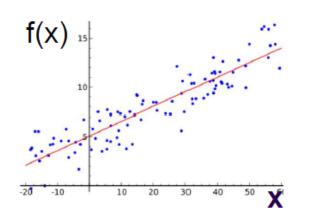
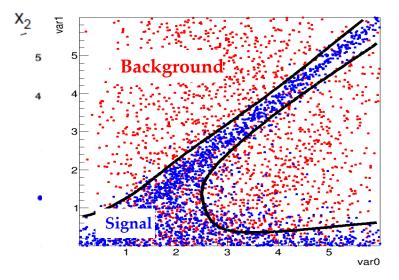
## INTRODUCTION TO DATA SCIENCE

## What are Multivariate Techniques

→ Many things ... starting from "linear regression" ...



to multivariate event classification

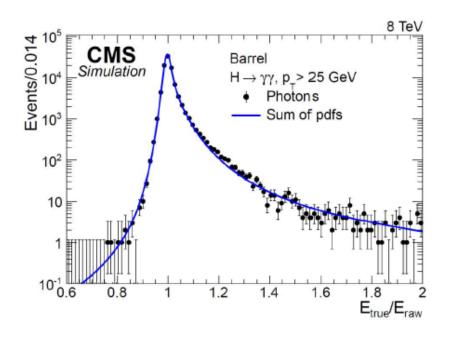


- → or w/o prior 'analytic' model
- typically "multivariate"
  - Parameters depend on the 'joint distribution' f(x<sub>1</sub>, x<sub>2</sub>)
- 'learning from experience' → known data points

#### Machine Learning - Multivariate Techniques

- fitted (non-)analytic function may approximate:
  - target value → 'regression'

(e.g. calorimeter calibration/correction function)

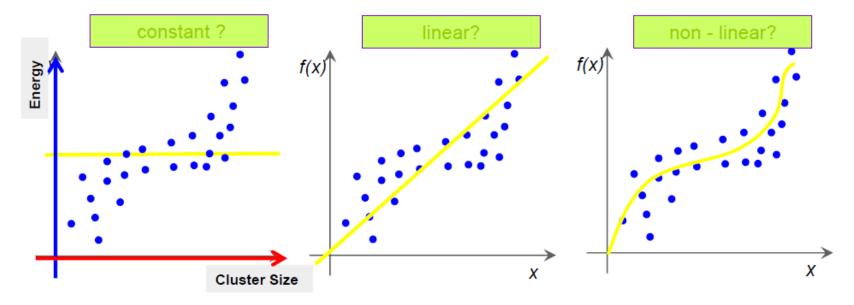


#### MC sample: $\gamma$ +jets

- Raw energy in crystals, η, Φ
- Cluster shape variables
- Local cluster position variables (energy leakage)
- Pile-up estimators
- → predict energy correction (i.e. parameters in crystal-ball: pdf for energy measurement)

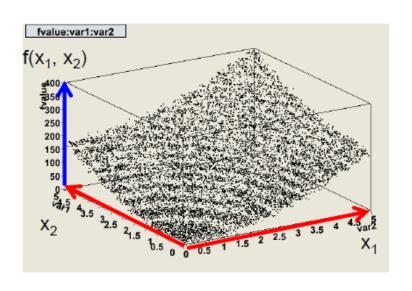
## Regression

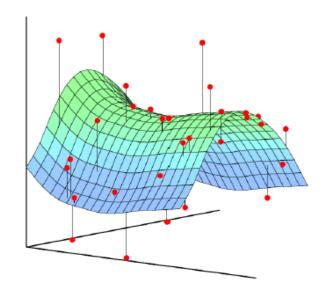
- 'known measurements" → model "functional behaviour"
- e.g. : photon energy as function "D"-variables: ECAL shower parameters + ...



- known analytic model (i.e. nth -order polynomial) → Maximum Likelihood Fit)
- no model ?
  - "draw any kind of curve" and parameterize it?
- seems trivial ? → human brain has very good pattern recognition capabilities!
- what if you have many input variables?

### Regression -> model functional behaviour





- "standard" regression → fit a known analytic function
  - e.g.  $f(\mathbf{x}) = ax_1^2 + bx_2^2 + c$
- BUT most times: don't have a reasonable "model" ? → need something more general:
  - e.g. piecewise defined splines, kernel estimators, decision trees to approximate f(x)

Note: we are not interested in the 'fitted parameter(s)', it is not: "Newton deriving  $F=m\cdot a$ "  $\rightarrow$  just provide prediction of function values f(x) for new measurements x

#### Multi-Variate Classification

Consider events which can be either signal or background events.

Each event is characterized by *n* observables:

$$\vec{x} = (x_1, ..., x_n)$$
 "feature vector"

Goal: classify events as signal or background in an optimal way.

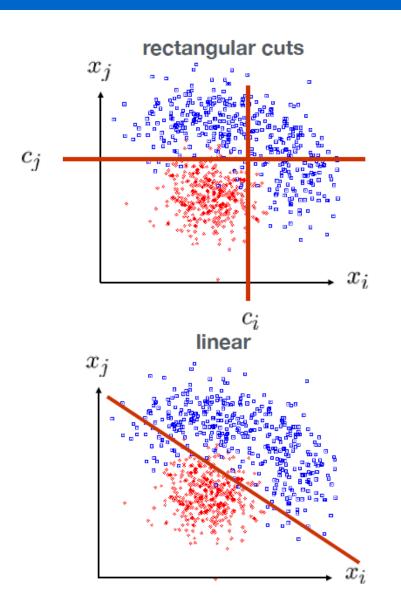
This is usually done by mapping the feature vector to a single variable, i.e., to scalar test statistic:

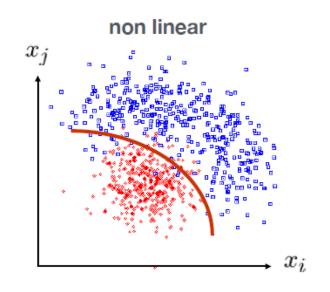
$$\mathbb{R}^n \to \mathbb{R} : y(\vec{x})$$

A cut y > c to classify events as signal corresponds to selecting a potentially complicated hyper-surface in feature space. In general superior to classical "rectangular" cuts on the  $x_i$ .

Problem closely related to machine learning (pattern recognition, data mining, ...)

## Classification: Different Approaches



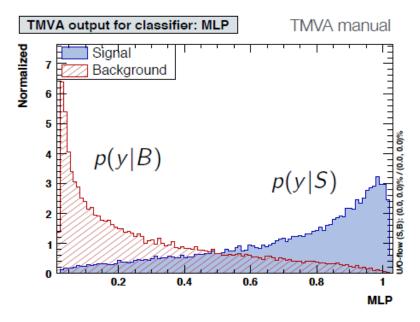


k-Nearest-Neighbor,Boosted Decision Trees,Multi-Layer Perceptrons,Support Vector Machines

. . .

#### Signal Probability Instead of Hard Decisions

Example: test statistic *y* for signal and background from a Multi-Layer Perceptron (MLP):



Instead of a hard yes/no decision one can also define the probability of an event to be a signal event:

$$P_s(y) \equiv P(S|y) = \frac{p(y|S) \cdot f_s}{p(y|S) \cdot f_s + p(y|B) \cdot (1 - f_s)}, \qquad f_s = \frac{n_s}{n_s + n_b}$$

## Machine learning: Basic terminology

The goal of machine learning is to predict results based on incoming data.

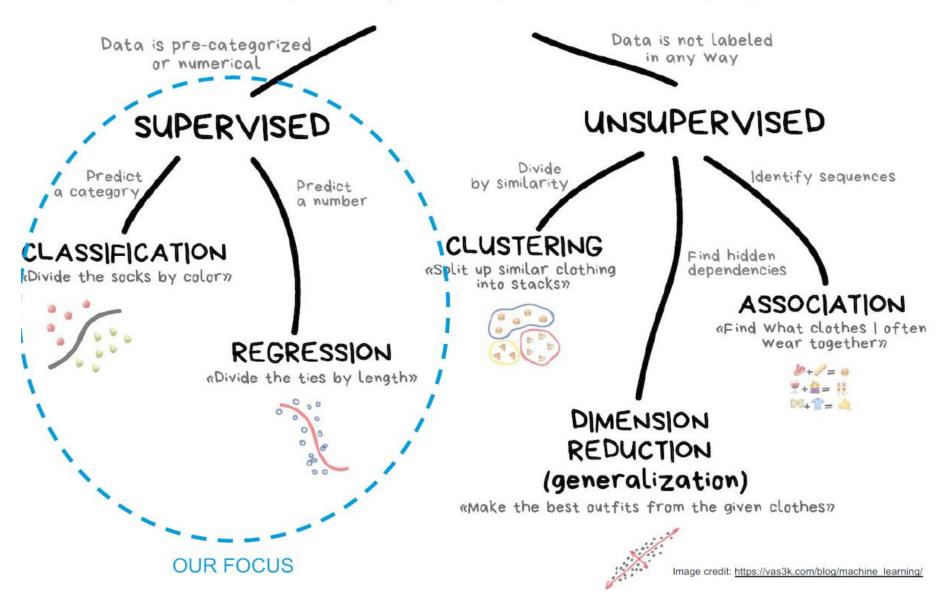
**Features** (also parameters, or variables): these are the factors for a machine to look at. E.g.: carthesian coordinates, pixel colors, a car mileage, user's gender, stock price, word frequency in the text.

- Quantitative (x = {1.02, 0.21, 0.12, 2})
- Qualitative discrete (x = {medium, small, large}) or categorical (x={red, blue, green})

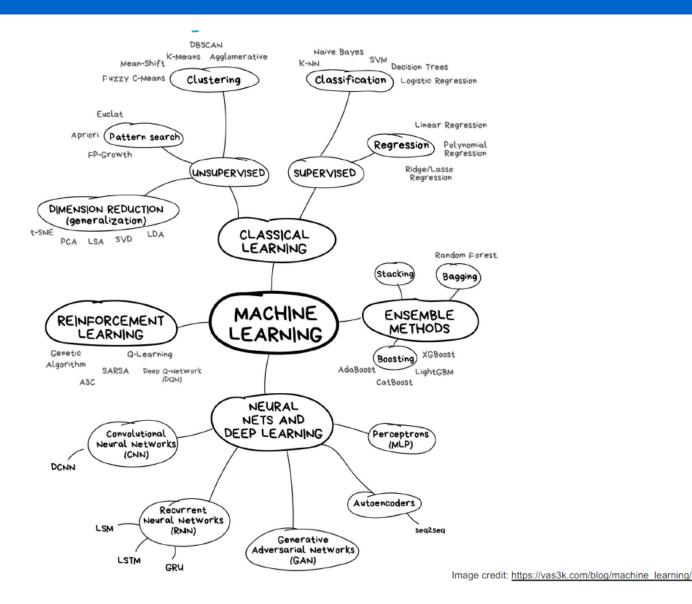
**Algorithms** (also models): Any problem can be solved in different ways. The method you choose affects the precision, performance, and size of the final model.

 If the data is insufficient/inapproriate (e.g. statistically limited or missing important features), even the best algorithm won't help. Pay attention to the accuracy of your results only when you have a good enough dataset.

#### CLASSICAL MACHINE LEARNING



#### Where are the neural networks?



#### **Neural Networks**

Any neural network is a collection of **neurons** and **connections** between them.

**Neuron** is a function with a set of inputs and one output. Its task is to take all numbers from its input, apply a function on them and send the result to the output.

Example: sum up all numbers from the inputs and if that sum is bigger than N give 1 as a result. Otherwise return zero.

**Connections** are like channels between neurons. They connect outputs of one neuron with the inputs of another so they can send digits to each other. Each connection has only one parameter the *weight*.

 These weights tell the neuron to respond more to one input and less to another. Weights are adjusted when training — that's how the network learns.

## Perceptron

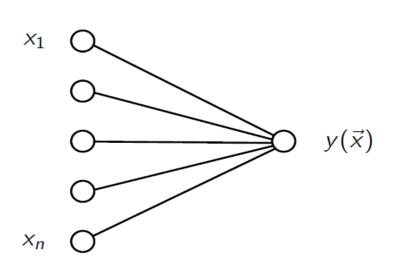
Discriminant:

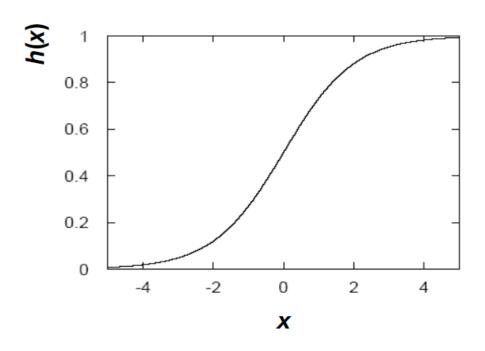
$$y(\vec{x}) = h\left(w_0 + \sum_{i=1}^n w_i x_i\right)$$

The nonlinear, monotonic function h is called activation function.

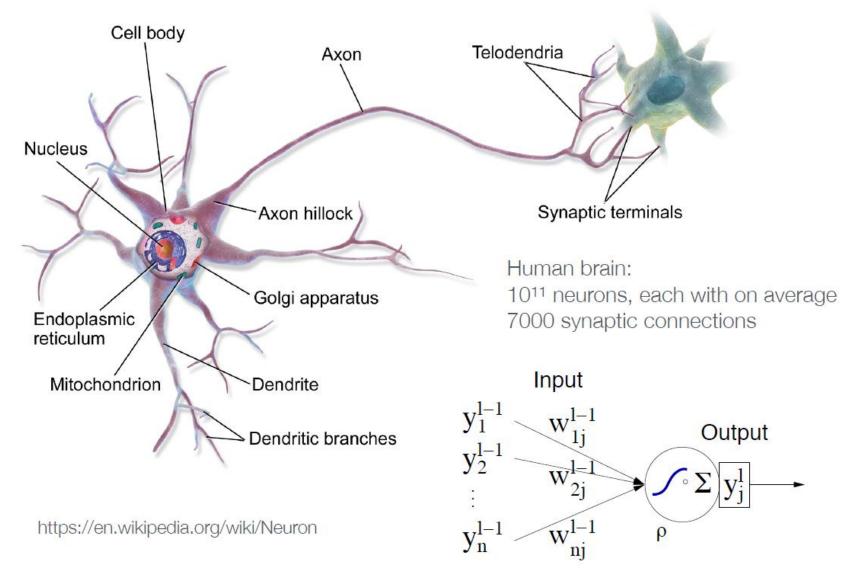
Typical choices for *h*:

$$\frac{1}{1+e^{-x}}$$
 ("sigmoid"), tanh x

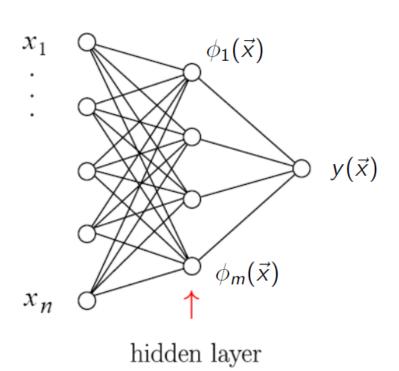




## The Biological Inspiration: the Neuron



#### Feedforward Neural Network with One Hiden Layer



superscripts indicates layer number

$$\phi_i(\vec{x}) = h\left(w_{i0}^{(1)} + \sum_{j=1}^n w_{ij}^{(1)} x_j\right)$$

$$y(\vec{x}) = h \left( w_{10}^{(2)} + \sum_{j=1}^{m} w_{1j}^{(2)} \phi_j(\vec{x}) \right)$$

Straightforward to generalize to multiple hidden layers

## Network Training

 $\vec{x}_a$ : training event, a = 1, ..., N

 $t_a$ : correct label for training event a

e.g.,  $t_a = 1$ , 0 for signal and background, respectively

 $\vec{w}$ : vector containing all weights

#### Error function:

$$E(\vec{w}) = \frac{1}{2} \sum_{a=1}^{N} (y(\vec{x}_a, \vec{w}) - t_a)^2 = \sum_{a=1}^{N} E_a(\vec{w})$$

Weights are determined by minimizing the error function.

## Backpropagation

Start with an initial guess  $\vec{w}^{(0)}$  for the weights an then update weights after each training event:

$$\vec{w}^{(\tau+1)} = \vec{w}^{(\tau)} - \eta \nabla E_a(\vec{w}^{(\tau)})$$
Learning rate

Let's write network output as follows:

$$y(\vec{x}) = h(u(\vec{x})) \text{ with } u(\vec{x}) = \sum_{j=0}^{m} w_{1j}^{(2)} \phi_j(\vec{x}), \ \phi_j(\vec{x}) = h\left(\sum_{k=0}^{n} w_{jk}^{(1)} x_k\right) \equiv h(v_j(\vec{x}))$$

Here we defined  $\phi_0 = x_0 = 1$  and the sums start from 0 to include the offsets.

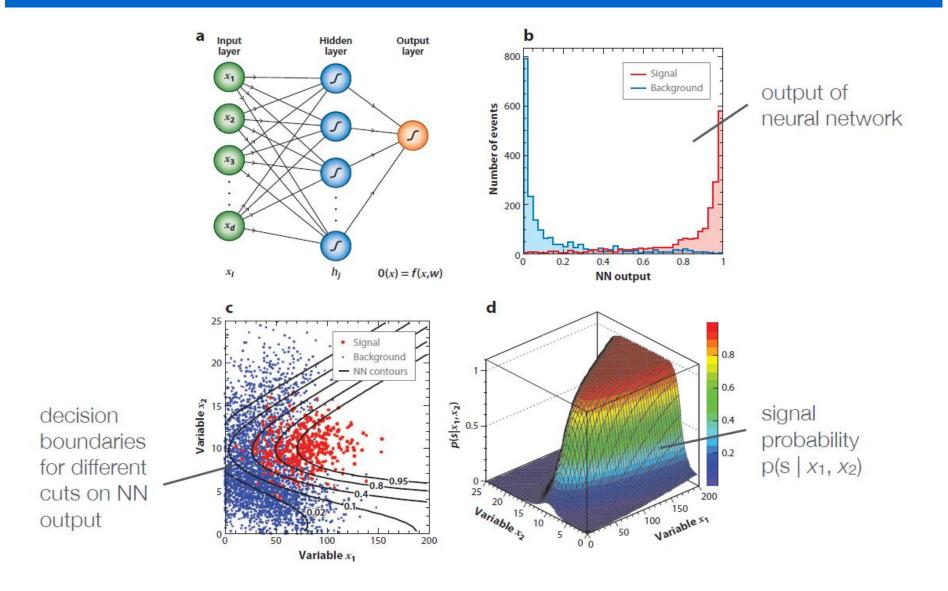
Weights from hidden layer to output:

$$E_{a} = \frac{1}{2}(y_{a} - t_{a})^{2} \rightarrow \frac{\partial E_{a}}{\partial w_{1j}^{(2)}} = (y_{a} - t_{a})h'(u(\vec{x}_{a}))\frac{\partial u}{\partial w_{1j}^{(2)}} = (y_{a} - t_{a})h'(u(\vec{x}_{a}))\phi_{j}(\vec{x}_{a})$$

Weights from input layer to hidden layer (→ further application of chain rule):

$$\frac{\partial E_a}{\partial w_{ik}^{(1)}} = (y_a - t_a)h'(u(\vec{x}_a))w_{1j}^{(2)}h'(v_j(\vec{x}_a))x_{a,k} \qquad \vec{x}_a \equiv (x_{a,1}, ..., x_{a,n})$$

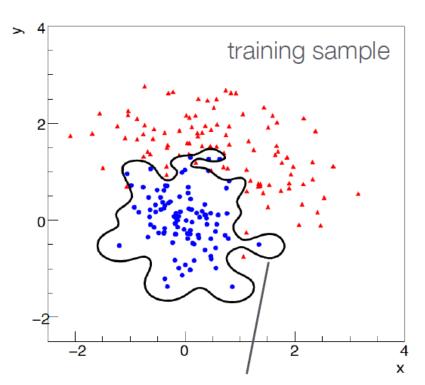
#### Neural Network Output and Decision Boundaries



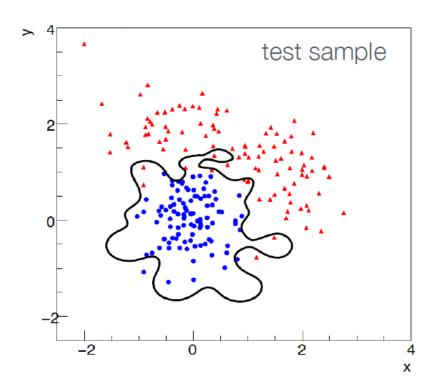
## **Example of Overtraining**

Too many neurons/layers make a neural network too flexible

→ overtraining

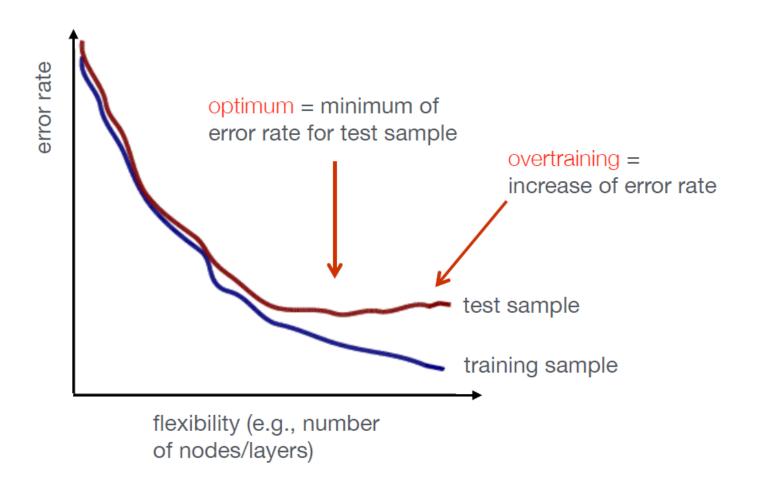






## Monitoring Overtraining

Monitor fraction of misclassified events (or error function:)



## Deep Neural Networks

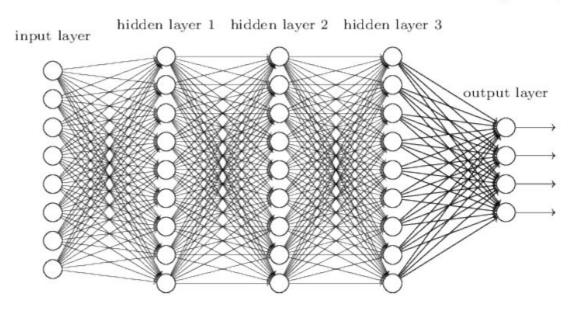
Deep networks: many hidden layers with large number of neurons

#### Challenges

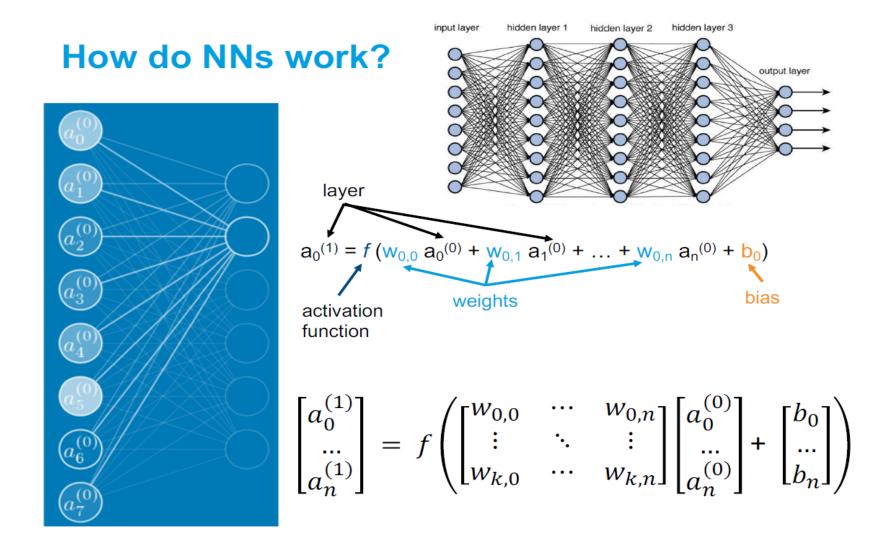
- Hard too train ("vanishing gradient problem")
- Training slow
- Risk of overtraining

#### Big progress in recent years

- Interest in NN waned before ca. 2006
- Milestone: paper by G. Hinton (2006): "learning for deep belief nets"
- Image recognition, AlphaGo, ...
- Soon: self-driving cars, ...



#### How do NNs work?



#### How do NNs learn?

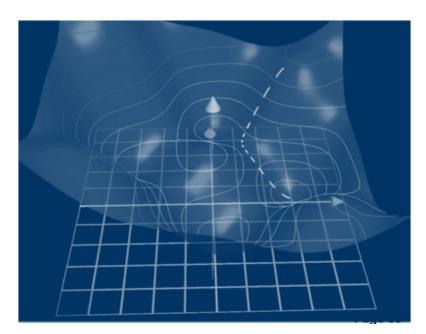
After we constructed a network, our task is to **assign proper weights** so neurons will react correctly to incoming signals.

define a loss function to measure how far the response is from the truth

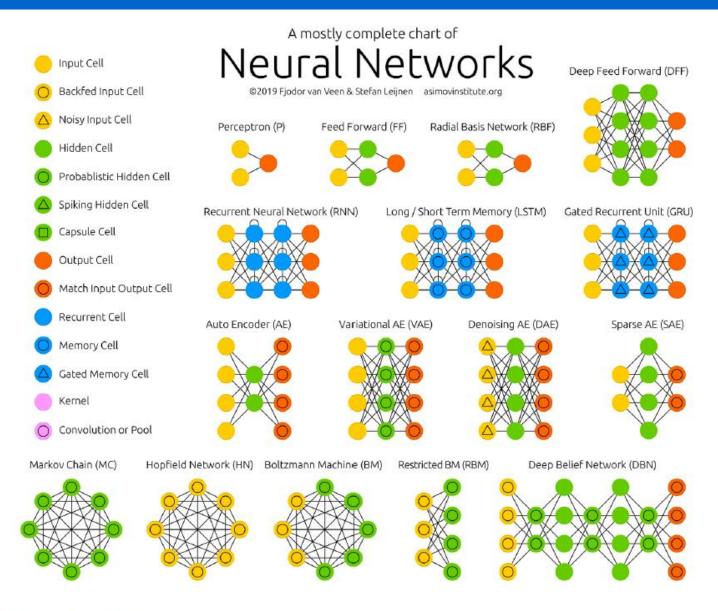
This function is a function of all the weights and biases in the NN (a priori a very large number), and the goal of training is to find its minimum.

- To start with, all weights are assigned randomly.
- After evaluating the NN on the training dataset, we can compute all the per-neuron differences with respect to the correct result.
- Computing the gradient of the loss, gives us a direction in which to tune the weights towards a local minimum

The process of correcting the weights is called backpropagation an error.



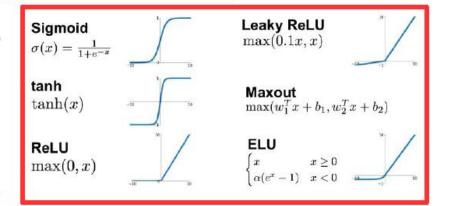
#### How do NNs learn?

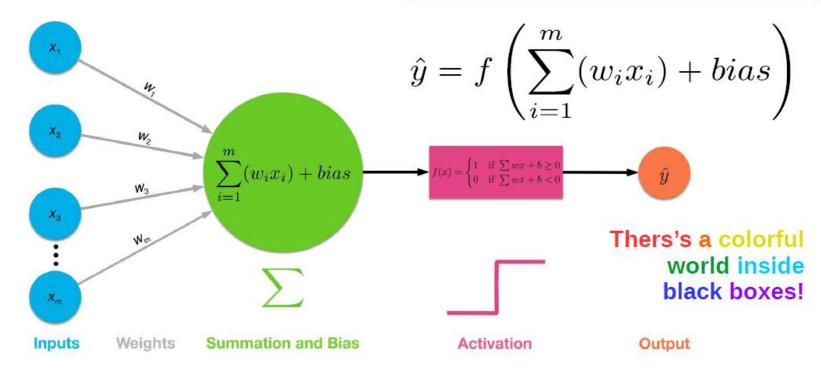


There are many more...

#### How do NNs learn?

- Each input is multiplied by a weight.
- The weighted values are summed and a bias is added
- The result is passed to an activation funciton (non liniarity).

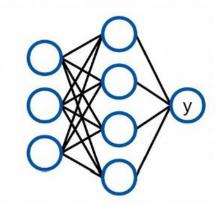


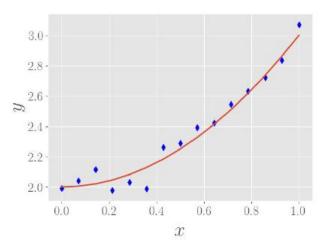


## **Typical Applications**

#### Regression:

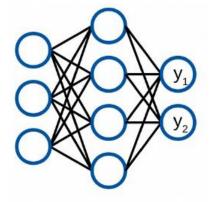
Predict a continuous label.

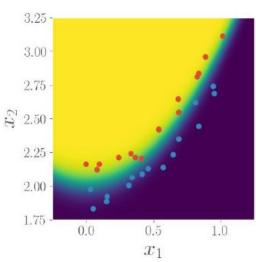




#### Classification:

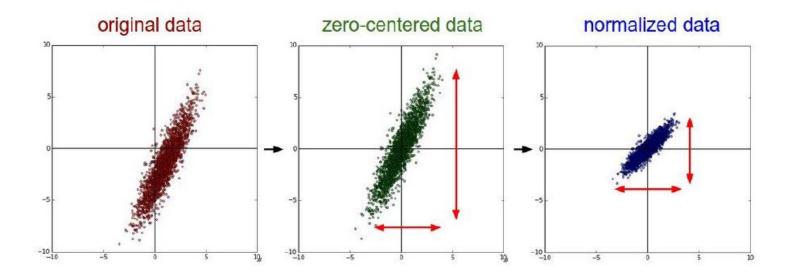
Separate events into multiple categories.





## Input Preprocesing

- Input features could have vastly different scales (e.g.  $p_{\tau}$  vs  $\eta$ ).
  - Difficult to find optimal values.
- Basic strategy: Normalize to mean=0 and variance=1.

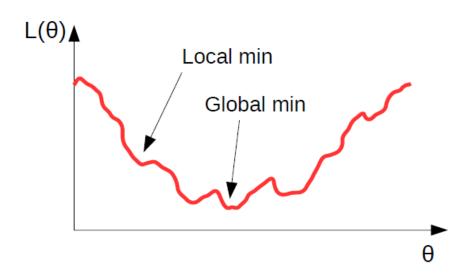


Other options possible: decorrelation, non-linear transformation, ...

## Training

- Training starts specifying an input and a target dataset.
  - For each input set, the target is what the network should learn for that input.
- A loss function is required L(θ):
  - The loss funtion quantifies the mistakes the NN makes.
     E.g. mean squared error can be used for regression.

Training is the minimization of the loss function w.r.t. the NN parameters.





#### Training: (Stochastic) Gradient Descent

 Given the increasing size of datasets and parameters, it is no more possible to directly minimize the loss function.

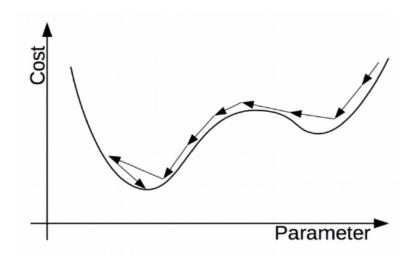
Iterative minimization by updating  $\theta$  in opposite direction of gradient.

$$\theta_i = \theta_{i-1} - lpha rac{\partial L}{\partial heta}$$
 , where  $lpha$  is the so-called « learning rate ».

 Evaluation and derivation of the loss function for the full dataset is costly:

#### Stochastic gradient descent:

Calculate gradient for a small stochastic subset of the training sample (batch). → This also helps to avoid local minima!

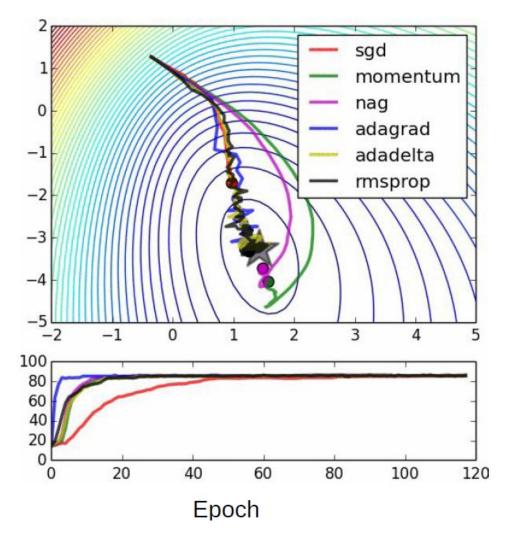




One iteration over the full training dataset is called *epoch*.

## Training: more optimisers

- More advanced options than fixed learning rate.
  - Momentum: past gradients used as « velocity »
  - Adaptive methods: different learning rates for each parameter and as a function of past gradients.



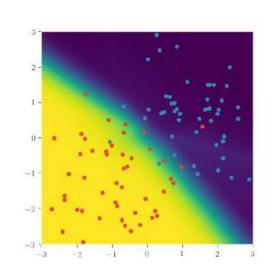


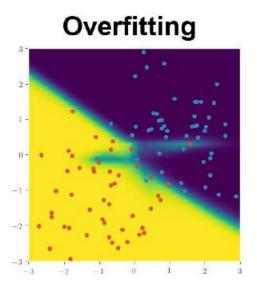
## Underfitting and overtraining

**Underfitting:** If model capacity is too low or if training is not enough

→ bad performance.

# Underfitting





Overfitting: If model capacity is too high, network can « memorize » training samples 

→ bad generalization.

## Overtraining solutions

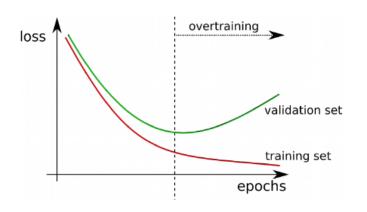
#### **Early stop:**

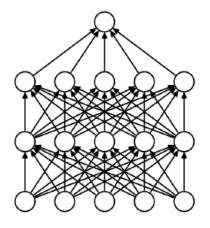
Evaluate the performance of the network on a validation dataset.

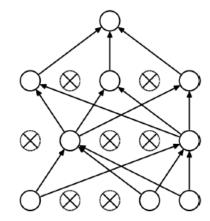
Stop when performance on validation set decreases

#### **Dropout:**

Randomly drop a percentage of nodes at each training step. Learn redundant representations, hence giving a more robust model.







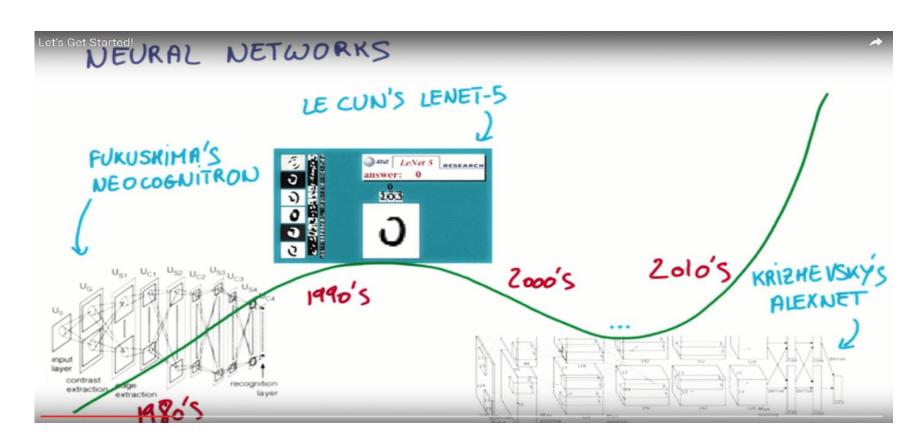
#### Deep-learning Neural Network

#### **TensorFlow**<sup>TM</sup>

MNIST example

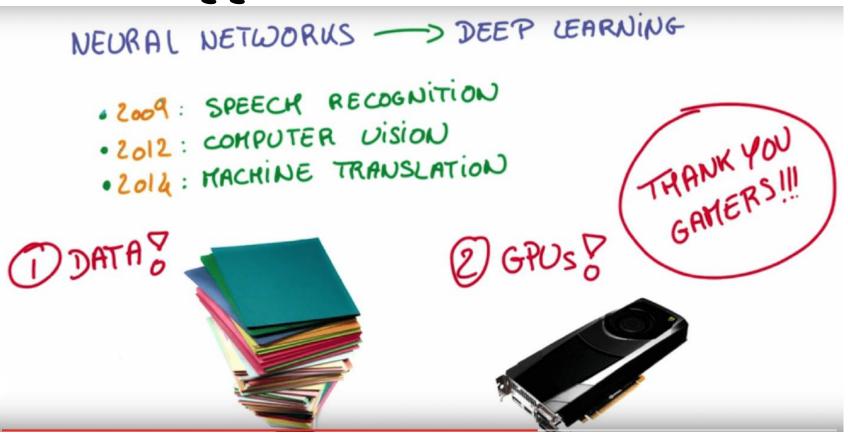
#### Neural network

## Since 2010 new era in Machine Learning: rapidly increasing areas of applications



#### Neural network

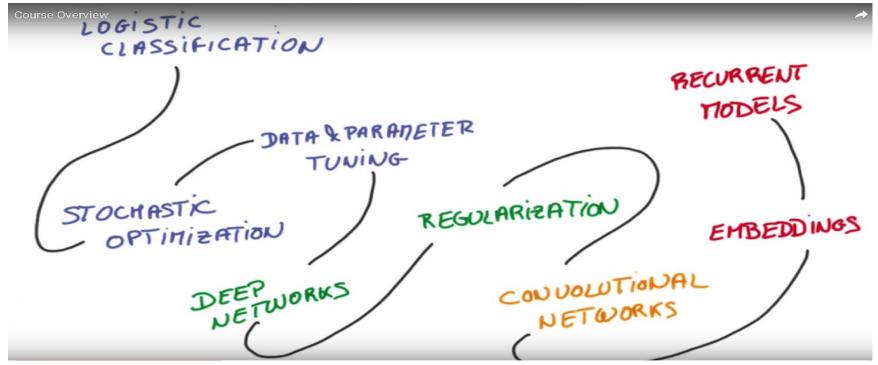
Since 2010 new era: rapidly increasing areas of applications



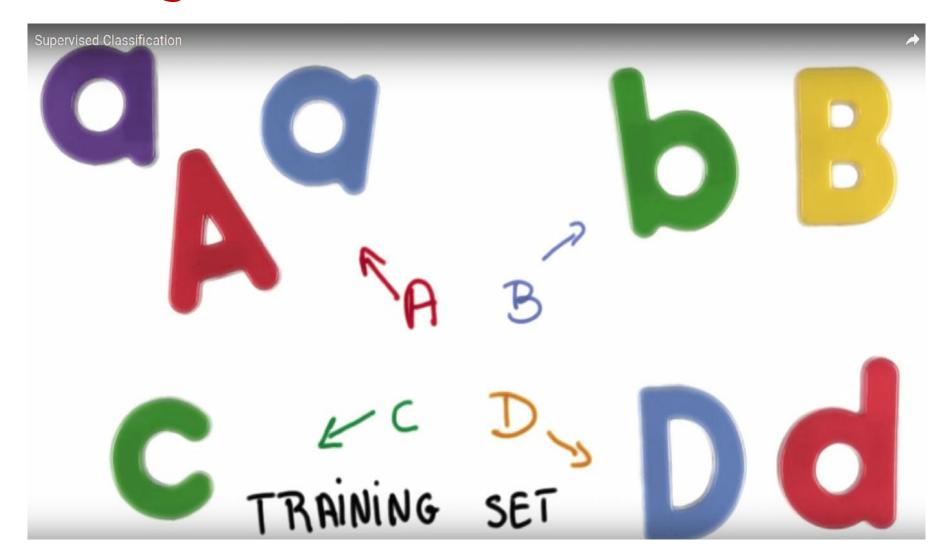
## Deep-learning tutorial @ udacity

https://www.udacity.com/course/deep-learning--ud730

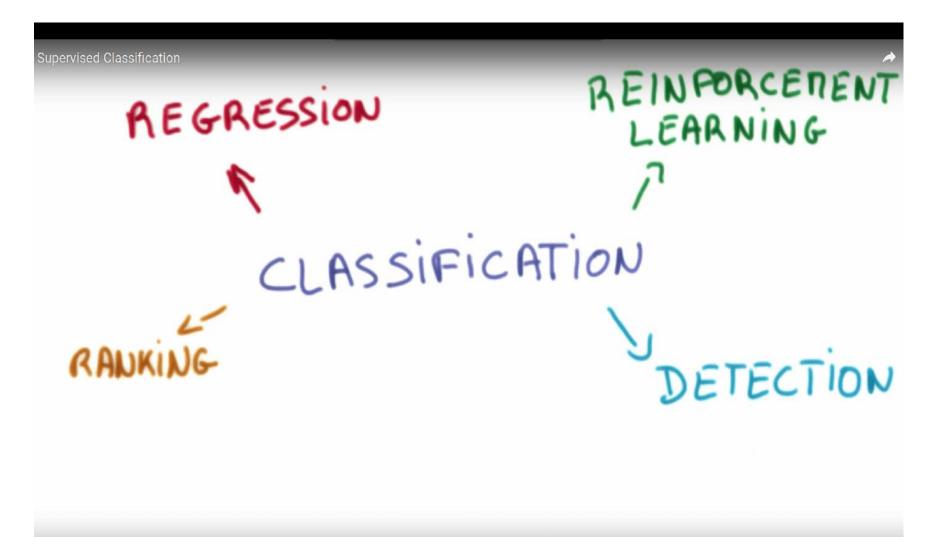




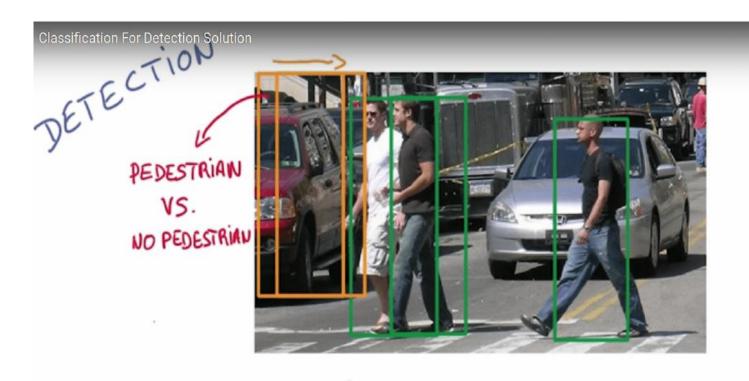
# Supervised Classifications



## Supervised Classifications

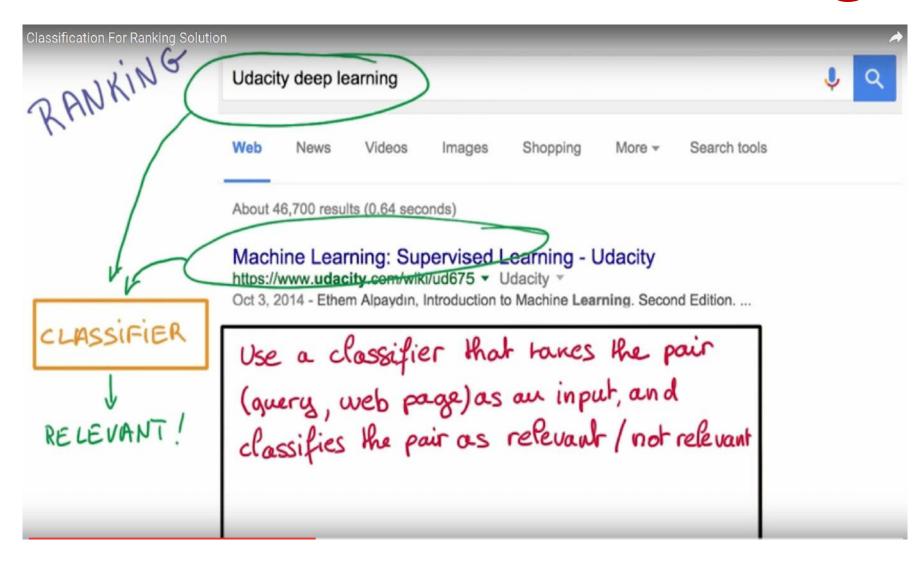


### Classifications for Detection

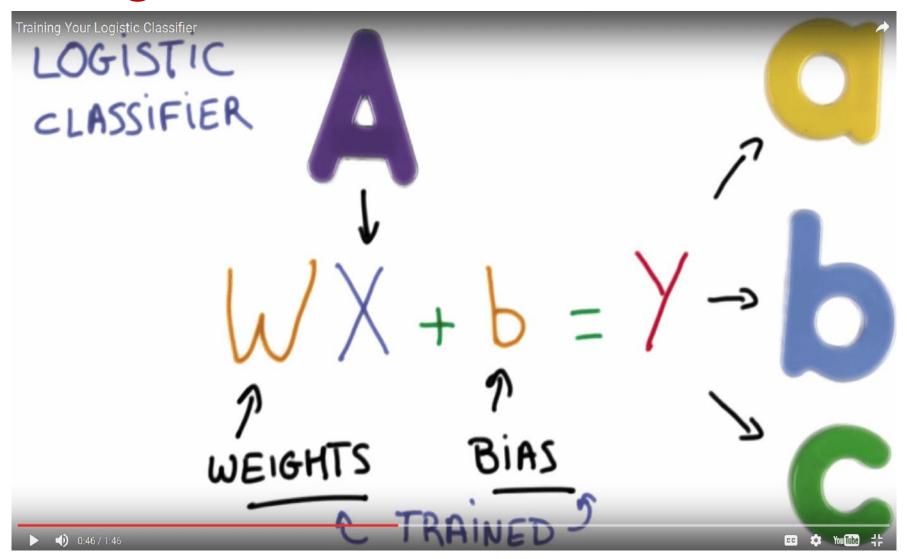


Use a binary pedestrian / no pedestrian classifier. Slide it over all possible locations in the image.

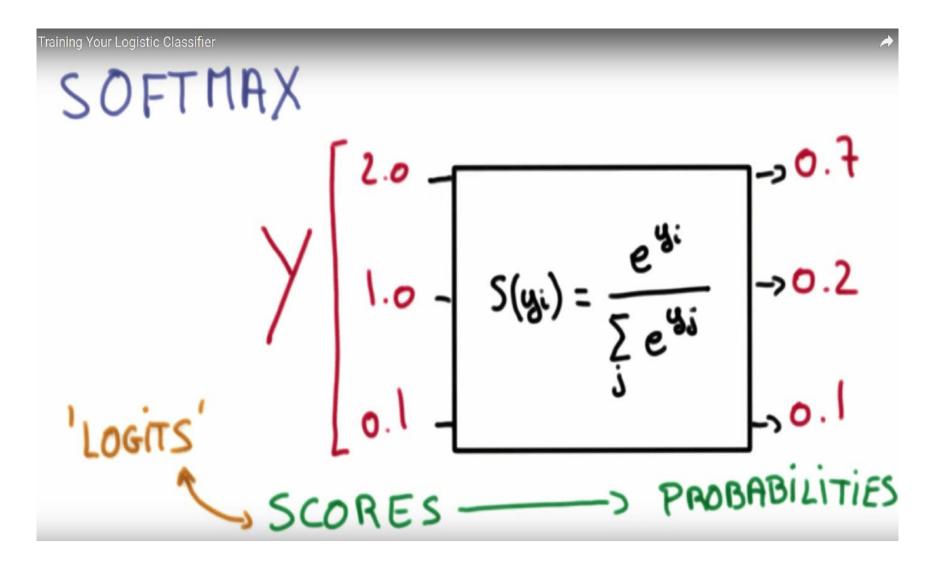
# Classifications for Ranking



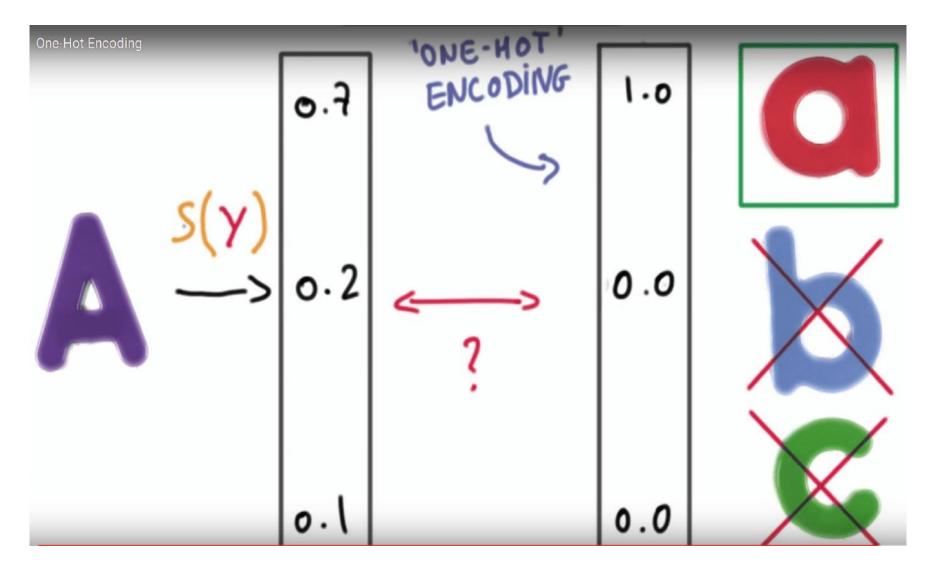
# Logistic classifier: Linear model



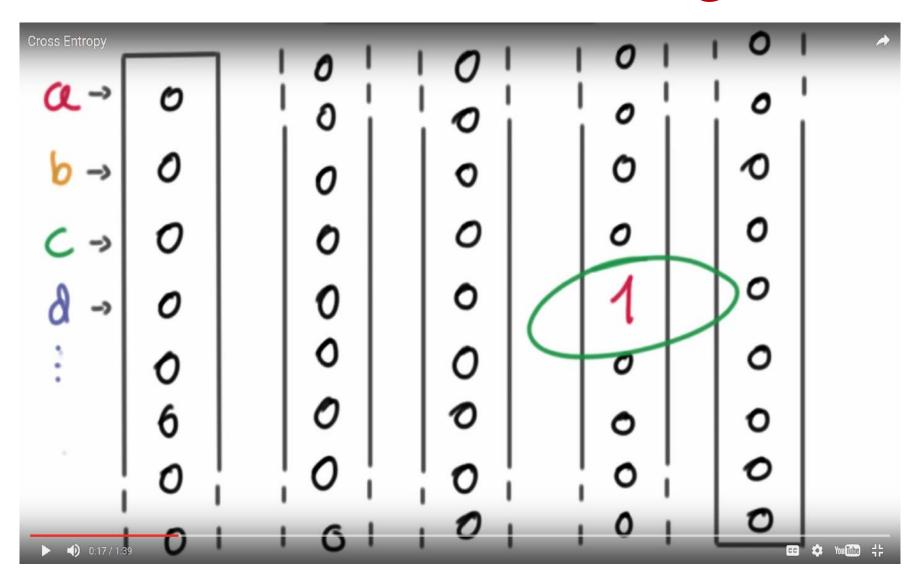
## Softmax



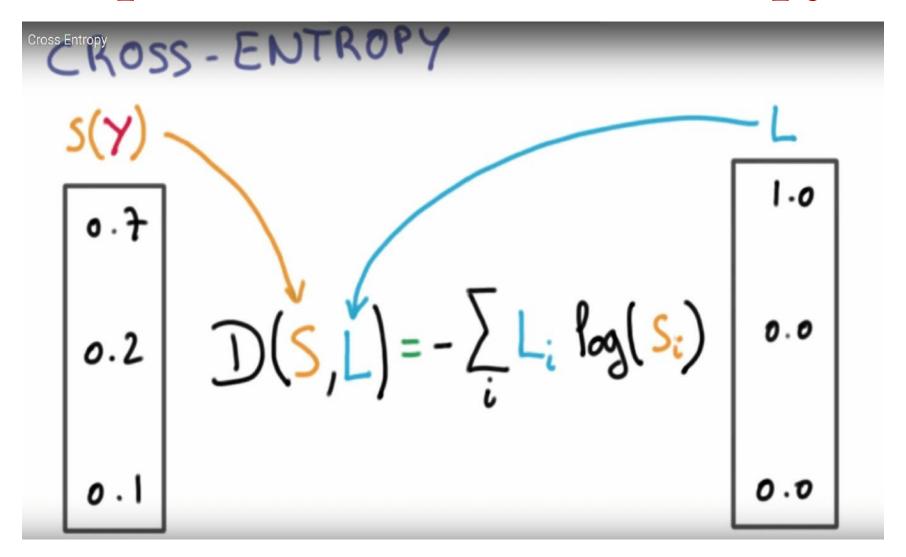
# "One hot" encoding



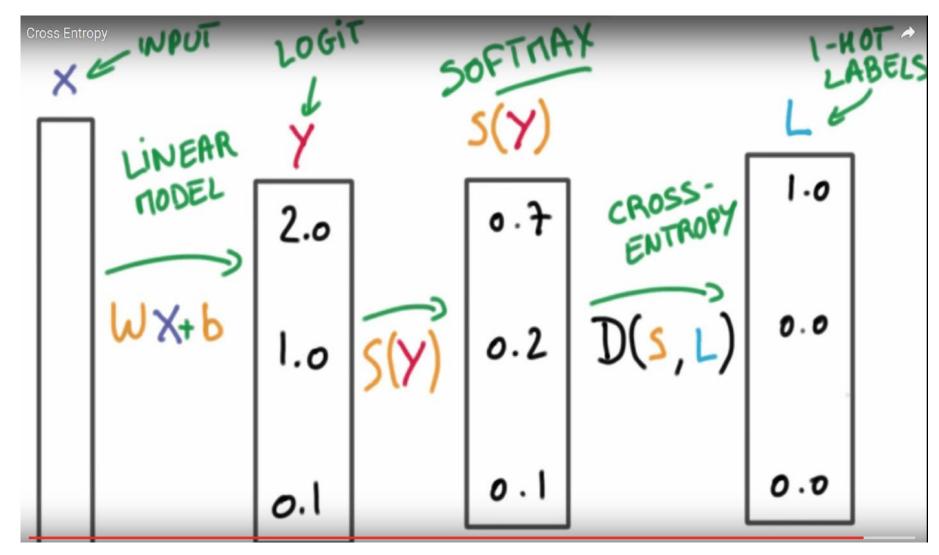
# "One hot" encoding



# **Optimisation: Cross-Entropy**

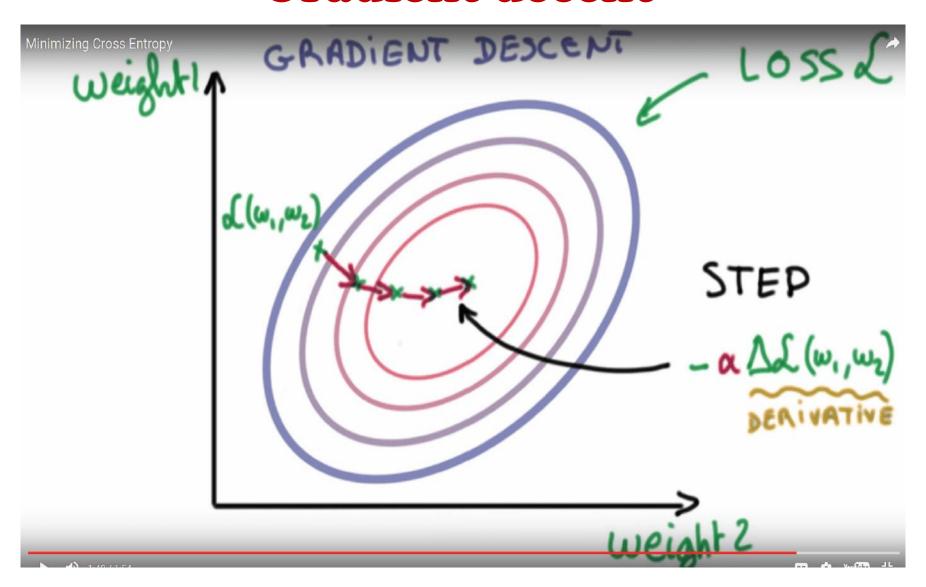


## Multinomial logistic classification

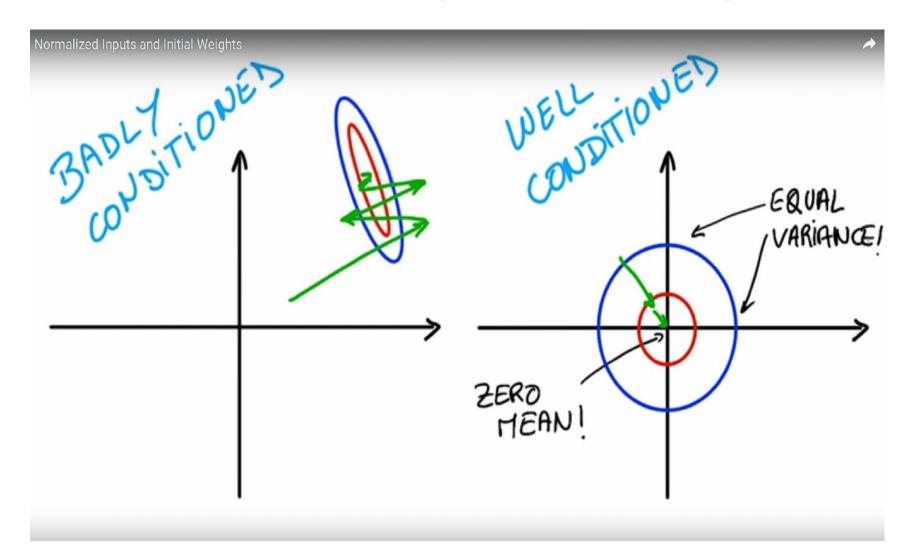


### Optimisation of average loss

### Gradient decent



### Normalised input and output



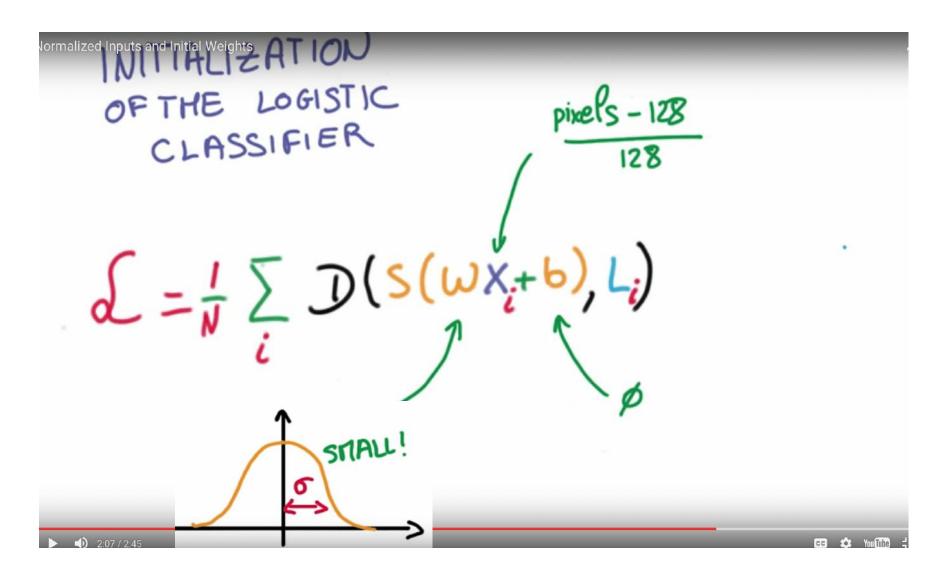
### Normalised input and output

# IMAGES

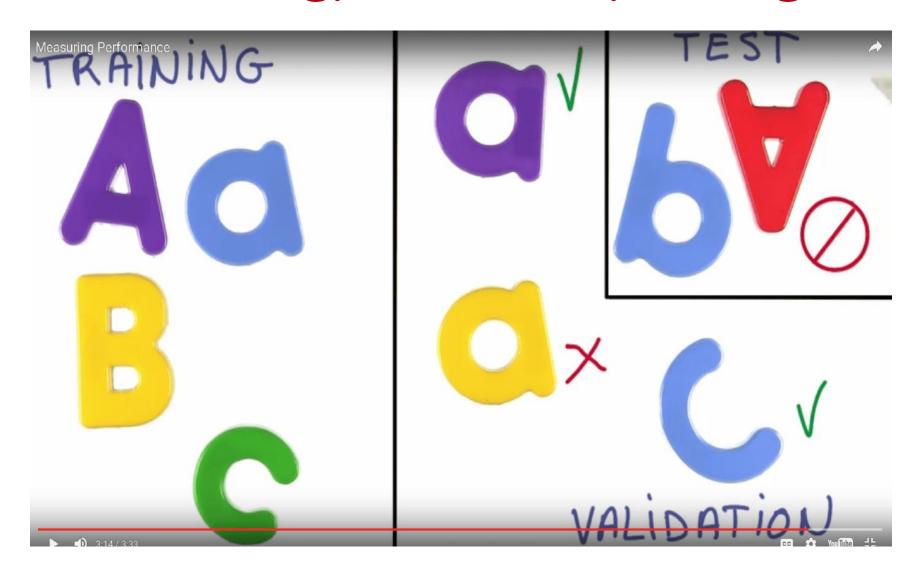
$$\frac{R - 128}{128} \qquad \frac{G - 128}{128} \qquad \frac{B - 128}{128}$$

$$128 \qquad 128$$

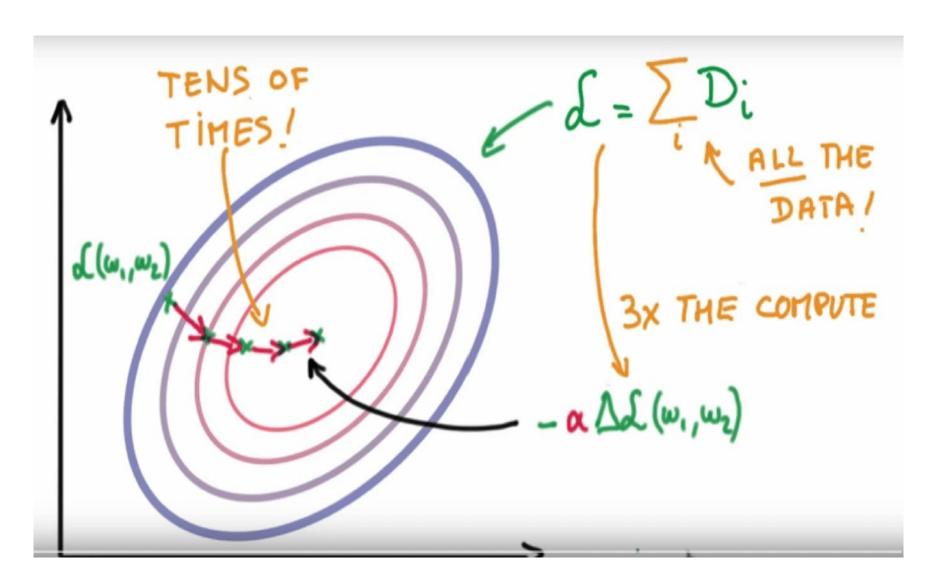
### Initialisation



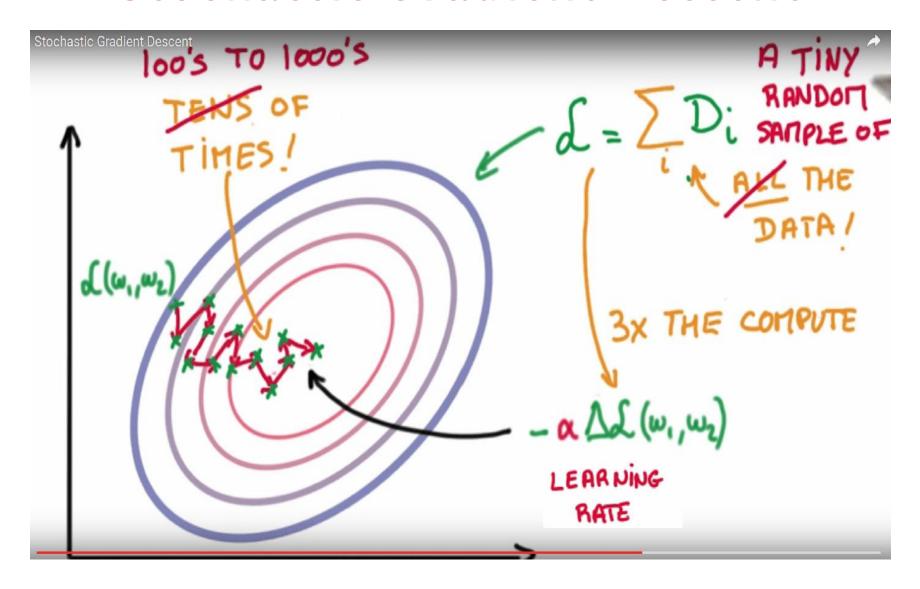
### Training, validation, testing



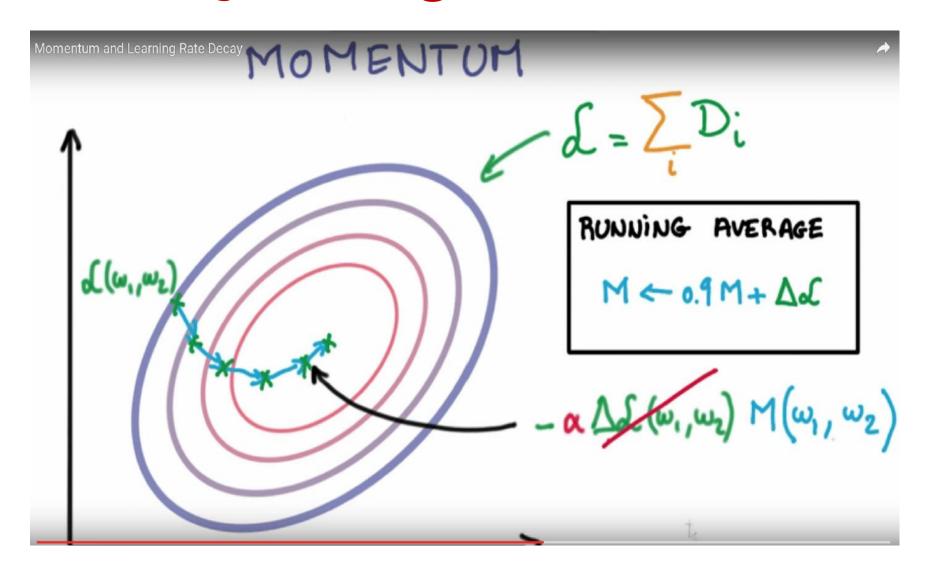
### **Gradient Descent**



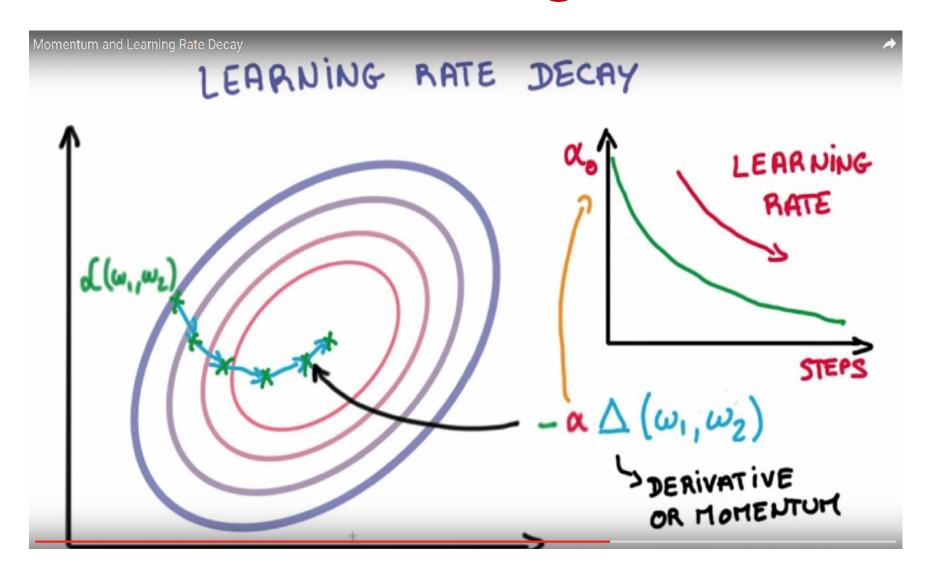
### Stochastic Gradient Descent



### SDG: optimising with momentum



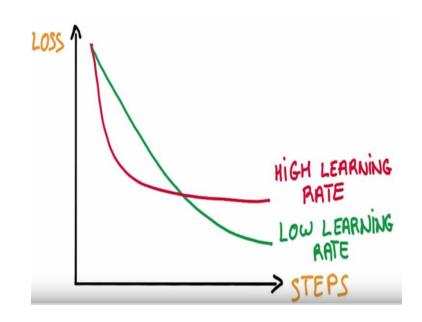
### SDG: learning rate



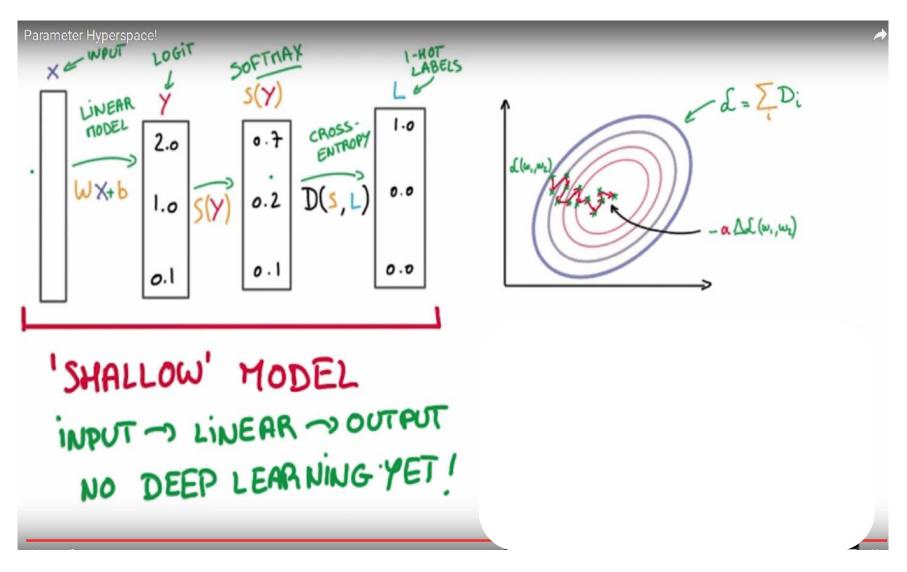
# SDG: "black magic"

# MANY HYPER-PARAMETERS

- · INITIAL LEARNING RATE
- · LEARNING RATE DECAY
- . MOMENTUM
- . BATCH SIZE
- . WEIGHT INITIALIZATION



# Input – linear - output



### Linear models are linear

LINEAR MODEL COMPLEXITY (N+1) K PARAMETERS

### Linear models are stable

$$Y = W \times \longrightarrow \frac{\Delta Y}{\Delta X} = W^{T}$$

$$\frac{\Delta Y}{\Delta W} = X^{T}$$

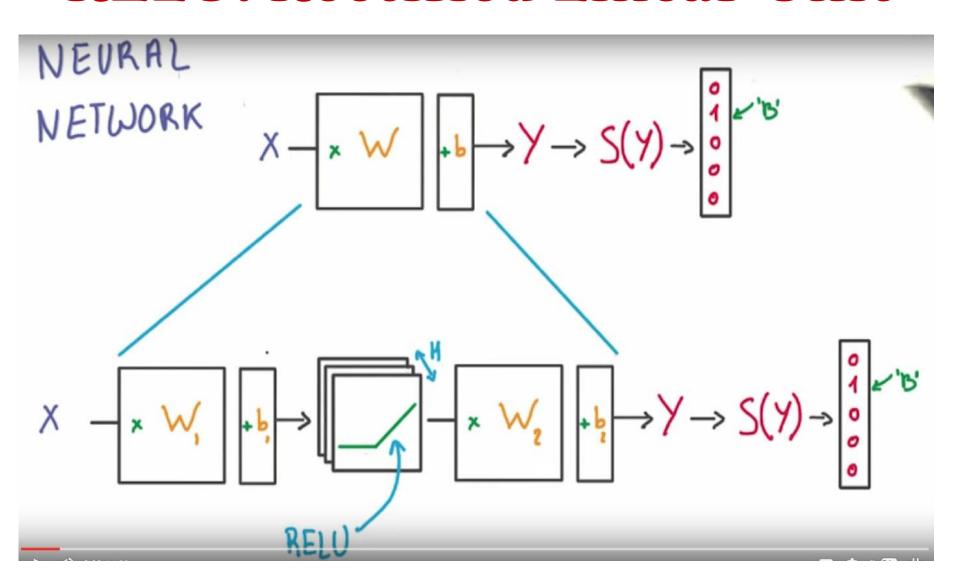
## Linear models are here to stay

This is still linear

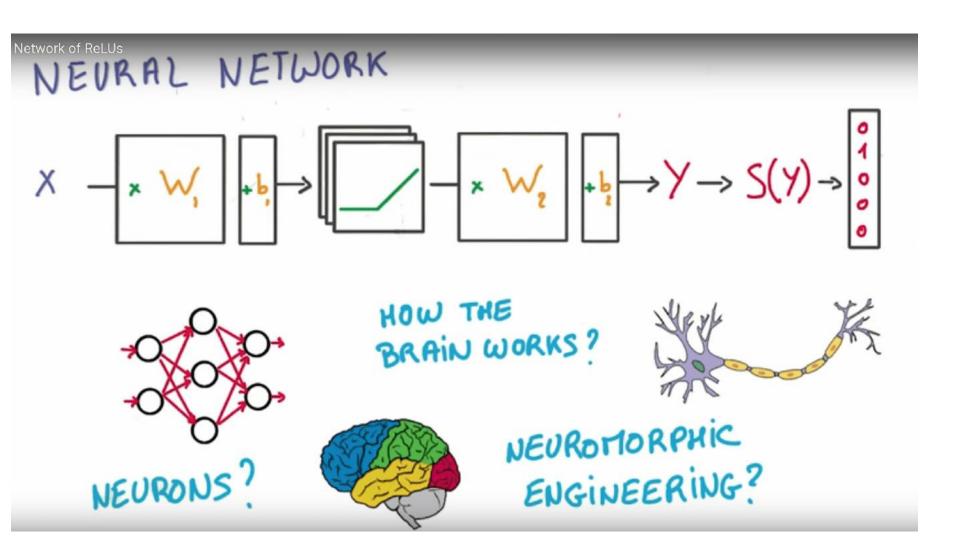
$$Y = W_1 W_2 W_3 X = W X$$

· Lets introduce non-linearity

### RELU: Rectified Linear Unit



### **Networks of RELU**

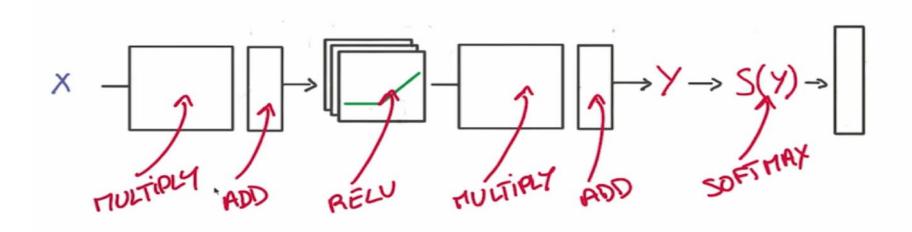


## The Chain Rule

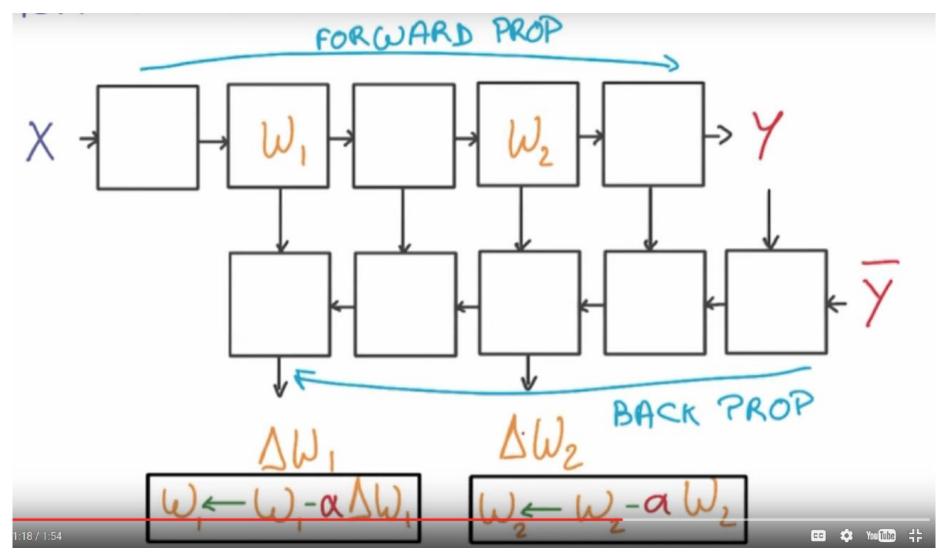




STACKING UP SIMPLE OPERATIONS

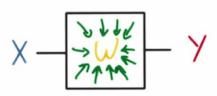


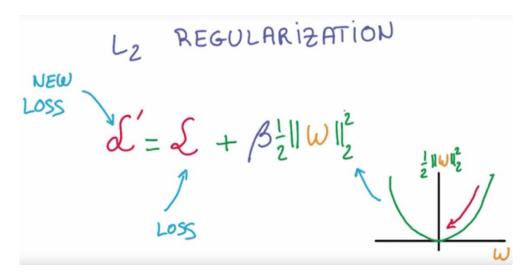
# Back - propagation

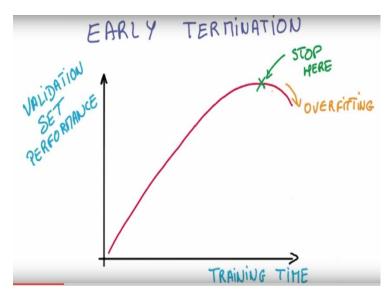


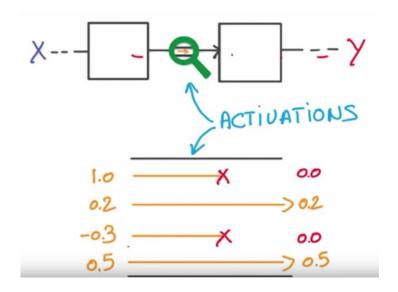
# Optimisation tricks

### REGULARIZATION

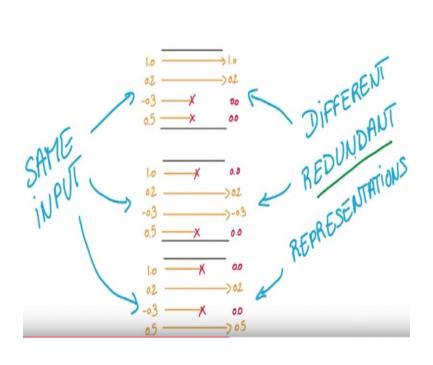


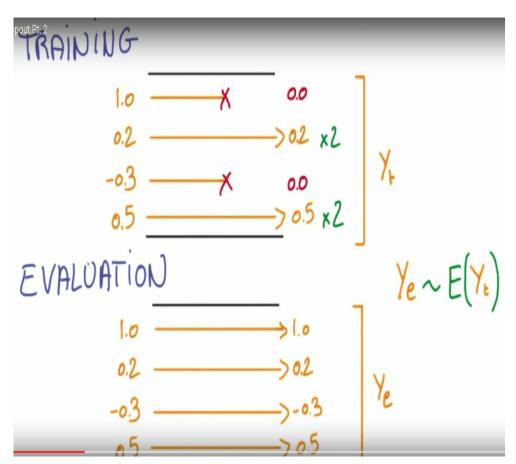




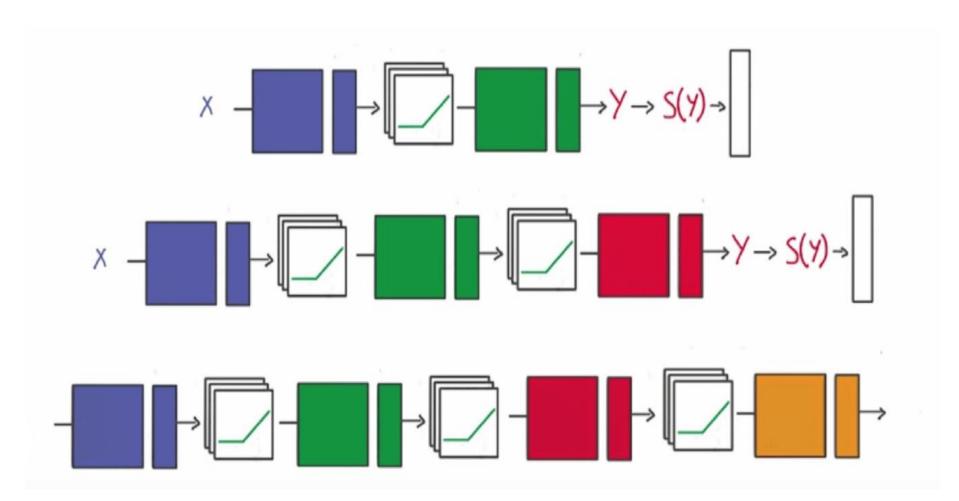


# Optimisation trick: dropout

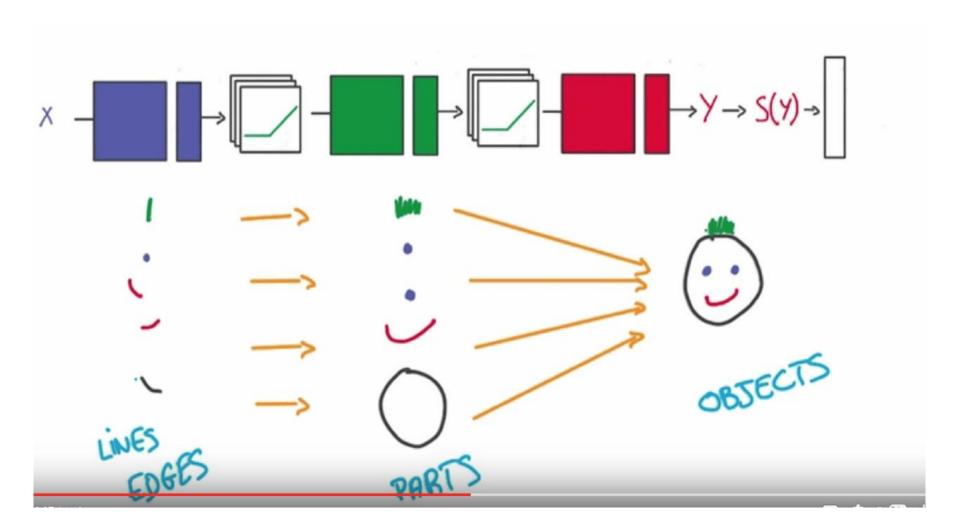




## Deep networks



## Deep networks



### tensorflow.org/paper/whitepaper2015.pdf

#### **TensorFlow:**

#### Large-Scale Machine Learning on Heterogeneous Distributed Systems

(Preliminary White Paper, November 9, 2015)

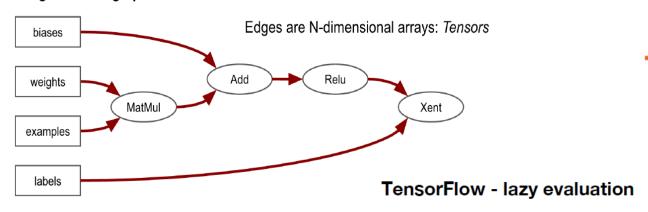
Martín Abadi, Ashish Agarwal, Paul Barham, Eugene Brevdo, Zhifeng Chen, Craig Citro, Greg S. Corrado, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Ian Goodfellow, Andrew Harp, Geoffrey Irving, Michael Isard, Yangqing Jia, Rafal Jozefowicz, Lukasz Kaiser, Manjunath Kudlur, Josh Levenberg, Dan Mané, Rajat Monga, Sherry Moore, Derek Murray, Chris Olah, Mike Schuster, Jonathon Shlens, Benoit Steiner, Ilya Sutskever, Kunal Talwar, Paul Tucker, Vincent Vanhoucke, Vijay Vasudevan, Fernanda Viégas, Oriol Vinyals, Pete Warden, Martin Wattenberg, Martin Wicke, Yuan Yu, and Xiaoqiang Zhen<sup>9</sup>
Google Research\*

#### Abstract

TensorFlow [1] is an interface for expressing machine learning algorithms, and an implementation for executing such algorithms. A computation expressed using TensorFlow can be executed with little or no change on a wide variety of heterogeneous systems, ranging from mobile devices such as phones and tablets up to large-scale distributed systems of hundreds of machines and thousands of computational devices such as GPU cards. The system is flexible and can be used to express a wide variety of algorithms, including training and inference algorithms for deep neural network models, and it has been used for conducting research and for deploying machine learning systems into production across more than a dozen areas of computer science and other fields, including speech recognition, computer vision, robotics, information retrieval, natural language processing, geographic information extraction, and computational drug discovery. This paper describes the TensorFlow interface and an implementation of that interface that we have built at Google. The TensorFlow API and a reference implementation were released as an open-source package under the Apache 2.0 license in November, 2015 and are available at www.tensorflow.org.



### TensorFlow is an open source software library for numerical computation using data flow graphs.





#### What is a Data Flow Graph?

Data flow graphs describe mathematical computation with a directed graph of nodes & edges. Nodes typically implement mathematical operations, but can also represent endpoints to feed in data, push out results, or read/write persistent variables. Edges describe the input/output relationships between nodes. These data edges carry dynamically-sized multidimensional data arrays, or tensors. The flow of tensors through the graph is where TensorFlow gets its name. Nodes are assigned to computational devices and execute asynchronously and in parallel once all the tensors on their incoming edges becomes available.

#### **Key Features**

- Deep Flexibility
- True Portability
- Connect Research and Production
- Auto-Differentiation
- Language Options
- Maximize Performance

#### **Parallel Execution**

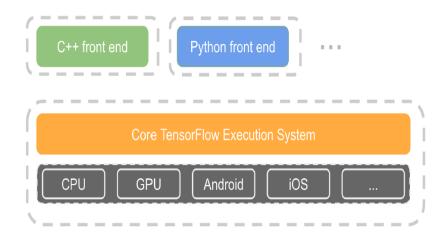
- Launch graph in a Session
- Request output of some Ops with Run API
- TensorFlow computes set of Ops that must run to compute the requested outputs
- Ops execute, in parallel, as soon as their inputs are available

### There are hundreds of predefined Ops (and easy to add more)

- · Basics: constant, random, placeholder, cast, shape
- Variables: assign, assign\_sub, assign\_add
- · Queues: enqueue, enqueue\_batch, dequeue, blocking or not.
- Logical: equal, greater, less, where, min, max, argmin, argmax.
- Tensor computations: all math ops, matmul, determinant, inverse, cholesky.
- Images: encode, decode, crop, pad, resize, color spaces, random perturbations.
- Sparse tensors: represented as 3 tensors.







#### And many neural net specific Ops

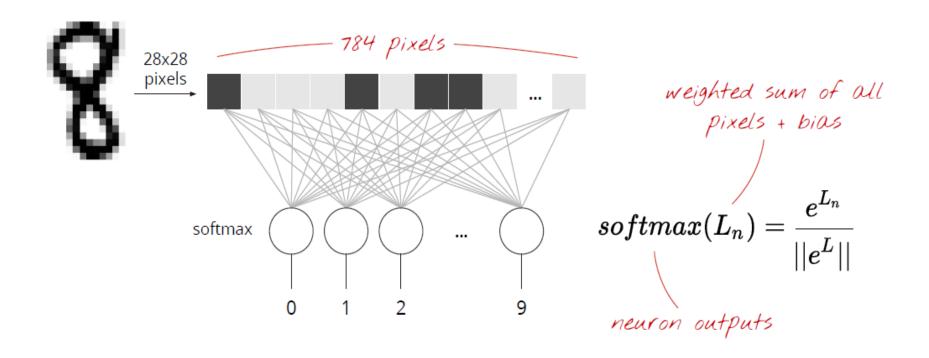
- Activations: sigmoid, tanh, relu, dropout, ...
- Pooling: avg, max.
- · Convolutions: with many options.
- · Normalization: local, batch, moving averages.
- Classification: softmax, softmax loss, cross entropy loss, topk.
- Embeddings: lookups/gather, scatter/updates.
- · Sampling: candidate sampler (various options), sampling softmax.
- Updates: "fused ops" to speed-up optimizer updates (Adagrad, Momentum.)
- · Summaries: Capture information for visualization.

# Hand-written diggits: MNIST



MNIST = Mixed National Institute of Standards and Technology - Download the dataset at <a href="http://yann.lecun.com/exdb/mnist/">http://yann.lecun.com/exdb/mnist/</a>

# Simple linear model

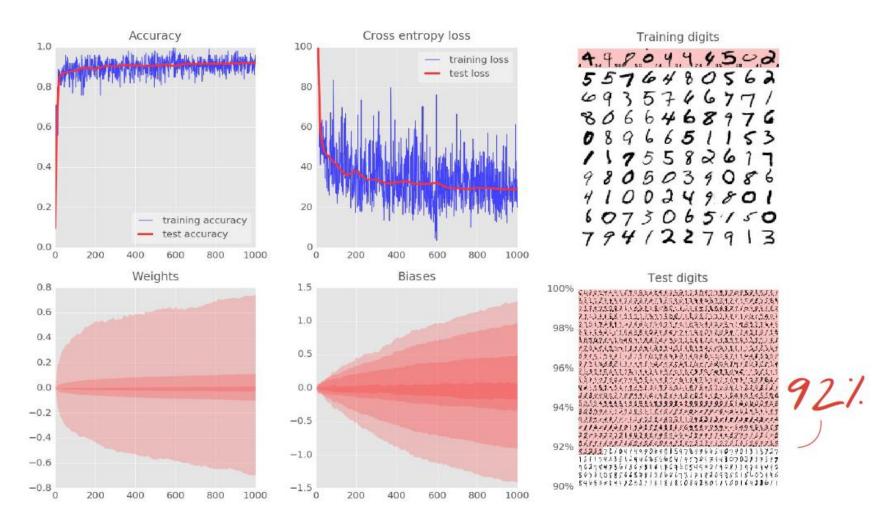


Slides from M. Gorner tutorial http://www.youtube.com/watch?v=vq2nnJ4g6NO

# TensorFlow full python code

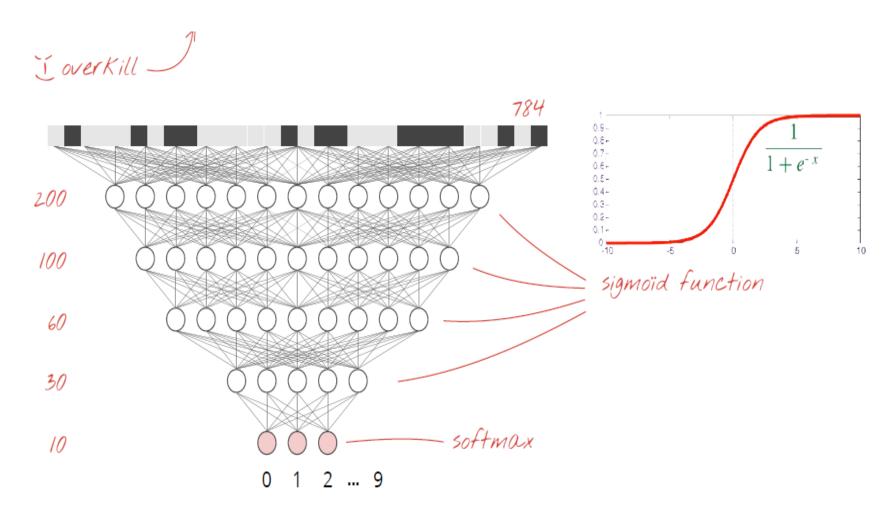
```
initialisation
import tensorflow as tf
X = tf.placeholder(tf.float32, [None, 28, 28, 1])
W = tf.Variable(tf.zeros([784, 10]))
b = tf.Variable(tf.zeros([10]))
init = tf.initialize all variables()
# model
Y=tf.nn.softmax(tf.matmul(tf.reshape(X,[-1, 784]), W) + b)
# placeholder for correct answers
Y = tf.placeholder(tf.float32, [None, 10])
                                  success metrics
# loss function
cross_entropy = -tf.reduce_sum(Y_ * tf.log(Y))
# % of correct answers found in batch
is correct = tf.equal(tf.argmax(Y,1), tf.argmax(Y,1))
accuracy = tf.reduce mean(tf.cast(is correct,tf.float32))
```

# Simple linear model



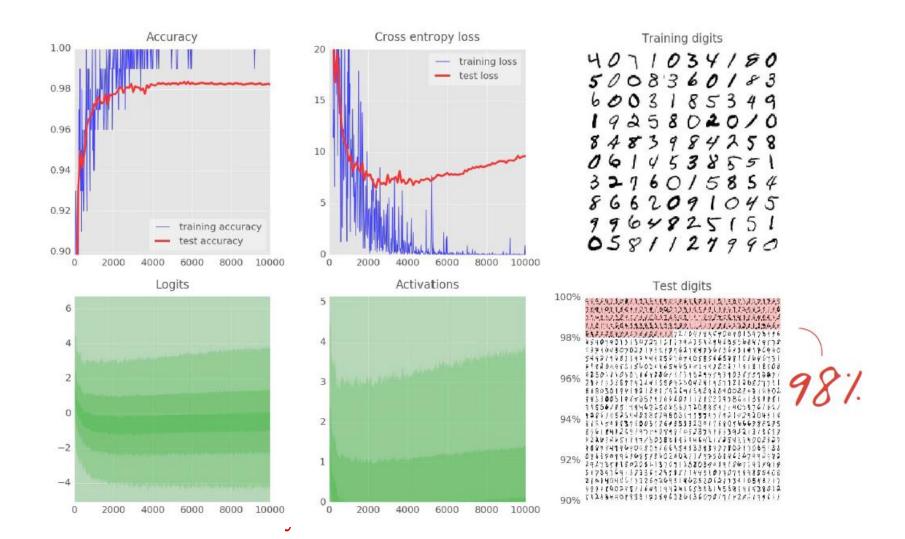
Slides from M. Gorner@youtube

# Multi-layer connected network



Slides from M. Gorner@youtube

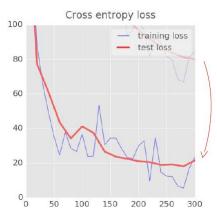
# Multi-layer connected network



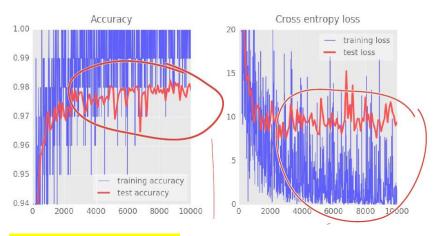
## All tricks count

#### **Use RELU**

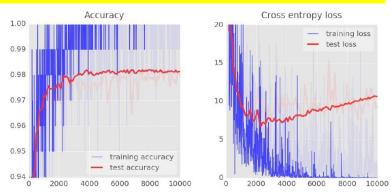




#### **But noisy accuracy**

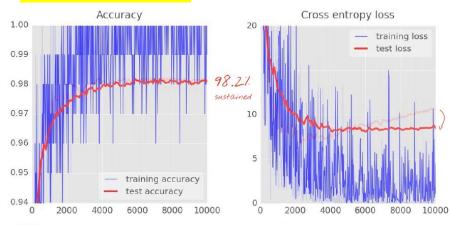


#### **Exponentialy reduce learning rates**



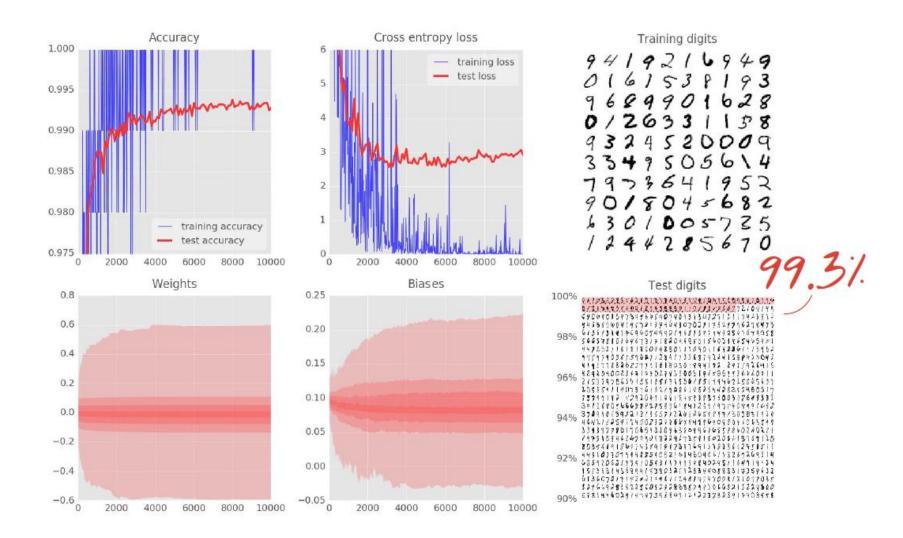
Learning rate 0.003 at start then dropping exponentially to 0.0001

### Add drop-out



RELV, decaying learning rate 0.003 -> 0.0001 and dropout 0.75

### Can do better with conv network



## References

http://www.deeplearning.book.org http://download.tensorflow.org/paper/whitepaper2015.pdf

https://www.tensorflow.org/

http://www.youtube.com/watch?v=vq2nnJ4g6NO

https://www.udacity.com/course/deep-learning--ud730