ML Overview in CMS, HEP, and beyond

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Outline

- I. Machine Learning beyond classification
- Π. Geometric Deep Learning
- Machine Learning in CMS
- Prospects of Deep Learning IV.





Machine Learning beyond classification

control, reconstruction, simulation, ...





AI in HEP

Role of AI: accelerator control, data acquisition, event triggering, anomaly detection, new physics scouting, event reconstruction, event generation, detector simulation, LHC grid control, analytics, signal extraction, likelihood free inference, background rejection, new physics searches, ...



LHC Computing Grid 200k cores pledge to CMS over ~100 sites



CERN Tier-0/Tier-1 **Tape Storage** 200PB total **CERN** Tier-0 Computing Center 20k cores Large Hadron Collider CMS L1 & High-40 MHz of collision Level Triggers 50k cores, 1kHz Up to date listing of references: **CMS** Detector 1PB/s





Producing the Data



A. Scheinker, C. Emma, A.L. Edelen, S. Gessner [2001.05461]

- Already successfully deployed on accelerator facilities.
- More promising R&D to increase beam time.
- Potential for detector control ?

Opportunities in Machine Learning for Particle Accelerators [1811.03172] Machine learning for design optimization of storage ring nonlinear dynamics [1910.14220] Advanced Control Methods for Particle Accelerators (ACM4PA) 2019 Workshop Report [2001.05461] Machine learning for beam dynamics studies at the CERN Large Hadron Collider [2009.08109]

> More of the relevant works at: https://iml-wg.github.io/HEPML-LivingReview/



. . .

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• Machine learning can be used to tune devices, control beams, perform analysis on accelerator parameters, etc.



Compressing Data



Deep Auto-Encoders for compression in HEP http://lup.lub.lu.se/student-papers/record/9004751

- Rich literature on data neural network.
- some loss of resolution.
- Saving on disk/tape cost.
- R&D needed to reach the

More of the relevant works at: https://iml-wg.github.io/HEPML-LivingReview/



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compression of image with

Make use of abstract semantic space for image compression.

Image compression can suffer

Potential in scouting strategies.

necessary level of fidelity.





Cleaning Data



- with automation.
- reducing workload.
- Continued R&D and experiment adoption.

A.A. Pol, G. Cerminara, C. Germain, M. Pierini, A. Seth [doi:10.1007/s41781-018-0020-1]

Towards automation of data quality system for CERN CMS experiment [doi:10.1088/1742-6596/898/9/092041] LHCb data quality monitoring <a>[doi:10.1088/1742-6596/898/9/092027 Detector monitoring with artificial neural networks at the CMS experiment at the CERN Large Hadron Collider [1808.00911] Anomaly detection using Deep Autoencoders for the assessment of the quality of the data acquired by the CMS experiment [doi:10.1051/ epiconf/201921406008]





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Data quality is a person power intensive task, and crucial for swift delivery of Physics

Machine learning can help

Learning from operators,



Managing Data



Cache Type	[hroughput] = Cost Read	l on hit ratio $ \mathbf{B}$	and sat.	CPU Eff.
SCDL	$\mathbf{79.43\%} \big \mathbf{50.68\%} \big $	21.22%	58.94%	58.75%
LFU	65.01% 104.73%	$\mathbf{33.29\%}$	51.00%	$\mathbf{60.92\%}$
Size Big	49.02% 111.73%	28.55%	54.40%	60.41%
LRU	47.15% 112.84%	27.64%	54.93%	59.90%
Size Small	46.71% 113.01%	27.39%	55.01%	59.73%



- Complex ecosystem with dedicated operation teams.
- Person power demanding, and inefficient in some corner of the phase space.
- Potential for Al-aided • operation.
- Lots of modeling and control challenges.
- R&D to increase operation efficiency.

Caching suggestions using Reinforcement Learning <u>_OD 2020</u>, in proceedings

More of the relevant works at: https://iml-wg.github.io/HEPML-LivingReview/



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[cds:2709338]

The LHC-grid is key to



Detecting New Data



- selected signatures.
- Further potential for reduction.
- Emerging opportunity for triggering on unknown
- experiment adoption.

Use of variational auto-encoders directly on data to marginalize outlier events, for anomalous event hotline operation. [doi:0.1007/JHEP05(2019)036]

More of the relevant works at: https://iml-wg.github.io/HEPML-LivingReview/



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More promising R&D and

signatures : "a la Hotline".

background trigger rate

Machine learning since long deployed in the trigger for

Data Triggering and Scouting



Phase-2 upgrade of the CMS L1-Trigger [cds:2714892]

- Trigger benefit from fast reconstruction algorithms
- L1 needs FPGA implementation. hls4ml-enabled algorithms.
- Quality of selection increases with refinement of object reconstruction
- Having the best reconstruction is particularly important in scouting
- Balance between speed and accuracy





Reconstructing Data



- techniques can help.
- or data.
- ground truth.
- new detector design.
- potential.

More of the relevant works at: https://iml-wg.github.io/HEPML-LivingReview/





Learn from the simulation, and/

 Learn from existing "slow reconstruction" or simulation

Automatically adapt algorithm to

 Image base methods evolving towards graph-based methods.

Accelerating R&D to exploit full



Simulating Data



Generative Adversarial Networks for LHCb Fast Simulation [2003.09762]

- computing intensive.
- Fast and approximate

- samples.
- starting.

More of the relevant works at: https://iml-wa.aithub.io/HEPML-LivinaReview/



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Fully detailed simulation is

simulators already in operation.

• Applicable at many levels : sampling, generator, detector model, analysis variable, etc

Generative models can provide multiple 1000x speed-up.

Careful study of statistical power of learned models over training

Many R&D, experiment adoption



Calibrating Data



- obvious use case.
- Learning calibrating models from simulation and data.
- Parametrization of scale factors using neural networks.
- Reducing data/simulation dependency using domain adaptation.
- Continued R&D

A deep neural network for simultaneous estimation of b jet energy and resolution [1912.06046]

More of the relevant works at: https://iml-wa.github.io/HEPML-LivingReview/



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• Energy regression is the most



Analyzing Data



- Machine learning has long classification.
- Increasing number of analysis with more complex DNN.
- Application to signal categorization, bkg modeling, kinematics reconstruction, decay product assignment, object identification, ...
- Breadth of new model agnostic methods for NP searches.
- Continued R&D and experiment adoption initiated.

Use of masked autoregressive density estimator with normalizing flow as model-agnostic signal enhancement mechanism. [doi:10.1103/PhysRevD.101.075042]



More of the relevant works at: https://iml-wg.github.io/HEPML-LivingReview/

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infiltrated analysis for signal/bkg



Theory Behind the Data



- of HEP analysis.

- of HEP simulator.
- R&D to bring this in the experiment.



More of the relevant works at: https://iml-wq.github.io/HEPML-LivingReview/

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• Hypothesis testing is the core

Intractable likelihood hinders solving the inverse problem.

Going beyond the standard approach using machine learning and additional information from the simulator.

More precise evaluation of the priors on theory's parameters.

• May involve probabilistic programming instrumentation



Geometric Deep Learning

Graph Neural Network ...





Graph Representation



Graph Neural Networks for Particle Physics reconstruction [2007.13681], [2012.01249]

Heterogenous data fits well in graph/set representation.

Multiple CMS ML Forum presentations on GNN applications [Sept 30, 2020], [Oct 20, 2021], [Nov 3, 2021] and reconstruction with ML [Feb 21, 2021], [Mar 10, 2021].



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Forewords on Graph



A graph is composed of

- Nodes that can be represented as a vector.
- Edges that can be represented with the adjacency matrix.
- \rightarrow Flowing of information using matrix operations.
- → With machine learning on graphs, edges and nodes might acquire internal representations.







Graph Neural Networks Formalism



Lots of possibilities to operate on a graph. Most available architectures can be expressed with Φ and ρ .

> Readily software: https://github.com/deepmind/graph nets https://github.com/rusty1s/pytorch_geometric



10/26/20

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Updated attributes

Updated attributes

Updated attributes



Geometric Deep Learning (I)





condensation, [2106.01832]. [1902.07987] [2002.03605]







Geometric Deep Learning (II)







Jet tagging in the Lund plane, [2012.08526]



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Lund coordinates

 $\mathcal{T}^{(j_0)}$

 ${\cal T}^{(i)}$

Lund tre

Geometric Deep Learning (III)

Pileup mitigation using graph neural network and transformers

ECAL superclustering with machine learning

Geometric Deep Learning (IV)

E/G energy regression using dynamic reduction network, [2003.08013]

Geometric Deep Learning (V)

Best models on all channels combined based on mean score

Anomalous jet detection using graph convolution network variational auto-encoder with normalizing flow in the latent space, [2110.08508]

Jet particle-based simulation with message passing GNN generative adversarial network, [2012.00173]

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ML in CMS

a selected pick of recent results ...

di-photon Mass Regression

Learn the a/di-photon mass from the energy deposition at the Ecal surface. Unprecedented reach at low mass.

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Ecal Regression

- [cds:2803235]
- Graph-based model with self-attention trained to :
 ✓ seed-cluster classification
 - ✓ super-cluster classification
 - ✓ super-cluster energy regression
- Promising work in progress for calorimeter reconstruction

Super-resolution Simulation

- Run GEANT4 with loose parameters as low-quality input
- Learn the full precision high-quality output with CNN
- Model able to "denoise" and approach full precision

Hadronic Tau Identification

- Combines jet features and particle-image features
- CNN model to classify hadronic tau
- Much reduced fake rate
- More hadronic taus in analysis

Vector-Like Lepton Pair Search

- At least 3b jets and two third generation leptons in final state
- DeepTau [cds:2800114] method used for tau identification.
- Attention-based graph model [2001.05311] working on final state objects acts as classifier used for signal categorization.
- State of the art deep-learning in state of the art NP search

Particle-Flow Reconstruction

Uses built-in dense matrix, reshape and scatter/gather operations in TF. Requires batch-mode graphs. No N² allocation or computation needed.

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Regress parton kinematics from candidate Model almost matching classical algorithm Execution time quasi-linear with pile-up

Particle Reconstruction at HL-LHC

- High-Granularity Calorimeter (HGCAL) provides fine-grained description of energy deposition
- Graph-based models [2106.01832] using object condensation loss [2002.03605] trained to perform cell-to-particle association
- Stepping stone towards ML-based particle reconstruction in HGCAL

Vertexing at L1 at HL-LHC

[cds:2801638]

- Tracks reconstructed at L1 used in input
- Model regress position of primary vertex and track-PV assignment
- Quantized/pruned model can efficiently ulletdeploy on FPGA

Prospects for Deep Learning

a few words of wisdom ...

Interpretability

Interplay between deep learning and science is key. Use Physics knowledge to produce better models. Use models to learn Physics knowledge.

Uncertainty Quantification

Propagation and estimation of uncertainties are keys. Uncertainty-aware models. Uncertainty-predicting models. Uncertainty-improving models.

Computation Aspect

Computational cost of Science is key. Adapt to heterogenous computing environment. Hardware-aware model optimization.

Publication Plans

Publishing in peer-reviewed journal is key. Importance of open-data samples. Flexibility in experiments to publish work in progress.

Summary

- Modern machine learning a.k.a Deep Learning goes much beyond classification.
- \rightarrow GDL is most promising for many applications.
- Novel Deep Learning are being adopted in CMS. Many more upcoming results.
- \rightarrow The future of AI4HEP is interpretable, quantifiable, runnable and publishable ...

A Definition

"Giving computers the ability to learn without explicitly programming *them*" A. Samuel (1959).

Is fitting a straight line machine learning? Models that have enough capacity to define its own internal representation of the data to accomplish a task : learning from data.

In practice : a statistical method that can extract information from the data, not obviously apparent to an observer.

Most approach will involve a mathematical model and a cost/ reward function that needs to be **optimized**.

→The more domain knowledge is incorporated, the better.

Supervised Learning

- Given a dataset of samples, a subset of features is qualified as target, and the rest as input
- Find a mapping from input to target
- The mapping should generalize to any extension of the given dataset, provided it is generated from the same mechanism

$$dataset = \{ (x_i, y_i) \}_i$$

find function f s.t. $f(x_i) = y_i$

- Finite set of target values : → Classification
- Target is a continuous variable :
 - → Regression

Unsupervised Learning

- Given a dataset of samples, but there is no subset of feature that one would like to predict
- Find mapping of the samples to a lower dimension manifold
- The mapping should generalize to any extension of the given dataset, provided it is generated from the same mechanism

$$dataset = \{ (x_i) \}_i$$

find f s.t. $f(x_i) = p_i$

- Manifold is a finite set → Clusterization
- Manifold is a lower dimension manifold :
 - → Dimensionality reduction, density estimator

Reinforcement Learning

- Given an environment with multiple states, given a reward upon action being taken over a state
- Find an action policy to drive the environment toward maximum cumulative reward

$$s_{t+1} = Env(s_t, a_t)$$

$$r_t = Rew(s_t, a_t)$$

$$\pi(a|s) = P(A_t = a|S_t = s)$$

find $\pi s.t. \sum_t r_t$ is maximum

Artificial Neural Network

- **Biology inspired** analytical model, but **not bio-mimetic**
- Booming in recent decade thanks to large dataset, increased computational power and theoretical novelties
- Origin tied to logistic regression with change of data representation
- Part of any "deep learning" model nowadays
- Usually large number of parameters trained with stochastic gradient descent

Neural Net Architectures

http://www.asimovinstitute.org/neural-network-zoo

> Does not cover it all : densenet, graph network, ...

Machine Learning in Industry

Deep Learning Everywhere

Speech Recognition

Language Translation

Language Processing Sentiment Analysis Recommendation

WEDICINE & BIOLOGY

Cancer Cell Detection Diabetic Grading Drug Discovery

Video Captioning Video Search Real Time Translation

MEDIA & ENTERTAINMENT

Face Detection Video Surveillance Satellite Imagery

& DEFENSE

Pedestrian Detection Lane Tracking Recognize Traffic Sign

AUTONOMOUS MACHINE

15 CINIDIA

https://www.nvidia.com/en-us/deep-learning-ai/

Rapidly Accelerating Use of Deep Learning at Google Number of directories containing model description files Used across products: 1500 1000 500 2013 2014 2015 2012

MACHINE INTELLIGENCE 3.0

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http://www.shivonzilis.com/machineintelligence

Prominent skill in industry nowadays. Lots of data, lots of applications, lots of potential use cases, lots of money. Knowing machine learning can open significantly career horizons.

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Learning to Control

Mastering the game of Go with deep neural networks and tree search, https://doi.org/10.1038/nature16961

> Modern machine learning boosts control technologies. AI, gaming, robotic, self-driving vehicle, etc.

Learning to Walk via Deep Reinforcement Learning https://arxiv.org/abs/1812.11103

Learning from Complexity

Machine learning model can extract information from complex dataset. More classical algorithm counter part may take years of development.

The Black-box Dilemma

Deep learning may yield great improvements. Having the "best classification performance" is not always sufficient. Forming an understand of the processes at play is often crucial.

Physics Knowledge

Machine Learning can help understand Physics.

Learning Observables

Search in the space of functions using decision ordering. Simplified to the energy flow polynomial subspace. Extract set of EFP that matches DNN performance.

1.75

1.50

1.25

Density

0.75

0.50

0.25

0.00

0.4

0.3

Density 70

0.1

0.8

0.7

Density 7.0

> 0.3 0.2 0.1

Use Physics

Let the model include Physics principles to master convergence

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Inductive Bias

Embed the symmetry and invariance in the model. Economy of model parameters.

Jet Tagging

Graph-based models have recently achieved state-of-the-art jet tagging performance on benchmarks, and in analysis. Still a very rich field, in particular in developing inductive bias in the model (symmetry, invariance, ...). Kinematic regression, substructure assignment, ... also possible thanks to model flexibility.

(c)

Operation Vectorization

ANN \equiv matrix operations \equiv parallelizable

$$\begin{bmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \\ w_{13} & w_{23} \end{bmatrix} \cdot \begin{bmatrix} i_1 \\ i_2 \end{bmatrix} = \begin{bmatrix} (w_{11} \times i_1) + (w_{21} \times i_2) \\ (w_{12} \times i_1) + (w_{22} \times i_2) \\ (w_{13} \times i_1) + (w_{23} \times i_2) \end{bmatrix}$$

Computation of prediction from artificial neural network model can be vectorized to a large extend.

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Hyper-Fast Prediction

Synthesizing FPGA firmware from trained ANN

https://fastmachinelearning.org/hls4ml/

J. Duarte et al.[1804.06913]

Artificial neural network model can be **executed efficiently on FPGA**, GPU, TPU, ...

Inference Engines

Growing list of deep learning accelerators. Location of the device is driven by the environment (Trigger, Grid, HPC, ...).

"Remote accelerator"

[<u>1811.04492</u>], [<u>2007.10359</u>], [<u>2007.14781</u>]

Model Compression

Model inference can be accelerated by reducing the number and size of operations.

The Standard Model

Well demonstrated effective model. Good amount of detailed, **"labelled" simulation available**.

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The Sea Beyond Standard Model

"Almost" Simple H₁

Focus on few sharply-defined alternative models (e.g., the Higgs)

Case-by-case design of **optimal test**

"Very" Composite H₁

Huge set of alternatives Case-by-case optimisation **unfeasible** The right H₁ likely not yet formulated

Slide: A. Wulzner [H&N]

Event Triggering

Select what is important to keep for analysis. Ultra fast decision in hardware and software.

Reconstruction of the event under limited latency / bandwidth. **Better resolution** help lowering background trigger rates, Faster algorithms helps making more refined decisions.

Reconstructing Collisions

Event Processing

Dimensionality reduction

Globalization of information

From detector signal to high-level features using mostly pattern recognition. Complex and **computing intensive** series of tasks. 63

Simulating Collisions

Madgraph, Pythia, Sherpa,	Event Generator : compute predictions of the standard r several orders of expansion in coupling constants (L NNLO,) using proton density functions.
Pythia,	Hadronization: phenomenological model of the evolutio hadrons under the effect of QCD.
GEANT 4, GEANT V	Material simulator: transports all particles throughout a detector, using high resolution geometrical description materials.
Homegrown software	Electronic emulator: converts simulated energy de sensitive material, into the expected electronic signal, noise from the detector.

Non-differentiable, **computing intensive** sequence of **complex simulators** of the signal expected from the detectors.

64

Reconstruction • Simulation ~ Identity

Simulation aims at predicting the outcome of collisions. Reconstruction aims at inverting it. Multiple ways to connect intermediate steps with deep learning.

The Computing Cost of Science

Ever growing needs for computing resource. Slowdown of classical architecture, over growth of GPU architecture.

Annual CPU Consumption [MHS06]

Possible Utilizations

Accuracy Speed

Interpretable

→ Fast surrogate models (trigger, simulation, etc); even better if more accurate. → More accurate than existing algorithms (tagging, regression, etc); even better if faster. Model performing otherwise impossible tasks (operations, etc)

