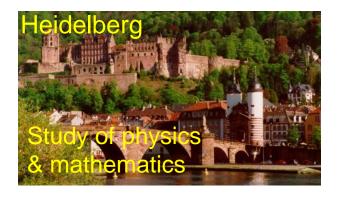
Machine Intelligence:: Deep Learning Week 1

Beate Sick, Oliver Dürr, Pascal Bühler

Institut für Datenanalyse und Prozessdesign Zürcher Hochschule für Angewandte Wissenschaften

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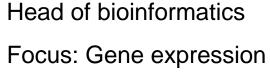
# Beate's Background













Researcher and Professor for applied statistics

Focus: deep learning

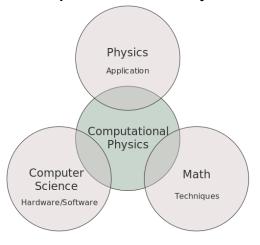


Researcher and lecturer

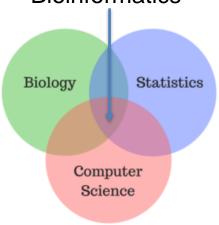
Focus: Biostatistics, DL

### Oliver's Background

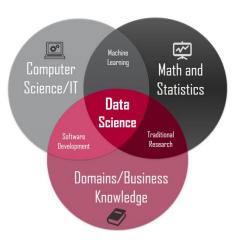
#### **Computational Physics**



**Bioinformatics** 



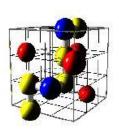
Data Science

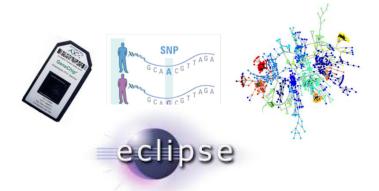


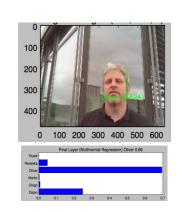
1990's Uni-Konstanz

2000's Genedata Basel

2010's ZHAW Winterthur HTWG Konstanz







### Tell us something about you

- Computer Science Background
  - Fluent in python?
- Statistics / Math
  - Who visited CAS StMo (statistisches Modellieren)?
  - What is a distribution?
  - Vector times Matrix?
    - Please make sure to check <a href="https://tensorchiefs.github.io/dl\_course\_2024/prerequistites.html">https://tensorchiefs.github.io/dl\_course\_2024/prerequistites.html</a>

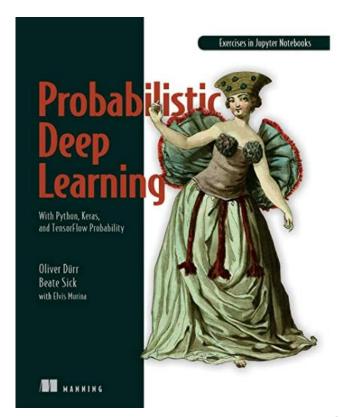
Any contacts with deep learning yet?

#### Technical details for this course

- Running the code:
  - Colab Notebooks
    - · needs no installation, only internet and google account
  - Anaconda
    - Installation by your own (no support)

#### Material for the course

- Website and Github repository
  - The CAS Deep Learning Course
    - https://tensorchiefs.github.io/dl\_course\_2024/
- Our Book "Probabilistic Deep Learning"
  - Can be used in addition to the course
  - https://github.com/tensorchiefs/dl\_book



### Organizational Issues: Test Projects

- Projects (2-3 People)
- Presented on the last day
  - Spotlight talk (5 Minutes)
  - Poster
- Topics
  - You can / should choose a topic of your own (please discuss your topic with us by week4 latest)
  - Possible Topics (see website)
    - Take part in a Kaggle Competition (e.g. Leaf Classification / Dogs vs. Cats)
    - Music classification
    - Polar bear detection
    - ...
- Computing: colab, laptop (or cloud computing)

#### Organizational Issues: Times

- Dates and times: see our webpage <u>CAS machine intelligence</u>
- Afternoon sessions
  - 13:30-17:00
- Theory and exercises will be mixed
  - Could be 50 minutes theory 30 minutes exercises
  - Could be vice versa
- Please interrupt us if something is unclear! The less we talk the better!

#### Outline of the DL Module (tentative)

- Day 1: Jumpstart to DL
  - What is DL
  - Basic Building Blocks
  - Keras
- Day 2: CNN I
  - ImageData
- Day 3: CNN II and RNN
  - Tips and Tricks
  - Modern Architectures
  - 1-D Sequential Data
- Day 4: Looking at details
  - Linear Regression
  - Backpropagation
    - Resnet
  - Likelihood principle

- Day 5: Probabilistic Aspects
  - TensorFlow Probability (TFP)
  - Negative Loss Likelihood NLL
  - Count Data
- Day 6: Probabilistic models in the wild
  - Complex Distributions
  - Generative modes with normalizing flows
- Day 7: Uncertainty in DL
  - Bayesian Modeling
- Day 8: Uncertainty cont'd
  - Bayesian Neural Networks
  - Projects

# Learning Objectives for today

- Get a rough idea what the DL is about
- Framework
  - Introduction to Keras

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

# Machine Perception

- Computers have been quite bad in things which are easy for humans (images, text, sound)
- A Kaggle contest 2012
- In the following we explain why

Kaggle dog vs cat competition

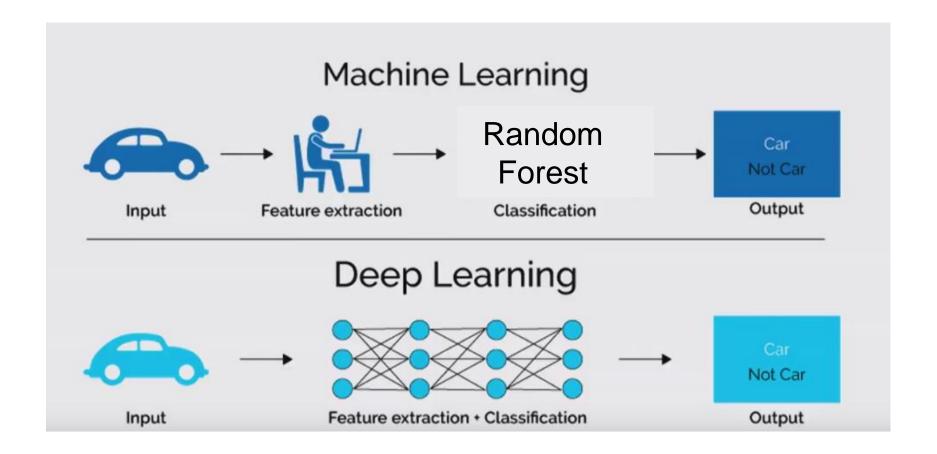


Deep Blue beat Kasparov at chess in 1997.

Watson beat the brightest trivia minds at Jeopardy in 2011.

Can you tell Fido from Mittens in 2013?

### Deep Learning vs. Machine Learning



# The most convincing case for DL (subjective view)

# Why DL: Imagenet 2012, 2013, 2014, 2015

1000 classes1 Mio samples

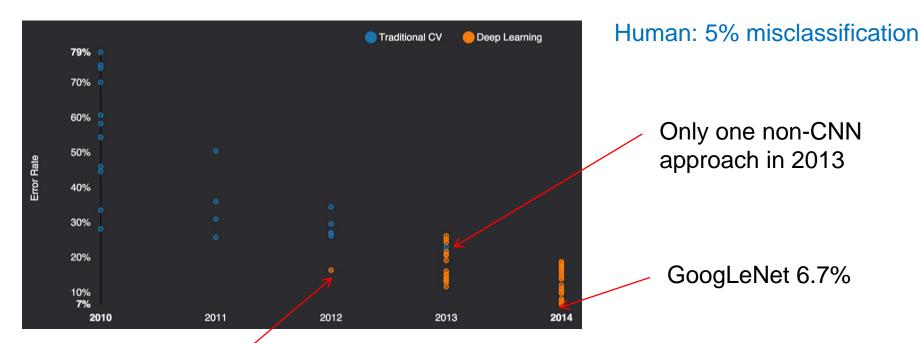








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A. Krizhevsky first CNN in 2012

Und es hat zoom gemacht

2015: It gets tougher

4.95% Microsoft (Feb 6 surpassing human performance 5.1%)

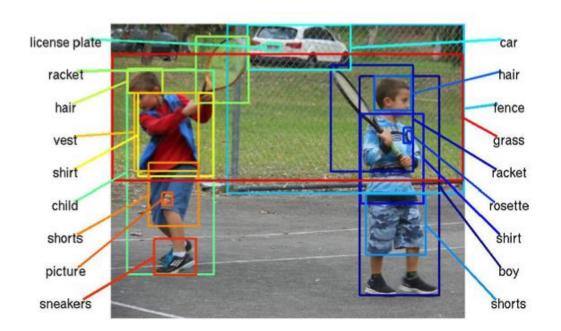
4.8% Google (Feb 11) -> further improved to 3.6 (Dec)?

4.58% Baidu (May 11 banned due too many submissions)

3.57% Microsoft (Resnet winner 2015) → task solved!

# The computer vision success story

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





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?



"man in black shirt is playing guitar."

# 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
Sequence (prompt) An astronaut riding a horse in a photorealistic style		Image Generation
Sequences (prompt) "Hallo, wie?"	Next word "geht"	Language Models
Simple number (age) age=52	Simple number (SPB) sbp = 152	Simple Regression Educational

Deep Learning öffnet Tür zu hören, sehen und Texten. Status Quo: kein Verstehen aber Erfassung statistische Zusammenhänge.

#### This is the new shit: LLM/ChatGPT



#### Die gefühlte Revolution

4. Dezember 2022, 18:51 Uhr | Lesezeit: 3 min



Turing-Test einen Menschen glauben, dass sie ein Mensch ist, im Stil von Kehinde Wiley." (Foto: Dall-E-Bild: SZ)



Marilyn Manson - This Is The New Shit (Official Music Video)

#### **GPT** (short for "Generative Pre-training Transformer")

is a type of language processing AI model developed by OpenAI. It is a large, deep learning model that has been trained on a diverse range of texts and can generate human-like text when given a prompt.

# First Neural Network

# The Single Neuron: Biological Motivation

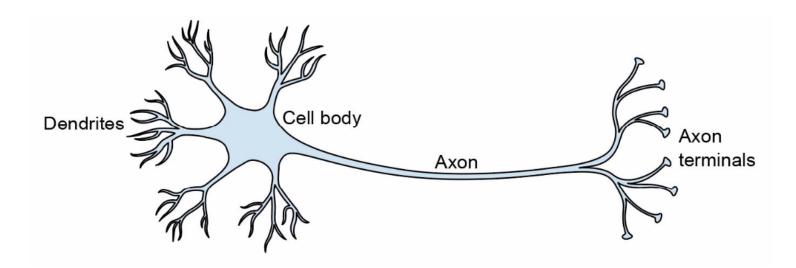
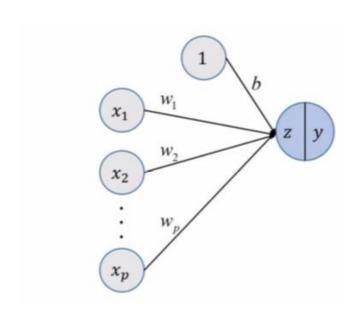
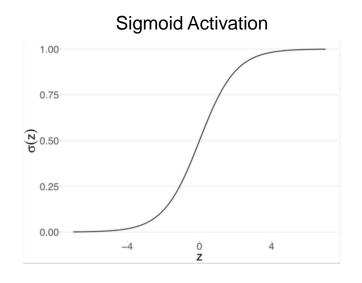


Figure 2.2 A single biological brain cell. The neuron receives the signal from other neurons via its dendrites shown on the left. If the cumulated signal exceeds a certain value, an impulse is sent via the axon to the axon terminals, which, in turn, couples to other neurons.

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

#### The Single Neuron: Mathematical Abstraction



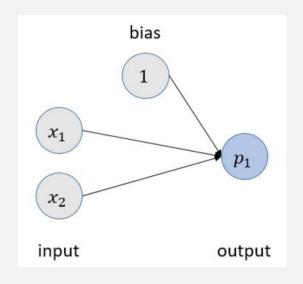


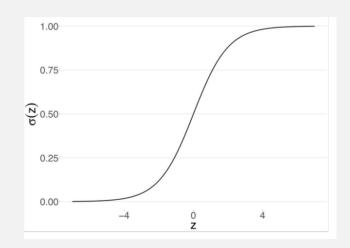
$$z = b + x_1 \cdot w_1 + x_2 \cdot w_2 + \dots + x_p \cdot w_p$$

$$y = \sigma(z) = \sigma(\beta_0 + \beta_1 x_{i1} + \dots + \beta_{ip} x_{ip}) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_{i1} + \dots + \beta_{ip} x_{ip})}}$$

The output after the sigmoid activation can be interpreted as probability for y=1

#### Exercise: Part 1







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

#### TASK (with pen and paper)

The weights (determined by a training procedure later) are given by  $w_1 = 0.3, w_2 = 0.1$ , and b = 1.0

What is the probability that a banknote, that is characterized by  $x_1$ =1 and  $x_2$  = 2.2, is a faked banknote?

#### GPUs love Vectors



In Math:

$$p_1 = \operatorname{sigmoid} \left( (x_1 \quad x_2) \cdot {w_1 \choose w_2} + b \right)$$

#### In code:

```
## function to return the probability output after the matrix multiplication
def predict_no_hidden(X):
    return sigmoid(np.matmul(X,W)+b)
```

# Toy Task

- Task tell fake from real banknotes
- Banknotes described by two features

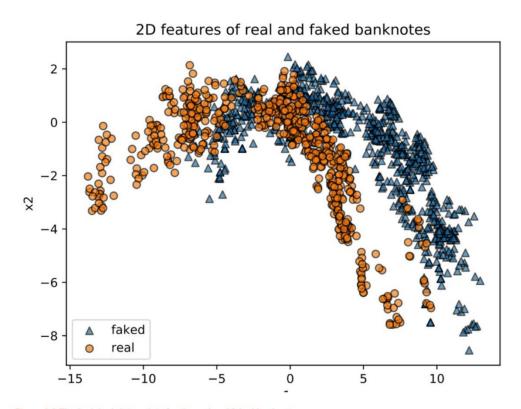
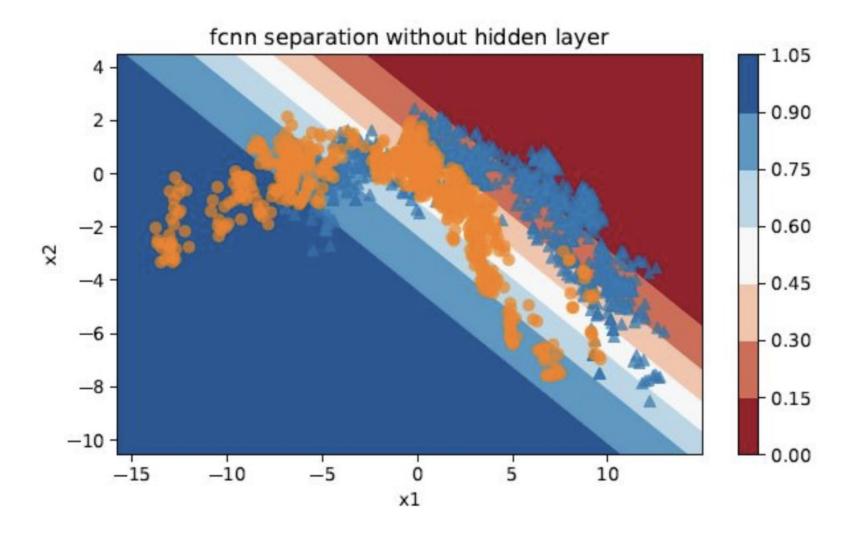


Figure 2.5 The (training) data points for the real and faked banknotes

#### Result (see later in the notebook)

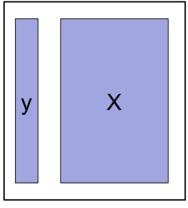


General rule: Networks without hidden layer have linear decision boundary.

# Our take on Deep Learning: Probabilistic Viewpoint

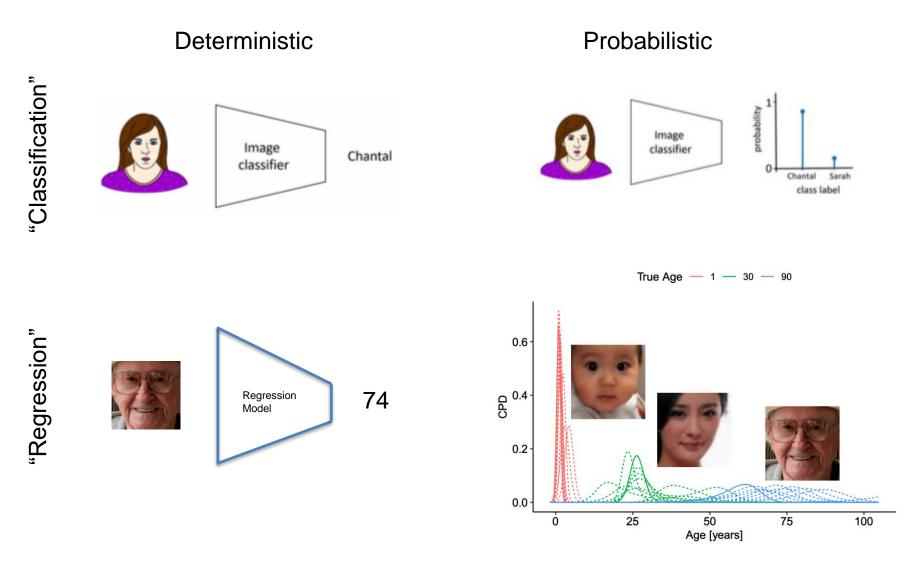
### Tasks in supervised DL

- 2 Main tasks in DL predict y given x
  - Classification
    - Point prediction: Predict a class label
    - Probabilistic prediction: predict a discrete probability distribution over all possible class labels
  - Regression
    - Point prediction: Predict a number
    - Probabilistic prediction: predict a continuous probability distributions over the possible Y value range
- The loss function depends on the task



**Supervised Learning** 

#### Probabilistic vs deterministic models



Conditional probability distribution (CPD) p(y|x)

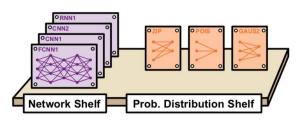
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### Guiding Theme of the course

- We treat DL as *probabilistic models*, as statistical model (logistic regression, ...) to predict the conditional probability distribution P(Y|x) for the outcome
- The models are fitted to training data with maximum likelihood (or Bayes)

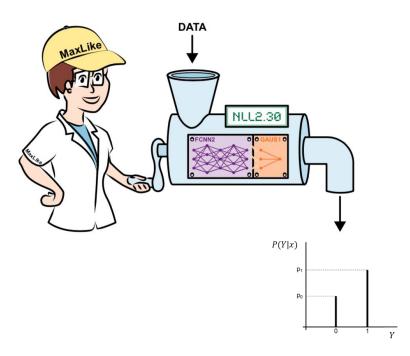
#### Special networks for x

- Vector FCNN
- Image CNN
- Text CNN/RNN



NN heads tailored for Y

- Probabilistic classification
- Probabilistic regression



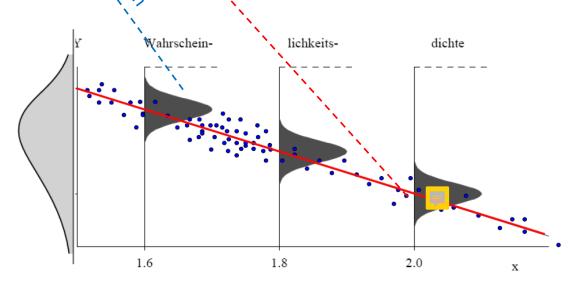
### Recall linear regression from statistics

 $(Y|X = x_i) \sim N(\mu(x_i), \sigma^2)$   $Y \in \mathbb{R},$   $\mu_x \in \mathbb{R}$ 

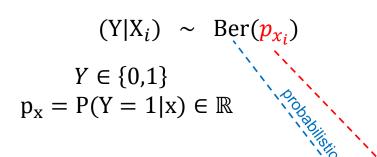
Y can have an arbitrary distribution.

 $y_i = \beta_0 + \beta_1 \cdot x_{i1} + \varepsilon_i$   $E(Y_{X_i}) = \mu_{X_i} = \hat{y}_{x_i} = \beta_0 + \beta_1 \cdot x_{i1}$   $Var(Y_{X_i}) = Var(\varepsilon_i) = \sigma^2$   $\varepsilon_i \sim N(0, \sigma^2)$ 

Probabilistic linear regression predicts for each input  $x_i$  a Gaussian conditional probability distribution for the output  $P(Y|x_i)$  that assigns each possible value of Y a likelihood.



### Recall logistic regression from statistics

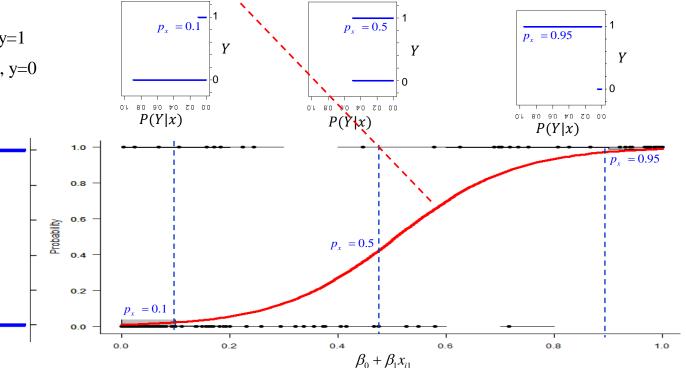


 $\log\left(\frac{p_{x_i}}{1-p_{x_i}}\right) = \beta_0 + \beta_1 x_{i1}$ 

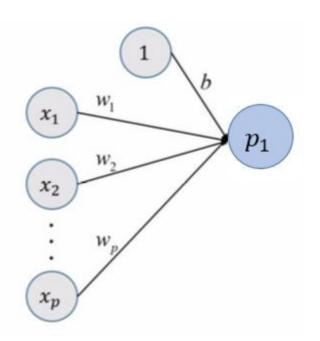
$$P(Y = 1 | x_i) = \frac{p_{x_i}}{p_{x_i}} = \sigma(\beta_0 + \beta_1 x_{i1}) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_{i1})}}$$

Logisic regression predicts a conditional Bernoulli  $P(Y|x_i)$ 

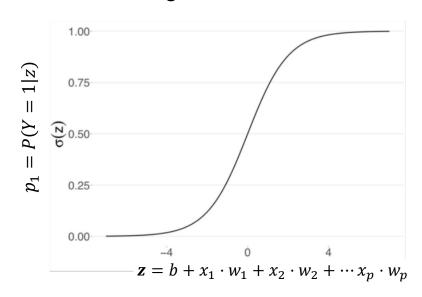
$$P(Y | X = x) = \begin{cases} p_x, & y=1\\ 1 - p_x, & y=0 \end{cases}$$



#### Logistic regression in DL view



#### **Sigmoid Activation**



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

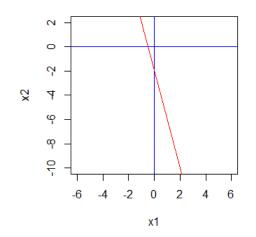
A NN for a binary outcome with only 1 neuron with sigmoid-activation (and no hidden layer) is nothing else than logistic regression!

### Logistic regression yield linear/planar decision curves

Logistic regression model: 
$$\ln\left(\frac{p}{1-p}\right) = 1 + 2x_1 + 0.5x_2$$

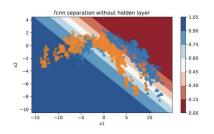
Determine the separation curve between Y=1 and Y=0 in the feature room which is spanned by  $x_1$  and  $x_2$  and draw it in the following plot  $x_2$  and  $x_3$ 

Hint: on the separation curve should hold: P(Y = 1|x) = 0.5-> plug in 0.5 for p and solve for  $x_2$ .



$$\ln\left(\frac{0.5}{1 - 0.5}\right) = 0 = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$
$$x_2 = -\frac{\beta_0}{\beta_2} - \frac{\beta_1}{\beta_2} \cdot x_1$$

$$x_2 = -2 - 4 \cdot x_1$$

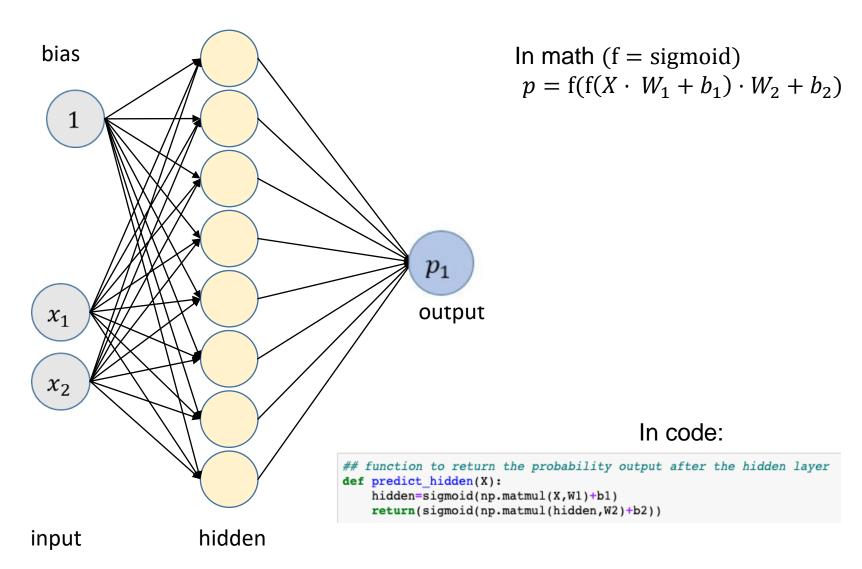


Hence a NN with 1 output neuron with sigmoid-activation w/o hidden layer have linear decision boundary



### A first deep network

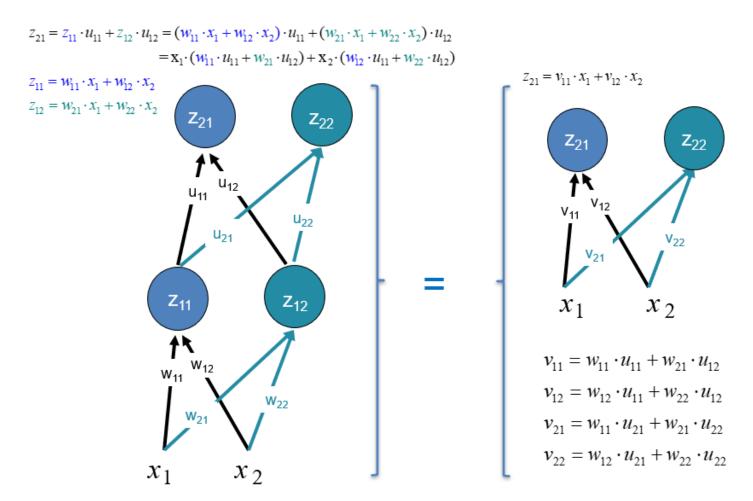
*W*<sub>from,to</sub>



# To go deep non-linear activation functions are needed

2 linear layers can be replaced by 1 linear layer -> can't go deep with linear layers!

$$z = (x \cdot W) \cdot U = x \cdot (W \cdot U) = x \cdot V$$



Remark: biases are ignored here, but do not change fact

#### Recap: Matrix Multiplication aka dot-product of matrices

We can only multiply matrices if their dimensions are compatible.

$$\mathbf{A} \times \mathbf{B} = \mathbf{C}$$
  
 $(\mathbf{m} \times \mathbf{n}) \times (\mathbf{n} \times \mathbf{p}) = (\mathbf{m} \times \mathbf{p})$ 

$$\begin{bmatrix} \mathbf{A}_{3x3} & \times & \mathbf{B}_{3x2} & = & \mathbf{C}_{3x2} \\ a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \mathbf{x} \begin{bmatrix} \mathbf{b}_{11} & \mathbf{b}_{12} \\ \mathbf{b}_{21} & \mathbf{b}_{22} \\ \mathbf{b}_{31} & \mathbf{b}_{32} \end{bmatrix} = \begin{bmatrix} \mathbf{c}_{11} & \mathbf{c}_{12} \\ \mathbf{c}_{21} & \mathbf{c}_{22} \\ \mathbf{c}_{31} & \mathbf{c}_{32} \end{bmatrix}$$

$$c_{11} = a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31}$$

$$c_{12} = a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32}$$

$$c_{21} = a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31}$$

$$c_{22} = a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32}$$

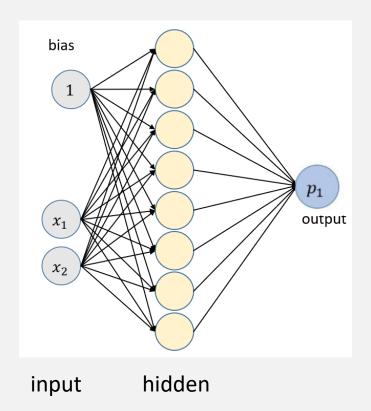
$$c_{31} = a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31}$$

$$c_{32} = a_{31}b_{12} + a_{32}b_{22} + a_{33}b_{32}$$

#### Example:

$$\mathbf{A}_{2x2} = \begin{pmatrix} 2 & 1 \\ \hline 0 & 3 \end{pmatrix} \qquad \mathbf{B}_{2x3} = \begin{pmatrix} 3 & 1 & 7 \\ 8 & 2 & 4 \end{pmatrix} \qquad \mathbf{C}_{2x3} = \mathbf{A}_{2x2} \cdot \mathbf{B}_{2x3} = \begin{pmatrix} 11 & 4 & 18 \\ 24 & 6 & 12 \end{pmatrix}$$

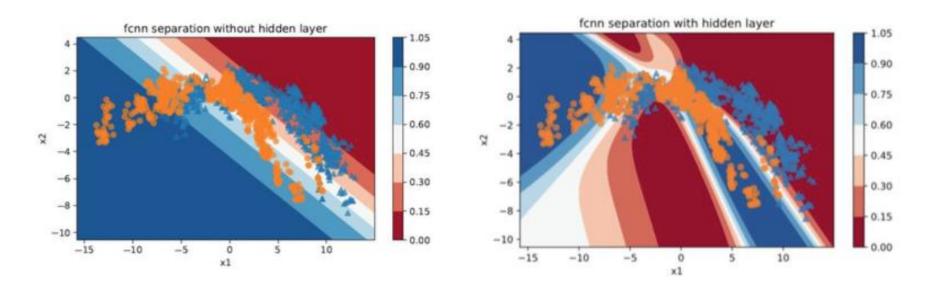
#### Exercise:



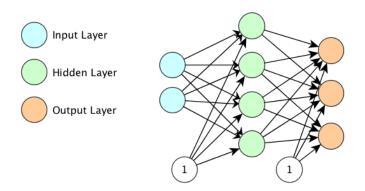


Open NB <u>01\_simple\_forward\_pass.ipynb</u> and do exercise <u>stop</u> before Keras

# Observations from NB: The benefit of hidden layers

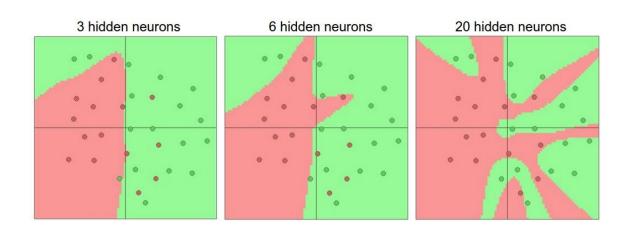


# One hidden Layer is "in theory" enough



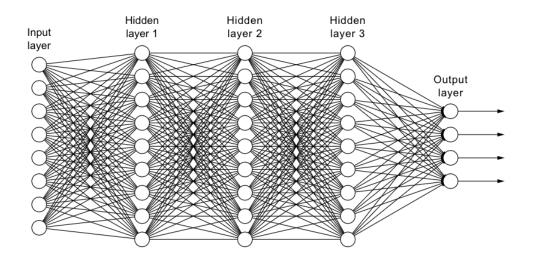
A network with one hidden layer is a universal function approximator!

→ Each decision curve can be fitted with a NN with large enough hidden layer

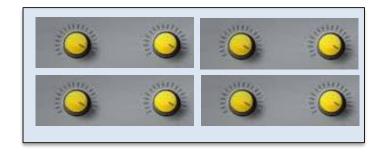


# Training NN: Minimize the loss function

# How to determine the weights



Given the input, the output of a NN is defined by the weights

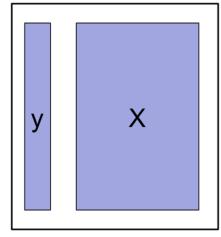


Typical >1 Mio. weights

During training the weights (including biases) are tuned so that the NN bests fulfils its specific tasks by minimizing a loss function.

#### Tasks in DL

- The loss function depends on the task
- 2 Main tasks in DL predict y given x



Supervised Learning

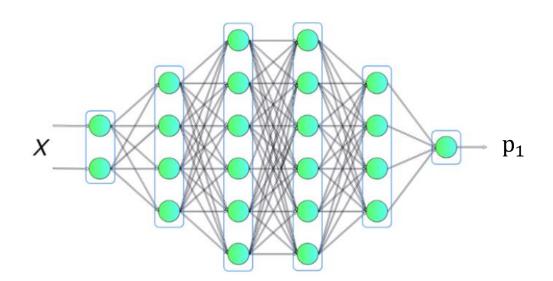
#### Classification

- Point prediction: Predict a class label
- Probabilistic prediction: predict a discrete probability distribution over the class labels
- First we focus on probabilistic binary classification where  $Y \in \{0, 1\}$

#### Regression

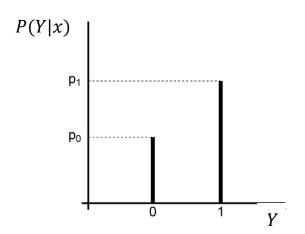
- Point prediction: Predict a number
- Probabilistic prediction: predict a continuous distributions

# Example of a NN for binary classification



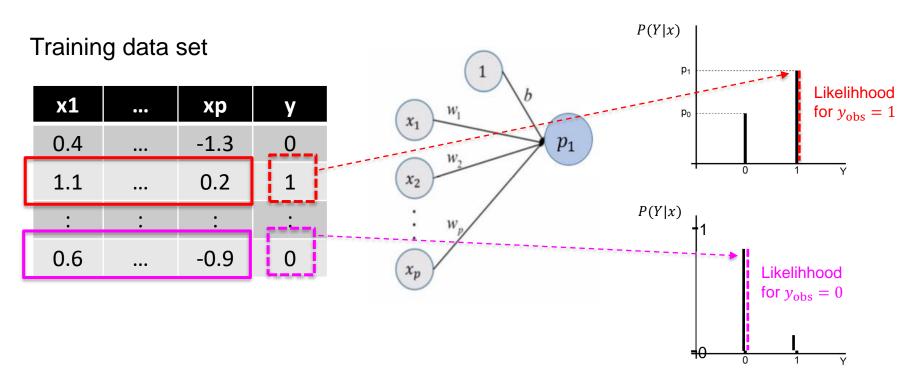
For binary classification we can use one neuron in the last layer with sigmoid activation yielding a conditional probability  $p_1$  for Y = 1

Given (=conditioned on) the input featurs x of an observation, the NN predicts as output the probability that this observation corresponds to class Y = 1 by  $p_1 = P(Y = 1|x)$ , and hence the probability for the Y = 0 is  $p_0 = P(Y = 0|x) = 1 - p_1$ .



# Probabilistic binary classification aka logistic regression

probabilistic prediction



Given (=conditioned on) the input featurs x of an observation i, a well trained NN

- should predict large  $p_1 = P(Y = 1|x)$  if the observed class is  $y_i = 1$
- should predict small  $p_1$  hence large  $p_0 = P(Y = 0|x)$  if observed is  $y_i = 0$
- → The likelihood (for the observed outcome) or LogLikelihood should be large

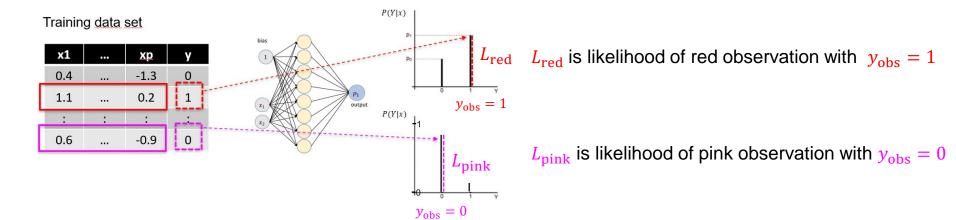


# Fitting a probabilistic binary classification

The Likelihood of an observation i is the likelihood (probability), that the predicted probability distribution  $P(Y|x_i)$  assigns to the observed outcome  $y_i$ .

Note: the predicted  $P(Y \mid x_i)$  and the corresponding likelihood for the observed  $y_i$  depends on the data-point  $(x_i, y_i)$  and the model parameter values

 $\rightarrow$  The higher the likelihood, the better is the model prediction P(Y|x)



#### Maximum likelihood principle:

Statistical models are fit to maximize the average LogLikelihood

$$L = \frac{1}{N} \sum L_i = \frac{1}{N} \sum [y_i \log(p_{1i}) + (1 - y_i) \log(1 - p_{1i})]$$

we often use the simplified notation average logLik :  $L = \frac{1}{N} \sum log(p_i)$ 

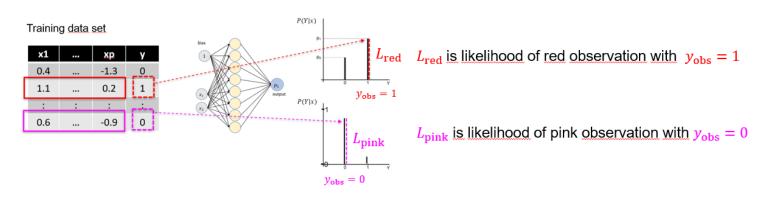
Predicted probability for the observed outcome  $y_{obs}$ 

# NLL Loss for probabilistic binary classification

In DL we aim to minimize a loss function L(data, w) which depends on the weights  $\rightarrow$  Instead of maximizing the average LogLikelihood

we minimize the averaged Negative LogLikelihood (NLL):

$$loss = NLL = -\frac{1}{N} \sum log(L_i)$$



The best possible value of the NLL contribution of an observation i is  $log(L_i) = -log(1) = 0$ The worst possible value of the NLL contribution of an observation i  $log(L_i) = -log(0) = \infty$ 

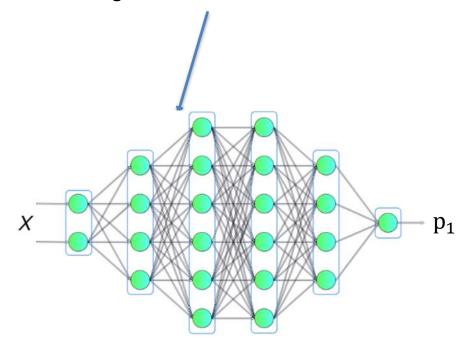
Note: In Keras we use the loss 'binary\_crossentropy', if we do probabilist binary classification with one output node with sigmoid activation.

# Optimization in DL

- DL many parameters
  - Optimization by gradient descent

- Algorithm
  - Take a batch of training examples
  - Calculate the loss of that batch
  - Tune the parameters so that loss gets minimized

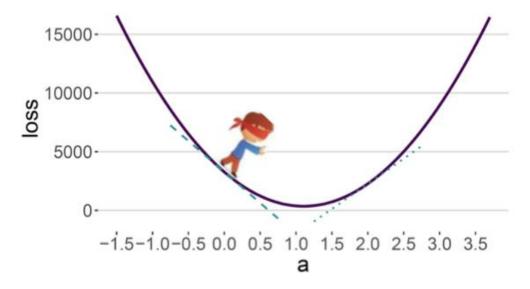
Parameters of the NN are the weights.



Modern Networks have Billions (10<sup>9</sup>) of weights. Record 2020 1.5E9 <a href="https://openai.com/blog/better-language-models/">https://openai.com/blog/better-language-models/</a>

#### Idea of gradient descent

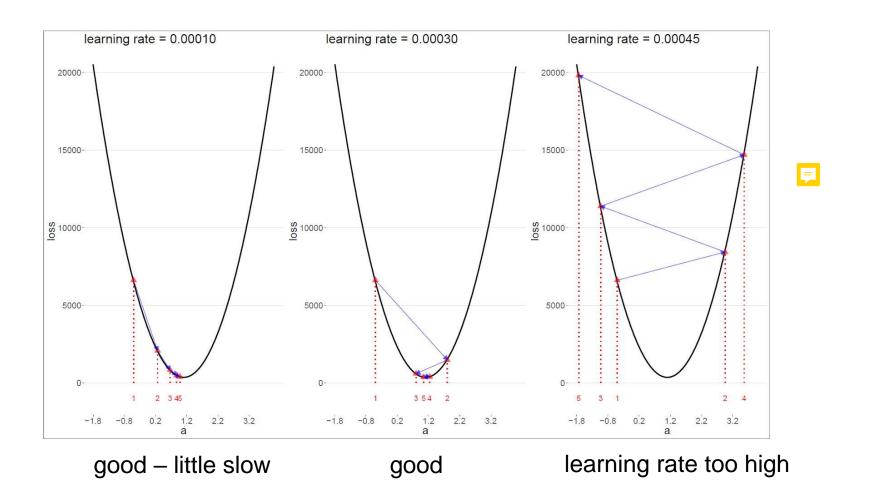
Shown loss function for a single parameter a



- Take a large step if slope is steep (you are away from minimum)
- Slope of loss function is given by gradient of the loss w.r.t. a
- Iterative update of the parameter a

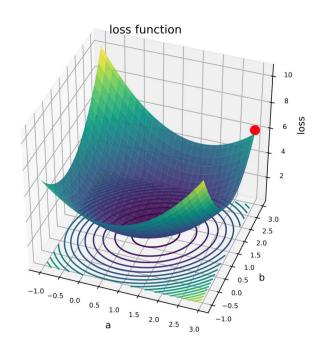
$$a^{(t)} = a^{(t-1)} - \varepsilon^{(t)} \frac{\partial L(a)}{\partial a} \bigg|_{a=a^{(t-1)}}$$
 learning rate

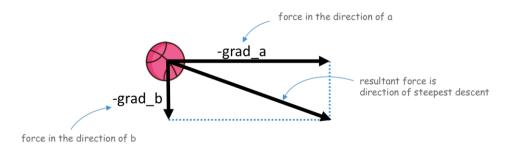
#### The learning rate is a very important parameter for DL



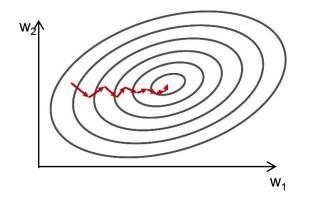
If the loss diverges to infinity: Don't panic, lower the learning rate!

#### In two dimensions





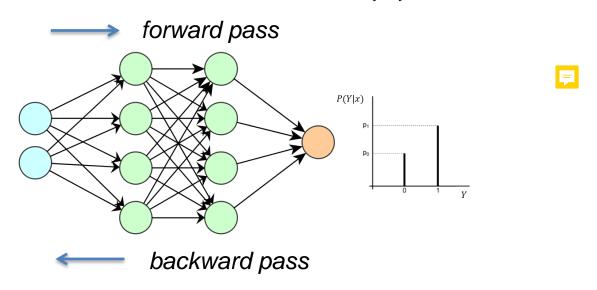
Gradient is perpendicular to contour lines



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

# Backpropagation

- We efficiently train the weights in a NN via forward and backward pass
  - Forward Pass propagate training example through network
    - Predicts as output  $P(Y|x_i)$  for each input  $x_i$  in the batch given the NN weights w  $\rightarrow$  With  $P(Y|x_i)$  and the observed  $y_i$  we compute the loss  $L = \left( \text{NLL} = -\frac{1}{N} \sum log(L_i) \right)$
  - Backward pass propagate gradients through network
    - Via chain rule all gradients  $\frac{\partial L(\mathbf{w})}{\partial w_k}$  are determined
      - $\rightarrow$  update the weights  $w_i^{(t)} = w_i^{(t-1)} \varepsilon^{(t)} \frac{\partial L(\mathbf{w})}{\partial w_i} \Big|_{w_i = w_i^{(t-1)}}$



# The miracle of gradient descent in DL



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

# Typical Training Curve / ReLU

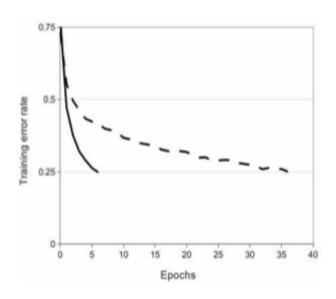
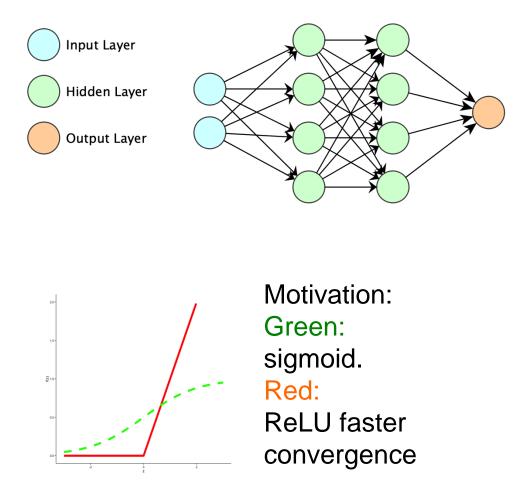


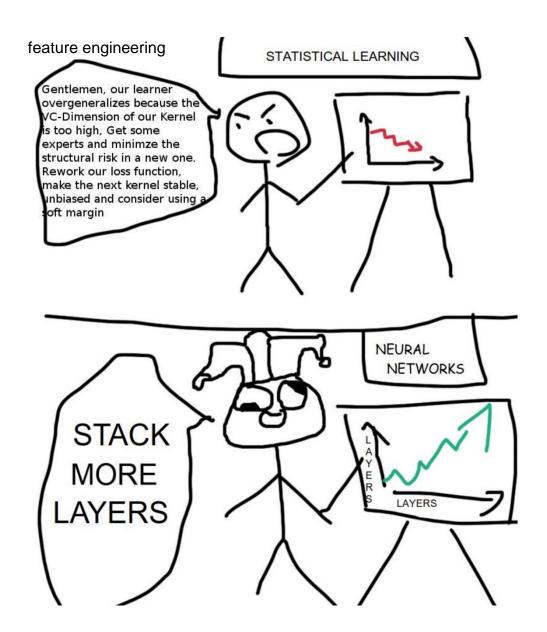
Figure 1: A four-layer convolutional neural network with ReLUs (solid line) reaches a 25% training error rate on CIFAR-10 six times faster than an equivalent network with tanh neurons

Source: Alexnet Krizhevsky et al 2012

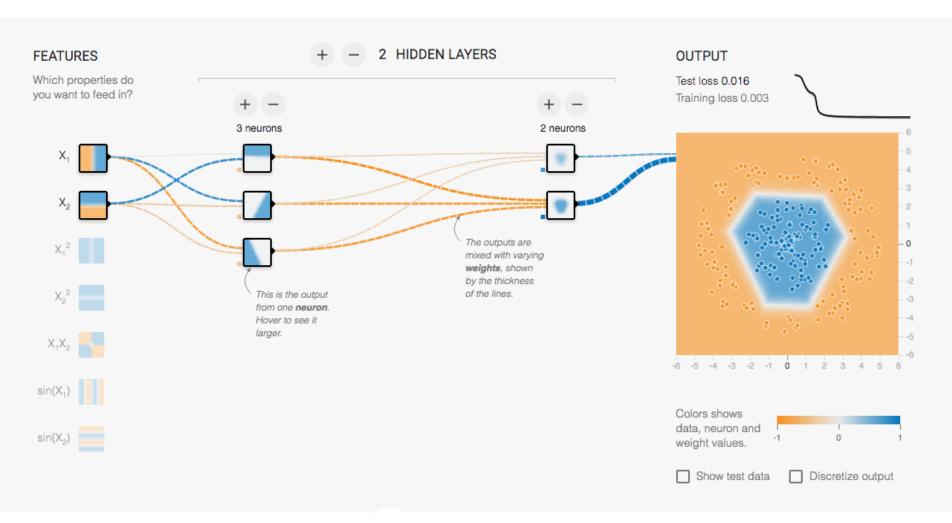


Epochs: "each training examples is used once"

#### Game time - Recall learing DL vs Statistical Learning



#### Experiment yourself (homework)



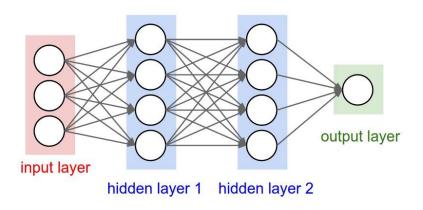
http://playground.tensorflow.org

Let's you explore the effect of hidden layers

# Introduction to Keras

# Keras as High-Level library to TensorFlow

- We use Keras as high-level library
- Libraries make use of the Lego like block structure of networks



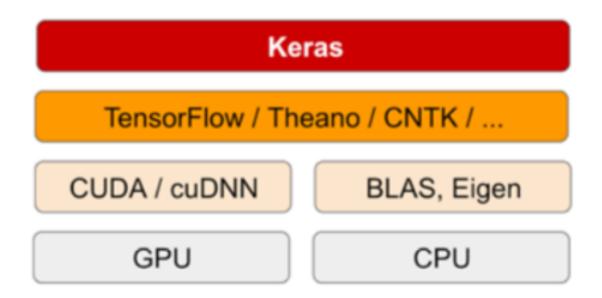




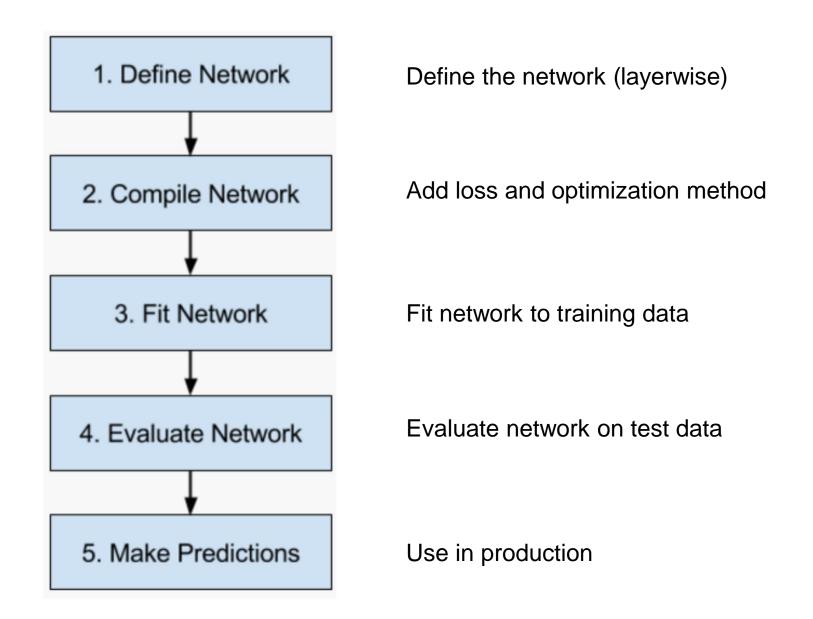


# High Level Libraries

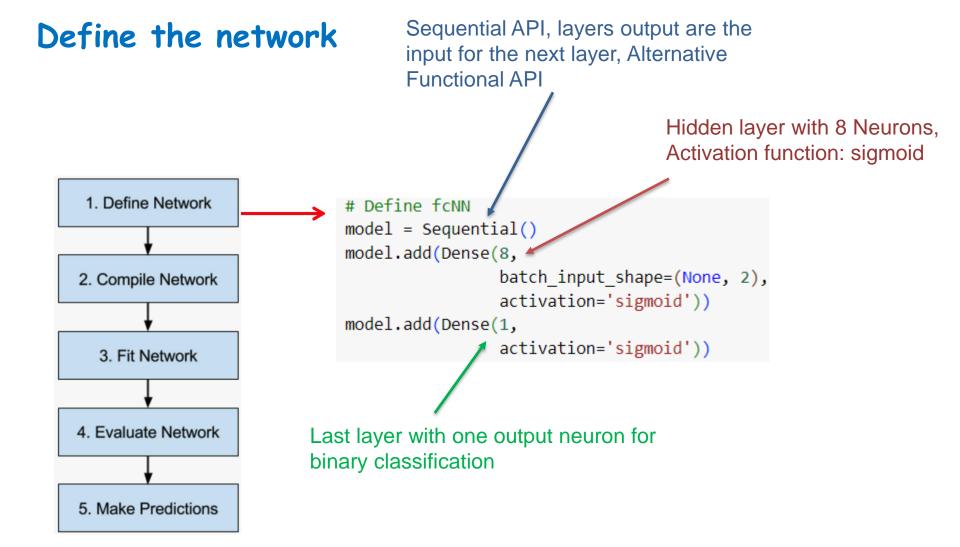
- Keras
  - Keras is now part of TF core
  - https://keras.io/



#### Keras Workflow



# A first run through

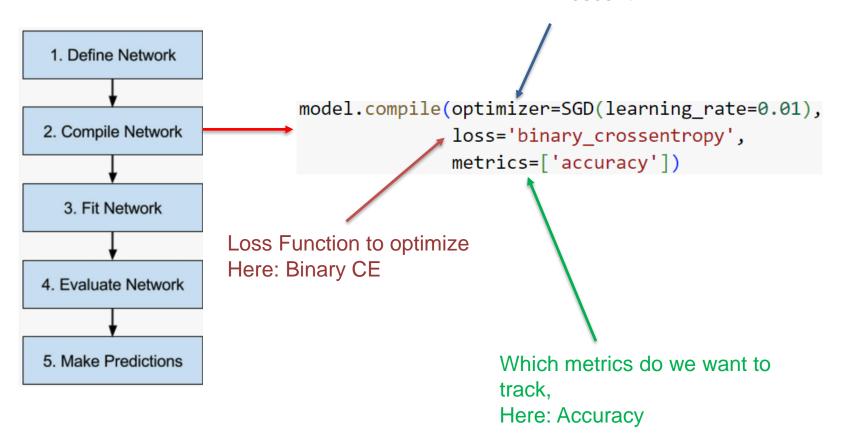


Input shape needs to be defined only at the beginning.

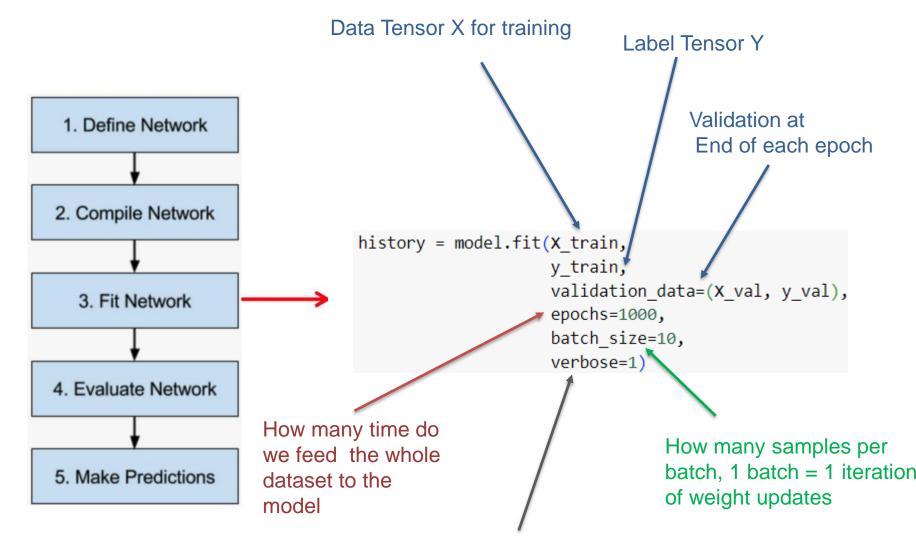
Alternative: input\_dim=2, Functional API or Sequential API

# Compile the network

Which optimizer should be used?
Here Stochastic Gradient
Descent

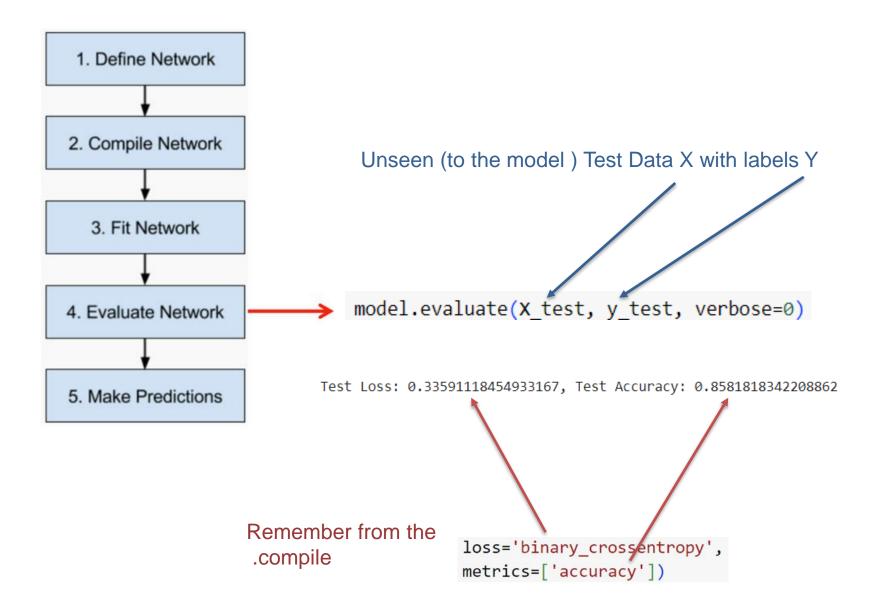


#### Fit the network

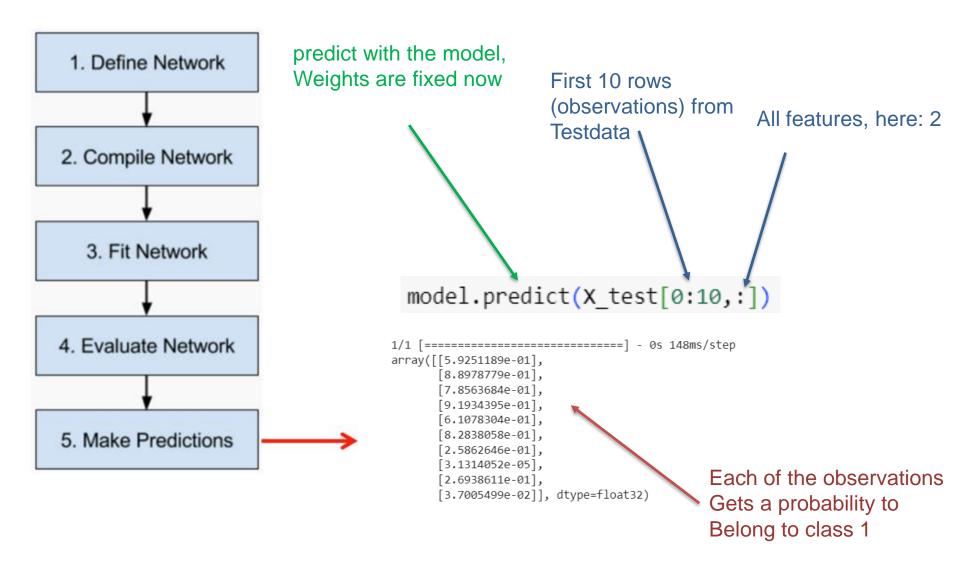


Should we see the whole output? If no verbose = 0

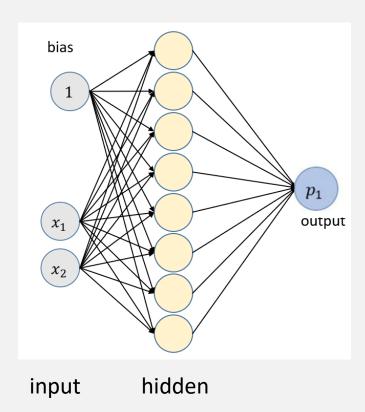
#### Evaluate the network



#### Make Predictions



#### Exercise:





Open NB <u>01\_simple\_forward\_pass.ipynb</u> and do the Keras part

#### Summary

- A neuron in a NN is loosely inspired by a neuron in the brain.
- The value of a neuron is computed by the weighted sum of the values in connected neurons of the previous layer, which is then passed through an activation function such as sigmoid or relu
- For a binary classification task we can use the sigmoid activation function for a single neuron in the last layer.
   As loss we use in Keras 'binary\_crossentropy' which is the NLL
- To achieve a non-linear (non-planar) decision boundary between the classes in binary classification, we need NNs with hidden layers.
- The weights of a NN are learned during the training via backprobagation minimizing the loss using SGD (Stochastic Gradient Descent)
- For efficient training use the relu activation function for hidden layers.
- If the loss diverges to infinity: Don't panic, lower the learning rate!