

### **Deep Neural Networks**



16 December 2019



Artificial Intelligence

> Machine Learning

Neural Networks

### **Deep Neural Networks**

- How are the Deep Neural Networks built?
- What can we do with them?
- Some simple examples in python

All examples from this lecture are available on g https://github.com/marcinwolter/DNN\_examples



#### 16.12.2019



Herbert Simon

Turing Award 1975

Nobel Prize in Economics 1978

# What is Machine Learning?



**Example**: Having input and the desired output (eg. calorimeter jet and it's energy) we can create a program (train our algorithm) to give us the desired output (the energies of other jets).



Herbert Alexander Simon:

with computer programs that automatically improve their performance through experience. "



Tom Mitchell

Carnegie Mellon University

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# What does "machine learning" mean?

 Machine learning is a field of computer science that gives computer systems the ability to "learn" (i.e. progressively improve performance on a specific task) with data, without being explicitly programmed.

### • Problems to which it's applied:

- Supervised learning (classification & regression)
- Clustering (unsupervised learning)
- Dimensionality reduction
- Reinforcement learning
- Many others....



### ≻Unsupervised Learning

Technique of trying to find hidden structure in unlabeled data

### ➤Supervise Learning

□Technique for creating a function from training data. The training data consist of pairs of input objects (typically vectors), and desired outputs.

### **Neural networks**





- At the input of each node a weighted sum of inputs is given. It is transformed by the activation function (typically sigmoid) and later send to the output.
- How to train the multilayer network? How to tune the weights in the hidden layers? This problem was unsolved for a long time...
  - Solution **backpropagation**. An error y-f(x,w) is propagated backward through the net using the actual weights ("revolution" of '80'ies).



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# **Machine Learning vs Deep Learning**

- Traditional ML (BDT, NN etc) the scientist finds good, well discriminating variables (~10), called "features", and performs classification using them as inputs for the ML algorithm.
- **Deep Learning** thousands or millions of input variables (like pixels of a photo), the features are *automagically* extracted during training.





### **Deeper network?**

Traditional Neural Networks have one or two hidden layers.

**Deep Neural Network:** a stack of sequentially trained **auto encoders**, which recognize different features (more complicated in each layer) and automatically prepare a new representation of data. This is how our brains are organized.

But how to train such a stack of layers?





http://www.andreykurenkov.com/writing/a-brief-history-of-neural-nets-and-deep-learning-part-4/



### **Training a Deep Neural Network**

- In the early 2000s, attempts to train deep neural networks were frustrated by the apparent failure of the well known back-propagation algorithms (backpropagation, gradient descent). Many researchers claimed NN are gone, only Support Vector Machines and Boosted Decision Trees should be used!
- In 2006, Hinton, Osindero and Teh<sup>1</sup> first time succeeded in training a deep neural network by first initializing its parameters sequentially, layer by layer. Each layer was trained to produce a representation of its inputs that served as the training data for the next layer. Then the network was tweaked using gradient descent (standard algorithm).
- There was a common belief that Deep NN training requires careful initialization of parameters and sophisticated machine learning algorithms.

<sup>1</sup>Hinton, G. E., Osindero, S. and Teh, Y., A fast learning algorithm for deep belief nets, Neural Computation 18, 1527-1554.



### Training with a brute force

- In 2010, a surprising counter example to the conventional wisdom was demonstrated<sup>1</sup>.
- Deep neural network was trained to classify the handwritten digits in the MNIST<sup>2</sup> data set, which comprises 60,000 28 × 28 = 784 pixel images for training and 10,000 images for testing.
- They showed that a plain DNN with architecture (784, 2500, 2000, 1500, 1000, 500, 10 HUGE!!!), trained using standard stochastic gradient descent (Minuit on steroids!), outperformed all other methods that had been applied to the MNIST data set as of 2010. The error rate of this ~12 million parameter DNN was 35 images out of 10,000.

The training images were randomly and slightly deformed before every training epoch. The entire set of 60,000 undeformed images could be used as the validation set during training, since none were used as training data.

<sup>1</sup> Cireşan DC, Meier U, Gambardella LM, Schmidhuber J. ,Deep, big, simple neural nets for handwritten digit recognition. Neural Comput. 2010 Dec; 22 (12): 3207-20.

<sup>2</sup> http://yann.lecun.com/exdb/mnist/

# Why it didn't work before?



- More data, clusters of GPU/CPU (computing power!)
- The particular non-linear activation function chosen for neurons in a neural net makes a big impact on performance, and the one often used by default is not a good choice.
- The old vanishing gradient problem happens, basically, because backpropagation involves a sequence of multiplications that invariably result in smaller derivatives for earlier layers: that is, unless weights are chosen with different scales according to the layer they are in! Making this simple change results in significant improvements.



# **DNN** – hierarchical feature extraction

Deep neural networks learn hierarchical feature representations





### Hand-writing recognition



### MNIST database of hand-written digits.



- With small and very simple MLP after a short training we got an accuracy of 98.3%
- Network has just two hidden layers very simple!

60000 train samples 10000 test samples

Layer (type)	Output Shape	Param #
dense_7 (Dense)	(None, 512)	401920
dropout_5 (Dropout)	(None, 512)	0
dense_8 (Dense)	(None, 512)	262656
dropout_6 (Dropout)	(None, 512)	0
dense_9 (Dense)	(None, 10)	5130

Total params: 669,706 Trainable params: 669,706 Non-trainable params: 0

#### Example:

https://github.com/marcinwolter/DNN\_e xamples/blob/master/mnist\_mlp.ipynb

Slightly updated example from net.

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### **Automated physicist?**

 Use of deep neural network to extract H->ττ and SUSY signals in simulated CMS data<sup>1,2</sup>.



ARTICLE

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# Searching for exotic particles in high-energy physics with deep learning

P. Baldi<sup>1</sup>, P. Sadowski<sup>1</sup> & D. Whiteson<sup>2</sup>

<sup>1</sup> P. Baldi, P. Sadowski, D. Whiteson, Searching for Exotic Particles in High-Energy Physics with Deep Learning, Nature Commun. 5 (2014) 4308
 <sup>2</sup> P. Baldi, P. Sadowski, D. Whiteson, Enhanced Higgs Boson to ττ Search with Deep Learning, PRL 114, 111801 (2015)



### **H->**τ τ searches







**Figure 2 | Low-level input features for Higgs benchmark.** Distributions in  $\ell v j j b \bar{b}$  events for simulated signal (black) and background (red) benchmark events. Shown are the distributions of transverse momenta ( $p_T$ ) of each observed particle (**a**-**e**) as well as the imbalance of momentum in the final state (**f**). Momentum angular information for each observed particle is also available to the network, but is not shown, as the one-dimensional projections have little information.



### **Higgs search**

 Physicists have built 7 well discriminating high-level variables (derived from 22 low level variables).



**Figure 3 | High-level input features for Higgs benchmark.** Distributions in simulation of invariant mass calculations in  $\ell v j j b \bar{b}$  events for simulated signal (black) and background (red) events.

# **Higgs searches**

- Data: 2 600 000 events for training, 100 000 for validation
- Deep NN: 5 layers, 300 nodes in each layer, fully connected

#### Table 1 | Performance for Higgs benchmark.

Technique	Low-level	High-level	Complete
AUC			
BDT	0.73 (0.01)	0.78 (0.01)	0.81 (0.01)
NN	0.733 (0.007)	0.777 (0.001)	0.816 (0.004)
DN	0.880 (0.001)	0.800 (<0.001)	0.885 (0.002)
Discovery sig	nificance		
NN	$2.5\sigma$	3.1 <i>o</i>	$3.7\sigma$
DN	$4.9\sigma$	$3.6\sigma$	$5.0\sigma$

Comparison of the performance of several learning techniques: boosted decision trees (BDT), shallow neural networks (NN), and deep neural networks (DN) for three sets of input features: low-level features, high-level features and the complete set of features. Each neural network was trained five times with different random initializations. The table displays the mean area under the curve (AUC) of the signal-rejection curve in Fig. 7, with s.d. in parentheses as well as the expected significance of a discovery (in units of Gaussian  $\sigma$ ) for 100 signal events and 1,000 ± 50 background events.



### doi:10.1038/ncomms5308

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### Convolutional Neural Network for pattern recognition





### **Convolutional NN**



Just connect only local areas, for example 10x10 pixels. Huge reduction of the number of parameters!

The same features might be found in different places => so we could train many filters, each recognizing another feature, and move them over the picture.

LeCun et al. "Gradient-based learning applied to document recognition" IEEE 1998



### **Example of pattern recognition** Top 9 patches that activate each filter

in layer 1

Each 3x3 block shows the top 9 patches for one filter.

















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# Pooling



**Pooling** – (in most cases **max pooling**) the group of outputs for a larger input area is replaced by a maximum (or average) for this given area:

- Data reduction,
- Lower sensitivity for the position of a given feature.



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# Quick test of hand-writing recognition

### MNIST database of hand-written digits.



### **Best results (Wikipedia):**

Deep neural network	6-layer 784-2500-2000-1500-1000-500-10	0.35 <sup>[23]</sup>	Max
Convolutional neural network	6-layer 784-40-80-500-1000-2000-10	0.31 <sup>[15]</sup>	
Convolutional neural network	6-layer 784-50-100-500-1000-10-10	0.27 <sup>[16]</sup>	
Convolutional neural network	Committee of 35 CNNs, 1-20-P-40-P-150-10	0.23 <sup>[8]</sup>	
Convolutional neural network	Committee of 5 CNNs, 6-layer 784-50-100-500-1000-10-10	0.21 <sup>[17]</sup>	Ţμ
Random Multimodel Deep Learning (RMDL)	30 Random Deep Leaning (RDL) models (10 CNNs, 10 RNNs, and 10 DNN)	0.18 <sup>[24]</sup>	

- With CNN we got after a short training an accuracy of 99.21%
- Our CNN neural net (small comparing to the winning nets):

https://github.com/marcinwolter/DN N\_examples/blob/master/mnist\_cnn. ipynb

### Slightly updated example from net.

DATA	DIMEN	SIONS	WEIGHTS(N)	WEIGHTS	5(%)
# 28	28	1			
			320	0.0%	
# 26	26	32			
			18496	1.0%	
# 24	24	64			
x			Θ	0.0%	
# 12	12	64			
			Θ	0.0%	
# 12	12	64			
			Θ	0.0%	
#	9216				
Х			1179776	98.0%	
#	128				
			Θ	0.0%	
#	128				
Х			1290	0.0%	
#	10				
ples, va	lidate	on 100	00 samples		
	DATA ## 28 ## 26 ## 24 ## 12 ## 12   ## 12   ## 24 X ## 24 X	DATA DIMEN ## 28 28 ## 26 26 ## 24 24 ## 12 12 ## 12 12 ## 12 12 ## 12 12 ## 128 ## 109 ## 1	DATA DIMENSIONS ## 28 28 1 ## 26 26 32 ## 24 24 64 ## 12 12 64 	DATA DIMENSIONS       WEIGHTS(N)         ##       28       28       1         ##       26       26       32         ##       26       26       32         ##       24       24       64         ##       12       12       64	DATA DIMENSIONS       WEIGHTS(N)       WEIGHTS         ##       28       28       1         //       26       26       32       0.0%         //       26       26       32       0.0%         //       26       26       32       0.0%         //       24       24       64       0       0.0%         //       12       12       64       0       0.0%         //       12       12       64       0       0.0%         //       12       12       64       0       0.0%         //       9216       0.0%       0.0%       0.0%         //       128       0       0.0%       0.0%         //       128       0       0.0%       0.0%         ///       10       10       0.0%       0.0%

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### **Figure recognition**



- Qualification project for IFJ PAN Ph.D. students
- https://github.com/marcinwolter/DNN\_examples/blob/master/figure\_cnn.ipynb



# CIFAR image classification Bonus example

### Classifies images into 10 classes

Very nice and advanced example, uses **data augmentation** (artificial replication)

runs on google Graphic Processor Units (GPU)



Example: cifar\_classifier\_gpu\_aug.ipynb

#### Source from net:

https://colab.research.google.com/drive/1zTYNJ3xtPeNsa5ARBw4Ufj8crPZJx-cp

https://github.com/marcinwolter/DNN\_examples/blob/master/ci far\_classifier\_gpu\_aug.ipynb

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#### M. Wolter, Deep Neural Networks

**Frue** label



Confusion matrix, without normalization



# **CNNs – quark-gluon jet classification**



Per pixel correlation between image intensity and CNN output. The four pixels at the core is highly correlated with jet being a quark jet

CNN as an entirely different approach than building likelihood from high level quantities show improvement of quark vs. gluon classification

"The image-based approach described in this note is a promising avenue for future research to confront a variety of tagging challenges."

# 4

From ATLAS-CONF-2016-057:

# **Example of CNN effort**

### ATLAS search for R-parity-violating SUSY gluino decays

Analysis from ATLAS-CONF-2016-057 used as a benchmark



https://indico.cern.ch/event/567550/contributions/2629673/attachments/1510135/2355667/ACAT-DeepNetworksForPhysicsAnalysis-1.pptx

# How could we get rid of simulated data?

- The Monte Carlo simulation used for training Machine Learning methods always differs to some extend from data.
- So, the best would be to train algorithms on data...
- ... => towards **unsupervised learning**?
- ... or maybe only **weakly supervised**?



No training datasets are provided, the data is clustered into different classes based on similarity.

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# Weakly Supervised Classification



- A new approach in Machine Learning: **weakly supervised** classification in which **class proportions are the only input** into the machine learning algorithm.
- Example problem from particle physics:
  - Quark versus gluon tagging weakly supervised classification can match the performance of fully supervised algorithms.
  - By design, the new algorithm is insensitive of MC mis-modelling trained on data.
- **Problem:** we have to find in data what is the proportion of gluon and quark jets.
- Maybe template fits in one/some variable/s using again MC?

arXiv:1702.00414



## Learning from Data Classification w/o Labeling



- A step even further is classification w/o labeling (CWoLa) https://arxiv.org/abs/1708.02949
- A classifier is trained to distinguish sample 1 from sample 2, which are mixtures of signal and background with different (and unknown) fractions.
- Such a classifier is optimal for distinguishing signal from background





### **Bayesian learning**

- All regression tools (neural networks, decision trees...) described here were returning the most probable output value.
- But a better thing is....

### - Probability distribution



### Machine vs. Bayesian learning



### **Machine learning**

We chose just one value of a parameter (or just one function).

### **Bayesian learning**

Each value of a parameter (or function) has a given probability.

### Implementation: Bayesian Neural Networks



Instead of one use many neural networks.

Having many networks we can get the probability distribution.



C.M. Bishop "Neural Networks for Pattern Recognition", Oxford 1995

Free software (used by D0 Collaboration): Radford Neal, http://www.cs.toronto.edu/~radford/fbm.software.html

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### **Example of BNN**



How does the 8-node, 1-hidden layer BNN works?

- Data generated from function:  $y=0.3+0.4x+0.5\sin(2.7x)+1.1/(1+x^2)$ with gaussian noise with **6**=0.1
- 400 neural networks, distribution => median and 10% Qnt i 90% Qnt
- Gal and Ghahramani (U. of Cambridge)<sup>1</sup> demonstrated that a DNN, in which nodes are randomly dropped during training (a procedure referred to as dropout), approximates variational inference in Bayesian neural networks.





### Mixture Density Network (MDN)





# Mixture Density Network (MDN)

- MDN is an interesting model formalism working on supervised learning problems in which the target variable cannot be easily approximated by a single standard probability distribution.
- Conditional probability distribution p(y|x) is modeled as a mixture of distributions (few Gaussians), in which the individual distributions and the corresponding mixture coefficients are parametrized by functions of the inputs x.

#### **Regression:**





Regular network - problems



Nice presentation: http://www.dbs.ifi.lmu.de/Lehre/DLAI/WS18-19/script/06\_uncertain.pdf

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### Mixture Density Network (MDN)



### MDN return not only maximum probability value, but the probability distribution: returns errors!

Example from https://github.com/cpmpercussion/keras-mdn-layer

Google Colaboratory runable adapted example:

https://github.com/marcinwolter/DNN\_examples/blob/master/MDN\_1D\_sine\_prediction.ipy nb

**Reference:** Bishop, Christopher M. Mixture density networks. Technical Report NCRG/4288,Aston University, Birmingham, UK, 1994 http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.120.5685&rep=rep1&type=pdf



# MDM example - ATLAS cluster position calculation

#### Currently uses a three-step process

- 1. Number Network: Determine the number of particles in this hit
- 2. Position Network: Determine the x-y position of each particle
- 3. Error Network: Estimate the error in x and y for each particle

### MDN: Feedforward network + Gaussian kernel(s)



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# Pattern Recognition in High Energy Physics



Seeding

**Track Building** 

**Track Fitting** 

- Track seeding finding the seeds (initial sets of hits) from which the track starts
- Track building = pattern recognition HEP jargon
  - Creating a 2- and 3-dimensional lines and assigning to them all the hits within a certain window
  - Fitted frequently with "robust fit"
- Track fitting final fitting of the track parameters (usually a Kalman filter used for tracking)

### **Usually this method works fine, is robust and efficient!**

# So, where is the problem?



CMS experiment simulation J.-R. Vlimant, Machine Learning for Charged Particle Tracking, MIT, 2018

- The time needed to process one event grows quickly (worse than quadratic) with luminosity (number of collisions).
- Huge part of CPU consumption is the track finding.

### **Deep Neural Network (DNN)?**

- Fast, parallel, in principle does pattern recognition "at once", without looping over hits.
- Also experiments with lower occupancy might profit from DNN's – higher precision and efficiency.
- There is a HEPTrkx group working on tracking for HEP experiments: https://heptrkx.github.io/

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### **Tracking in 2D toy model**



- CNN returns track parameters (regression)
- What about many tracks?
  - Solution: add Mixture Density Network(MDN) layer to process many tracks.
  - Straight tracks described by two parameters. Each parameter has associated MDN Gaussian
  - If a number of tracks lower than expected some MDN outputs have very low amplitude.
  - Important we are getting errors of track parameters



Track described by to interception parameters  $b_1$  and  $b_2$ .



### **Mixed Density Network**



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### **MDN Tracking – error estimation**



Pull plots have a width not far from 1.

If a random variable x is generated repeatedly with a Gaussian than the pull distribution:

$$g = \frac{x-\mu}{\sigma}$$

will be distributed as a standard Gaussian with mean zero and unit width.



- GANs were introduced Ian Goodfellow and others in 2014. Yann LeCun called adversarial training "the most interesting idea in the last 10 years in ML." https://arxiv.org/abs/1406.2661
- GANs' can learn to mimic any distribution of data. They can be taught to create worlds similar to our own in any domain: images, music, speech, prose. They are robot artists!





### How do GANs work?

- **Discriminative algorithms** classify input data; given the features, they predict a label or category to which that data belongs (*signal* or *background*)
- **Generative algorithms** do the opposite, assuming the event is *signal*, how likely are these features?
- Another way to distinguish discriminative from generative like this:
  - Discriminative models learn the boundary between classes
  - Generative models model the distribution of individual classes





### **Blind forger and detective**



R: Real Data

G: Generator (Forger)

I: Input for Generator

The forger has never seen Mona Lisa, but gets the judgments of detective and tries to fool him (i.e. paint something that looks like Mona Lisa).

They both (forger and detective) have to train in parallel (important), since if detective is to clever the forger will never paint anything acceptable.



- **Training set** MNIST: hand-written digits supplied by US post.
- **Discriminator** convolutional neural network labeling images as real or fake.
- **Generator** inverse convolutional network (while a standard convolutional classifier takes an image and downsamples it to produce a probability, the generator takes a vector of random noise and upsamples it to an image).

Implementation: Python code using Keras interface and TensorFlow backend.



2400 cycles 8000 cycles Each cycle digits look more and more realistic. 19900 cycles

Updated code from the net:

https://github.com/marcinwolter/DNN\_examples/blob/master/gan\_generate\_letters.ipynb

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# Conclusions

- Many new methods were developed recently.
- Machine Learning approach becomes to be used not only for classification, but also for other tasks.
- Each month new application appear!

- Artificial intelligence is no match for natural stupidity.
- The development is driven by AI applications (image recognition, autonomous cars etc). But the physics community can profit!
- More and more advanced ML techniques have application in HEP. Try to find a new one!

### **GANs give profits!!!!**



"Edmond de Belamy" is part of a fictitious family created by a "generative adversarial network," of which there's ten other paintings. "Edmond" is one of the most striking of the paintings, and will likely become an important part of art history going forward thanks to its huge selling price. The generator behind the painting created new portraits based on 15,000 from the last 600 years, taking existing art and crafting something wholly original and quite alien.

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