Machine Learning













- The LHC challenge
- A little bit of history of ML in HEP
- The CERN ML-LHC community
- Deep Learning at LHC by a few examples (biased selection)
 - Local reconstruction: clustering in calorimeters
 - Supervised Learning: jet tagging
 - Unsupervised searches: (re)discovering particles
 - Real time inference on FPGAs



• Generative models: jet generation [Not Covered for lack of time]







The LHC and its big-data challenge







LHC: Energy frontier exploration

- Discover the Higgs boson or exclude its existence
- Characterize the nature of EW symmetry breaking
- Help answering the big questions *left in particle physics*
 - What stabilises physics at EW scale?
 - What's the nature of Dark Matter?
 - Origin of cosmological matter/ antimatter asymmetry
 - Are there unexpected phenomena at the energy frontier













• The LHC collides protons at unprecedented energy (equivalent to 13,000 times their mass)

• one collision every 25 ns (= 40 Millioncollisions/sec)

• Thousands of particles emerging from each collision

● 1 MB of data recorded at each collision by big detectors





The LHC collisions



European Research











Big Data @LHC



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• The amount of produced data is too much to be stored

● 1,000 times the data generated by google searches+youtube+facebook back in 2013

 Reduced to 5x(google) searches+youtube+facebook) after first filtering

• Can only store 5% of those



Big Data (20HC









Things will get worse









More sensors, more RECO troubles

9

• To disentangle 200 collisions happening at once, we will build new detectors with more (smaller) sensors

• Event complexity grows non linearly

• To profit of that, computing resources for data processing will have to increase



We are off by a factor ~10 if we project to 2027











• We know how to get from the data the answers we want

physics + intuition + computing

• But the process is slow



• We can use DL solutions as a shortcut: we teach neural networks how to give us the answer we want directly from the raw data









It started with NNs & Pattern Recognition

• First papers proposing NNs applications in HEP date back to end of 80s

 Pattern
 recognition (particle tracking)

• Object identification (classification)

Bruce H. Denby (Orsay, LAL) Nov, 1987

35 pages

DOI: 10.1016/0010-4655(88)90004-5 Report number: LAL-87-56 View in: ADS Abstract Service

[→ cite

Abstract: (Elsevier) Within the past few years, two novel computing techniques, cellular automata and neural networks, have shown considerable promise in the solution of problems of a very high degree of complexity, such as turbulent fluid flow, image processing, and pattern recognition. Many of the problems faced in experimental high energy physics are also of this nature. Track reconstruction in wire chambers and cluster finding in cellular calorimeters, for instance, involve pattern recognition and high combinatorial complexity since many combinations of hits or cells must be considered in order to arrive at the final tracks or clusters. Here we examine in what way connective network methods can be applied to some of the problems of experimental high energy physics. It is found that such problems as track and cluster finding adapt naturally to these approaches. When large scale hard-wired connective networks become available, it will be possible to realize solutions to such problems in a fraction of the time required by traditional methods. For certain types of problems, faster solutions are already possible using model networks implemented on vector or other massively parallel machines. It should also be possible, using existing technology, to build simplified networks that will allow detailed reconstructed event information to be used in fast trigger decisions.

Carsten Peterson (Lund U.) Apr, 1988

16 pages Published in: Nucl.Instrum.Meth.A 279 (1989) 537 DOI: 10.1016/0168-9002(89)91300-4 Report number: LU-TP-88-8

⊡ cite

Abstract: (Elsevier) A neural network algorithm for finding tracks in high energy physics experiments is presented. The performance of the algorithm is explored on modest size samples with encouraging results. It is inherently parallel and thus suitable for execution on a conventional SIMD architecture. More important, it naturally lends itself to direct implementations in custom made hardware, which would permit real time operations and hence facilitate fast triggers. Both VLSI and optical technology implementations are briefly discussed.













And it's still about MMs & Pattern Recognition

Most of these applications are still the core of ML applications in HEP nowadays

• but Deep Learning is broadening the use case list







eatured Prediction Competi

TrackML Particle Tracking Challenge

High Energy Physics particle tracking in CERN detectors

CERN · 651 teams · 3 years ago









Dealing with HEP data

- **Sparse data:** HEP data are sets of detector hits. Popular DL architectures (CNNs, RNNs) might work but with a cost (wasted memory) and could be improvable
- Custom edge computing: inference will have to run on our resources, going from front-end chips to custom electronic boards, dedicated computer centres, to the GRID (i.e., full support of sitedependent heterogenous computing)
- <u>Real-time:</u> (with real data) inference has to happen within the time boundaries of the trigger (as fast as <1 µsec)









<u>ML in HEP before DL</u>

• Classification:

- identify a particle & reject fakes
- identify signal events & reject background

• Regression:

• Measure energy of a particle

• We typically use BDTs for these task

- moved to Deep Learning for analysis-specific tasks
- same will happen for centralised tasks
 (eventually)



Centralised task (in online or offline reconstruction) Analysis-specific task (by users on local computing infrastructures) 14















Deep Learning and LHC Big Data

- In this seminar, I will highlight a few examples of this
- will make a difference
- to adapt techniques



• Possible solution to the HL-LHC Big-data problem: Deep Learning to be <u>faster</u> and <u>better</u> in what we do today, freeing resources for new ideas

• One BIG challenge: DL deployment needs to happen in between collisions and data analysis (trigger, reconstruction, ...), where freeing resources

• Other issue: our data are not mainstream Deep Learning data. Work needed









Research



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CERN: a worldwide community

- International community that goes beyond CERN research staff
 - We (CERN physicists) are a minority
 - Most physicists at CERN visit from other universities
 - Organized in independent scientific collaborations (the experiments: ATLAS, CMS, LHCb, ALICE, DUNE, ...)

MEMBER STATES ASSOCIATE MEMBER STATES ASSOCIATE MEMBERS IN THE PRE-STAGE TO MEMBERSHIP OBSERVERS OTHER STATES

● O(1000) people in each



• Across experiments, a growing control to many problems

Across experiments, a growing community of researchers applying ML







on in dedicated workshops

- <u>DS@LHC</u> (then <u>DS@HEP</u>) from 2015 to 2017
- ML4Jets (since 2017)
- DarkMachines (with astro)
 • • • •
- In special sessions at dedicated conferences
 - <u>CHEP</u>, <u>ACAT</u>, etc.
- And in workshops @ML conferences
 And



• …

ML4PS workshop @NeurIPS • <u>AI & Physics</u> @AMLD



• Within years, DL discussion in our community has been carried











• The iML group is a crossexperiment forum at CERN

• representative from all LHC experiments + Theory

Monthly meetings on various subjects

• Yearly workshop with invited talks from ML community



The inl group

82. Machine Learning in Procter and Gamble

Left Michele Floris (University of Derby (...

O 20/10/2020, 10:25

Plenary

(no recording)

rocter & Gamble (P&G) is one of the oldest and largest "consumer goods" companies in the world. It is present in abo

83. Using Topological Data Analysis to Disentangle Complex Data Sets

Maurizio Sanarico (SDG Group) **O** 20/10/2020, 10:55

Plenary

A recent new branch of the, currently called AI, is the Topological Data Analysis (TDA). TDA was born as an extension of algebraic topology to discrete data and, therefore, is a combination of algebraic topology, geometry, statistics and

81. Zenseact : Deep learning and computer vision for self-driving cars

L Christoffer Petersson **O** 20/10/2020, 11:25 Plenary

(no recording)

e mission of Zenseact is to develop a world-leading software platform for autonomous driving, with the main goal to

74. Solving Inverse Problems with Invertible Neural Networks

Logither Content Conte

() 20/10/2020, 14:00

Plenary

Interpretable models are a hot topic in neural network research. My talk will look on interpretability from the perspective of inverse problems, where one wants to infer backwards from observations to the hidden characteristics of a system.

72. Structured models of objects, relations, and physics

Logian Dr Peter Battaglia (DeepMind) O 20/10/2020, 15:00 Data Science Seminar











- In recent years, data challenges served as opportunity to attract attention of ML community on our problems
 - <u>Higgs Kaggle</u> challenge (classification)
 - <u>TrackML</u> Kaggle challenge (pattern recognition)
 - <u>Flavor</u> Kaggle challenge (classification)
 - <u>LHC 01ympics</u> (anomaly detection)
 - DarkMachines (anomaly detection)



• <u>40 MHz Anomaly detection</u> (anomaly detection)

Data Challenges



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• This meeting is about CERN and ELLIS

• For this reason, I focused on what CERN physicists in the experiments are working on

• You should keep in mind that the ML effort for ML experiments goes beyond this

• Many more groups all over the world developing MLbased solutions for the LHC experiments, neutrinos, etc.

• By joining ELLIS, CERN would act as a bridge between the ELLIS community and this large HEP-ML worldwide community









Local Reconstruction









Dealing with Real Life Detectors

- Most of HEP-related DL literature
 uses ConvNNs
- In practice, little of that made it to production so far
- Main issue (IMO): difficult to fit an irregular array of sensors (unordered set of dots in some feature space) in a regular array of pixels
- Several solutions attempted
 - pixelate the data with a coarser binning
 - use recurrent networks (imposing some use-casespecific ordering criterion)
 - use graph networks













EdgeConv for Particle Physics

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• Graphs can be very functional to process raw data

• each detector hit represented as coordinates + energy



• EdgeConv used as a baseline

• Pros: no assumption on the underlying geometry

• Cons: large memory consumption (large number of connections)















Reducing m

Introduce step to learn an (a) optimized spatial distribution (a)

FIN

(C)

as coordinates of a new space (b)

• as distances from a fixed number of aggregators (c)

Ise customised architectures to keep resources under control

• Gravnet: weight connection by potential of euclidean distance









Reducing memory consumption

Introduce step to learn an optimized spatial distribution

• as coordinates of a new space (b)

• as distances f (a) number of aggr

• Use customised a to keep resource control

> • Gravnet: weigh by potential c distance

• Garnet: keep numbers $O^{\nu_k} f_{4}^{i}$ connections small through V_{4} small number of $f_{a}^{i}ggr_{3}egators$ f_{4}^{i}













https://arxiv.org/abs/1902.07987













Separating overlapping showers



(a) Truth

(b) Reconstructed











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+ (44)

0

-50

-100

European



GraphMets for Calorimetry

• Good performance achieved, comparable to more traditional approaches

• Using a potential (V(d)) to weight up the near neighbours allows to keep memory footprint under control (with respect to other graph approaches)







Jet Tagging





European





- You have a jet at LHC: spray of hadrons coming from a "shower" initiated by a fundamental particle of some kind (quark, gluon, W/Z/H bosons, top quark)
- You have a set of jet features whose distribution depends on the nature of the initial particle
- You can train a network to start from the values of these quantities and guess the nature of your jet

Jet taqqinq

q/g t→Wq→qqq h/W/Z→qq









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- 10²
- 10¹
- 10-1
- 10-2





0.08

0.06

0.04

0.02

0.00

-0.02

-0.04

Doosted Doson Type Tagging One problem, martines olutions Convolved Feature Layers Convolutions

• Data as images

• can use computing vision techniques

s as proatgess sequences

 ϕ) to a rectangular grid that allows for an imageergy from particles are deposited in pixels in (η, ϕ) em as the pixel in a greyscale analogue. st introduced by our group [JHEP 02 (2015) 118] echniques s event reconstruction and computer vision.. We ne jet-axis, and normalize each image, as is often scriminative difference in pixel intensities.

• can use graph

Difference reater orks, as in

mage between signal - media analyses

• Data as graphs of n top of Jet Images to distinguish between a standard model background, QCD.

signal and background image after applying the learned c difference-visualization technique helps understand what the network learns.



. Nachman	(SLAC)	Boosted Boson Type Tagging



















	AUC	Acc	1,	$\epsilon_B (\epsilon_S = 0)$
			single	mean
CNN [16]	0.981	0.930	$914{\pm}14$	$995{\pm}15$
$\operatorname{ResNeXt}[31]$	0.984	0.936	1122 ± 47	1270 ± 28
TopoDNN [18]	0.972	0.916	295 ± 5	$382\pm$ 5
Multi-body N -subjettiness 6 [24]	0.979	0.922	$792{\pm}18$	798 ± 12
Multi-body N -subjettiness 8 [24]	0.981	0.929	867 ± 15	918 ± 20
TreeNiN [43]	0.982	0.933	1025 ± 11	1202 ± 23
P-CNN	0.980	0.930	732 ± 24	845 ± 13
ParticleNet [47]	0.985	0.938	$1298 {\pm} 46$	1412 ± 45
LBN [19]	0.981	0.931	$836{\pm}17$	$859{\pm}67$
LoLa [22]	0.980	0.929	$722{\pm}17$	768 ± 11
LDA [54]	0.955	0.892	$151 {\pm} 0.4$	151.5 ± 0.5
Energy Flow Polynomials [21]	0.980	0.932	384	
Energy Flow Network [23]	0.979	0.927	633 ± 31	729 ± 13
Particle Flow Network [23]	0.982	0.932	891 ± 18	1063 ± 21
GoaT	0.985	0.939	1368 ± 140	

0.0 0.1 0.2 0.3 • Several architectures tried on problem Signal efficiency ε_S

• CNNs, physics motivated custom architectures, PointCloud, etc.

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• Best results achieved with graph architectures

Example: Top Taggers















• Rather than specifying a signal hypothesis upfront, we could start looking at our data

• Based on what we see (e.g., clustering alike objects) we could formulate a signal hypothesis

• EXAMPLE: star classification was based on observed characteristics

Class	Effective temperature ^{[1][2]}	Vega-relative chromaticity ^{[3][4][a]}	Chromaticity (D65) ^{[5][6][3][b]}	Main-sequence mass ^{[1][7]} (solar masses)	Main-sequence radius ^{[1][7]} (solar radii)	Main-sequence Iuminosity ^{[1][7]} (bolometric)	Hydrogen lines	Fraction of all main-sequence stars ^[8]
0	≥ 30,000 K	blue	blue	≥ 16 <i>M</i> ⊙	≥ 6.6 R ⊙	≥ 30,000 <i>L</i> ⊙	Weak	~0.00003%
В	10,000–30,000 K	blue white	deep blue white	2.1–16 <i>M</i> ⊙	1.8–6.6 R ⊙	25–30,000 L _☉	Medium	0.13%
Α	7,500–10,000 K	white	blue white	1.4–2.1 <i>M</i> ⊙	1.4−1.8 R ⊙	5–25 L _☉	Strong	0.6%
F	6,000–7,500 K	yellow white	white	1.04−1.4 <i>M</i> ⊙	1.15–1.4 <i>R</i> ⊙	1.5–5 <i>L</i> ⊙	Medium	3%
G	5,200–6,000 K	yellow	yellowish white	0.8–1.04 <i>M</i> ⊙	0.96–1.15 R ⊙	0.6−1.5 <i>L</i> _☉	Weak	7.6%
К	3,700–5,200 K	light orange	pale yellow orange	0.45–0.8 <i>M</i> ⊙	0.7–0.96 R _☉	0.08–0.6 <i>L</i> ⊙	Very weak	12.1%
М	2,400–3,700 K	orange red	light orange red	0.08–0.45 <i>M</i> ⊙	≤ 0.7 R ⊙	≤ 0.08 L _☉	Very weak	76.45%



• Afterwords, it was realised that different classes correspond to different temperatures







• Anomaly detection is one kind of data mining technique

- One defines a metric of "typicality" to rank data samples
- Based on this ranking, one can identify less typical events, tagging them as anomalies
- By studying anomalies, one can make hypotheses on new physics mechanisms **Object ID: 960415** 20





Learning from Anomalies













DeepLearning from Anomalies

- Use semi/weakly/un supervised learning techniques to learn from data a metric
- Use that metric to replace physics motivate features (or supervised ML scores)
- Could be useful
 - Online, to select events that we should keep but we are not (human bias in defining what is *interesting*)



• Offline, to enhance signals from unexpected signatures

Detection of "expected" signal events



ML classifier score or physics motivated discriminating quantity











• A few given for strategy design

• A few kept "black" and opened after submissions collected

High-level features AE Density Estimation (GIS)

Latent Dirchlet Allocation

High-level features AE **Density Estimation (GIS)**

Latent Dirchlet Allocation

• Several methods designed, now being considered for real LHC analyses

Figure 51. Results of unblinding the first black box. Shown are the predicted resonance mass (top left), the number of signal events (top right), the mass of the first daughter particle (bottom left), and the mass of the second daughter particle (bottom right). Horizontal bars indicate the uncertainty (only if provided by the submitting groups). In a smaller panel the pull (answertrue)/uncertainty is given. Descriptions of the tested models are provided in the text.













• Similar scope, different setup

• no specific event topology

• generic event representation (list of reconstructed particles)

• Use unsupervised algorithms to define anomaly score

 mainly autoencoders, with various
 architecture and training setup

 High performance on benchmark
 examples, not always generalising to black boxes (optimization is an issue)



DarkMachine Challenge



Figure 11: Box plots for each of the physics signals in the hackathon dataset. These summarize the span of results for the many anomaly detection models trained on background only samples. Channel 2a has the tightest pre-selection cuts, and therefore less data, which leads to the signals looking less anomalous.



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PORTUGUES AND AND MARKING ARRESTS PORTUGUES AND ARRESTS PORTUGUES ARE SOLUTION		

DL as an electronic circuit







• Tool to deploy NNs to FPGA

- reads as input models trained on standard DeepLearning libraries
- comes with implementation of common ingredients (layers, activation functions, etc)
- Uses HLS libraries to deliver a firmware implementation of a given network on FPGA
- Could also be used to design AI-specific ASICs for future experiments













Lowier Duarta Lbl c/ml

The full model





Model Compression: reuse



Fully serial

reuse = 4use 1 multiplier 4 times



mult

reuse = 2use 2 multipliers 2 times each



Reuse factor: how much to parallelize operations in a hidden layer

erc

Less resources/ Less throughput









Model Compression: pruning

 Remove parameters that don't
 really contribute to performances

• For DNN, can remove up to 70% of a network with little impact on performance

 Resources saving exploited
 easily at HLS conversion

More complicated with other architectures (requires dedicated pruning strategies)





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FPGA used to compute them, require more Model Compression: QUathese bits. Zallow the binary p

- Quantization: reduce the number of bits used to represent numbers (i.e., reduce used memory)
 - models are usually trained at 64 or 32 bits
 - this is not necessarily needed in real life
 - one can go down to 16 bits w/o performance loss
 - one can do more quantising the model WHILE training
 - One could go as down as binary/ ternary precision with further computational advantage











Tuning the throughput with reuse factor Awill reduce the DSP^sugantization down to ~ 13 bits for DNNs Latency well within the constraints

<u> IFast-inference</u>





Quantization-aware Training

• Post-training quantisation can affect accuracy

• for a given bit allocation, the loss minimum at floating-point precision might not be the minimum anymore

• One could specify quantisation while look for the minimum

• Maximize accuracy for minimal FPGA resources



• We teamed up with Google to exploit this strategy in a QKeras+h1s4m1 bund1e



Model	Accuracy [%]	Latency [ns]	Latency [clock cycles]	DSP [%]	LUT [%]
Baseline	74.4	45	9	56.0 (1826)	5.2 (48321)
Baseline pruned	74.8	70	14	7.7 (526)	1.5 (17577)
Baseline heterogeneous	73.2	70	14	1.3 (88)	1.3 (15802)
QKeras 6-bit	74.8	55	11	1.8 (124)	3.4 (39782)
QKeras Optimized	72.3	55	11	1.0 (66)	0.8 (9149)



https://arxiv.org/abs/2006.10159













One can push quantisation to extremes

• binary & ternary networks

Multiplications can be replaced by bit manipulations, saving resources

• Can achieve low latencies at small accuracy cost and minimal resource consumption



Extreme Quantization







https://arxiv.org/abs/2003.06308





Fast CNN inference on 1 - o

Drastic drop of DSP consumption and overall only ~ % of FPGA resources used

lock 5:	<u>Output:</u> Dense output (n-10)	Layer name	Layer type	Input shape	Weights	MFLOPs	Energy [nJ]
atch Norm.	Softmax	Conv 0	Conv2D	(32, 32, 3)	432	0.778	1,795
eLU		Conv 1	Conv2D	(15, 15, 16)	2,304	0.779	1,802
		Conv 2	Conv2D	(6, 6, 16)	3,456	0.110	262
		Dense O	Dense	(96)	4,032	0.008	26
		Dense 1	Dense	(42)	2,688	0.005	17
		Output	Dense	(64)	65	0.001	4
	Softmax	Model total			12,858	1.71	3,918

Fast CNN inference on FPGAs

Execution time reduced to 5 µsec to basically no accuracy loss down to 6 bits

GraphNets on FF

Model	V_{\max}	R_{reuse}	Latency (cycles)	$\frac{\text{Interval}}{(\text{cycles})}$	DSP (10^{3})	LUT (10^3)	$FF (10^3)$	BRAM (Mb)	ROC AUC	Response RMS
Continuous	128	32	155	55	3.1 [56%]	$57 \; [9\%]$	39 [2.9%]	1.8 [2.3%]	0.98	0.23
Quantized	128	32	148	50	1.6 $\left[29\% ight]$	70 $[11%]$	$41 \ [3.1\%]$	$1.9 \ [2.4\%]$	0.98	0.24
Quantized	64	16	99	34	1.6 [29%]	$63 \ [9\%]$	38 [2.9%]	1.8 [2.3%]	0.96	0.24
Quantized	32	8	75	26	1.4 [25%]	$52 \ [8\%]$	33[2.5%]	1.8[2.3%]	0.86	0.37
Quantized	16	4	63	22	1.5~ig[27%ig]	57 $[9%]$	37~[2.8%]	$1.8\;ar{2.3\%}$	0.64	0.36

Regression

• ML has a long tradition in HEP, dating CERNCOURIER back to the end of the 80s

• ML has been functional to discoveries (e.g., Higgs but not only)

• ML popularity is increasing with Deep Learning opening new directions

• Latest issue of CERN Courier dedicated to AI@CERN

• A community eager to learn & do more, for which CERN joining ELLIS would be a great opportunity

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Conclusions

ARTIFICIAL INTELLIGENCE

