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# New developments in Nachine Learning in particle

# Spåtind 2023



Inspire: ("machine learning" or "deep learning" or neural) and (hep-ex or hep-ph or hep-th)



Selected Papers: 420 Total Papers: 420 Year: 2022







#### <u>Nature Review</u>



Dataset increase factor for 5o discovery

#### <u>Nature Review</u>

Analysis	Years of data collection	Sensitivity without machine learning	Sensitivity with machine learning	Ratio of <i>P</i> values	Additional data required
$\frac{CMS^{24}}{H \to \gamma\gamma}$	2011–2012	2.2 $\sigma$ , <i>P</i> = 0.014	2.7 $\sigma$ , <i>P</i> = 0.0035	4.0	51%
$\begin{array}{l} {\rm ATLAS^{43}} \\ {\rm \textit{H}} \rightarrow \tau^+ \tau^- \end{array}$	2011–2012	2.5 $\sigma$ , $P = 0.0062$	3.4 $\sigma$ , P = 0.00034	18	85%
$ATLAS^{99}$ $VH \rightarrow bb$	2011–2012	1.9 $\sigma$ , P = 0.029	2.5 $\sigma$ , P = 0.0062	4.7	73%
${ m ATLAS^{41}}$ VH $ ightarrow$ bb	2015–2016	2.8 $\sigma$ , $P = 0.0026$	3.0 <i>σ</i> , <i>P</i> = 0.00135	1.9	15%
${ m CMS^{100}}\ VH  ightarrow bb$	2011–2012	1.4 $\sigma$ , P = 0.081	2.1 $\sigma$ , P = 0.018	4.5	125%



Google	chat gpt X 🕹 🔍				
	Q All 🗉 News 🖾 Images 🕞 Videos 🖺 Books : More	Tools			
	About 10,700 results (0.31 seconds)				
	👅 The New York Times	J. CO			
	Opinion   ChatGPT Has a Devastating Sense of Humor				
	The chat bot makes a lot of mistakes. But it's fun to talk to, and it knows its limitations.	TSA			
	5 weeks ago				
	The New York Times	1 4 <sup>-1</sup>			
	Can ChatGPT Make This Podcast?				
	It's writing podcast scripts, finishing students' homework and correcting mistakes in computer code: ChatGPT, the A.I. chatbot from OpenAI,				
	4 weeks ago				
	The New York Times				
	How to Use ChatGPT and Still Be a Good Person				
	It's a turning point for artificial intelligence, and we need to take advantage of these tools without causing harm to ourselves or others.				
	2 weeks ago				
	The New York Times	The Daily is a sh			
	Did Artificial Intelligence Just Get Too Smart?	Hosted by Michael E			
	The power and potential of a technology called ChatGPT have led some to claim it heralds a new era in computing.	Their team of journa They cover the news			
	3 weeks ago				
	The New York Times				
	ChatGPT is Social Media's Newest Star				
	Social media's newest star is a robot: a program called ChatGPT that tries to answer questions like a person. Since its debut last week				











<u>GPT-3: 175 billion parameters (0.16% of the human brain)</u>





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T1037 / 6vr4 90.7 GDT (RNA polymerase domain) **T1049 / 6y4f** 93.3 GDT (adhesin tip)

Experimental resultComputational prediction

#### AlphaFold nature cover











T1037 / 6vr4 90.7 GDT (RNA polymerase domain) **T1049 / 6y4f** 93.3 GDT (adhesin tip)

Experimental resultComputational prediction

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### <u>100 million jets for training</u>

"Particle Transformer For Jet Tagging" H. Qu, C. Li, S. Qian







I'm a bit late with my presentation, could you summarise the latest progress in Machine Learning for Particle Physics?

Learning for Particle Physics?

山豆 Sure! In recent years, there has been significant progress in the application of machine \$ learning techniques to particle physics. Some key areas where machine learning has made significant contributions include:

- leptons (such as electrons and muons).
- accurately reconstruct the events that occurred.
- are produced in each collision event.
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Overall, machine learning has made significant contributions to particle physics and is expected to continue to play a major role in this field in the future.

1. Classification of particles: Machine learning algorithms, particularly deep learning algorithms, have been successfully used to classify different types of particles based on their properties and characteristics. For example, they can be used to identify and distinguish between different types of hadrons (such as protons and neutrons) or

2. Event reconstruction: Machine learning algorithms have also been used to improve the accuracy of event reconstruction in particle physics experiments. Event reconstruction refers to the process of reconstructing the collision events that occurred in a particle accelerator from the raw data collected by detectors. Machine learning algorithms can be used to identify patterns and correlations in the data that can help scientists more

Particle identification: Machine learning algorithms have been used to identify and classify particles based on their properties and characteristics. This can be particularly useful in the context of high-energy particle colliders, where large numbers of particles

4. Simulation and modeling: Machine learning algorithms have also been used to improve the accuracy of simulations and models in particle physics. For example, they have been used to model the interactions between particles and the underlying physical

5. Data analysis and interpretation: Machine learning algorithms have been used to analyze and interpret large datasets generated by particle physics experiments. For example, they have been used to identify patterns and correlations in the data that can help scientists better understand the underlying physical processes at play.

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## What makes particle physics special?

 $dP_{data}^n = |M_S + M_B|^2 dp_1 dp_2 \dots dp_n$ 



 $M_S M_B * + M_B M_S *$ 





Dijet invariant mass



#### ~40 quadrillion collisions recorded at LHC

















### 0.4 -







<u>arXiv:1511.05190</u>











![](_page_25_Picture_1.jpeg)

#### SOTA: Graph Neural Networks acting on point cloud data

<u>ParticleNet</u> (GNN on point cloud)
 <u>LundNet</u> (GNN,Lund plane)
 <u>ABCNet</u> (GNN, attention)
 <u>Point Cloud Transformers</u> (transformer, attention)
 <u>ParticleNeXt</u> (GNN, attention, Lund)
 <u>ParT</u> (transformer, attention)

![](_page_26_Figure_2.jpeg)

#### SOTA: Graph Neural Networks acting on point cloud data

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![](_page_27_Figure_2.jpeg)

![](_page_27_Figure_3.jpeg)

### SOTA: Graph Neural Networks acting on point cloud data

 ParticleNet (GNN on point cloud) LundNet (GNN,Lund plane)
 ABCNet (GNN, attention) Point Cloud Transformers (transformer, attention) ParticleNeXt (GNN, attention, Lund) ParT (transformer, attention)

![](_page_28_Figure_2.jpeg)

### (Self-)Attention

- Allows inputs to interact with each other ("self") and find out who they should pay more attention to ("attention").
- Outputs: aggregates of interactions and attention scores

![](_page_29_Figure_6.jpeg)

The	The
animal	animal
didn't	didn't
cross	cross
the	the
street	street
because	because
it	it
was	was
too	too
wide	wide
	· Goo

![](_page_29_Picture_9.jpeg)

### (Self-)Attention

- Allows inputs to interact with each other ("self") and find out who they should pay more attention to ("attention").
- Outputs: aggregates of interactions and attention scores

![](_page_30_Picture_6.jpeg)

### Weighted sum over all input vectors:

$$y_i = \sum_j w_{ij} x_j$$

Weight (how related inputs are):

$$w'_{ij} = x_i^T x_j$$

Map to [0,1]:

### (Self-)Attention

- Allows inputs to interact with each other ("self") and find out who they should pay more attention to ("attention").
- Outputs: aggregates of interactions and attention scores

![](_page_31_Picture_6.jpeg)

### Weighted sum over all input vectors:

![](_page_31_Figure_8.jpeg)

Weight (how related inputs are):

![](_page_31_Picture_10.jpeg)

$$w'_{ij} = \mathbf{x}_i^{\mathsf{T}} \mathbf{x}_j$$

Map to [0,1]:

### (Self-)Attention

- Allows inputs to interact with each other ("self") and find out who they should pay more attention to ("attention").
- Outputs: aggregates of interactions and attention scores

#### Attention weights: weighted importance between each pair of particles

- Determine relationship between all particles of point cloud
- Jet features become parameters of the model
- Several attention layers  $\rightarrow$  different important features (multi-head attention)

![](_page_32_Figure_12.jpeg)

#### Weighted sum over all input vectors:

$$y_i = \sum_j w_{ij} x_j$$

Weight (how related inputs are):

![](_page_32_Picture_16.jpeg)

$$w'_{ij} = x_i^T x_j$$

Map to [0,1]:

### (Self-)Attention

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#### **Transformer:**

• Only set of interaction between units is self-attention!

![](_page_33_Figure_14.jpeg)

#### Weighted sum over all input vectors:

$$y_i = \sum_j w_{ij} x_j$$

Weight (how related inputs are):

![](_page_33_Picture_18.jpeg)

$$w'_{ij} = x_i^T x_j$$

Map to [0,1]:

### (Self-)Attention

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#### **Transformer:**

• Only set of interaction between units is self-attention!

#### Example prompt

Rigor [adj.] Something for scientists to aspire to, a state of mind that would not be required if scientists could be trusted to do their job.

View next definition

#### GPT-3's output: 1 of 10

The Literature [noun] A name given to other people's published papers, referred to by scientists without actually reading them.

<u>Gwern.net</u>

Weight (how related inputs are):

![](_page_34_Picture_21.jpeg)

 $w'_{ii} = x_i' x_j$ 

Map to [0,1]:

![](_page_34_Picture_26.jpeg)

![](_page_35_Figure_1.jpeg)

#### **ABCNet:**

Pixel intensity = particle importance w.r.t most energetic particle in jet, from attention weights No substructure information given, learned through attention layers!

![](_page_35_Picture_4.jpeg)


# Train on simulation, test on data





# If data and simulation differ, this is sub-optimal!



# Semisupervised: Classification without Labels







**CWola hunting in ATLAS** 

MJJ







#### CWola hunting in ATLAS

MJJ





# Hybrid approaches - NoVa



#### <u>Aurisano et al</u> <u>K. Sachdev</u>





# Hybrid approaches - NoVa



Efficiency of selecting electron neutrinos improved by 40%







# Hybrid approaches - NoVa



Efficiency of selecting electron neutrinos improved by 40%

#### <u>Aurisano et al</u> K. Sachdev

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(c) A simulated electron is inserted in place of the muon to make an MRE event.



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Analysis	Years of data collection	Sensitivity without machine learning	Sensitivity with machine learning	Ratio of <i>P</i> values	Additional data required
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			$\begin{array}{c} 100\\ \hline \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	(a) A 400 (b) The m 400	candidate $\nu_{\mu}$ CC in $_{600}$ 800 <b>40% increa</b> nuon removed or MR( $_{600}$ 800



# ML for higher sensitivity↔ ML for higher efficiency



# High Luminosity LHC

#### New Physics is produced 1 in a trillion

• Need <u>more collisions</u> to observe rare processes

# High Luminosity LHC

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• Need <u>more collisions</u> to observe rare processes

#### High Luminosity LHC

- $\bullet$   $\times 10$  increase in data size
- ×3 collisions per second

#### How

- ×2 protons per bunch
- Squeeze beam at interaction point (B\*)





/m

### ructure $\rightarrow$ pile-up of ~ 60 events/x-ing (s/x-ing)





# High Luminosity LHC

200 vertices (average 140)



# High Luminosity LHC

Must maintain physics acceptance  $\rightarrow$  better detectors

CMS High Granularity (endcap) calorimeter

• 85K (today)  $\rightarrow$  6M (HL-LHC) readout channels

More collisions More readout channels





CMS HGCAL TDR

# **Computing resources**



Need innovation and new techniques to maintain physics reach while staying within throughout requirements!

#### **CMSOfflineComputingResults**

... flat computing budget



# Todays algorithms will not be sustainable in HL-LHC! → Utilise modern Machine Learning to become

f b nd

- faster
- better
- and do more



# CMS Experiment at the LHC, CERN

Data recorded: 2010-Nov-14 18:37:44.420271 GMT(19:37:44 CEST) Run / Event: 151076/1405388

10 billion collisions per second ~10 PB of data per second -











# CMS CT

Geneva Lake



### High Level Trigger: Latency 0(100) ms

# CMS

DATA 99.75% of events rejected! 750 kHz ~Tb/s

Geneva



# ATLAS ~0.02% of collision events remaining ATLAS

DATA 99.982% of events rejected 7.5 kHz ~Gb/s

Geneva

LHC

LHCh



### High Level Trigger: Latency 0(100) ms

(intel)

Xeon\* 7500

Genev

# CMS

## DATA 100 kHz ~Tb/s

**Detector:** 40 MHz ~Pb/s

Level-1 trigger: Latency O(1) µs

LHCh





### Fast inference on specialised hardware

**ASIC inference** 

**Detector:** 40 MHz ~Pb/s

**FPGA** inference

LHCb

Level-1 trigger: Latency O(1) µs







# Ideally



# Reality

# Efficient NN design for edge compute

#### Before deploying any DNN on chip (CMS trigger, iPhone), must make it efficient!

• Big engineering field in its own right

#### **During training**

- Quantization: do you really need 32-bit FP precision?
- Pruning: removal insignificant synapses
- Knowledge distillation

#### Post-training

Parallelisation (lower latency ↔ more resources)

#### From 8 GPU server to tiny FPGA!







# Quantization





### Nature Machine Intelligence 3 (2021)

www.nature.com/natmachintell/August 2021 Vol. 3 No. 8

# nature machine intelligence

#### Quantized neural networks on the edge





## Google AI





# FPGA performance



#### Nature Machine Intelligence 3 (2021)



64

#### CMS High Granularity calorimeter

• 6.5 million readout channels, 50 layers





CMS High Granularity calorimeter

• 6.5 million readout channels, 50 layers

# BUT: Cannot read out all these channels fast enough for L1 to trigger!







# Variational Autoencoder

<u>ECON-T, D. Noonan</u>




### ML for compression



### <u>ECON-T, D. Noonan</u>



### ML for compression



#### ECON-T, D. Noonan



## ML for compression



<u>ECON-T, D. Noonan</u>



#### **16 ReLU activated nodes**



### ML for reconstruction



On FPGA: 3.5 µs to cluster energy deposits

### ML for reconstruction



On FPGA: 3.5 µs to cluster energy deposits

• Graph Neural Networks (GarNet/GravNet) for fast clustering of irregular geometry detectors





## Bias in particle physics



Some variable of interest



Need to exploit the full capabilities of the LHC and be more generic!



## Limitations of current trigger



Trigger threshold

Energy (GeV)

### Level-1 rejects >99% of events! Is there a smarter way to select?

76



Trigger threshold

Energy (GeV)

# Look at data rather than defining signal hypothesis a priori Can we "classify" objects/events?



# ML for anomaly detection

### Autoencoders: Learns from data

- Trains unsupervised
- Learns to compress, then reconstruct data
- Often used for financial fraud detection
  - Low rate of anomalous events versus high rate "background"



### Real data X





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### • Difference $\mathbf{X}$ - $\hat{\mathbf{X}}$ defines "degree of abnormality"







## ML for anomaly detection



Nature Machine Intelligence 4, 154 (2022)

### Select based on degree of abnormality!

80



### Data challenge on real-time anomaly detection

• Dataset: Nature Scientific Data (2022) 9:118

#### Tutorial: Anomaly detection on FPGA with hls4ml

Help us find new physics!

mpp-hep.github.io/ADC2021/

Welcome to the Anomaly Detection Data Challenge 2021!



## Real-time ML in other experiments



Taking plasma accelerators to market



<u>F. Capel et al.</u>





## Real-time ML in other experiments





### <u>F. Capel et al.</u>





## Real-time ML in other experiments

### Signals and backgrounds



<u>F. Capel et al.</u>



#### **CMS***Public* Total CPU HL-LHC (2031/No R&D Improvements) fractions 2022 Estimates



### **CMS Offline Computing Results**



### **CMS Offline Computing Results**



HL-LHC, Simulation of CMS HGCAL with 140 PU







 $O(10^3)$ 

 $10^{-18}$ m







detector response simulation [Hard & Slow]



81%

DIGI+RECO



Energy deposits→digital signals→reconstructed by the reconstruction software [Hard & Slow]













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Overall, machine learning has made significant contributions to particle physics and is expected to continue to play a major role in this field in the future.

G Regenerate response

PT Dec 15 Version. Free Research Preview. Our goal is to make AI systems more natural and safe to interact with. Your feedback will help us imp

≻

# Backup

### FPGAs as Al accelerators

At LHC, DAQ FPGAs are idle ~50% of the time (no collisions)

- Could these be utilised for co-processing?
- Running AI inference for reconstruction tasks!





<u>C. Beteta, I. Bezshyiko, N. Serra</u>



## Hardware: Al engines

#### More and more dedicated AI processors on the market

• We should explore these to speed up our inferences!

#### Xilinx Versal AI processors

- Example Xilinx ACAP board: 400 AI processors, ~2M logic cells (FPGA), 2k DSPs, Arm CPU, Arm RPU
- Data can move back and forth between AI Engines and FPGA

Currently explored for real-time tracking in trigger application

- Interaction Network for pattern recognition (similar to **DeZoort et al**)
- Deployed on Xilinx Versal VC1902 ACAP





### ...and more!

### Semantic segmentation for autonomous vehicles



N. Ghielmetti et al.

#### Other examples

- For fusion science phase/mode monitoring
- <u>Crystal structure detection</u>
- <u>Triggering in DUNE</u>
- Accelerator control
- Magnet Quench Detection
- MLPerf tinyML benchmarking
- Food contamination detection
- etc....





## Quantization-aware training

### Lossless quantization for deep neural networks!



<u>arxiv:2103.13630</u>





#### arXiv:1804.09720

## Hybrid approaches - MicroBooNE



# DNN likelihood

#### Alternative approach: End-to-end DNN search

- How do we get around defining a signal hypothesis?
- What is alternate hypothesis to test reference?

Idea: Assume alternate model n(x|w) can be parametrised in terms of reference model n(x|R)

$$n(x \mid \overrightarrow{w}) = n(x \mid R)e^{f(x; \overrightarrow{w})}$$
 - Set of real functions

• Let DNN parametrise alternative model

$$f(x; \vec{w}) = NN$$

unctions

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 - Set of real full

• Let DNN parametrise alternative model

$$f(x; \vec{w}) = NN$$

Formulate loss as log likelihood.
 → Trained DNN is the maximum likelihood fit to data and reference log-ratio
 → best approximate of true data distribution

$$f(x, \widehat{\mathbf{w}}) \simeq \log \left[ \frac{n(x|\mathbf{T})}{n(x|\mathbf{R})} \right]$$
 — True underlying d

unctions

lata distribution

101

### **INPUTS** - any high level features



 $f(x, \widehat{\mathbf{w}}) \simeq \log \left[ \frac{n(x|\mathbf{T})}{n(x|\mathbf{R})} \right]$  — True underlying data distribution

### **OUTPUTS**

-tobs and  $f(x; \hat{w})$ 

hypothesis test + p-value Data  $\rightarrow$  toys under R, repeat


## ML on FPGA for tracking

### In HL-LHC, will need to do track finding at L1

• O(1000) hits, O(100) tracks, 40 MHz rate, ~5 µs latency

Graph Neural Networks for fast charged particle tracking

Design	(n <sub>nodes</sub> , n <sub>edges</sub> )	RF	Precision	Latency [cycles]	ll [cycles]	DSP [%]	] LUT [%]	FF [%]	BRAM [%]
Throughput-opt.	(28, 56)	1	ap_fixed<14,7>	> 59	1	99.9	66.0	11.7	0.7
The target FPGA BRAM (Xilinx, Inc.,	is a Xilinx Virtex UltraSca 2021). A 5 ns clock period	le+ VU9P is used.	FPGA (part number )	xcvu9p-flga2104-2L-e),	which has	6,840 DSPs,	1,182,240 LUTs,	2,364,480 FFs,	and 75.9Mb of

#### DOI:10.3389/fdata.2022.828666





# Probing algorithm response: t-SNE for NoVA



**Nature Review** 





Can we have the best of both worlds?

# Knowledge Distillation



## Inference





۹

**\*** 





is cat
is dog









### Train student to learn both true and predicted (teacher) labels!

 $L_{total} = \beta \times L_{Distillation} + \alpha \times L_{student}$ 

Student learns subtle learned features from teacher!

