# Introduction to Deep Learning and its applications to the LHC

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"Machine Learning at LHC" KMI Nagoya

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# The AI Revolution is Here



The past decade has seen remarkable advances in machine learning and artificial intelligence.

These technological breakthroughs are reshaping the world around us.

Deep learning also has the potential to revolutionize physics at the LHC.

# Deep Learning Breakthrough

### ImageNet Challenge

# IMAGENET

- 1,000 object classes (categories).
- Images:
  - o 1.2 M train
  - 100k test.



## Deep Learning Breakthrough

In 2012, a deep convolutional neural network won the "ImageNet" image classification competition by a huge margin (Krizhevsky, Sutskever, Hinton)

This dramatic breakthrough inaugurated the modern revolution in deep learning.



# of parameters 1000 x LeNet (60M). Required training on a GPU.

### Deep Learning Breakthrough



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airplane	- 1	X	-	×	*	*	1	-17-		-
automobile			E		-	Tel			-	*
bird	S.	ſ	2			4	1		12	4
cat	-		4	54			Z.	Å_	A.S.	1
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dog	17	1	-	<b>N</b> .	1	(A)	9	13	3	The second
frog		1	1					5		5
horse	-	The second	P	2	P	ICAN	-	20	6	1
ship		Carden	10	-	44	-	2	120	1	
truck			1					1	0 3	den







# Natural language

# Google

HomePod

Echo †

Yoruba-**Translate from English** 

dog dog dog dog dog dog dog dog dog

dog dog dog dog dog dog dog dog

+

English -

Doomsday Clock is three minutes at twelve We are experiencing characters and a dramatic developments in the world, which indicate that we are

increasingly approaching the end

times and Jesus' return



Invoke

Follow

Sure Abby

Baby\*

Read 8:59 PM

Feedback

When auto correct hates you and your

### Generative modeling

#### **Painting created by AI sells for** stunning \$432K

By Tamar Lapin

October 26, 2018 | 2:38am | Updated

there is no one else in the world. there is no one else in sight. they were the only ones who mattered. they were the only ones left. he had to be with me. she had to be with him. i had to do this. i wanted to kill him. i started to cry. i turned to him.

this was the only way. it was the only way. it was her turn to blink . it was hard to tell. it was time to move on . he had to do it again. they all looked at each other. they all turned to look back. they both turned to face him. they both turned and walked away.



"Portrait of Edmond de Belamy"

#### Automatically captioned





2015

2016

2017

# Game playing











# Game playing











# Plan of the lecture

- I. Machine Learning Basics
- 2. Intro to Deep Learning
- 3. Deep Learning at the LHC

I will assume most of you know some collider physics.

I will not assume any familiarity with machine learning or neural networks.

# I. Machine learning basics

#### "ML is glorified function fitting"

Want to fit a function  $f(x; \theta)$  with some parameters  $\theta$  ("weights") to a collection of examples  $\{x_i\}$  in order to achieve some objective.

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 $\mathbf{x} \in \mathbb{R}^d$  is called the feature space

i=1,...N indexes the training dataset.

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#### Some typical objectives:



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- Classification
- Regression
- Clustering
- Anomaly detection
- Density estimation

$$P(x) = 0.5 * \mathcal{N}(x|\mu = (0, -1.5), \sigma = (1, 1)) + 0.5 * \mathcal{N}(x|\mu = (0, +1.5), \sigma = (1, 1))$$

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"supervised ML"

- Classification
- Regression
- Clustering
- Anomaly detection
- Density estimation
- Generation

# MNIST example

image database of 70,000 handwritten digits



# MNIST example



 $\mathcal{X}$ 

heta parameters of fitting function

 $\begin{pmatrix}
P_0(x;\theta) \\
P_1(x;\theta) \\
\vdots \\
P_9(x;\theta)
\end{pmatrix}$ 

Input: handwritten digit image 28x28 pixel intensities from MNIST database  $\sum_{i} P_i(x;\theta) = 1$ 

Output: probability it's a 0, 1, ...,9

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How to perform the fit?

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How to perform the fit?

Minimize a loss function! Loss function quantifies how well the objective has been achieved.

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$\sum_{(x,y)} L(P(x;\theta), y)$	$\sum_{x} L(P(x;\theta))$
Data is labeled	Data is not labeled
supervised ML	unsupervised ML

#### Examples of loss functions

$$L = (P(x;\theta) - y)^2$$

"mean-squared error" used for regression

$$L = -\left(y\log P(x;\theta) + (1-y)\log(1-P(x;\theta))\right)$$

"binary cross entropy" used for binary classification

 $L = -y_j \log P_j(x;\theta)$ 

"categorical cross entropy" used for multi-class classification

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MNIST example: labels "one-hot encoding"  $0 \rightarrow [1,0,...,0]$  $1 \rightarrow [0,1,...,0]$ ...  $9 \rightarrow [0,0,...,1]$  "categorical cross entropy" used for multi-class classification
#### Minimizing the loss function



Highly nonconvex function over a many-dimensional space. Many local minima.

#### Gradient descent

$$\langle L \rangle(\theta) \equiv \sum_{(x,y)} L(P(x;\theta),y)$$

Want to minimize wrt  $\theta$ .

**Obvious idea:**  $\theta \to \theta - \alpha \, \partial_{\theta} \langle L \rangle(\theta)$ 

 $\alpha$ : "learning rate"

"gradient descent method"

(generalization of Newton-Raphson method)



#### Gradient descent: problems

Downsides to gradient descent:

- average over full dataset  $< L(\theta) >$  can be expensive to compute
- poor initial guess or learning rate can lead to becoming stuck in poor local minimum



#### Stochastic Gradient Descent



- Batch gradient descent
- Mini-batch gradient Descent
  - Stochastic gradient descent

Can actually improve convergence by using noisy estimator of gradient!

 $L(P(x;\theta),y)$  $(x,y) \in \text{full dataset}$ 

 $\sum L(P(x;\theta),y)$  $(x,y) \in \text{minibatch}$ 

#### Stochastic Gradient Descent

#### Method:

- I. Divide up training data into minibatches.
- 2. Update weights minibatch by minibatch

 $\theta \to \theta - \alpha \,\partial_{\theta} \langle L \rangle(\theta)$ 

(average computed on each minibatch)

3. Repeat until convergence.



minibatch I minibatch 2 minibatch 3

. . .

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3. Repeat until convergence.

#### "one epoch"



minibatch 1 minibatch 2 minibatch 3

. . .

# Overfitting

The fitting function (especially if it is a neural network) may be overparametrized. So overfitting is a major concern.



# Overfitting

Many ways to mitigate overfitting problem. Eg early stopping. Key concept: train/val/test split



#### Brief (re)fresher on machine learning

#### "ML is glorified function fitting"

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Finally, what functions to use?

Current trend: deep neural networks!

# 2. Intro to Deep Learning

#### What is a (deep) neural network?

#### Basic building block of a neural network:



#### Activation functions

NNs need a source of non-linearity so they can learn general functions.

This is usually implemented with the activation function.



Sigmoid used to be standard. But this led to the vanishing gradient problem. The ReLU activation was invented to solve this problem. Now it is the standard.

#### "Fully connected" or "Dense" Neural Network



$$P = A^{(3)}(w_k^{(3)}A^{(2)}(w_{kj}^{(2)}A^{(1)}(w_{ji}^{(1)}x_i + b_j^{(1)}) + b_k^{(2)}) + b^{(3)})$$

# Expressiveness

One reason why NNs "work" is that they are <u>universal function approximators</u> (asymptotically) Math. Control Signals Systems (1989) 2: 303-314

Mathematics of Control, Signals, and Systems © 1989 Springer-Verlag New York Inc.

#### Approximation by Superpositions of a Sigmoidal Function\*

#### G. Cybenko†

Abstract. In this paper we demonstrate that finite linear combinations of compositions of a fixed, univariate function and a set of affine functionals can uniformly approximate any continuous function of n real variables with support in the unit hypercube; only mild conditions are imposed on the univariate function. Our results settle an open question about representability in the class of single hidden layer neural networks. In particular, we show that arbitrary decision regions can be arbitrarily well approximated by continuous feedforward neural networks with only a single internal, hidden layer and any continuous sigmoidal nonlinearity. The paper discusses approximation properties of other possible types of nonlinearities that might be implemented by artificial neural networks.

Key words. Neural networks, Approximation, Completeness.



Can fit any function with a single, infinitely-wide hidden layer

#### Deep neural networks



Expressivity of a neural network increases exponentially with the number of layers (Delalleau and Bengio, 2011, Montufar et al 1402.1869, Ganguli et al 1606.05336, 1606.05340)

### End-to-end learning



Universal function approximation and high expressivity means that deep NNs can learn abstract concepts from low-level, high-dimensional inputs

"Automated feature engineering"

"End-to-end learning"

#### Example: MNIST in more detail



Output: probability it's a 0, 1, ...,9

#### Example: MNIST in more detail

Layer (type)	Output Shape	Param #
dense_1 (Dense)	(None, 512)	401920
dropout_1 (Dropout)	(None, 512)	0
dense_2 (Dense)	(None, 512)	262656
dropout_2 (Dropout)	(None, 512)	0
dense_3 (Dense)	(None, 10)	5130
Total params: 669,706 Trainable params: 669,706 Non-trainable params: 0		



Test accuracy: 0.9831





Principal neural network architecture for image recognition. Invented in 1998 (LeCun, Bottou, Bengio, Haffner)

Achieved 99% accuracy on MNIST!

However, CNNs fell out of favor (until AlexNet in 2012) when they did not immediately generalize well to more complex image recognition tasks such as ImageNet.

Main idea: features in an image (edges, curves, corners,...eyes, noses,...) are the same no matter where they occur.

Goal: Want to find these features in a translationally invariant way.

Solution: Drag or convolve a "filter" across the image that selects out interesting features.



Main idea: features in an image (edges, curves, corners,...eyes, noses,...) are the same no matter where they occur.

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Finds features in the image in a translation invariant way

Can apply multiple filters to image to produce a stack of feature maps





CNNs typically end with fully connected layers.

These are thought to extract the highest level information and to perform the actual classification task on the feature maps found by the convolutional layers.

What does the machine learn?



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

### Generative Adversarial Networks (GANs)

Breakthrough method in generative modeling and unsupervised learning (Goodfellow et al. 2014)



Idea: train two neural networks: a "generator" that attempts to generate fake, random images, and a "discriminator" that tries to tell them apart from a database of real images.

#### Generative Adversarial Networks (GANs)

$$L_{GAN} = \sum_{x \in \text{real}} \log D(x) + \sum_{z \in \text{random}} \log(1 - D(G(z)))$$

Training is performed "adversarially"

- Discriminator tries to minimize loss
- Generator tries to **maximize** loss
- Take turns training discriminator and generator to optimize fake image generator

#### Generative Adversarial Networks (GANs)



#### Real or fake?

# 3. Deep Learning at the LHC





• 600 million collisions per second



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- Raw data rate ~ I PB/s (I PB=10^6 GB)



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### LHC and Big Data

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### LHC and Big Data

#### The data is

- large (billions of events on tape)
- complex (hundreds of particles per event)
- well-understood (Standard Model of particle physics).

Also, it is relatively easy to generate realistic simulated data.



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# The LHC is a great setting for deep learning!

# Deep Learning Papers



#### An explosion of interest in machine learning!

# The Landscape of DL @ LHC



# The Landscape of DL @ LHC



See talks by Michael Kagan and Tilman Plehn



slide credit: J.Thaler

### A popular example: boosted top tagging





#### Some obvious ideas:



#### State of the art with cuts on kinematic quantities:



Can deep learning do better??

#### Jet images Cogan et al 1407.5675, Almeida et al 1501.05968, de Olivera et al 1511.05190



Jets are naturally images in eta and phi.

Should be able to apply "off-the-shelf" NNs developed for image recognition to classify jets at the LHC! de Oliveira et al 1511.05190

### Other jet representations

Many other ways to represent a jet besides jet images!

#### Lists of 4-vectors



#### Sequences

- View anti- $k_T$  sequence as a binary tree
- Order using depth-first traversal prioritizing jets with 'parents' whose d<sub>ii</sub> is smaller









From Wikipedia, the free encyclopedia

### Community top tagging comparison

#### Kasieczka, Plehn et al 1902.09914



Q:There are many papers developing jet taggers with different jet representations and architectures. How can we evaluate their relative strengths and weaknesses?

A: Let's perform an applesto-apples comparison of various top taggers on a common dataset!

### Community top tagging comparison

Kasieczka, Plehn et al 1902.09914

	AUC	Acc	$1/\epsilon_B \ (\epsilon_S = 0.3)$			#Param	
			single	mean	median		
CNN [16]	0.981	0.930	$914{\pm}14$	$995{\pm}15$	$975 \pm 18$	610k	
ResNeXt [31]	0.984	0.936	$1122 \pm 47$	$1270\pm28$	$1286 \pm 31$	1.46M	
TopoDNN [18]	0.972	0.916	$295\pm5$	$382\pm 5$	$378\pm8$	59k	
Multi-body $N$ -subjettiness 6 [24]	0.979	0.922	$792{\pm}18$	$798{\pm}12$	$808 \pm 13$	57k	
Multi-body $N$ -subjettiness 8 [24]	0.981	0.929	$867 \pm 15$	$918{\pm}20$	$926 {\pm} 18$	58k	
TreeNiN $[43]$	0.982	0.933	$1025 \pm 11$	$1202\pm23$	$1188 \pm 24$	34k	
P-CNN	0.980	0.930	$732 \pm 24$	$845 \pm 13$	$834 \pm 14$	348k	
ParticleNet [47]	0.985	0.938	$1298 {\pm} 46$	$1412{\pm}45$	$1393 \pm 41$	498k	
LBN [19]	0.981	0.931	$836 {\pm} 17$	$859{\pm}67$	$966{\pm}20$	705k	
LoLa [22]	0.980	0.929	$722 \pm 17$	$768{\pm}11$	$765 \pm 11$	127k	
LDA $[54]$	0.955	0.892	$151 \pm 0.4$	$151.5{\pm}0.5$	$151.7 {\pm} 0.4$	184k	
Energy Flow Polynomials [21]	0.980	0.932	384			1k	
Energy Flow Network [23]	0.979	0.927	$633 \pm 31$	$729 \pm 13$	$726 \pm 11$	82k	
Particle Flow Network [23]	0.982	0.932	$891 \pm 18$	$1063 \pm 21$	$1052\pm29$	82k	
GoaT	0.985	0.939	$1368 \pm 140$		$1549 \pm 208$	35k	

#### Have we found the optimal tagger??

#### CMS performance study JME-18-002-PAS



#### CMS performance study JME-18-002-PAS



### Beyond top tagging

Many other classification tasks at LHC are enhanced with deep learning:

- quark/gluon tagging (Komiske, Metodiev & Schwartz '16, et seq)
- b and c tagging (DeepCSV)
- boosted W/Z tagging (Oliveira et al '15, et seq)
- strange tagging (Nakai, Thomas & DS to appear)
- u vs d tagging using jet charge (Fraser & Schwartz '18)
- boosted W+/Z/W- tagging using jet charge (Chen, Chiang, Cottin & DS 1908.08256)
- ....

#### Beyond classification — decorrelation

Raw tagger performance not the only consideration.

For robust background estimation, generally need to ensure tagger does not sculpt the background mass distribution.



Two approaches with deep learning:

- adversarial decorrelation (Louppe et al 1611.01046, Shimmin et al 1703.03507)
- DisCo decorrelation (Kasieczka & DS 2001.05310)

See talks by Michael Kagan and DS

#### Beyond classification — decorrelation

Raw tagger performance not the only consideration.

For robust background estimation, generally need to ensure tagger does not sculpt the background mass distribution.

This would greatly underestimate the background in the SR

Two approaches with deep learning:

- adversarial decorrelation (Louppe et al 1611.01046, Shimmin et al 1703.03507)
- DisCo decorrelation (Kasieczka & DS 2001.05310)



Could have real-world applications, e.g. in designing fairer

Als?

### Beyond classification — pileup regression

PileUp Mitigation with Machine Learning (PUMML) (Komiske, Metodiev, Nachman & Schwartz 1707.08600)



Leading vertex

neutral particles

#### Can measure

- 1. Leading vertex charged particles
- 2. Pileup charged particles
- 3. Total neutral particles

#### Beyond classification — GemANs for everything

Can use GANs for event generation, fast detector simulation, unfolding, ...



See talks by Tao Liu, Ben Nachman and DS

#### Way beyond classification: anomaly detection



from Nachman & DS 2001.04990

See talks by Tao Liu, Ben Nachman and DS

#### Way beyond classification: anomaly detection



from Nachman & DS 2001.04990

(a) Signal sensitivity

(b) Background specificity

Many interesting new ideas for model-independent searches being proposed

### Summary/Outlook

Deep learning is revolutionizing nearly every aspect of high-energy physics.

- Tagging
- Pileup
- Event generation
- Detector simulation
- Triggering
- Searches for NP
- ....

Exciting times are ahead!

### Thanks for your attention!

# Supplementary material

## **Disappearing Gradient**



Chain rule for gradient of network involves multiple factors of the derivative multiplied together

 $(0.25)^4 = 0.0039$ 

Deep networks with Sigmoid activations have exponentially hard time training early layers

## Disappearing Gradient



Using the Rectified Linear Unit (ReLU) solves this problem. ReLU(x) =  $\{0 \text{ if } x <=0, x \text{ if } x >0\}$ 

# Still has nonlinearity which allows network to learn complicated patterns

Nodes can die (derivative always 0 so cannot update)

## Disappearing Gradient



Leaky Rectified Linear Unit (LeakyReLU) solves this problem.

LeakyReLU(x) = {alpha\*x if  $x \le 0$ , x if  $x \ge 0$ }

I have never had to use this in practice

### Convolutional neural network (CNN)

Dealing with multiple channels is straightforward — just enlarge filter to include channel dimension (3d filter) and perform element-wise multiplication along channel dimension as well.



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### Convolutional neural network (CNN)

"Max pooling"

12	20	30	0			
8	12	2	0	$2 \times 2$ Max-Pool	20	30
34	70	37	4		112	37
112	100	25	12			

Reduces image size, reducing parameters and mitigating overfitting

Allows NN to find spatially larger, often higher-level features

Popular architecture for natural language processing (sentence completion, autocorrect, translation, speech recognition...)

Starting point: sequence of numbers  $x_1, x_2, x_3, ...$ 

Suppose we want to predict the next number in the sequence? Idea of RNN:

- feed data sequentially to NN
- after each time step update hidden state. Hidden state encodes "memory" of sequence.
- Use hidden state to make predictions.

Basic RNN architecture



 $s_t = f(Ux_t + Ws_{t-1})$  hidden state after time step t



sequence classification, regression

#### Different modes/uses of RNNs



real-time prediction
### Recurrent Neural Networks (RNNs)

### Different modes/uses of RNNs



sequence-to-sequence

### Recurrent Neural Networks (RNNs)

Simple RNNs applied to long sequences have a very serious exploding/ vanishing gradient problem.

Prevents them from "remembering" relevant information from earlier in the sequence.



"Long-short term memory" and "Gated recurrent units" are two methods commonly used to solve the gradient problem and improve performance.

## Normalizing flows

Rezende & Mohamed 1505.05770

Recently a lot of excitement and progress in the problem of density estimation with neural networks.

Idea: map original distribution to normal distribution through series of invertible transformations.



Examples: RealNVP, NICE, Glow, ...

### Autoregressive flows

$$p(x)=\prod_i p(x_i\,|\,x_{1:i-1})$$

Special type of normalizing flows. Learn probability density of each coordinate conditioned on previous coordinates.

Transformation upper triangular — automatically invertible. Allows for more expressive transformations.



Examples: MADE, MAF, IAF, NAF, PixelRNN, Wavenet, ...

#### Macaluso & DS 1803.00107



#### Individual images very sparse

QCD

20

10

30



Building on previous "DeepTop" tagger of Kasieczka et al 1701.08784

#### Macaluso & DS 1803.00107



Average images clearly different

Building on previous "DeepTop" tagger of Kasieczka et al 1701.08784

#### Macaluso & DS 1803.00107



#### AdaDelta

 $\eta=0.3$  with annealing schedule

minibatch size=128

cross entropy loss

#### Macaluso & DS 1803.00107



Can achieve factor of ~3 improvement over cut-based approaches and BDTs!

#### Macaluso & DS 1803.00107



Can achieve factor of ~3 improvement over cut-based approaches and BDTs!



robust against different orderings

# Sequences

Egan et al 1711.09059

- View anti-k<sub>T</sub> sequence as a binary tree
- Order using depth-first traversal prioritizing jets with 'parents' whose d<sub>ii</sub> is smaller



Turn jet into a sequence, e.g. using jet clustering history.

Feed sequence to RNN/LSTM, etc.





### Trees

Louppe et al 1702.00748, Cheng 1711.02633



Use jet clustering history to build binary tree

Train recursive neural net on jet tree to learn "embedding" for classifier.

## Graphs / Point clouds

### Hu & Gouskos 1902.08570

Particle cloud

- particles are intrinsically unordered
- primary information:
  - 2D coordinates in the  $\eta$ - $\phi$  space
- but also additional "features":
  - energy/momenta
  - charge/particle type
  - track quality/impact parameters/etc.





