International Center for
Quantum-field Measurement Systems for
Studies of the Universe and Particles
WPI research center at KEK

Machine Learning at LHC

Yu Nakahama (KEK IPNS & QUP)

Quposium 2023, December 12nd at Epochal Tsukuba

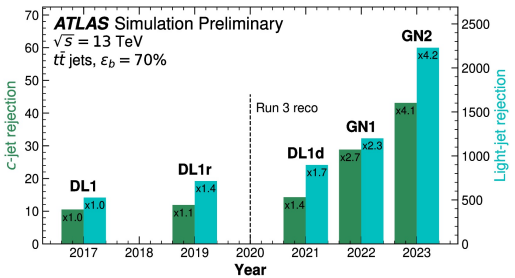
Introduction

- Machine Learning has been in High Energy Physics since early 2000
  - Signal-Background separation in physics data analysis, and
  - Object reconstruction and identification such as flavour tagging

- More attractions all from science, industry, and society

What's new recently

- Significant increase in compute power (GPU) and data available for ML training
- Dramatic increase in ML architectures for different applications:
  - Transformers/large-language models (LLMs), graph neural networks (GNNs), convolutional neural networks (CNNs), etc
- ML advancements have already affected HEP
  - e.g. drastic improvement in flavour tagging using Graph Neural Network (by a factor of 3)
    → in physics sensitivity as well
    e.g. H→cc, di-Higgs search



[Transformer- based GN2, FTAG-2023-01]

Why use ML

- ML to exploit high-dimensional correlations
  - Our multidimensional distributions are rarely rectangular
  - Rectangular cuts won't maximize signal efficiency and background rejection
  - Maximizing our performance is essential in luminosity era.
- ML as a surrogate model: fast and/or can run many types of hardware: e.g., ML-based track reconstruction, fast simulation
- ML for non-standard data: data that is less confined than our offline physics objects (e.g., operational & trigger data), variable length input, etc.

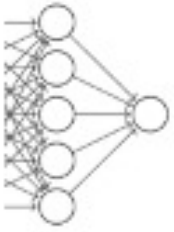
Let's focus on the areas as well as the areas QUP and its network colleagues are involved in.
Disclaimar: This talk is not comprehesive summary.

Adapting ML to HEP
- Evolving data representations

Credit: M. Kagan (SLAC)

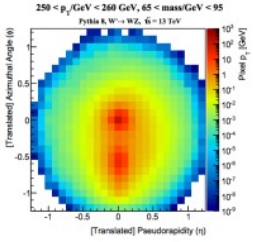
Arbitarary inputs

Feedforward Neural Network



early 2000's

Images



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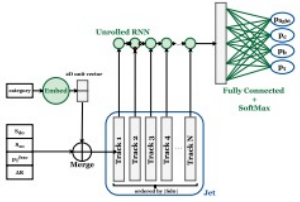
Sequences



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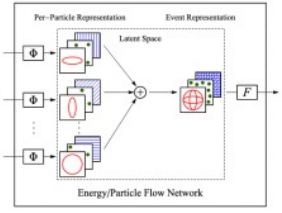
Sets



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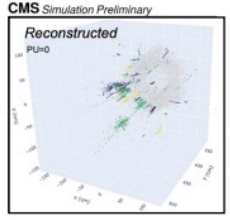
Graphs
(& Transformers)



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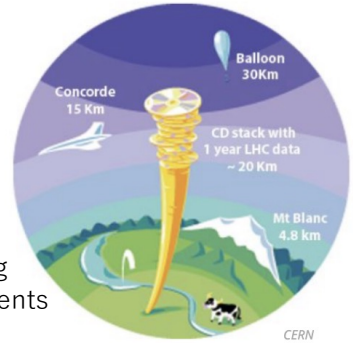
Our “big science” challenges at LHC

- Too much data at LHC to handle quickly

→Considered as a severe issue already.

- Too large-sized & complex detector

After selecting interesting events

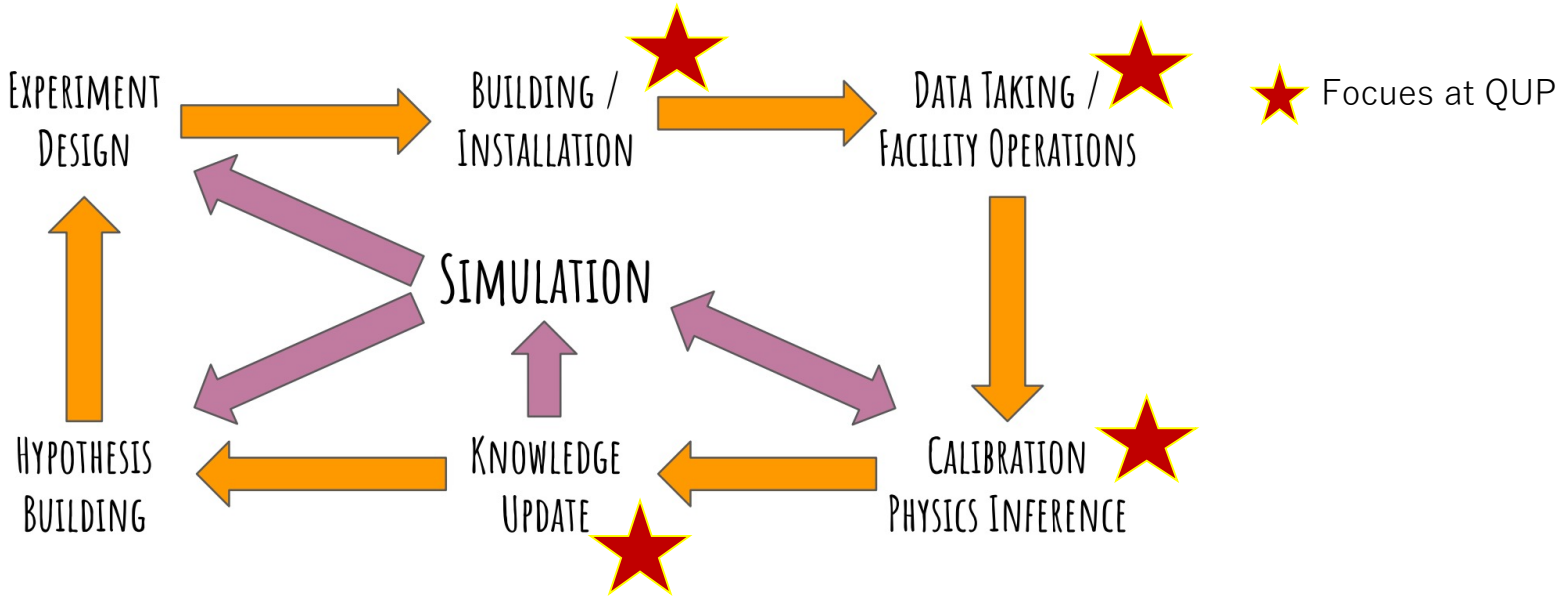


- Too specialized and sub-divided
  – Only specialized experts can handle each.

→ Not easily scalable for future with available resources.

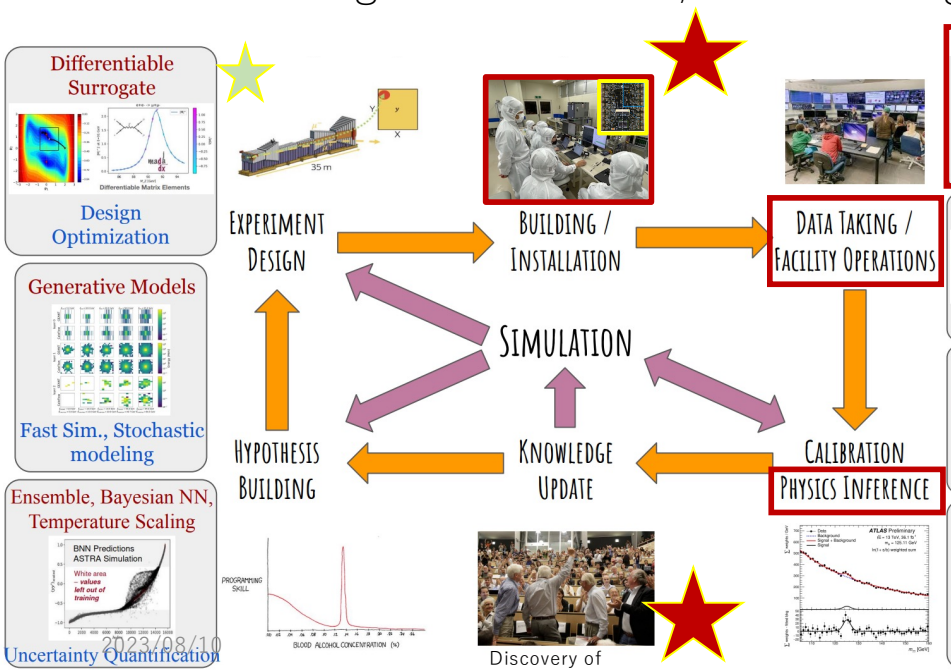
Today: ML everywhere in our HEP workflow

- Optimization, automation, quality improvement, efficiency, precision
  - Including hardware work, brainstorming, communications



Today: AI/ML everywhere in our HEP workflow

- Optimization, automation, quality improvement, efficiency, precision
  - Including hardware work, brainstorming, communications



Focues at QUP

Interests at QUP

- Several studies on going
- Will focus on those where PoC is demonstrated as achievement and the integration to actual system is in progress.

Credit (original sketch): K. Terao (SLAC)

QUP/KEK's approach

- Leveraging machine learning for automating & accelerating "Scientific Discoveries" in the area on the early universe and Dark Matter in collider physics and cosmology.
  - ML applications
    - to physics analyses in our interests for maximising scientific outputs
    - to facilities in our responsibilities for smart automation
  - Developments of Anomaly Detection techniques

Core members on ML at QUP

2 PIs


Yu Nakahama


Daniela Bortoletto

1 senior scientist
/1 affiliate
/ 1 PD


Yuji Chinone


Javier Montejo


Louis Vaslin

Collaborators with facility-type expertise inside QUP


Nanae Taniguchi (Belle, FPGA)


Kazuki Ueno (J-PARC COMET, FPGA)

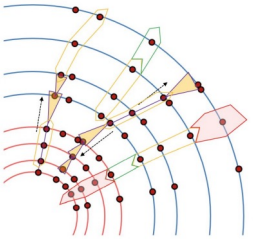

Maurice Garcia-Sciveres (Micro-electronics)


Masaya Miyahara (Micro-electronics)

Collider physics
Cosmology

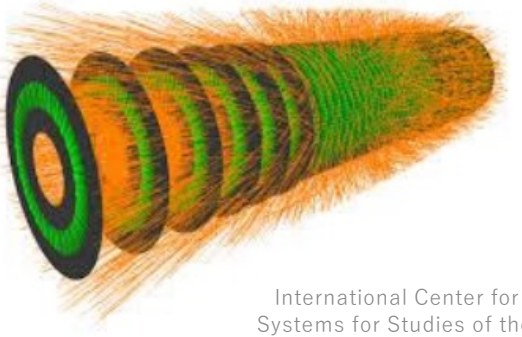
with ~100 international/domestic collaborators through our JSPS core-to-core research network "AI-Smart" in HEP.

Particle tracking for the upgraded LHC

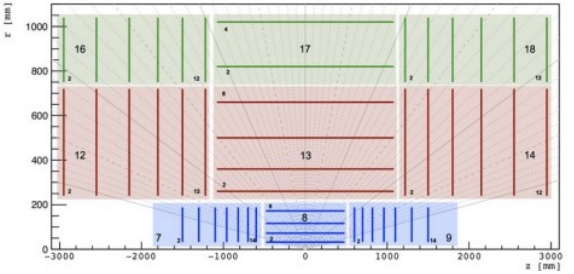


- Track reconstruction: find trajectories from space-points
  - Single most computationally intensive algorithm
  - Enormous challenge in the upgraded LHC:
    5k charged particles and 100k hits per event with lots of noise hits!
    → challenging pattern recognition problem

New all-silicon tracking detector (ITk) for the upgraded LHC: Demonstration of charged tracks and hits

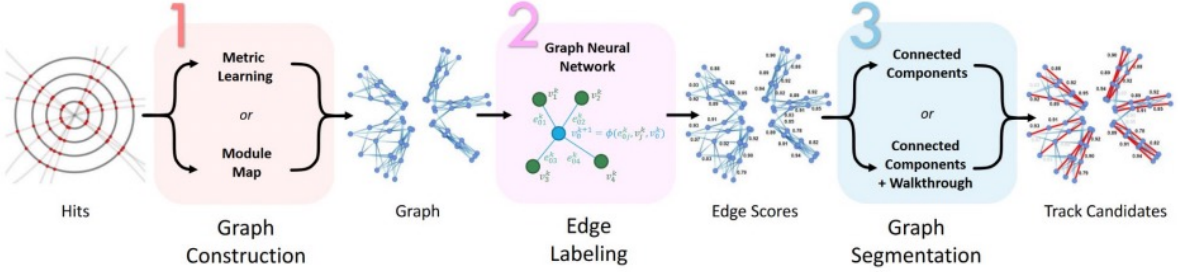


Detector layout



Particle tracking with Graph Neural Network

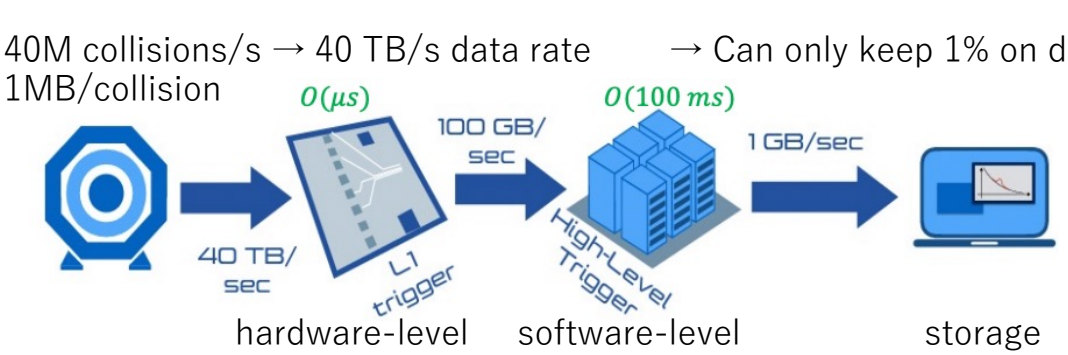
- Transform global pattern recognition problem into a local problem
- The pipeline consists 3 discrete steps: graph construction, edge labeling, graph segmentation
  - Graph construction: module map and Metric Learning
  - Edge labeling: Graph Neural Network
  - Graph Segmentation: Connected Components & Walkthrough



Credit: X. Ju (LBL)

- Very competitive performance on realistic ATLAS ITk data

Triggering physics events



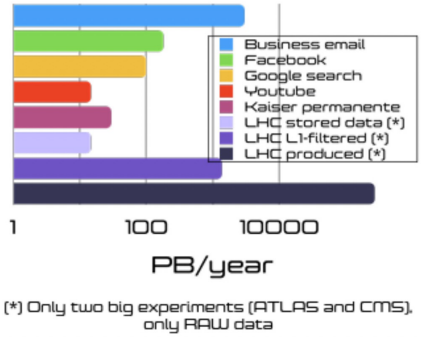


Image credit: Wired 2013

- Triggering physics events at HL-LHC is challenging (x10 in rate).
- Current algorithms and computing model is not sustainable.

→ Solutions are strongly desired from

- new algorithmic paradigms e.g. ML and new technologies e.g. accelerators

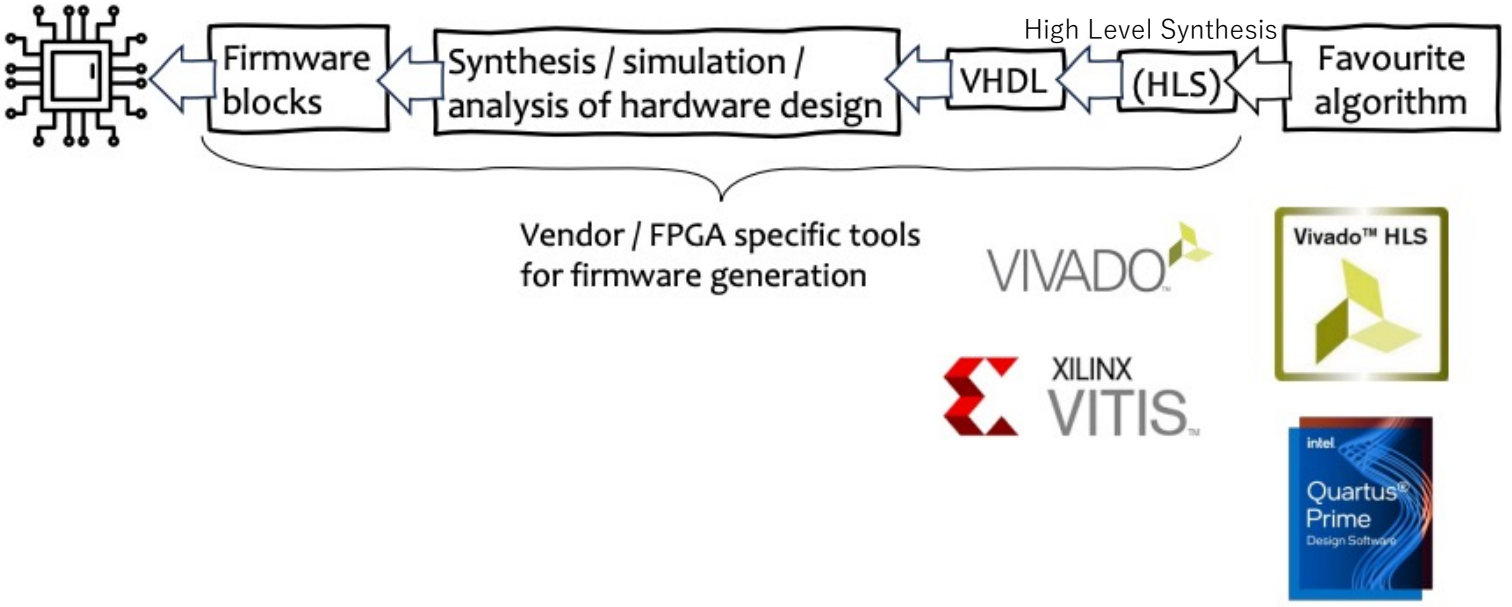
Fast (i.e. Low-latency) Machine Learning

- Move improvements from ML for reconstruction to online.
- Why “ML on FPGA” (*)?
  - Taylored Hardware with ML-specific components
    - Relevant for hardware-trigger-level and software-level applications
  - Taylored PCIe cards with FPGAs for power-efficient acceleration
    - x10 compared to GPUs. Relevant for software-level applications

- Tools available to ease implementation of state-of-the-art ML algos (pioneered by HEP community)

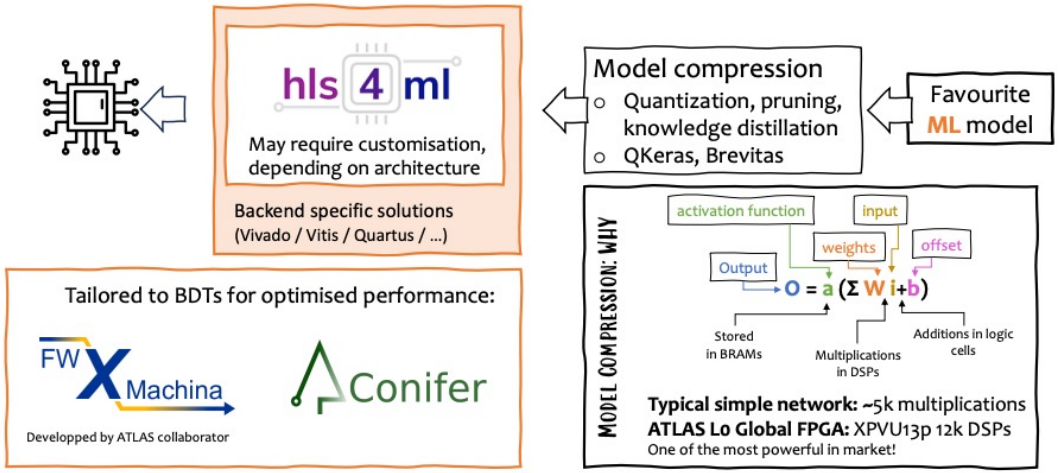
(*) “ML on FPGA” refers to ML inference ONLY. GPUs are typically used for training.

How to implement algorithms to FPGAs



Credit: A. Sfryla (Geneva)

Tools for ML on FPGAs - pioneered by HEP



Credit: A. Sfryla (Geneva)

- ML-specific tools developed from vendors as well as HEP communities (e.g. hls4ml, fwXmachina)
- Opportunities opened up for explorations of how to use FPGAs as accelerators
  - For tracking, quantised & prunned GNN Implementation on FPGA in progress.

→ Extremely active area at HEP, along with trigger developments for HL-LHC.

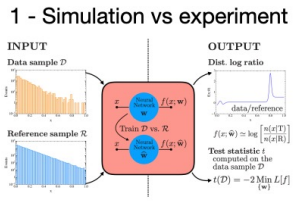
ML for physics analyses

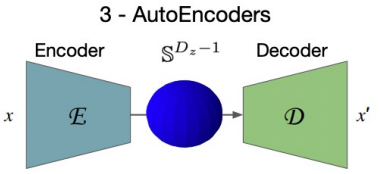
- Event classification, statistical analysis and inference.

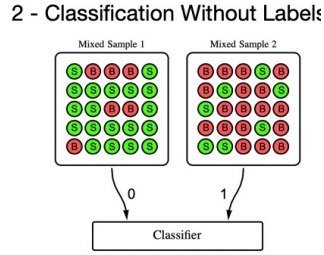
- Anomaly detection
  - Given no clear BSM signals found, how can we search for many new signatures?
  - There are exciting new ideas on data-driven searches to expand search space
    - Sensitive to data representation. Some minimal model assumptions, e.g. bump-hunt, can be used.
    - Recent algorithm release by Louis, inspired by AEs and generative models that allows for both anomaly detection and data-driven background modeling

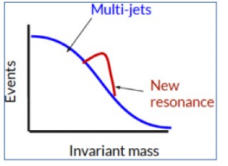
ML-based anomaly detection

Image credit: B. Dillon







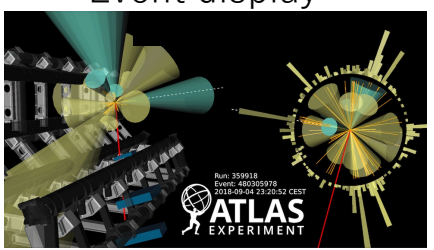


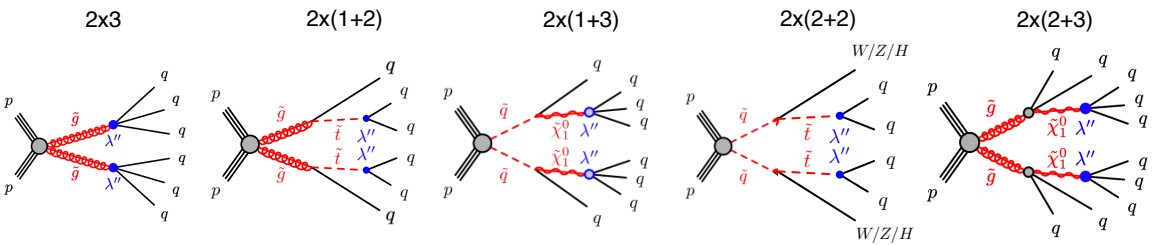
GAN-AE: an anomaly detection algorithm for New Physics search in LHC data, Eur. Phys. J. C 83, 1008 (2023)

Example: Anomaly search in multi-jet final state

- Search for R-Parity Violating SUSY in many jet final state
- Minimal assumption is pair-production of BSM particles that decays identically.

Event display



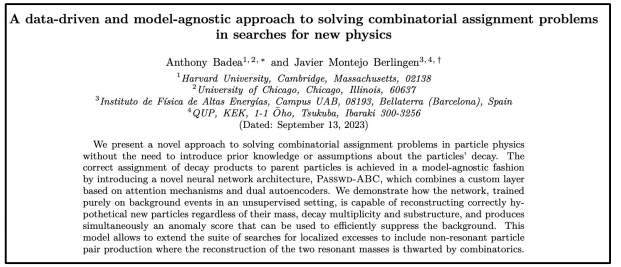


- Big problem dealing with combinatorics
  - For events with 10 jets, there are 10k+ combinations.

→ Solve by ML-based data-driven & model-agnostic methodology

Proof of concept

- Successfully built a NN that
  - splits events into two (three) sets: BSM1, BSM2 (and ISR)
  - earns by itself useful features and a metric to compute similarity between both sets, and minimizes that metric.
  - Can be trained directly on data.
  - Is permutation invariant, no impact from permuting jets within a set, or the two sets among them.
- In validation, the NN reconstructs correctly the peak of the different signals, despite not having seen any signal during the training.



A data-driven and model-agnostic approach to solving combinatorial assignment problems in searches for new physics

Anthony Badea[1,2,*] and Javier Montejo Berlingen[3,4,†]
[1] *Harvard University, Cambridge, Massachusetts, 02138*
[2] *University of Chicago, Chicago, Illinois, 60637*
[3] *Instituto de Física de Altas Energías, Campus UAB, 08193, Bellaterra (Barcelona), Spain*
[4] *QUP, KEK, 1-1 Oho, Tsukuba, Ibaraki 300-3256*
(Dated: September 13, 2023)

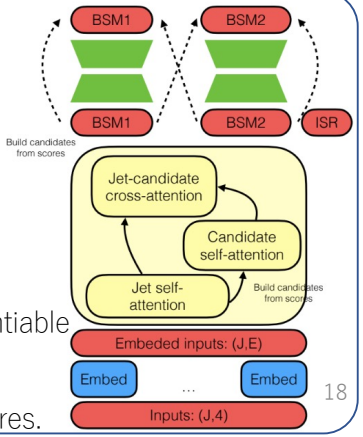
We present a novel approach to solving combinatorial assignment problems in particle physics without the need to introduce prior knowledge or assumptions about the particles' decay. The correct assignment of decay products to parent particles is achieved in a model-agnostic fashion by introducing a novel neural network architecture, PASSWD-ABC, which combines a custom layer based on attention mechanisms and dual autoencoders. We demonstrate how the network, trained purely on background events in an unsupervised setting, is capable of reconstructing correctly hypothetical new particles regardless of their mass, decay multiplicity and substructure, and produces simultaneously an anomaly score that can be used to efficiently suppress the background. This model allows to extend the suite of searches for localized excesses to include non-resonant particle pair production where the reconstruction of the two resonant masses is thwarted by combinatorics.

https://arxiv.org/abs/2309.05728 , submitted to PRL.

Also a related pheno. paper "The ABC of RPV", J. High Energ. Phys. 2023, 215 (2023).

NN model details

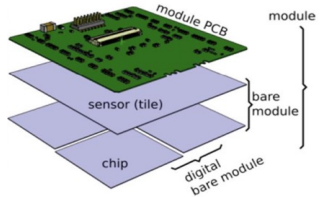
- Embedding
  - Per-jet, maps into a new feature space (J, 4) → (J, E)
- Transformers and attention mechanisms
  - Combines 3 vectors into a new vector. No learnable parameters, permutation equivariant
    E.g. jet self-attention: (J,E) →(J,E)
- Building candidates by grouping jets
  - Interpret the 3 first features per jet as a multiclass score to be assigned to BSM1, BSM2, ISR
  - Use Gumbel-Softmax to get a discrete choice of which jet to assign to each candidate, but still differentiable
- Autoencoders
  - NN that reduces for each candidate into a small latent space and tries to reconstruct the original features.



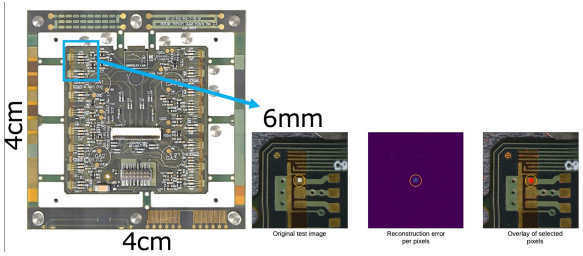
Louis Vaslin (QUP)
→ See his poster for the details

ML for Detector Building

Module components



- For the LHC upgrade, we build ~3k pixel-detector modules in Japan for coming few years.
  - Strict Quality Control requires Visual Inspection at each O(10) stages.
- Instead of manual inspection by eyes, developed new tool of defect detections “Anomaly Detection”.
  - Focus on FLEX Printed Circuit Boards made in Japan (Time: 10min→1min / sheet).
    - Unsupervised for unknown defects and
    - Supervised for known labelling.
  - Integrating in production workflow in progress.



- Plan to transfer the tool for other applications

Sharing ML expertise & building connections with communities around

- First “ML at HEP” workshop (2023 Feb)
  - 120 registrants
  - Second annual event (2024 Jan)
    - Focus: HEP, cosmology, achievements
      https://conference-indico.kek.jp/event/253/

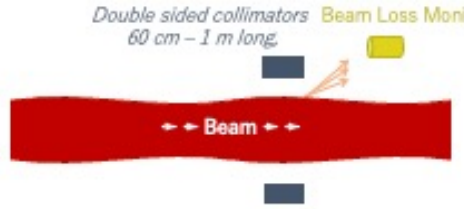
- “AI-Smart x TDAQ” workshop (2023 Sep)
  - Focus: fast ML, tracking, operation, facilities
  - 50 registrants from colliders (ATLAS, BelleII, ALICE), muons, and accelerators

  → Based on strong interests & future potentials, launching a school series e.g. ”ML on FPGA” school (2024 Feb)

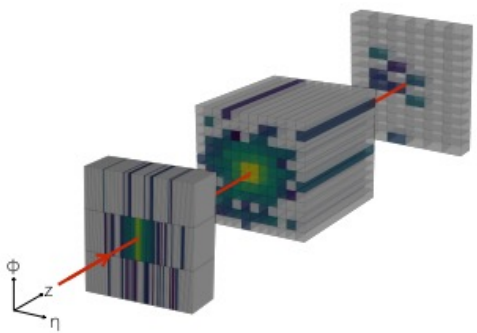
Other applications with large interests

D. Mirarchi (CERN)

- ML applications in LHC acceralator operation
  - Fully automated collimator alignment based on ML operationally (alignment time: 1/10 wrt Run1)
  - Anomaly detection in loss pattern for early detection of collimation hierarchy breakage



- ML application in detector simulation
  - Using deep generative models for critically slow simulation components e.g. calorimeters using Generative Adversarial Network (speed: 100,000x wrt full simulation. Critical for HL-LHC.
  - Surrogate modeling to efficiently model complex systems.



Summary

- ML applications at HEP and LHC continues success stories

- A QUP, leveraging machine learning for automating and accelerating “Scientific Discoveries” in the area on the early universe and Dark Matter in collider physics and cosmology.
  - ML applications
    - to physics analyses in our interests for maximising scientific outputs
      e.g. New Physics search and Higgs property measurements
    - to facilities for smart automation and operation e.g. detector building and triggering
  - ML algorithm developments such as Anomaly Detection techniques.

End

International Center for
Quantum-field Measurement Systems for
Studies of the Universe and Particles
WPI research center at KEK