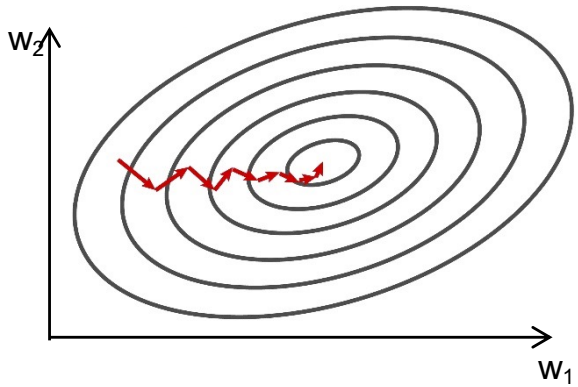
See: https://developers.google.com/machine-learning/crash-course/fitter/graph

In two dimensions





Gradient is perpendicular to contour lines



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

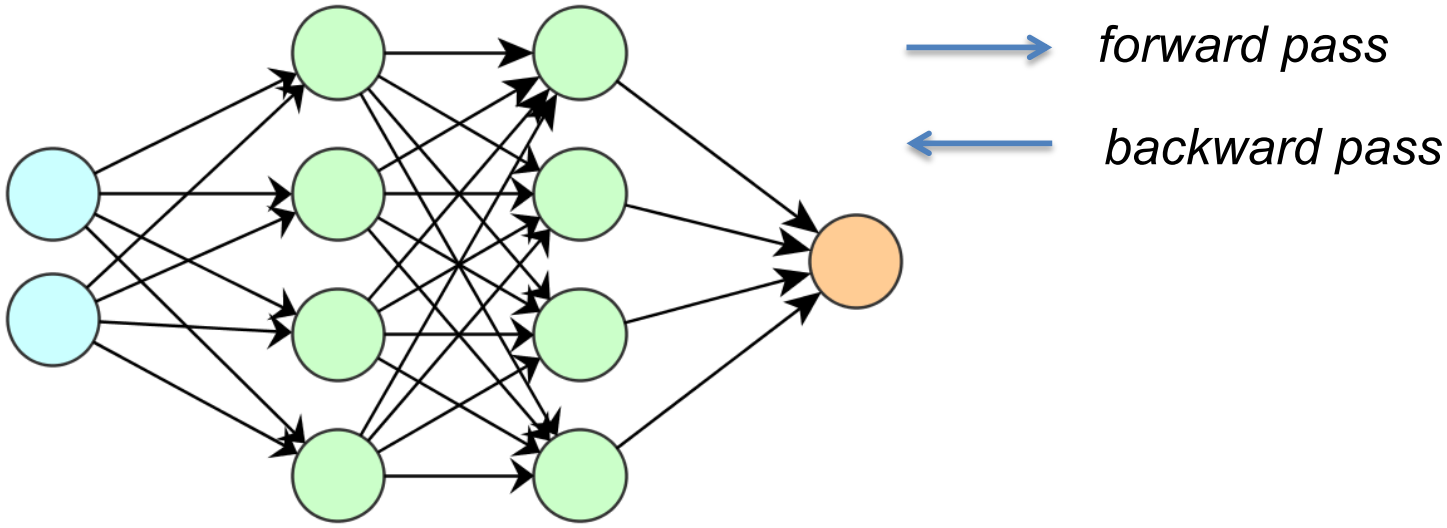
The miracle of gradient descent in DL

Loss surface in DL (is not convex) but SGD magically also works for non-convex problems.

Modern deep learning: No distinction between network (model) and training (SGD)

Backpropagation

- We need to calculate the derivative of the loss function $loss(\{X_i, Y_i\}, W)$ w.r.t. all weights W
- Efficient way backpropagation (chain rule)
  - Forward Pass propagate training example through network
    - Gives output for current configuration of network
  - Backward pass propagate training example through network
    - Chain rule all gradients can be calculated in a single flow from the “end”



For more see e.g. chapter 3 in Probabilistic deep learning

Typical Training Curve / ReLU

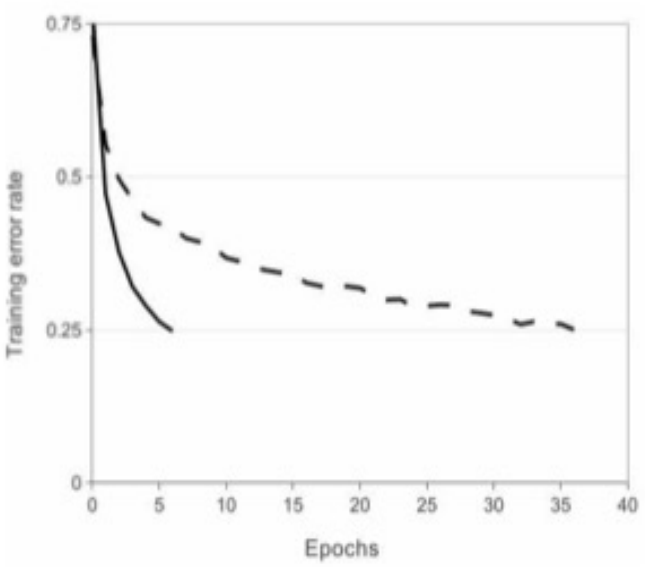
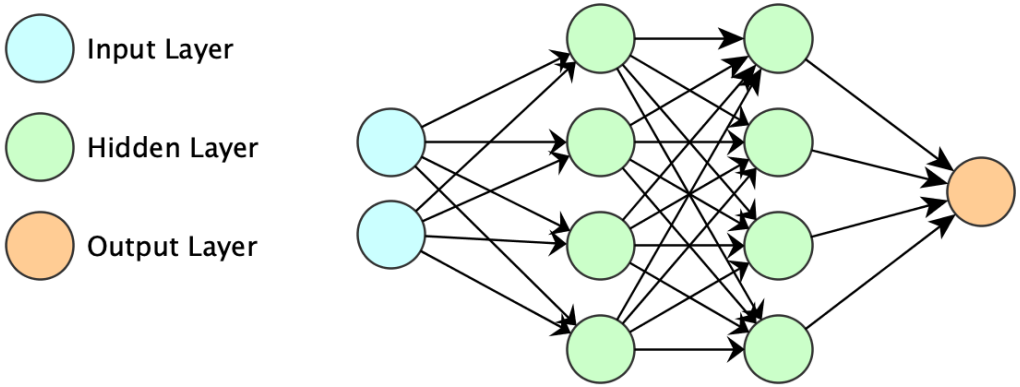
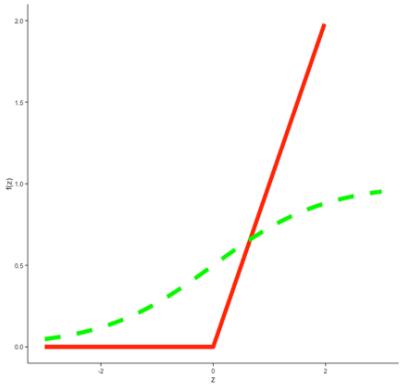


Figure 1: A four-layer convolutional neural network with ReLUs **(solid line)** reaches a 25% training error rate on CIFAR-10 six times faster than an equivalent network with tanh neurons

Source:
Alexnet
Krizhevsky et al 2012



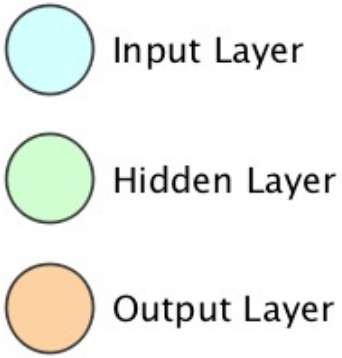


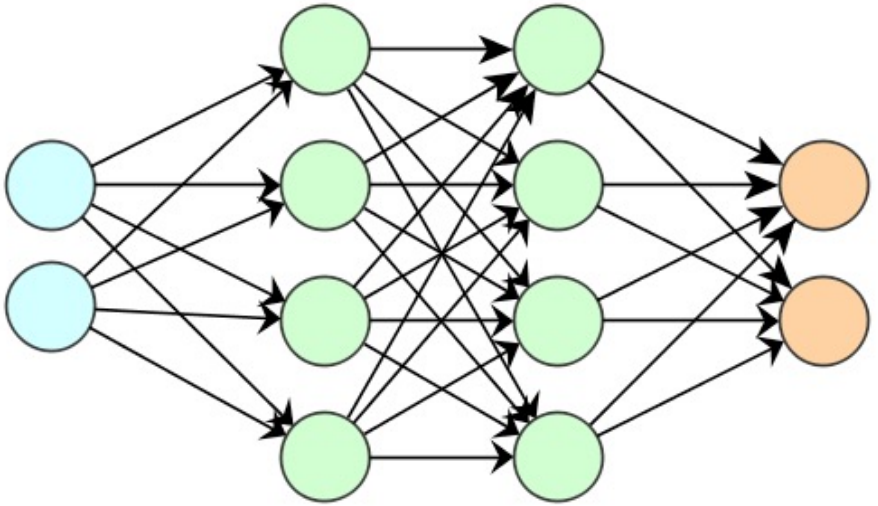
Motivation:
Green:
sigmoid.
Red:
ReLU faster
convergence

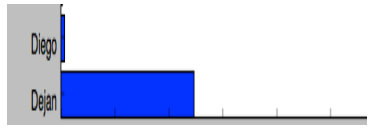
Epochs: ”each training examples is used once”

Deep Learning Frameworks

Recap: The first network



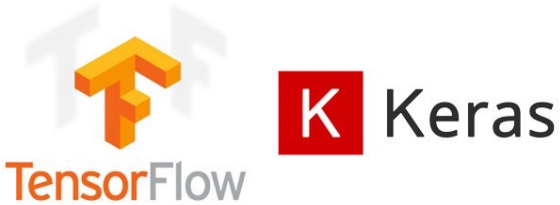




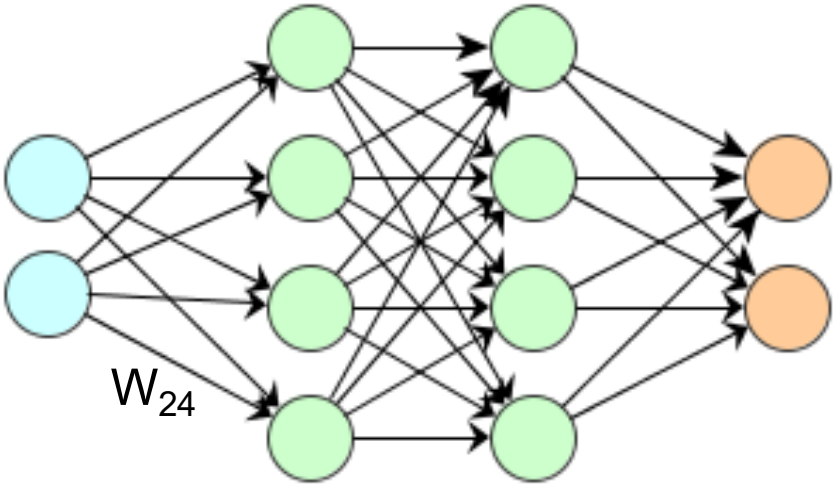
- The input: e.g. intensity values of pixels of an image
  - (Almost) no pre-processing
- Output: probability that image belongs to certain class
- Information is processed layer by layer from building blocks
- Arrows are weights (these need to be learned / training)
- Training requires gradients of loss w.r.t weights

Deep Learning Frameworks (common)

- Computation needs to be done on GPU or specialized hardware (compute performance)
- Data Structure are multidimensional arrays (*tensors*) which are manipulated
- Automatic calculation of the gradients
  - Static: computational graph (see chapter 3 in probabilistic deep learning)
  - Dynamic: reverse mode auto diff
- In this course: TensorFlow with Keras



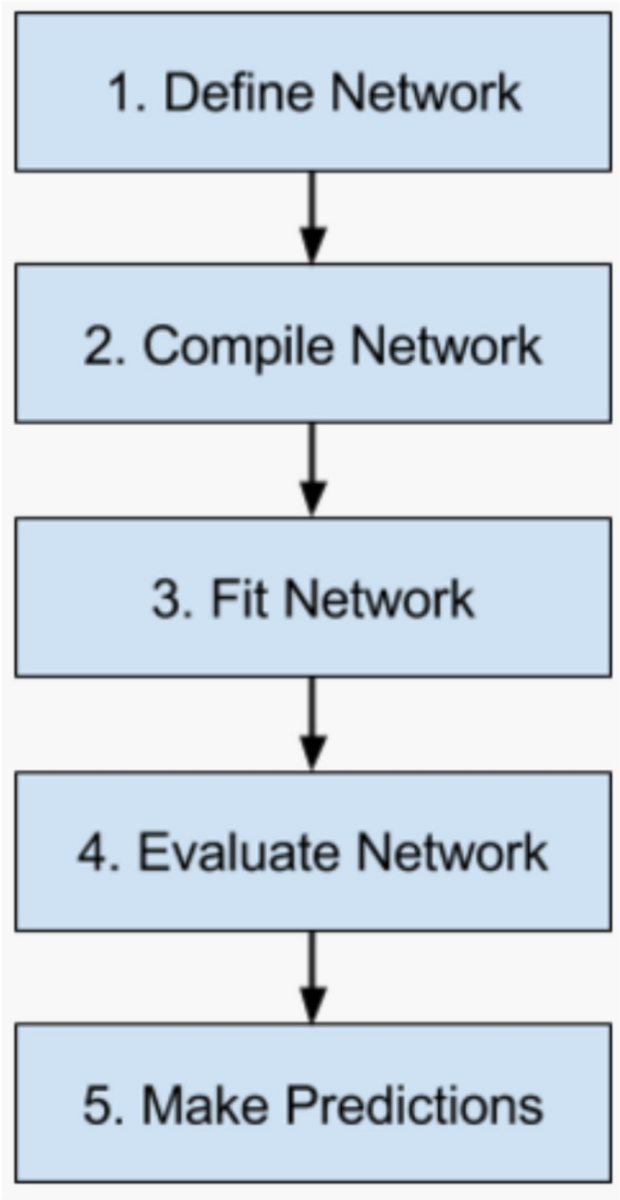
Typical Tensors in Deep Learning



- The input can be understood as a vector
- A mini-batch of size 64 of input vectors can be understood as tensor of order 2
  - (index in batch, x_j)
- The weights going from e.g. Layer L_1 to Layer L_2 can be written as a matrix (often called W)
- A mini-batch of size 64 images with 256,256 pixels and 3 color-channels can be understood as a tensor of order 4.

Introduction to Keras

Keras Workflow



Define the network (layerwise)

Add loss and optimization method

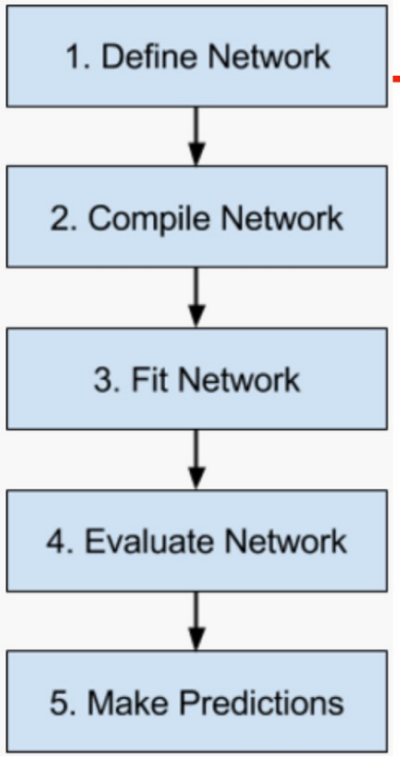
Fit network to training data

Evaluate network on test data

Use in production

A first run through

Define the network



Number of neurons in first hidden layer

Dimension of input, here vector size 784

```
model <- keras_model_sequential()
model %>%
  layer_dense(units = 256, activation = 'relu', input_shape = c(784)) %>%
  layer_dropout(rate = 0.4) %>%
  layer_dense(units = 128, activation = 'relu') %>%
  layer_dropout(rate = 0.3) %>%
  layer_dense(units = 10, activation = 'softmax')
```

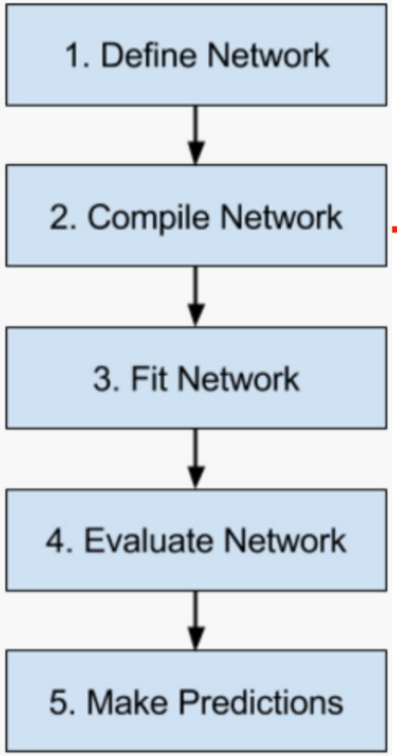
Alternative version w/o pipe

```
model <- keras_model_sequential()
model = layer_dense(model, units = 256, activation = 'relu', input_shape = c(784))
model = layer_dropout(model, rate = 0.4)
...
```

Input shape needs to be defined only at the beginning.

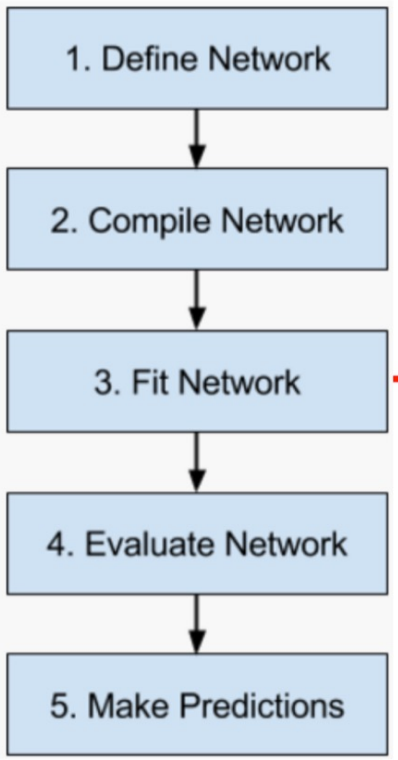
Alternative: `input_dim=784`

Compile the network




```
model %>% compile(loss = 'categorical_crossentropy',
                  optimizer = 'sgd',
                  metrics = c('accuracy'))
```

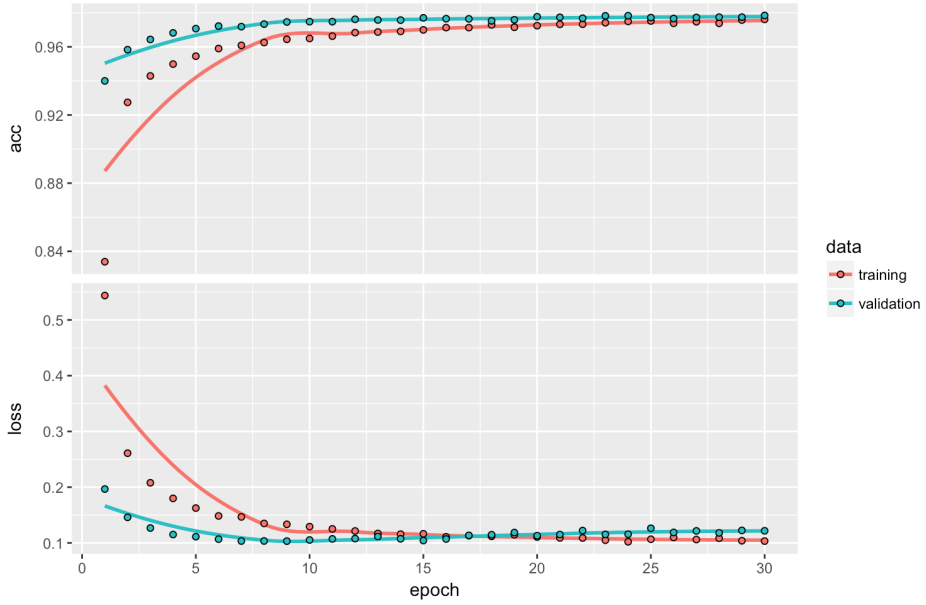
Fit the network



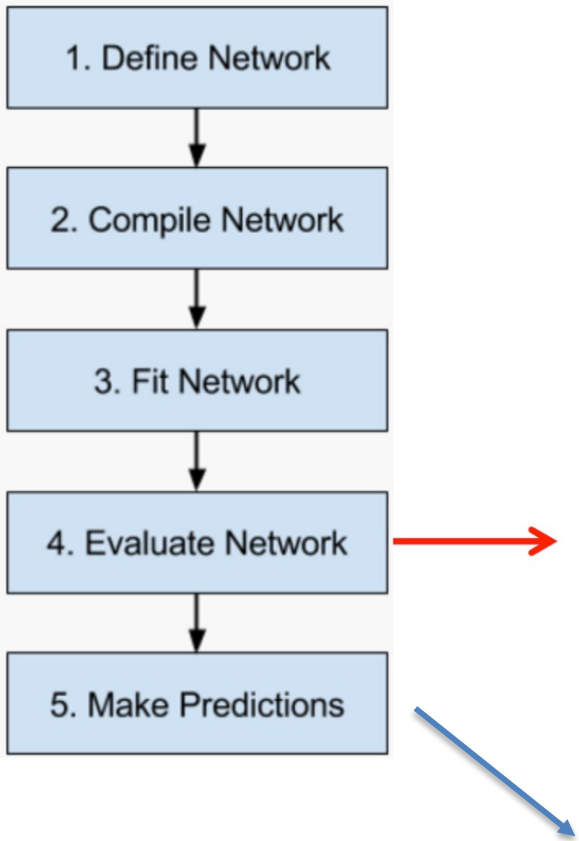

```
history <- model %>% fit(
  x_train, y_train,
  epochs = 30, batch_size = 128,
  validation_split = 0.2
)
```

20% of the data is not use for fitting the weights.

```
plot(history)
```



Evaluate the network



Evaluate the model's performance on the test data:

```
model %>% evaluate(x_test, y_test)
```

```
$loss
[1] 0.1149

$acc
[1] 0.9807
```

```
model %>% predict_classes(x_test)
```

```
 [1] 7 2 1 0 4 1 4 9 5 9 0 6 9 0 1
```

More layers

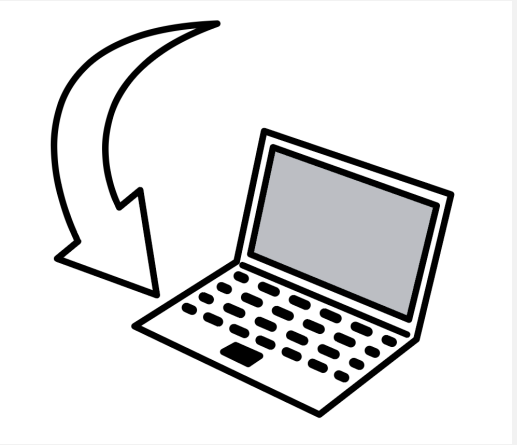
- Dropout
  - keras.layers.Dropout
- Convolutional (see lecture on CNN)
  - keras.layers.Conv2D
  - keras.layers.Conv1D
- Pooling (see lecture on CNN)
  - keras.layers.MaxPooling2D
- Recurrent (not in course)
  - keras.layers.SimpleRNNCell
  - keras.layers.GRU
  - keras.layers.LSTM

How to use TF and Keras in the course

- Use google colab
  - Free resource with preinstalled (kind of) jupyter notebooks
  - Usually for python
  - To start R notebook (not possible over GUI)
    - https://colab.research.google.com/notebook#create=true&language=r

- Use RStudio
  - Installation a bit tedious, especially for tfprobability
  - You might by lucky though

Excercise



For this lecture:

Play around with code, answer questions ask questions if you have any. See also https://tensorchiefs.github.io/dl_rcourse_2022/

1. Check installation colab 00_R_Keras_TF_TFP.ipynb
   https://colab.research.google.com/github/tensorchiefs/dl_rcourse_2022/blob/main/notebooks/00_R_Keras_TF_TFP.ipynb

2. Banknote example (01_nb_ch02_01.ipynb):
   https://colab.research.google.com/github/tensorchiefs/dl_rcourse_2022/blob/main/notebooks/01_nb_ch02_01.ipynb

3. MNIST with simple FCNN (02_nb_ch02_02a.ipynb)
   https://colab.research.google.com/github/tensorchiefs/dl_rcourse_2022/blob/main/notebooks/02_nb_ch02_02a.ipynb