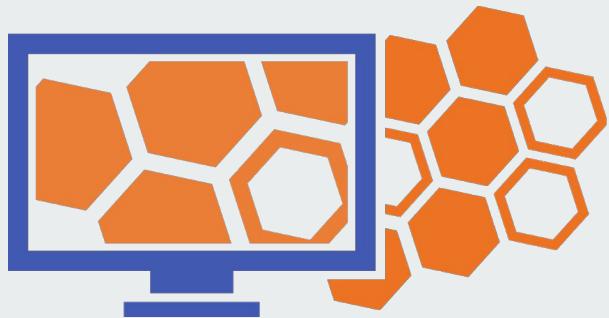


# *Deep Learning Workshop*

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January 16th & 17th 2019



**CompCancer**



# Agenda

1. Provide **theoretical** and **practical** hands-on knowledge on Deep Learning
2. Provide domain expert knowledge on **Deep-Learning interpretability**, **image-classification** and **'omics data analysis**



# Aim

1. Improve/ establish programming skills
2. Gain theoretical insights into the keynote topics
3. Motivate your Deep-Learning-based publications

# Context



- Today CompCancer PhD Graduate School
- First workshop offshoot Berlin Social Bioinformatics Meetings
- Next meeting January 29th



Bioinformatics Social Meetings Berlin



2018

# Workshop Organizers

*Manuela Bernary*



- CompCancer organizer
- Blüthgen Lab
- [manuela.benary@cms.hu-berlin.de](mailto:manuela.benary@cms.hu-berlin.de)

*Teresa Domaszewska*

- Bioinformatician
- Robert Koch Institute
- [domaszewskat@rki.de](mailto:domaszewskat@rki.de)



*Raik Otto*

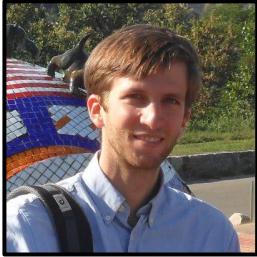
- Bioinformatician
- AG Leser
- [raik.otto@hu-berlin.de](mailto:raik.otto@hu-berlin.de)



# Schedule

Today

1. Session 1 - Introduction
  - a. Programming basics
  - b. Theoretical basics
2. Session 2- Interpretability of DL



Keynote 1  
Grégoire Montavon

Tomorrow

3. Session 3 - Image Analysis
4. Session 4 - Transcriptomics & Drug response



Keynote 2  
Dagmar Kainmüller



Keynote 3  
Jonathan Ronen

# Contributors & Supporters

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*Lisa Mais*

*Timon Hick*



*Maryam Habibi*



*Sven Giese*



*Peter Hirsch*

# Photography

We would like to take pictures.

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Let us know if you would like to opt-out from being shown in pictures.



2018



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# Session 1

# Programming Basics &

# Theory of Deep Learning

# Aim Session 1



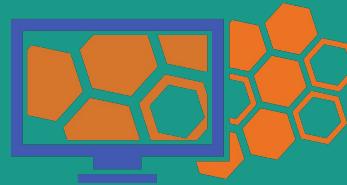
## Programming

- Hardware & software requirements
- How to connect to and monitor GPU servers
- How to train Deep Learning models
- Empower participants to train models independently
- Essential terminology

# Agenda of Programming session



1. Connecting to & monitoring of server
2. First DL model - Diabetes prediction
  - a. Guided
  - b. General theory of DL
  - c. Explanation source code
3. Second model - Number classification
  - a. Apply skills from 1 independently
  - b. Basic concepts
4. Mini-Hackathon - Melanoma classification
  - a. Real-world challenge
  - b. Advanced concepts



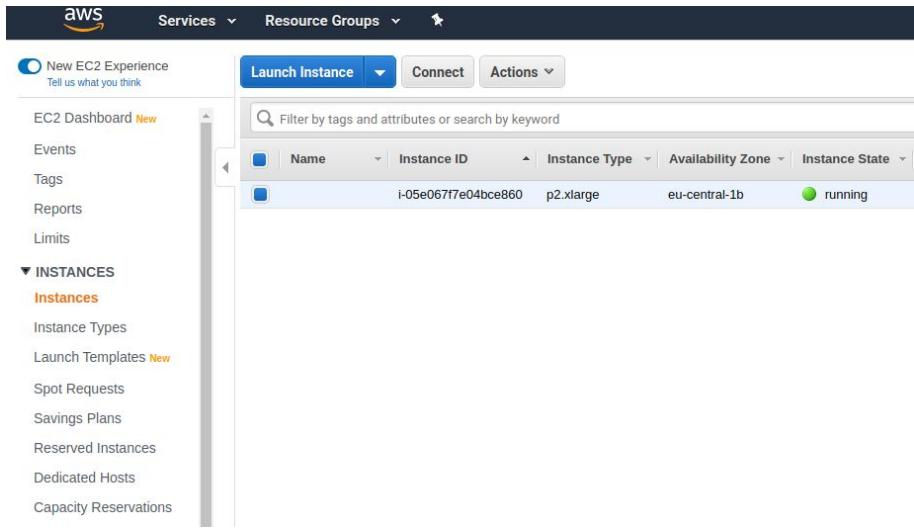
CompCancer

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# Connecting & Monitoring

# Amazon Web Service GPU-Server Cloud

- Model creating (training) takes place on a GPU server
- Server has to have access to data
- Sudo rights!
- Amazon Web Services (AWS) sponsors the GPU servers for this workshop
- We connect to virtual cloud instances

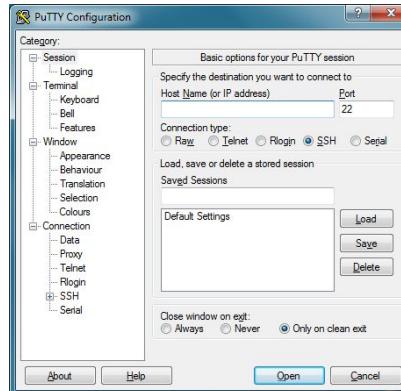


# SSH and Port Forwarding

## Secure SHell (SSH)

- Encrypted communication protocol
- Authenticates remote users and remote systems
- Commonly consists of public and private key

PuTTY Client



## Port Forwarding

Ports are 'gateways' where software can communicate with another system's software

- Avoids collisions of software communication
- Fixed ports for important software exists

Aim: Redirect the port of the DL programming software from the AWS Server to your laptop

# Connecting to your server from POSIX systems

Updated!

1. Go to [github.com/RaikOtto/CompCancer](https://github.com/RaikOtto/CompCancer)
2. Look up your IP **XYZ** -> number on post-it
3. Download key **.pem** file
4. Open terminal and *cd* to download folder
5. > `chmod 400 Workshop_SSH_Key.pem`
6. > `ssh -i "Workshop_SSH_Key.pem" -Y -L 8889:localhost:8889 -L 6014:localhost:6014 XYZ -l ubuntu`

↓ Updated!

# Connecting to your server from MS Windows

Updated!

1. Go to [github.com/RaikOtto/CompCancer](https://github.com/RaikOtto/CompCancer)
2. Look up your IP **XYZ** -> number on post-it
3. Download key **.ppk** file
4. Start PuTTY
5. Hostname: **XYZ**
6. Auth - autologin username: ubuntu
7. Auth - private key file -> **.ppk** file
8. Tunnels
  - a. Source port: 8889
  - b. Destination: localhost:8889 (click 'Add')
  - c. Source port: 6014
  - d. Destination: localhost:6014 (click 'Add') ← Updated!
9. 'Open', accept button

# Session control via Servlet

Screen version 4.00.03 (FAU) 23-Oct-06

Copyright (c) 1993-2002 Juergen Weigert, Michael Schroeder  
Copyright (c) 1987 Oliver Laumann

- Setup server-sided application
- Facilitates simultaneously working in different screens
- Prevents scripts from terminating due to disconnects

```
> screen + 'space bar' # new session
> Ctrl + a
> Ctrl + c # create new screen
> Ctrl + 1 # move back to screen 1

> screen -rd # pickup disconnected session
```

# NVIDIA-smi



Monitoring of the GPU

- Monitor GPU status

```
> Ctrl + a  
> 2  
> Watch -n 1 nvidia smi
```

```
Every 1.0s: nvidia-smi

Sat Jan 11 15:08:04 2020
+-----+
| NVIDIA-SMI 418.87.01      Driver Version: 418.87.01      CUDA Version: 10.1 |
+-----+
| GPU  Name      Persistence-M| Bus-Id      Disp.A  | Volatile Uncorr. ECC
| Fan  Temp     Perf  Pwr:Usage/Cap| Memory-Usage | GPU-Util  Compute M.
|-----+
|  0  Tesla K80          On  | 00000000:00:1E.0 Off |                    0
| N/A  54C     P0    74W / 149W | 11032MiB / 11441MiB |     0%     Default
+-----+
+-----+
| Processes:
| GPU  PID  Type  Process name                  GPU Memory
| Usage
|-----+
|  0    22440   C  ...conda3/envs/tensorflow2_p36/bin/python  11019MiB
+-----+
```

# Tensorflow & CUDA



## Tensorflow

- Differential programming library
- Trains Deep-Learning models
- Google open source software
- Based on Google-internal *DistBelieve*
- Developed by Geoffrey Hinton and Jeffrey Dean



## CUDA

- Compute Unified Device Architecture (CUDA)
- Application programming interface (API)
- Requires correct CUDA Toolkit version
  - > nvcc --version

CUDA Toolkit	Linux x86_64 Driver Version
CUDA 10.2 (10.2.89)	>= 440.33
CUDA 10.1 (10.1.105)	>= 418.39
CUDA 10.0 (10.0.130)	>= 410.48
CUDA 9.2 (9.2.88)	>= 396.26

# Keras

---

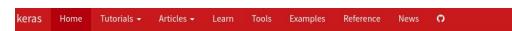
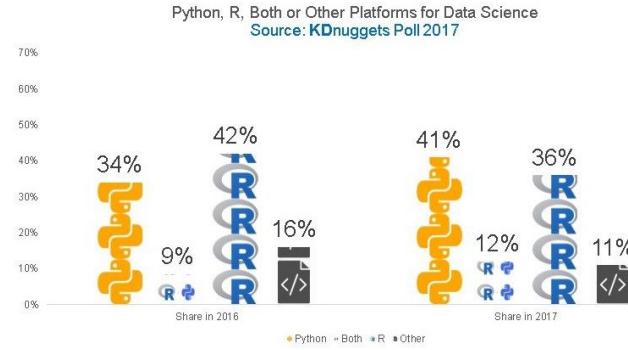
- High-level neural network API
- Focus on eager execution
- Supports arbitrary network architectures
- Built-in support for most common architectures
  - Convolutional networks
  - Recurrent networks etc.
- Supports different backends
  - TensorFlow
  - CNTK
  - Theano (deprecated)



# Python versus R



- Python dominant over R for DL modeling
  - Other languages exist
- DL model three will cover DL in R



## R interface to Keras

Keras is a high-level neural networks API developed with a focus on enabling fast experimentation. Being able to go from idea to result with the least possible delay is key to doing good research. Keras has the following key features:

- Allows the same code to run on CPU or on GPU, seamlessly.
- User-friendly API which makes it easy to quickly prototype deep learning models.
- Built-in support for convolutional networks (for computer vision), recurrent networks (for sequence processing), and any combination of both.
- Supports arbitrary network architectures: multi-input or multi-output models, layer sharing, model sharing, etc. This means that Keras is appropriate for building essentially any deep learning model, from a memory network to a neural Turing machine.
- Is capable of running on top of multiple backends including TensorFlow, CNTK, or Theano.

For additional details on why you might consider using Keras for your deep learning projects, see the [Why Use Keras?](#) article. This website provides documentation for the R Interface to Keras. See the main Keras website at <https://keras.io> for additional information on the project.

## Getting Started

### Installation

First, install the keras R package from GitHub as follows:

```
devtools::install_github("rstudio/keras")
```

[Copy to clipboard](#)

# Preparation Tensorflow Python models



Testing the installed software

```
> python
```

```
> import tensorflow
```

```
ubuntu@ip-172-31-41-43:~$ python
Python 3.6.6 |Anaconda, Inc.| (default, Jun 28 2018, 17:14:51)
[GCC 7.2.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ModuleNotFoundError: No module named 'tensorflow'
>>> █
```

Tensorflow software required

# Install software: BioConda & PIP



Large bioinformatics repository

```
> conda install -c anaconda tensorflow-gpu
```



Generic Python repository

```
> pip install tensorflow-gpu --user
```

# Selecting the correct software environment

---



Software environment

- Different versions of the same software exist on the same system
- Activation of environment required

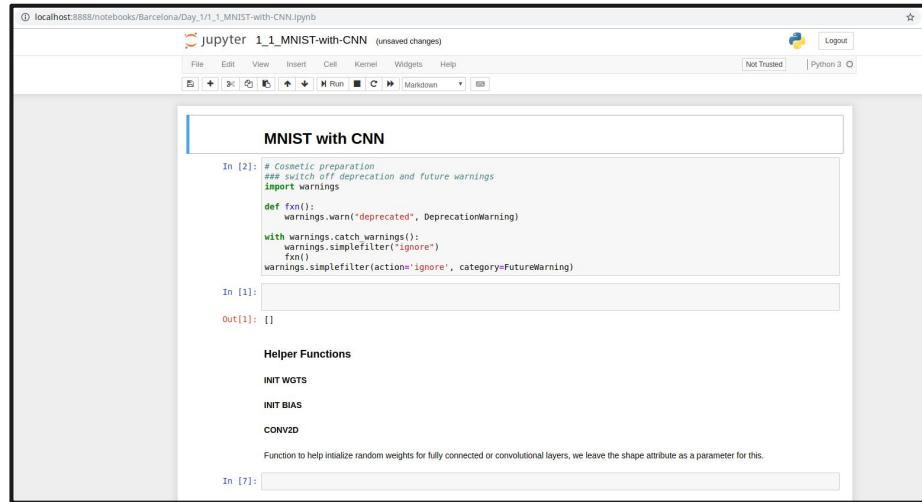
```
> conda env list
```

```
> conda activate tensorflow2_p36
```

```
ubuntu@ip-172-31-41-43:~$ conda activate tensorflow2_p36
(tensorflow2_p36) ubuntu@ip-172-31-41-43:~$ python
Python 3.6.5 |Anaconda, Inc.| (default, Apr 29 2018, 16:14:56)
[GCC 7.2.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow
>>> █
```

# Jupyter Server

- Programming Graphical User Interface (GUI)
- MS Word for Machine-Learner
- Based on IPython
- Uses 'Notebooks'
  - Integrates source code and comments



The screenshot shows a Jupyter notebook window titled "jupyter 1\_1\_MNIST-with-CNN (unsaved changes)". The notebook contains a single code cell (In [2]) with Python code for cosmetic preparation and setting warning filters. Below the code cell is a "Helper Functions" section containing four function names: INIT\_WOTS, INIT\_BIAS, CONV2D, and a description of the CONV2D function. The notebook interface includes a toolbar at the top with various icons for file operations, a status bar indicating "Not Trusted" and "Python 3", and a progress bar at the bottom.

```
# Cosmetic preparation
## switch off deprecation and future warnings
import warnings

def fmx():
    warnings.warn("deprecated", DeprecationWarning)

with warnings.catch_warnings():
    warnings.simplefilter("ignore")
    fmx()
warnings.simplefilter(action='ignore', category=FutureWarning)
```

In [2]:

Out[1]: []

Helper Functions

INIT\_WOTS  
INIT\_BIAS  
CONV2D

Function to help initialize random weights for fully connected or convolutional layers, we leave the shape attribute as a parameter for this.

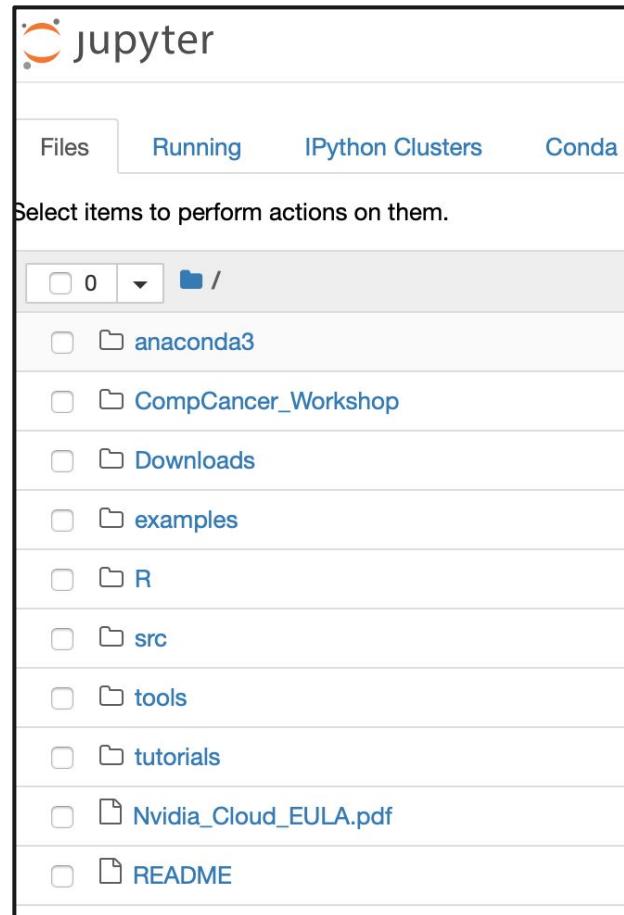
In [7]:

Jupyter notebook

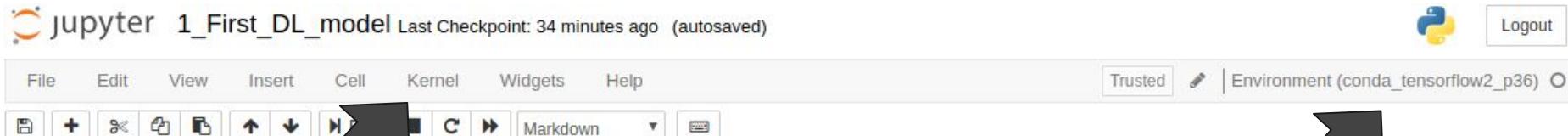
- Text files with .ipynb ending
- JSON format

# Start Jupyter server

- > Ctrl + a
  - > 1
  - > jupyter-notebook --port=8889
- 
- **Password: 'CompCancer'**
  - Start server in servlet session to avoid stopping the server on logout



# Interaction & Keyboard Shortcuts



Set Kernel

- Kernels governs communication with GPU and software
- Cells either contain source code or Markdown
- Markdown ~= Website CSS

Conda environment

- Enter = enter cell
- Esc = leave cell
- Shift + enter = execute cell & move
- Ctrl + enter= execute cell & stay
- A insert cell above
- B insert cell above below
- M transform cell Markdown
- D + D delete

# Mini-Hackathon

---

- Apply your learned Deep-Learning skills
- Real-world Stanford-created challenge
- Melanoma-classification
- Employs advanced concepts
- Announcement of winner at the end of Session 1

## Hackathon Challenge



## Melanoma-classification Hackathon



CompCancer

---

# General Theory Deep-Learning

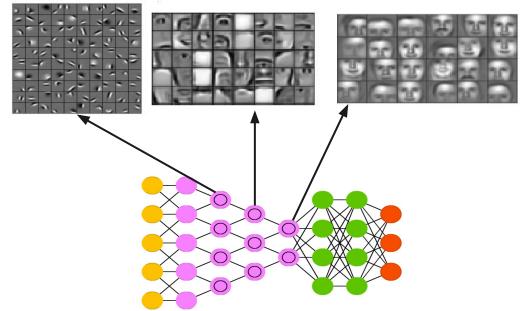
# Actual name of Deep-Learning



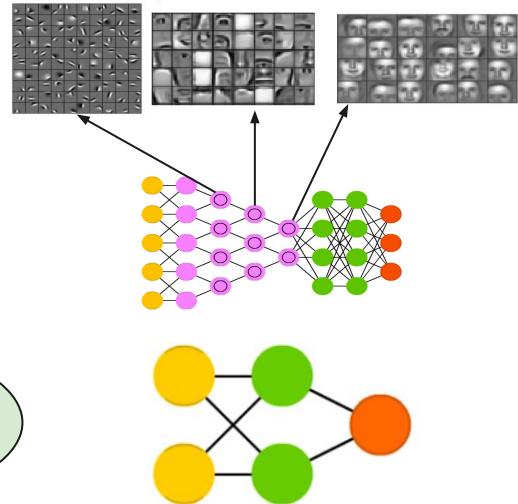
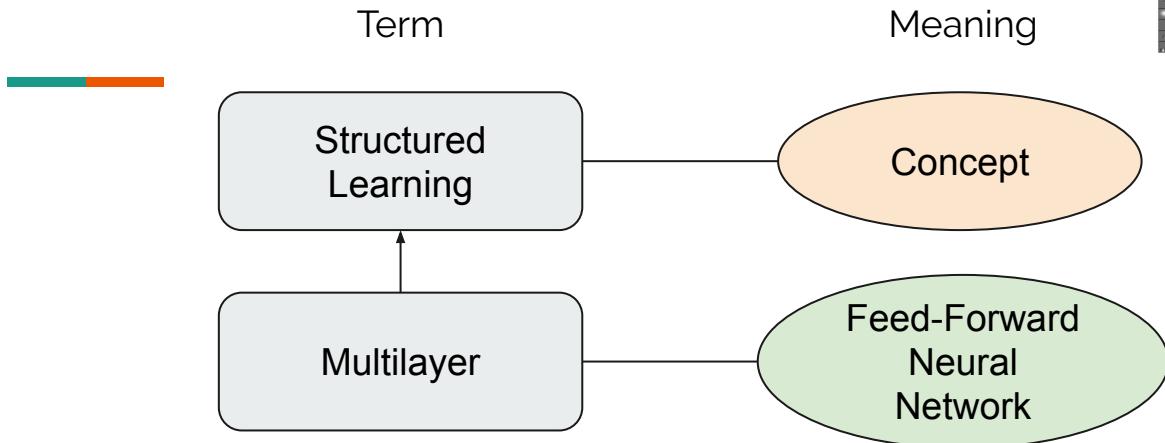
## ***Structured Learning Feed-Forward Multilayer Perceptron Artificial Neural Network***

(in general parlance)

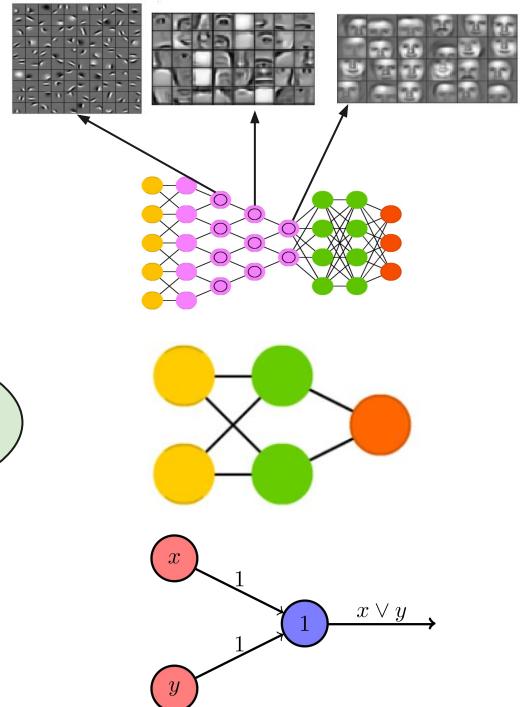
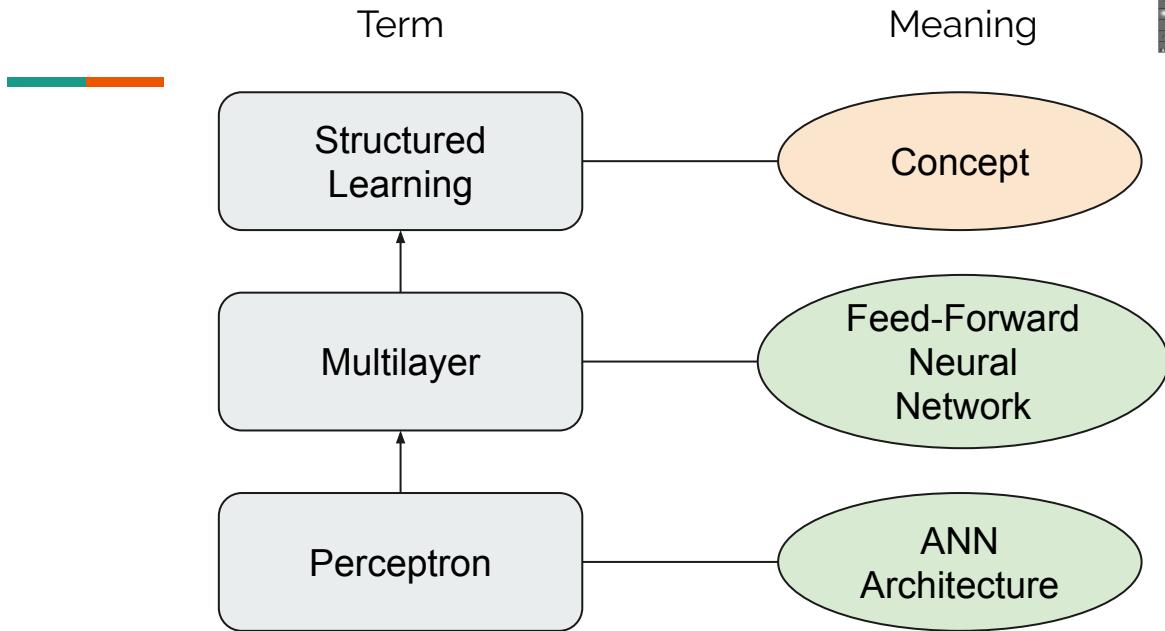
# Structured Learning Multilayer Perceptron Network



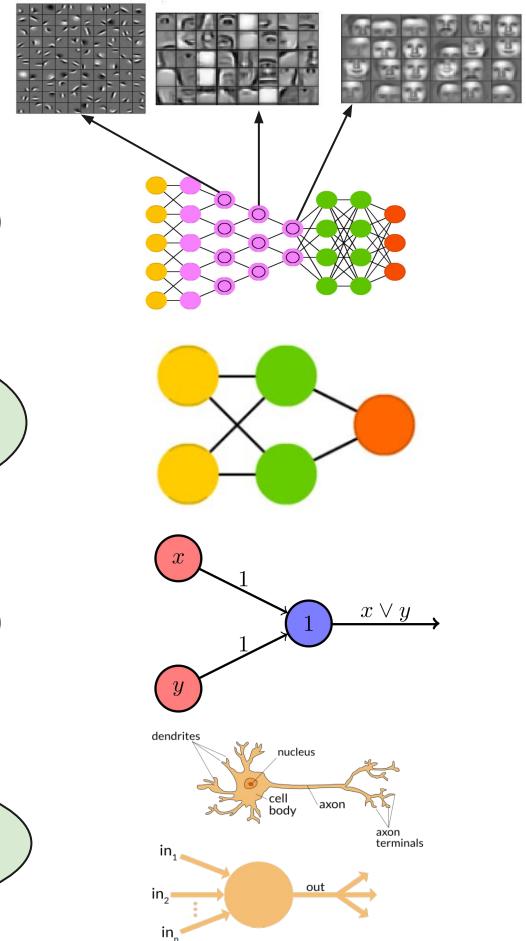
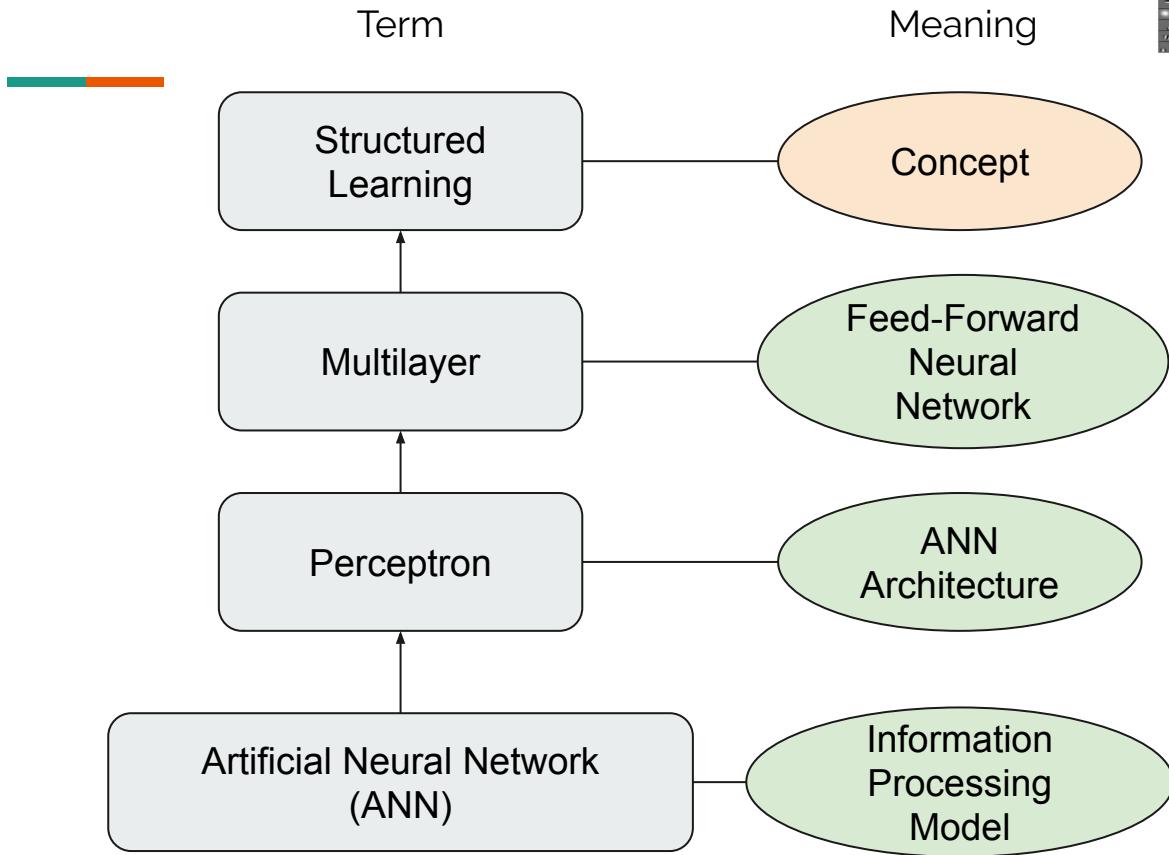
# Structured Learning Multilayer Perceptron Network



# Structured Learning Multilayer Perceptron Network



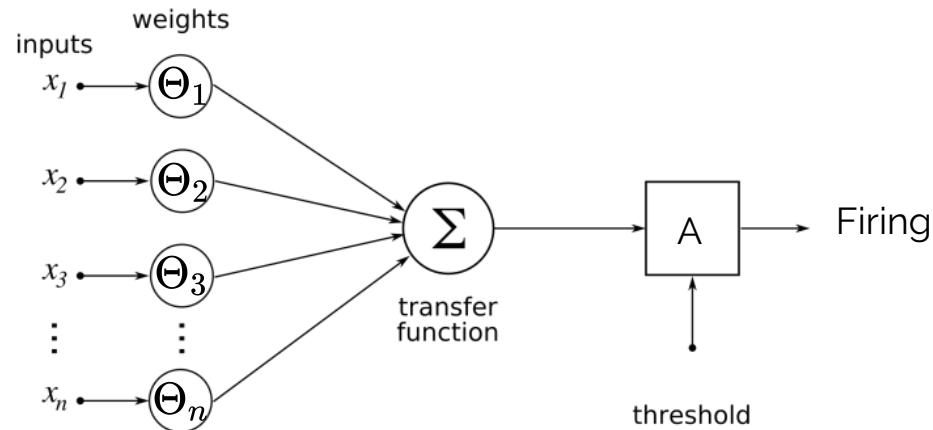
# Structured Learning Multilayer Perceptron Network



# Artificial Neural Networks

## Artificial Neural Network (ANN)

- Information processing model
- Set of **nodes**  $V$  connected by **edges**  $E$
- Firing of node depends on **activation function**  $A$
- Weights of edges  
 $\Theta$



Artificial Neuron

$$\text{Firing} = A(\sum(\text{weights } \Theta \cdot \text{input } x) + \text{bias})$$

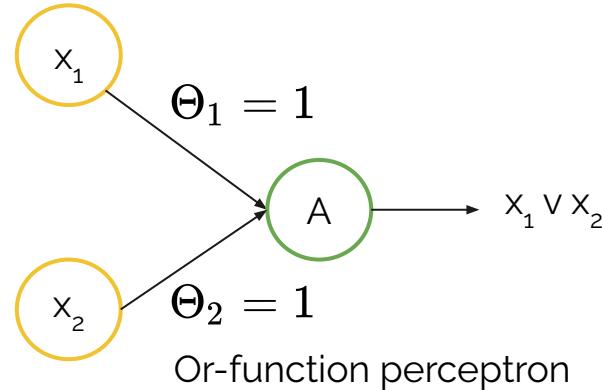
# Perceptron



Single-layer Perceptron

- Input layer labeled as  $x$ 
  - Binary
- No hidden layers
- Weight convergence ensured for one layer
  - Delta rule
- Prediction is matrix operation
  - (Historically) binary

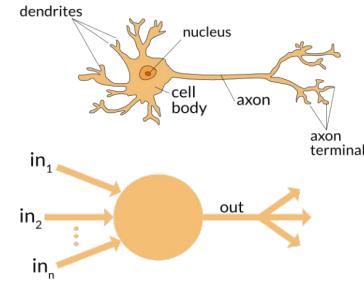
$$h_{\Theta}(x) = A(\Theta \cdot x)$$



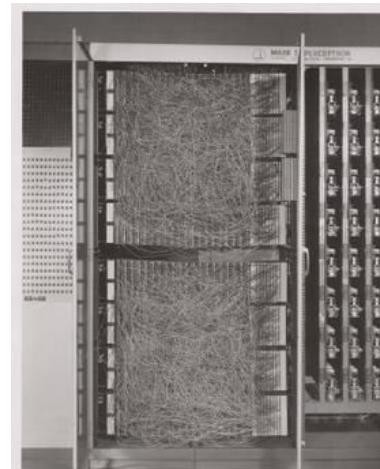
$x_1$	$x_2$	$h_{\Theta}(x)$
0	0	0
1	0	1
0	1	1
1	1	1

# History of perceptron / Deep-Learning

- Loosely inspired by biological neural networks
- Developed by Frank Rosenblatt in 1958
  - US Navy
  - Classify images of numbers
- DL Winter
  - 1969, Minsky & Papert
  - XOR-function impossible for one-layer perceptron



Edge weight via potentiometer



'Perceptron Machine'

# Motivation Machine-Learning

- Hypothesis

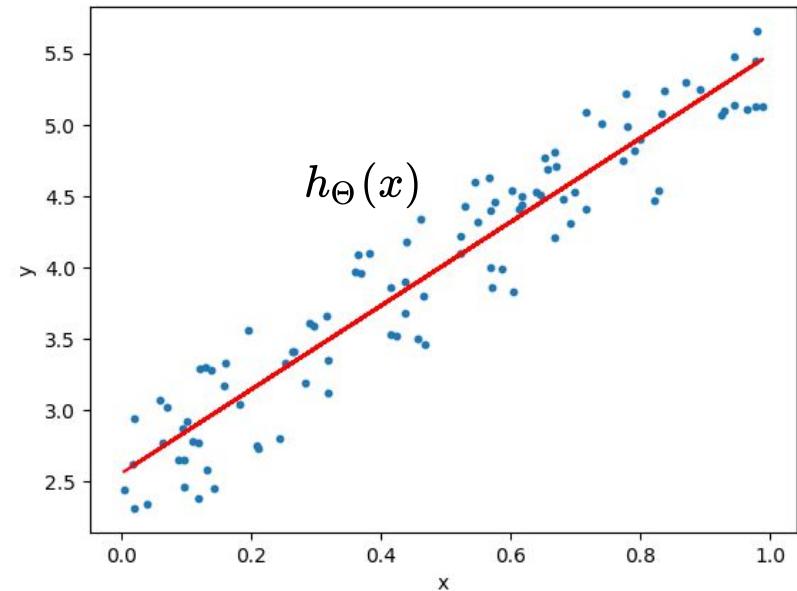
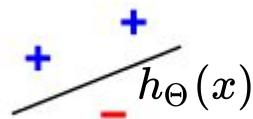
$$h_{\Theta}(x) = \Theta_0 + \Theta_1 \cdot x$$

- Parameters

$$\Theta_0, \Theta_1$$

- Cost Function

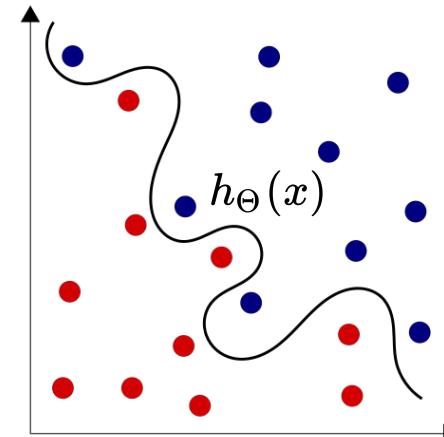
$$J(\Theta_0, \Theta_1) = \frac{1}{2m} \sum_{i=1}^m (h_{\Theta}(x_i) - y_i)^2$$



Regression

# Non-linearity

- Non-linearity defies linear hypothesis
- Addition of non-linear features  $x^2$
- (Generally) require complex hypothesis functions
- Utilization of 'Kernel-trick'
  - Projection into higher-dimension
  - Requires fine-tuning of model and/or domain knowledge



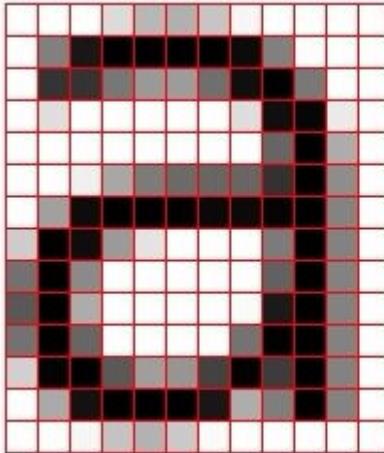
Non linear separability

$$h_{\Theta}(x_1, x_2) = (x_1, x_2, x_1^2 + x_2^2)$$

Non-linear hypothesis function  $h_{\Theta}(x)$

# Complex hypothesis: Combinatorial Explosion

- Complex problem require complex pattern recognition
  - Inefficient or infeasible
- 'Classical' ML models challenged by input dimension



=

1.0	1.0	1.0	1.0	0.9	0.6	0.6	0.6	1.0	1.0	1.0	1.0	1.0
1.0	0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	1.0	1.0	1.0
1.0	0.2	0.2	0.5	0.6	0.6	0.5	0.0	0.0	0.5	1.0	1.0	1.0
1.0	0.9	1.0	1.0	1.0	1.0	1.0	0.9	0.0	0.0	0.9	1.0	1.0
1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.0	0.5	1.0
1.0	1.0	1.0	0.5	0.5	0.5	0.5	0.5	0.4	0.0	0.5	1.0	1.0
1.0	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	1.0
0.9	0.0	0.0	0.6	1.0	1.0	1.0	1.0	0.5	0.0	0.5	1.0	1.0
0.5	0.0	0.6	1.0	1.0	1.0	1.0	1.0	0.5	0.0	0.5	1.0	1.0
0.5	0.0	0.7	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.5	1.0	1.0
0.6	0.0	0.6	1.0	1.0	1.0	1.0	0.5	0.0	0.0	0.5	1.0	1.0
0.9	0.1	0.0	0.6	0.7	0.7	0.5	0.0	0.5	0.0	0.5	1.0	1.0
1.0	0.7	0.1	0.0	0.0	0.0	0.0	1.0	0.9	0.8	0.0	0.5	1.0
1.0	1.0	1.0	0.8	0.8	0.9	1.0	1.0	1.0	1.0	1.0	1.0	1.0

Example: 50 x 50 pixel image

$$h_{\Theta}(x_1, x_2) = (x_1, x_2, x_1 \cdot x_2)$$

> choose(2500,2)

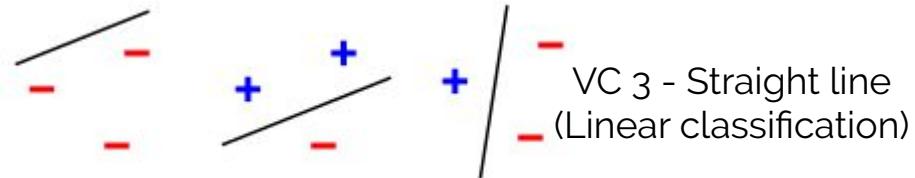
[1] 3123750

# Vapnik–Chervonenkis Dimension

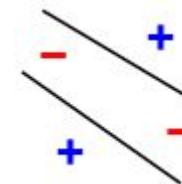
Vapnik–Chervonenkis Dimension (VC)

- 'Measure of complexity'
- Upper error bound calculation possible
- **Cardinality** of the largest shatterable set of points

#Variables	#Boolean Function	#BF Linearly separable
2	16	14
3	256	104
4	65536	1882



VC 3 - Straight line  
(Linear classification)



VC 4 - Two  
Straight lines

# Multilayer Perceptron

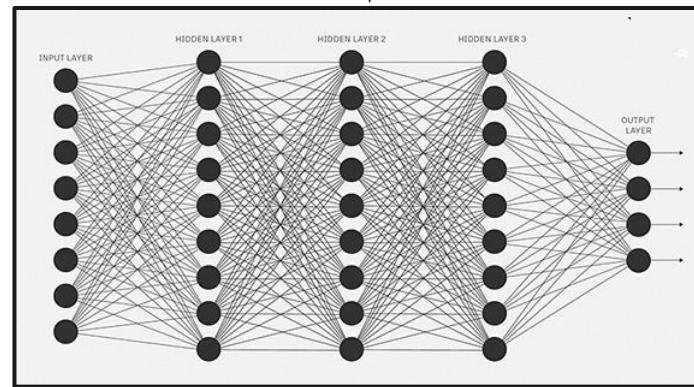
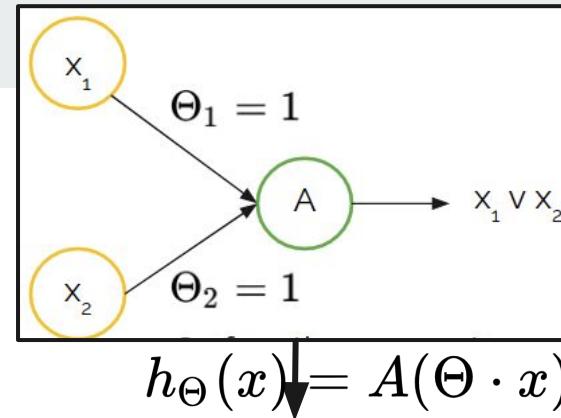
- VC dimension dynamic
- Deep-Learning architecture parameters
  - $|E|$  number edges
  - $|V|$  number nodes
- Computationally expensive

VC Sign-Activation  
Function

$$O(|E| \cdot \log(|E|))$$

VC Sigmoid-Activation  
Function

$$O(|E|^2 \cdot |V|^2)$$

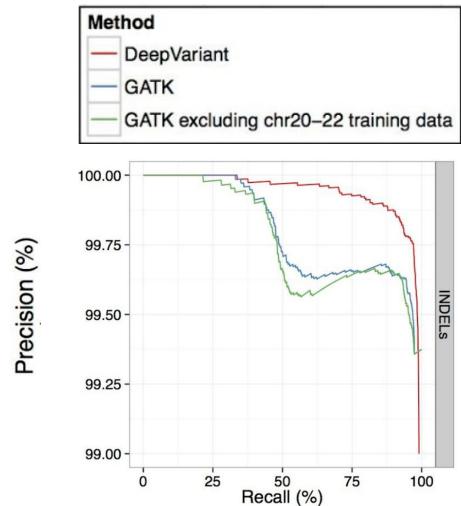
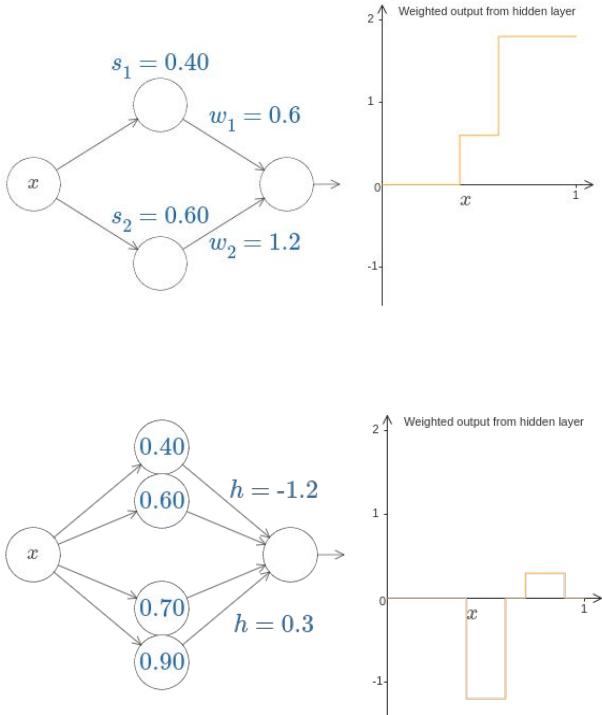


Increased number of layers

$$h_{\Theta}(x) = A_k(\Theta_{k-1} \cdot, \dots, A_2(\Theta_1 \cdot x))$$

# Universal Function Approximation

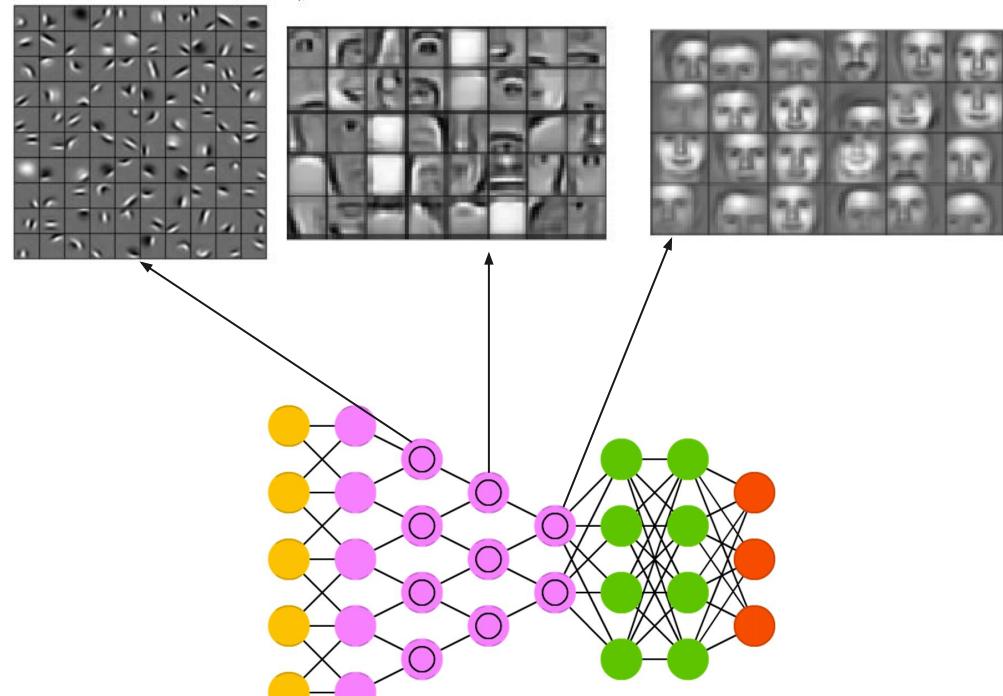
- Approximation of any Lebesgue-integrable function
- $h_{\Theta}(x)$  can be latent
- Google's DeepMind beat GATK by learning a latent error function
- Error function (almost) intractable
  - Approximated by GATK with mixed gaussian models



DL beats GATK gold-standard

# Definition Structured Learning

- Abstract concept of how to learn
- Each layer learns different level of abstraction
- Independent from ANNs
- Automatic feature selection
- Analogy to PCA: layers are an analogy to eigenvectors of matrix



Different degrees of abstractions in different layers

Credit Image: NVIDIA



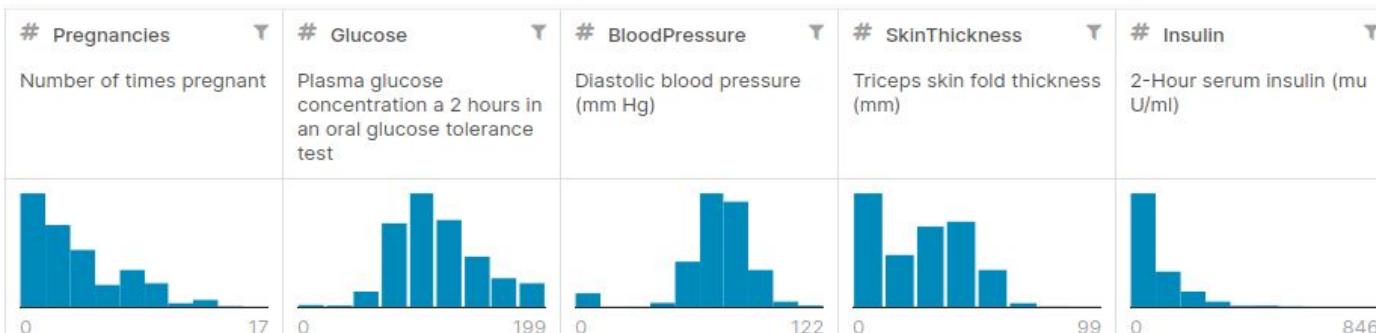
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# First Deep Learning model

## Diabetes prediction

# Deep-Learning model 1

- Predict Diabetes status of Pima Indians
- Numeric matrix
  - Columns 1-8: data
  - Column 9: Phenotype





CompCancer

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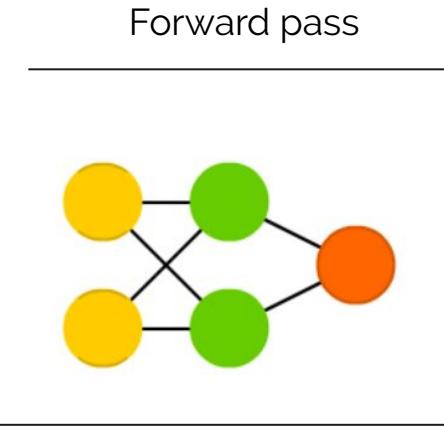
# Theory Model 1

# Feed Forward Artificial Neural Network



Feed Forward Artificial Neural Network (FFNN)

- Propagate an input signal through network
  - From **input** to **output** layer with intermediate **hidden** layers
- Prediction by forward pass
- Learn edges during backward propagation



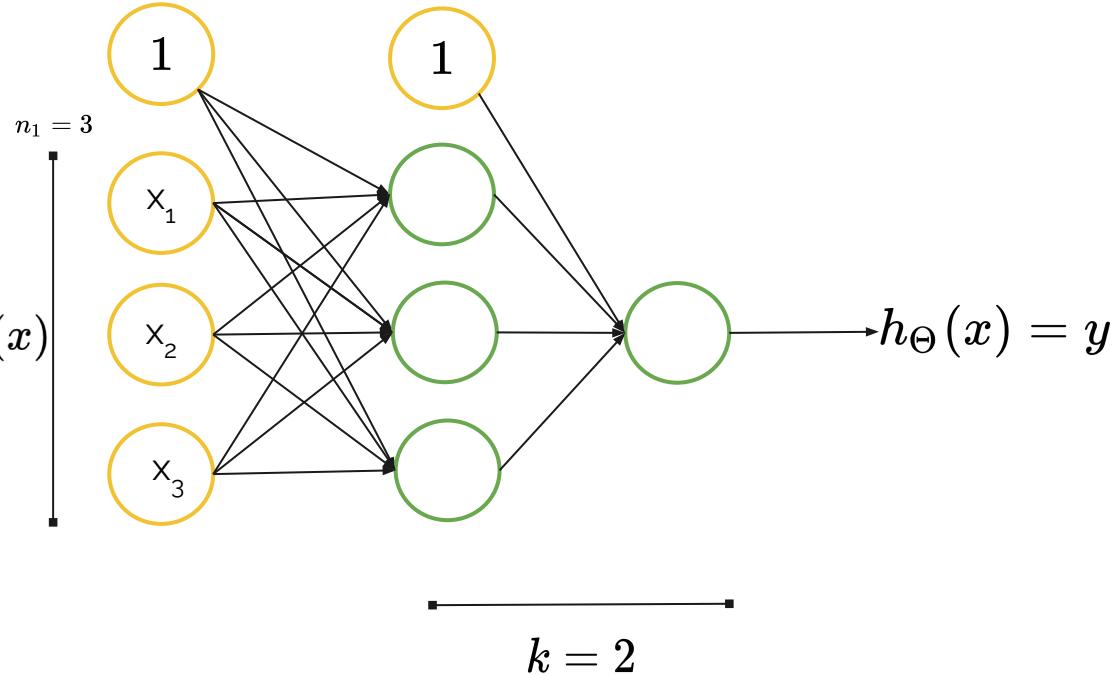
Backward  
propagation

Input Cell   Output Cell  
 Hidden Cell

$$\text{Output network} = f_{\text{act}}(\sum (a_i \text{ final layer}))$$

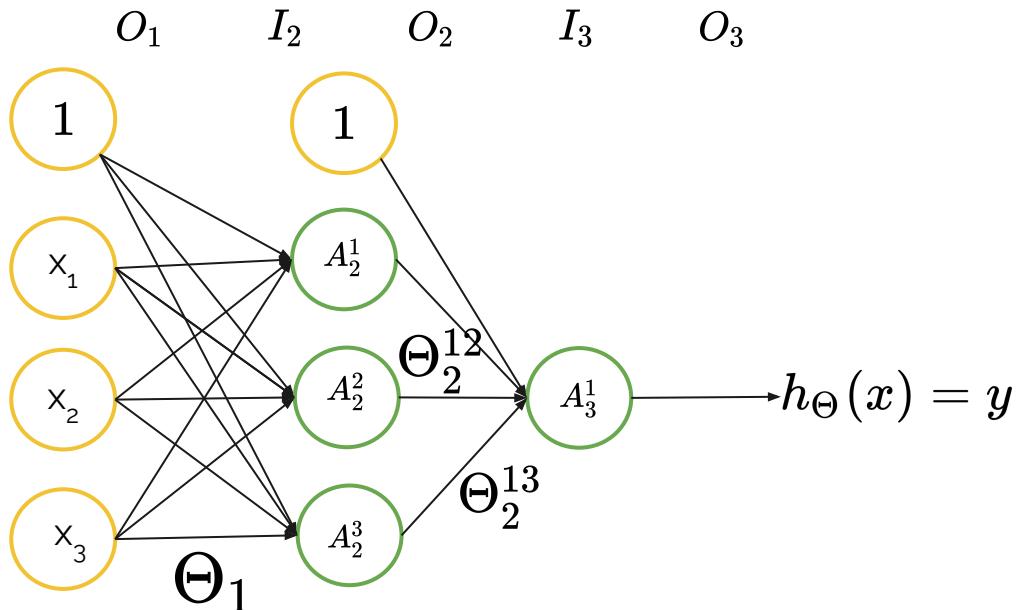
# Parameters FFNN Network

- Input  $x = [x_1, x_2, \dots, x_n]$
- Output  $y = [y_1, y_2, \dots, y_n] = h_\Theta(x)$
- Number layers (depths)  $k$
- Width  $n$



# Parameters FFNN Layer

- Input layer  $I_i$
- Output layer  $O_i$
- Activation function layer  $A_i$
- Weights edges  $\Theta_{layer}^{to\ from}$



#weights fully connected layer:  $a_n \cdot (a_{n-1} + 1)$

# Feed Forward Pass

- Pass input through network
- From **input** to **output** layer
- *Forward pass == Forward propagation*

$$O_1 = x$$

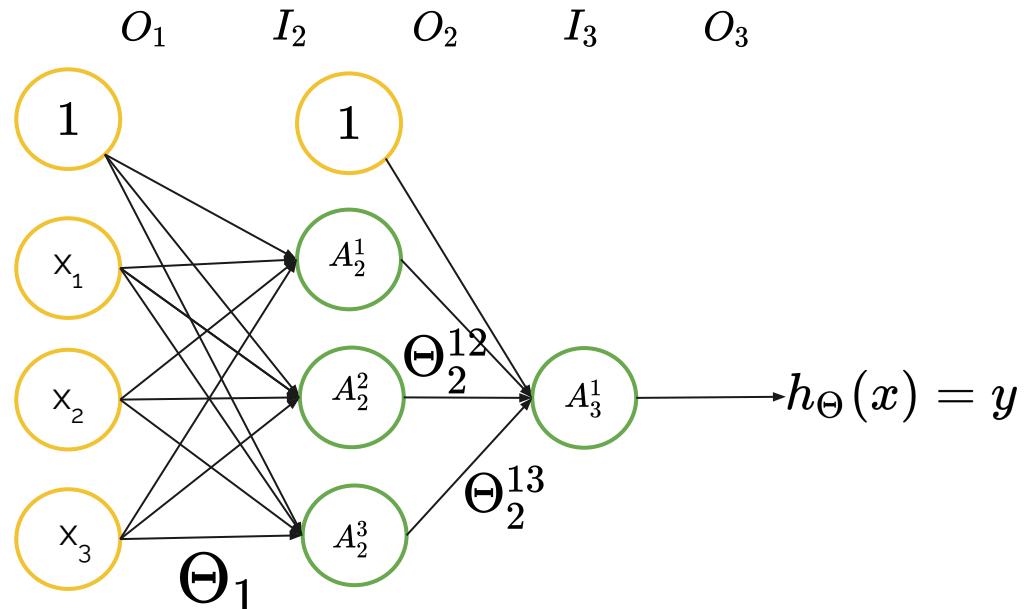
$$I_2 = \Theta_1 \cdot O_1$$

$$O_2 = A(I_2) \text{ (add } O_0^1/x_0)$$

$$I_3 = \Theta_2 \cdot O_2$$

$$O_3 = A(I_3) \text{ (add } O_0^2)$$

$$h_{\Theta}(x) = O_3$$

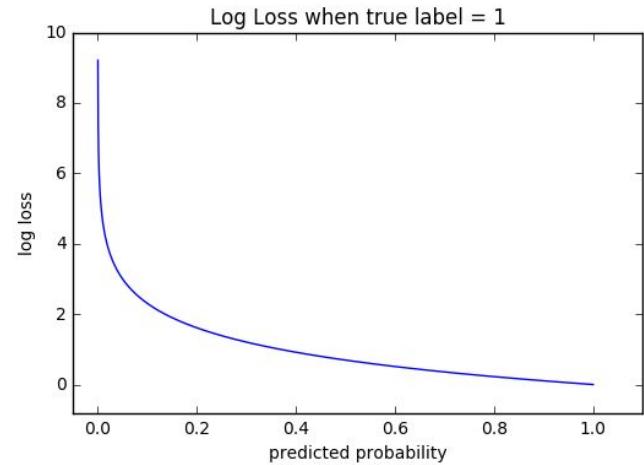


$$h_{\Theta}(x) = A_3(\Theta_2 \cdot A_2(\Theta_1 \cdot x))$$

Recursive formulation  
Biases nodes omitted

# Cost / loss function

- Quantification of difference prediction to truth y
- Partial derivatives required
- Cross-entropy function for classification
- RMSE for regression

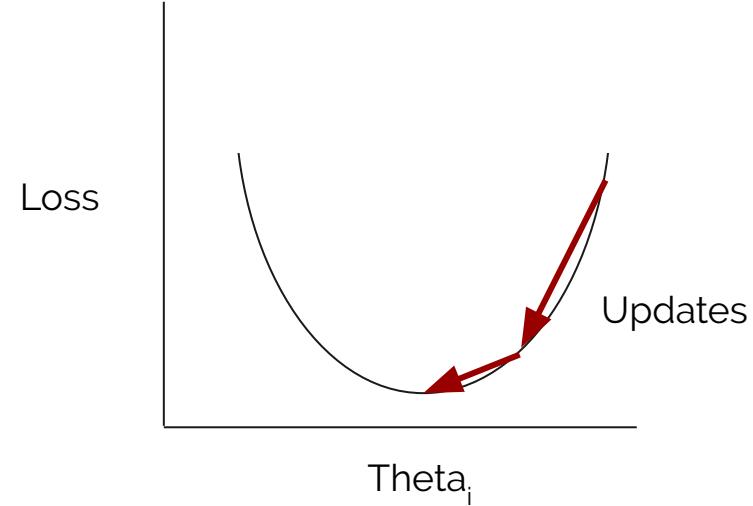


Error Quantification

$$J_{\Theta}(x, y) = -\frac{1}{m} \left[ \sum_{i=1}^m y_i \cdot \log(h_{\Theta}(x_i)) + (1 - y_i) \cdot \log(1 - (h_{\Theta}(x_i))) \right]$$

# Gradient descent

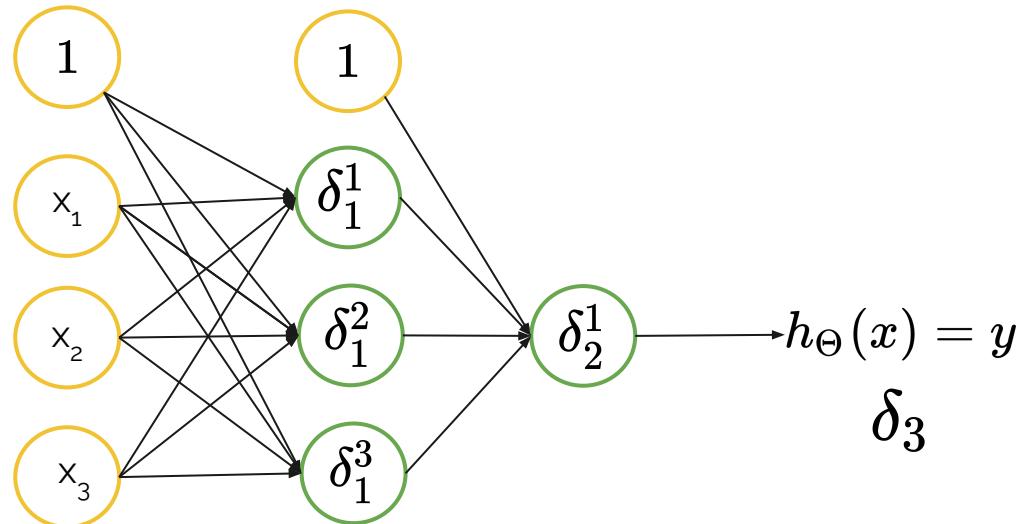
- Calculate minimum of  $J$
- Not necessarily global optimum
- Optimizers
  - Adam, Adadelta, RMS Prop
  - Global optimum not ensured



$$J_{\Theta}(A_3(\Theta_2 \cdot A_2(\Theta_1 \cdot x)), y) = J(x, y, \Theta) = J(x, y, \Theta_k, \Theta_{k-1}, \dots, \Theta_1)$$

# Intuition Backpropagation

- Error for node  $j$  in layer  $i$   $\delta_i^j$
- Quantify error for every node
- Calculate partial derivatives  $-\frac{\partial}{\partial \Theta} J_\Theta(x)$
- Update weights by error gradient with learning rate



$$\delta_3 = J_\Theta(x) = y_{truth} - A_3(I_3)$$

$$\delta_2 = \Theta_2 \cdot \delta_3 \cdot A'_2(I_2)$$

$$\delta_1 = \Theta_1 \cdot \delta_2 \cdot x$$

Total derivative shown

# Outline Mathematics Backpropagation



$$(1) J_\Theta(A_3(\Theta_2 \cdot A_2(\Theta_1 \cdot x)), y) \quad \text{Chain rule}$$

$$(2) \frac{\delta J_\Theta}{\delta x} = \frac{\delta J_\Theta}{\delta O_3} \cdot \frac{\delta O_3}{\delta I_2} \cdot \frac{\delta I_2}{\delta O_1} \cdot \frac{\delta O_1}{\delta x} \quad \frac{\delta a}{\delta c} = \frac{\delta a}{\delta b} \cdot \frac{\delta b}{\delta c}$$

$$(3) \frac{\delta J_\Theta}{\delta A_3} \cdot (A_3)' \cdot \Theta_2 \cdot (A_2)' \cdot \Theta_1 \quad (f(g(x)))' = f'(g(x)) \cdot g'(x)$$

...

$$(4) \delta_i := (A_i)' \cdot (\Theta_{i+1})^T \cdot \dots \cdot (\Theta_{k-1})^T \cdot (A_{k-1})' \cdot (\Theta_k) \cdot (A_k)' \nabla_{O_k} J_\Theta(x)$$

$$(5) \nabla_{\Theta_i} J_\Theta(x) = \delta_i (O_{i-1})^T$$



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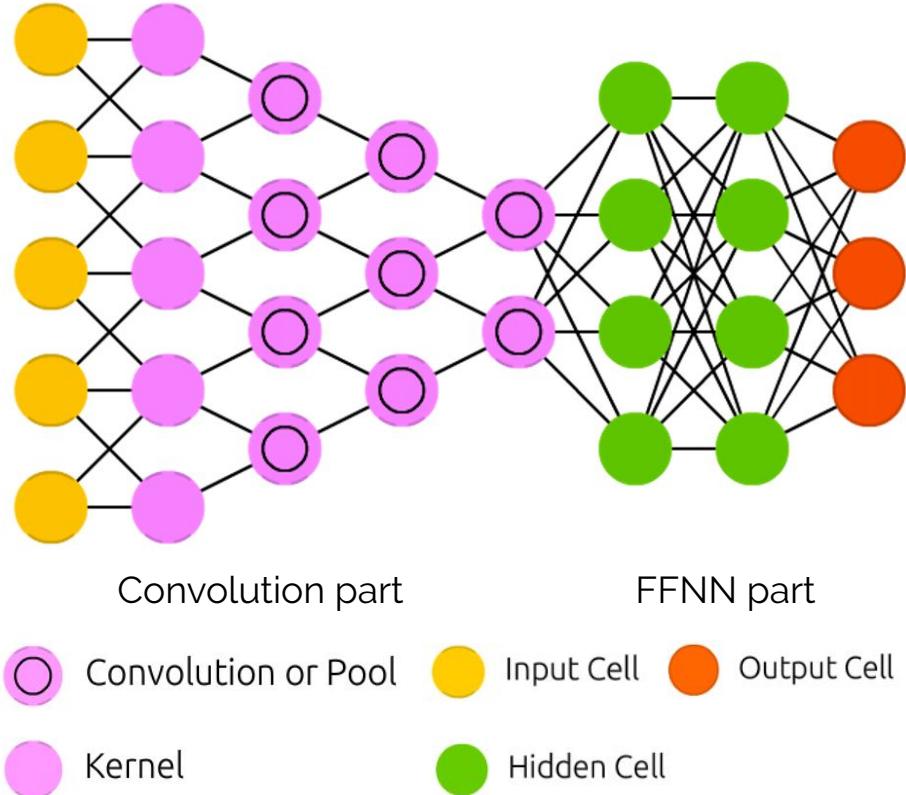
# Second model

# Convolutional Neural Network

# Number recognition

# Convolutional Neural Networks

- Image classification
- **Convolve** pixels into decision units
  - $200 \times 200$  pixels -> 40 000 input units ->  
e.g. 20 decision units
- Project abstract patterns into higher and smaller layers
- Optional combination with FFNN for non-linear behavior

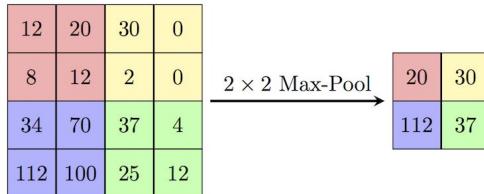


# Max Pooling & Striding & Padding



## (Max)-Pooling

- Kernel filter function
- Reduce features
- Induces abstract pattern recognition



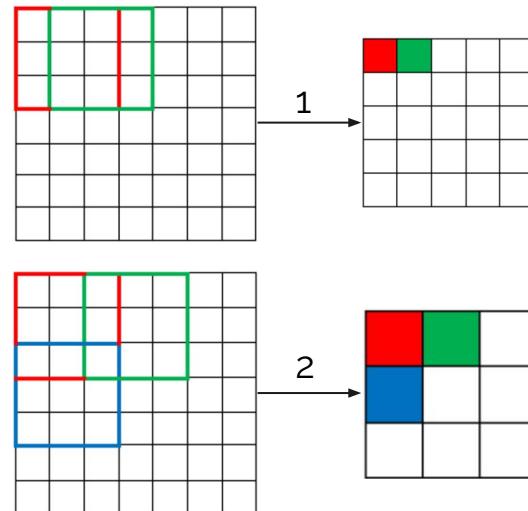
## Padding

- Addition to outer pixels
- Ensure desired kernel coverage of pixels

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

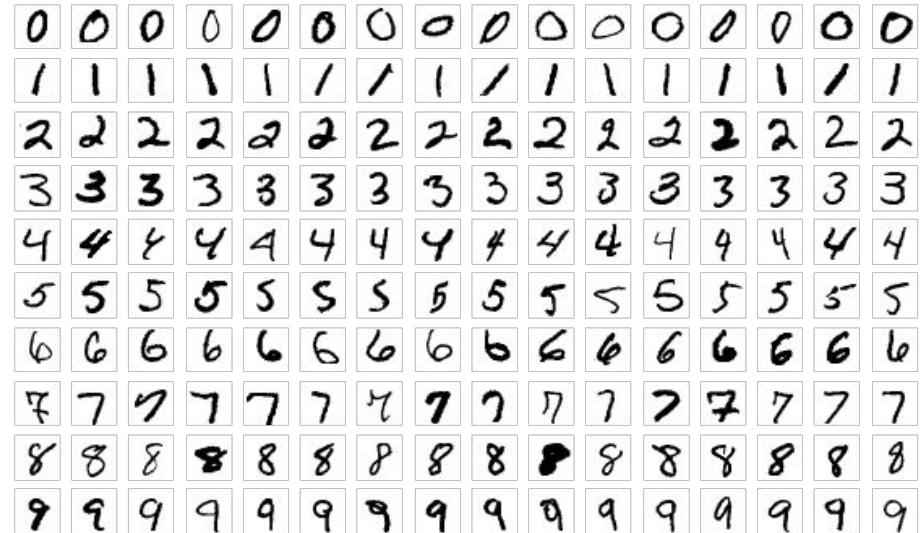
## Striding

- Movement control of filter kernel
- Amount of skipped pixels



# MNIST dataset

- Very well known tutorial dataset
- Used to be real-world challenge before being 'solved'
- 60,000 samples
- 28x28 pixels
- You will solve MNIST via DL convolutional network



Hand-written number classification



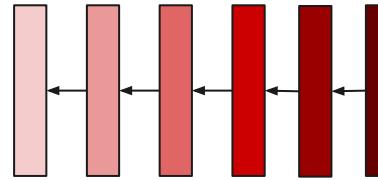
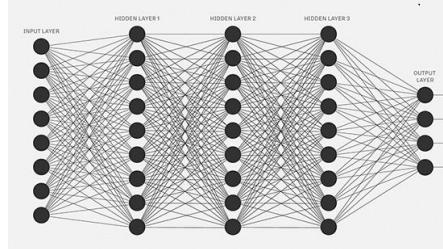
CompCancer

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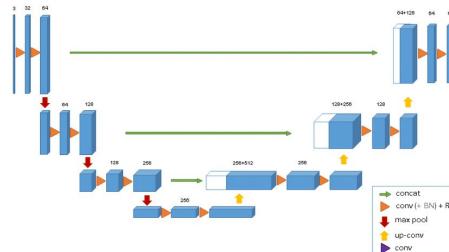
# Theory model 2

# Vanishing gradient problem

- Partial derivatives decay through layers
- Slows down or stops model training
  - Contributed to AI winter
- Remedies:
  - More computational power
  - ANN architecture adaptation
  - Residual ANNs



Decay of partial derivative  $-\frac{\partial}{\partial \Theta} J_{\Theta}(x)$



Note high-level edges

Credit Image: Google, Perceptron. Mitchell, Machine Learning, p87.

# Weight initialization

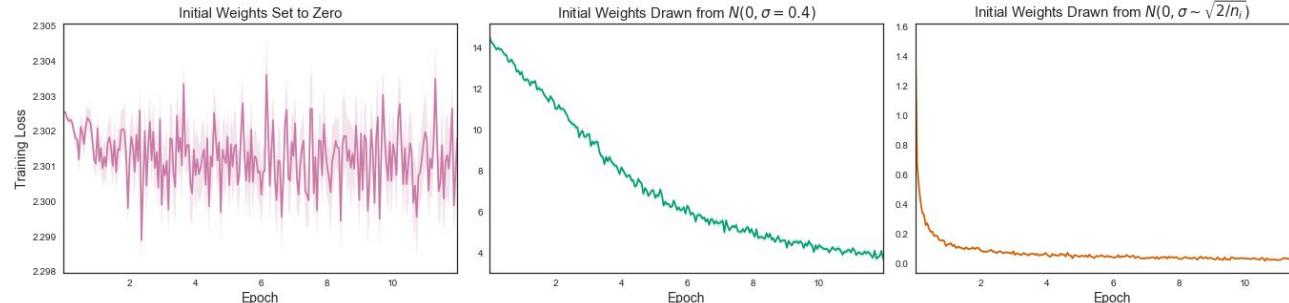


## Properties

- Critical for effective model training
- Each edge has weight parameter
- Avoiding symmetries necessary

## Initialization types

- $[0, \dots, 1]$ ,  $\mathbb{R}$ , uniform
- $N(\mu, \sigma)$
- Orthogonal
  - Weights drawn from orthogonal matrix
- All zeros
- All ones



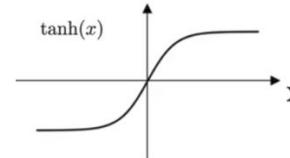
Impact weight initialization on loss

Credit Image: Perunicic et al. 2018

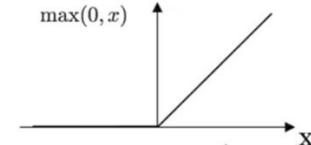
# Activation functions

- Key for non-linearity
- Influences multiple behaviors
  - Vanishing gradient
  - Prediction performance
- Frequently utilized functions
  - Hyper Tangent  $\rightarrow [-1, 1]$
  - Sigmoid  $\rightarrow [0, 1]$
- Last layer
  - Binary - Logistic
  - Multinomial - Softmax

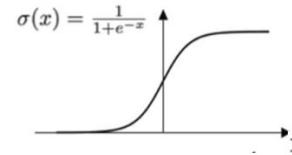
Hyper Tangent Function



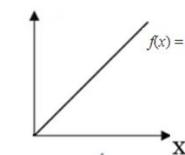
ReLU Function



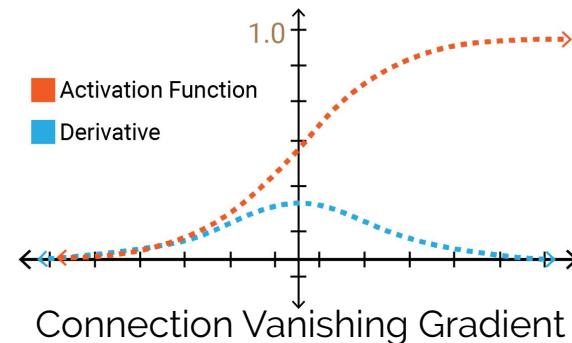
Sigmoid Function



Identity Function

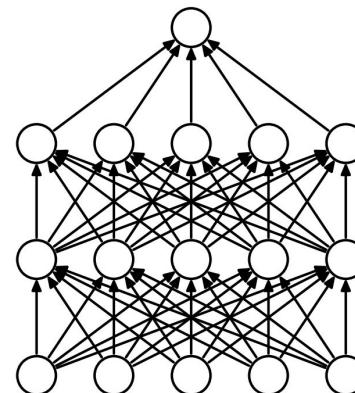


Types of activation functions

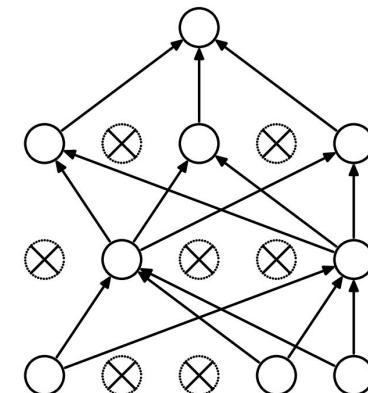


# Dropout layer

- Avoids overfitting
- Enforce redundancy
- Increases training time
- Can be problematic for Convolutional Neural Networks (CCN) - Model 2



(a) Standard Neural Net



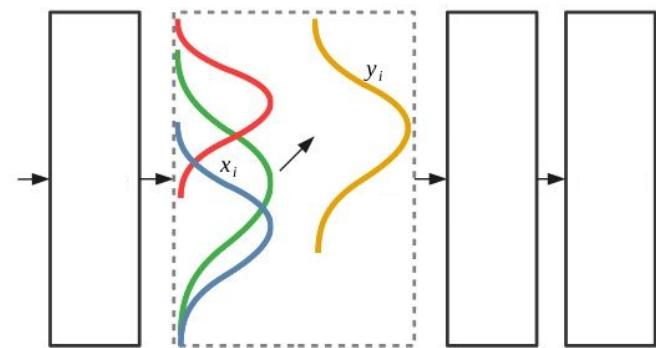
(b) After applying dropout.

Dropout application on architecture

# Definition 'Batch size' and 'Epoch'

## Epoch & Batch

- **Batch** partition of dataset
  - Batch size # of samples per batch
- **Epoch** complete iteration over batches
- **Batch normalization** Solves '*internal covariate shift*'
  - Distribution of input features differs for different batch
- **Assumption** batches independently and identically distributed

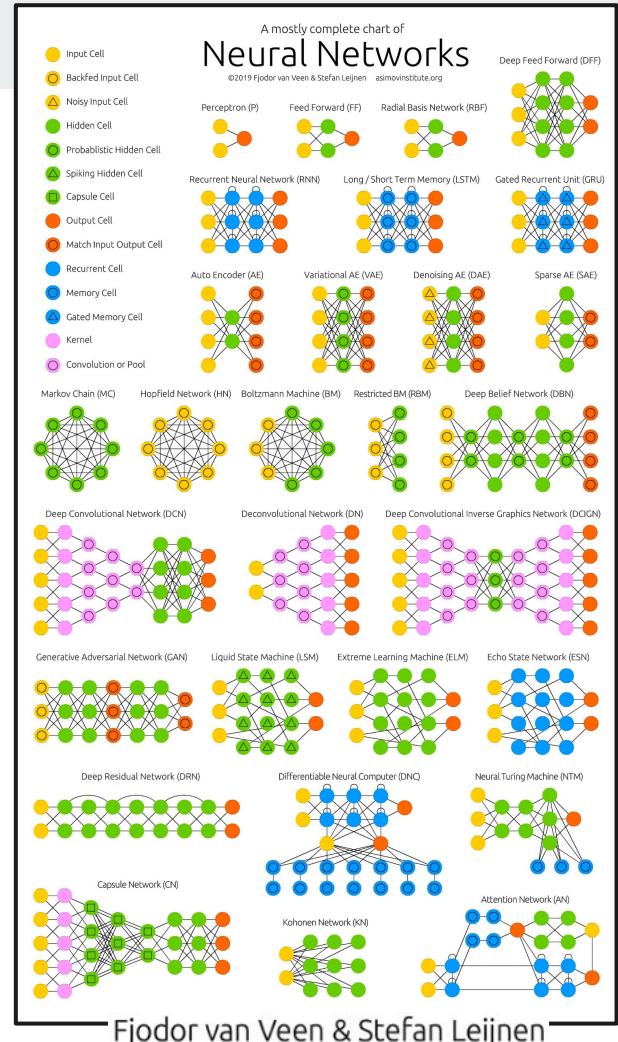


Ensure same mean and variance  
for  $x$  and  $y$

# Network Architectures



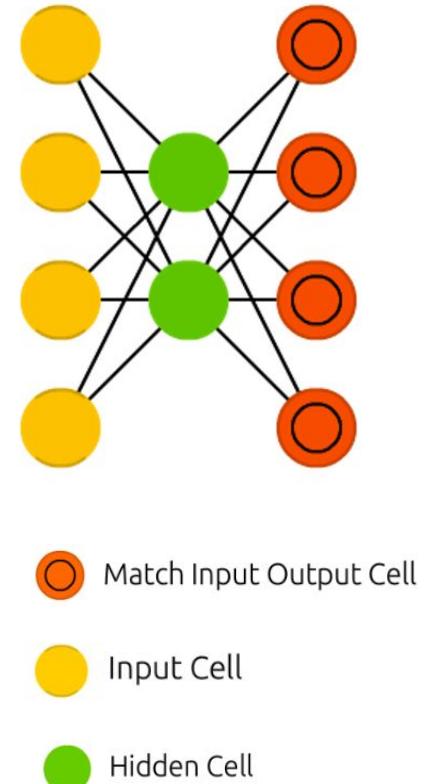
1. Feed forward neural networks **FFNN**
2. Convolutional Neural Network **CNN**
3. Recurrent neural networks **RNN**
4. Long / short term memory **LSTM**
5. Gated recurrent units **GRU**
6. (Variational) Autoencoders (**V**)**AE**
7. Deep belief networks **DBN**
8. Capsule Networks **CapsNet**
9. ...



# Autoencoders

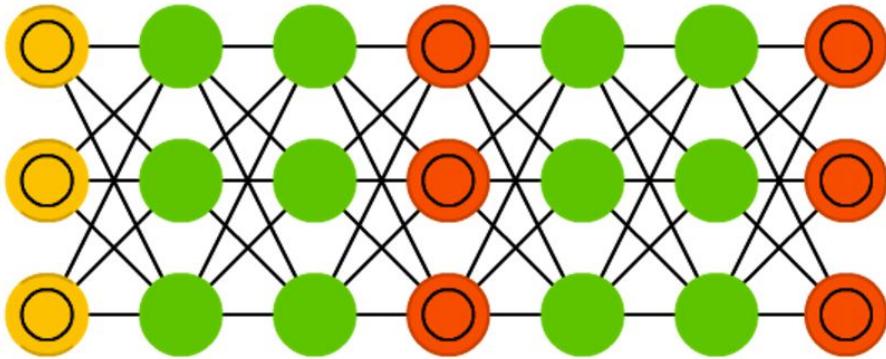
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- Encode/ compress information
- Smallest layer (almost) always in the center
  - Layers before: **encoding** layers
  - Central layer: **coding** layer
  - Layers after: **decoding** layers
- Enforce 'meaningful' central units that cover the abstract representation of the input to output transformation
- Can conduct a PCA by SVD on coding layers



# Generative Adversarial Networks

- Combination of two networks
- One generates content
- Other classifies content
  - Generated or real content?
- Competitive approach, train both networks simultaneously



Portrait of Edmond Belamy  
432,500\$

○ Match Input Output Cell

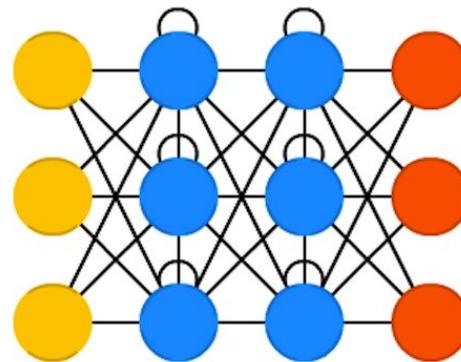
○ Backfed Input Cell

● Hidden Cell

# Recurrent Neural Network

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- Introduce nodes states as memory
- Nodes process information from **previous layer** and **themselves** from previous pass
- Order of input changes output
- Susceptible for vanishing gradient problem
- State information lost over time
- Utilized for data with a sequence
  - Speech understanding
  - Image processing
  - Autocompletion

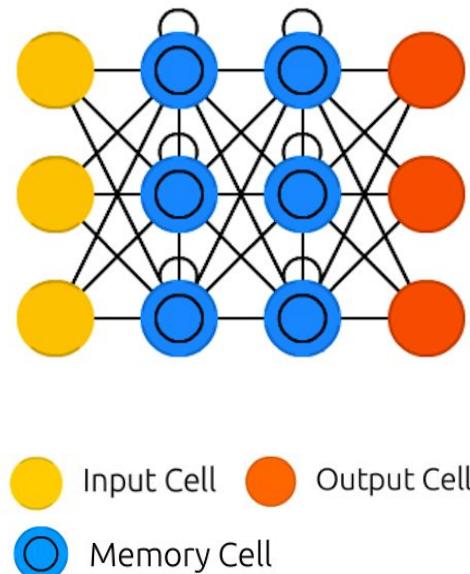


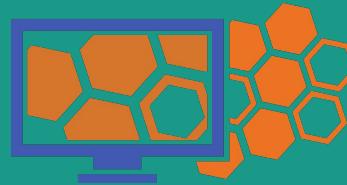
Central memory layer

Input Cell   Recurrent Cell   Output Cell

# Long-Short Term memory

- Combat the vanishing gradient problem with **gates** and **memory cells**
- Three types of gates
  - Input, output and forget
- Gates safeguard information by stopping or allowing information flow
- Able to learn complex sequences:
  - Shakespeare
  - Composing primitive music
- Resources intensive





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Third model

Keras and R

# Keras and R

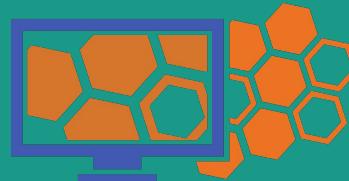


## Requires

- R-studio Server
- Jupyter notebook
  - Kernel installation
- According to Keras documentation same performance

The screenshot shows a Jupyter Notebook interface with the title "jupyter 3\_Keras\_in\_R Last Checkpoint: 6 hours ago (autosaved)". The toolbar includes File, Edit, View, Insert, Cell, Kernel, Widgets, and Help, along with various icons for file operations and cell execution. The code cell In [7] contains the following R script:

```
In [7]: #' Train a simple deep CNN on the CIFAR10 small images dataset.  
#'  
#' It gets down to 0.65 test logloss in 25 epochs, and down to 0.55 after 50 epochs,  
#' though it is still underfitting at that point.  
  
library(keras)  
install_keras(tensorflow = "gpu")  
  
# Parameters -  
  
batch_size <- 32  
epochs <- 5  
data_augmentation <- TRUE
```



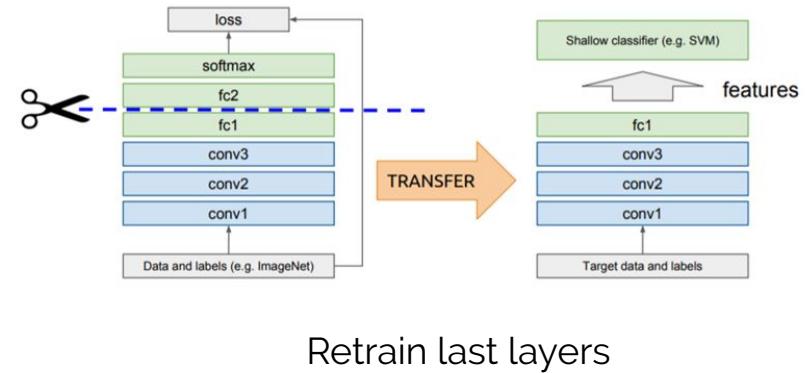
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# Third model Mini-Hackathon Melanoma Classification

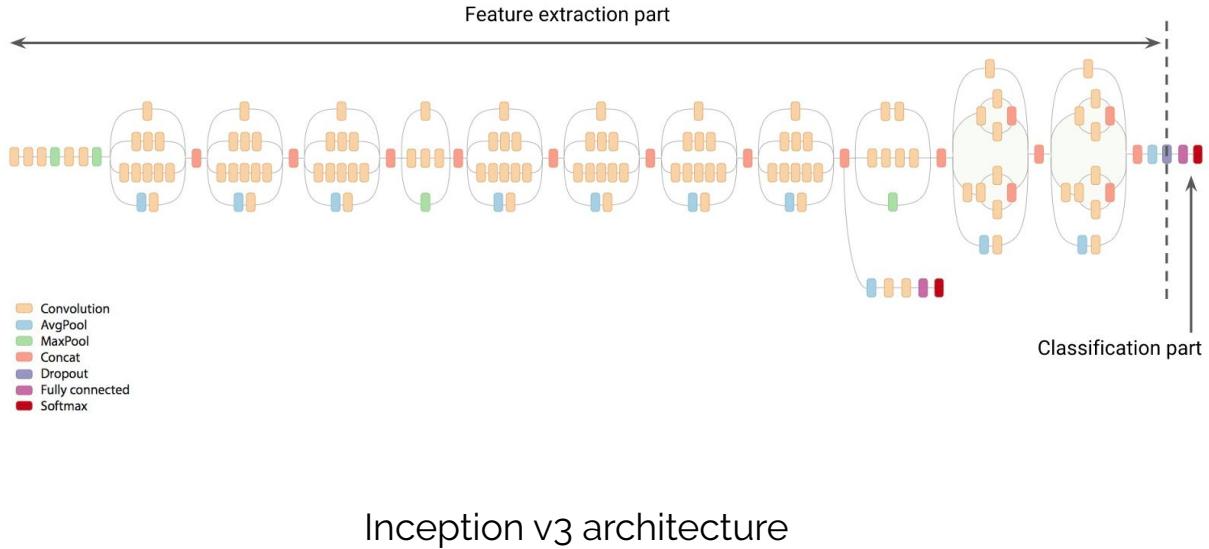
# Transfer learning

- Pre-trained model
- Adapt model to new task
  - Add new or retrain last layer(s)
- Reduces data usage and training time
- Powerful models available
  - E.g. BioBert



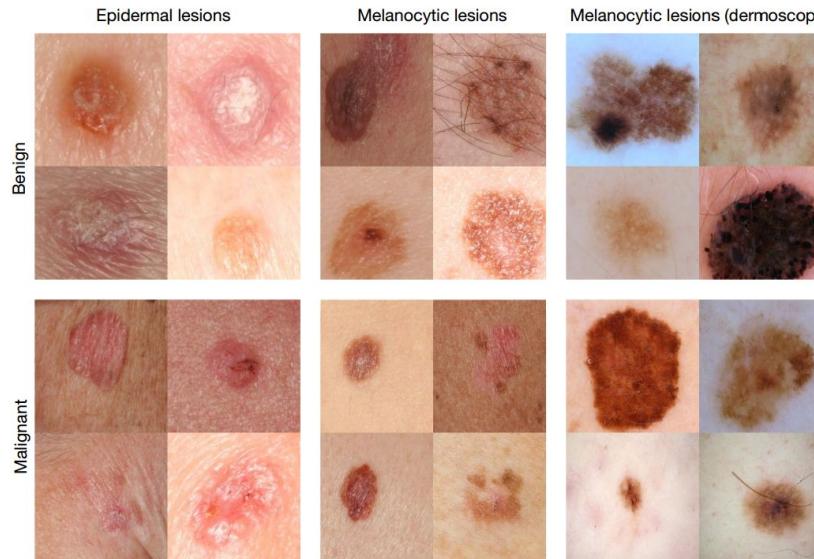
# Inception v3 pre-trained model

- Trained on various types of images
- Comprises of two parts
- Skip feature part and train classification part
- Won ImageNet classification
  - 14 million images
  - 1,000 classes



# Melanoma classification challenge

- Real-world Kaggle challenge
- Designed by Stanford researchers
- Task is to classify lesions



Credit Image: Esteva, Kuprel et. al, 2017

# Summary Deep Learning models



Positive



Negative **X**

- Neural networks flexible
- Transfer-learning powerful
- Non-linearity
- Large dimension input possible
- Dynamically adaptable architecture
- Parallelization possible

- Complex
- Slow
- Black-box
- Hardware requirements high
- (Generally) requires significant amounts of data

# However



"It's not who has the best algorithm that wins. It's who has the best data."