在ATLAS实验研究进展和在未来对撞器量子机器学习应用计划

第三届高能所深度学习研讨会, 2023年6月15日

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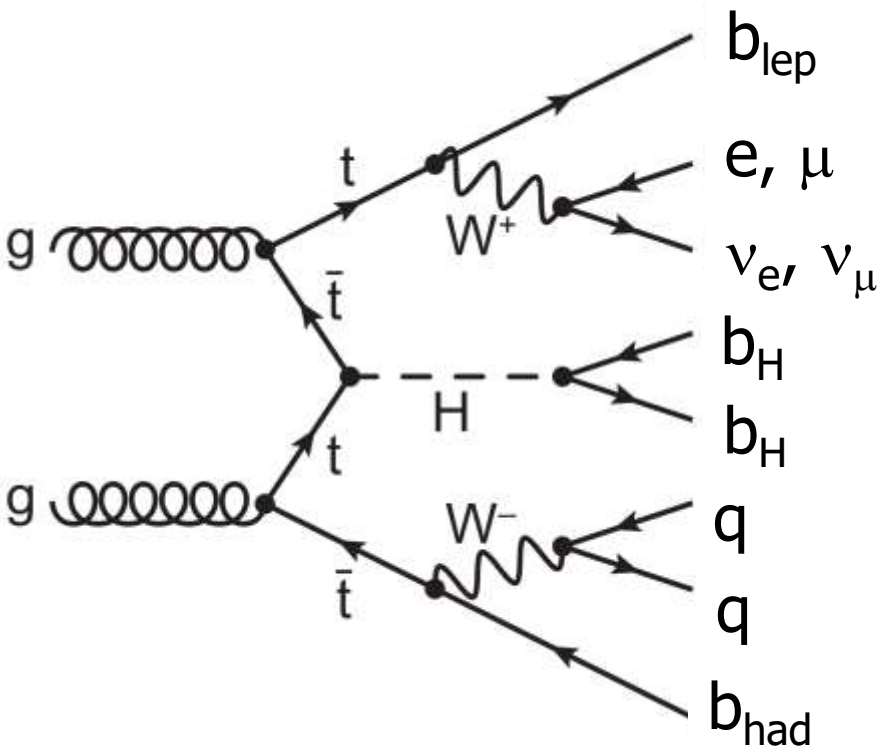
Introduction

- Dedicated ML groups exists in the ATLAS Collaboration.
- IHEP is actively contributing to the ATLAS ML activities.
  - Symmetry Preserving Attention Networks for jet-parton assignment (大川英希)
  - Boosted W-jet tagging using ParticleTransformer & ParticleNet (王书栋，徐达，李刚，方亚泉)
  - Both presented at ATLAS ML Workshop this year. 3 talks from China (2 from IHEP☺)
- Future colliders, especially the High Luminosity LHC will face major computing challenges.
  - ML will be the baseline to cope with the situation
  - Quantum computing may bring in a big leap. Various studies ongoing at IHEP: e.g. quantum transformers (Abdualazem Mohammed，王书东，沙其雨，大川英希，方亚泉等), quantum tracking (大川英希), quantum GAN (黄晓忠，大川英希，李卫东)

I will cover these items today

Michael Fenton, Alexander Shmakov, 大川英希 (IHEP), Yuji Li, Ko-Yang Hsiao, Shih-Chieh Hsu, Daniel Whiteson, Pierre Baldi

Symmetry Preserving Attention Networks



- Collaboration w/ UC Irvine & Washington
- Jet-parton assignment (i.e. top reconstruction) is a crucial component in $t\bar{t}$ & $t\bar{t}H$ analyses.
- Standard algorithms compare all possible permutations of jets per event & systematics
  - Combinatoric diverges with jet multiplicity.

Unsorted list of jets

$j_1, j_2, j_3, j_4, j_5, j_6, j_7, j_8$

Target partons

$b_{lep}, b_H, b_H, \varnothing, b_{had}, \varnothing, q, q$

Attention for Top Reconstruction

- Attention mechanisms are superceding RNNs & LSTMs in neuro linguistic programming.
  - Permutation invariant & can handle variable-length lists
- **Tensor Attention: generalization of attention to encode symmetries** ($t\leftrightarrow\bar{t}$, $b\leftrightarrow\bar{b}$ in H, $q\leftrightarrow\bar{q}'$ in W)

e.g. Two-body decay symmetries (W→$q\bar{q}'$, H→$b\bar{b}'$)

$$S^{ijk} = \frac{1}{2}(\theta^{ijk} + \theta^{jik})$$

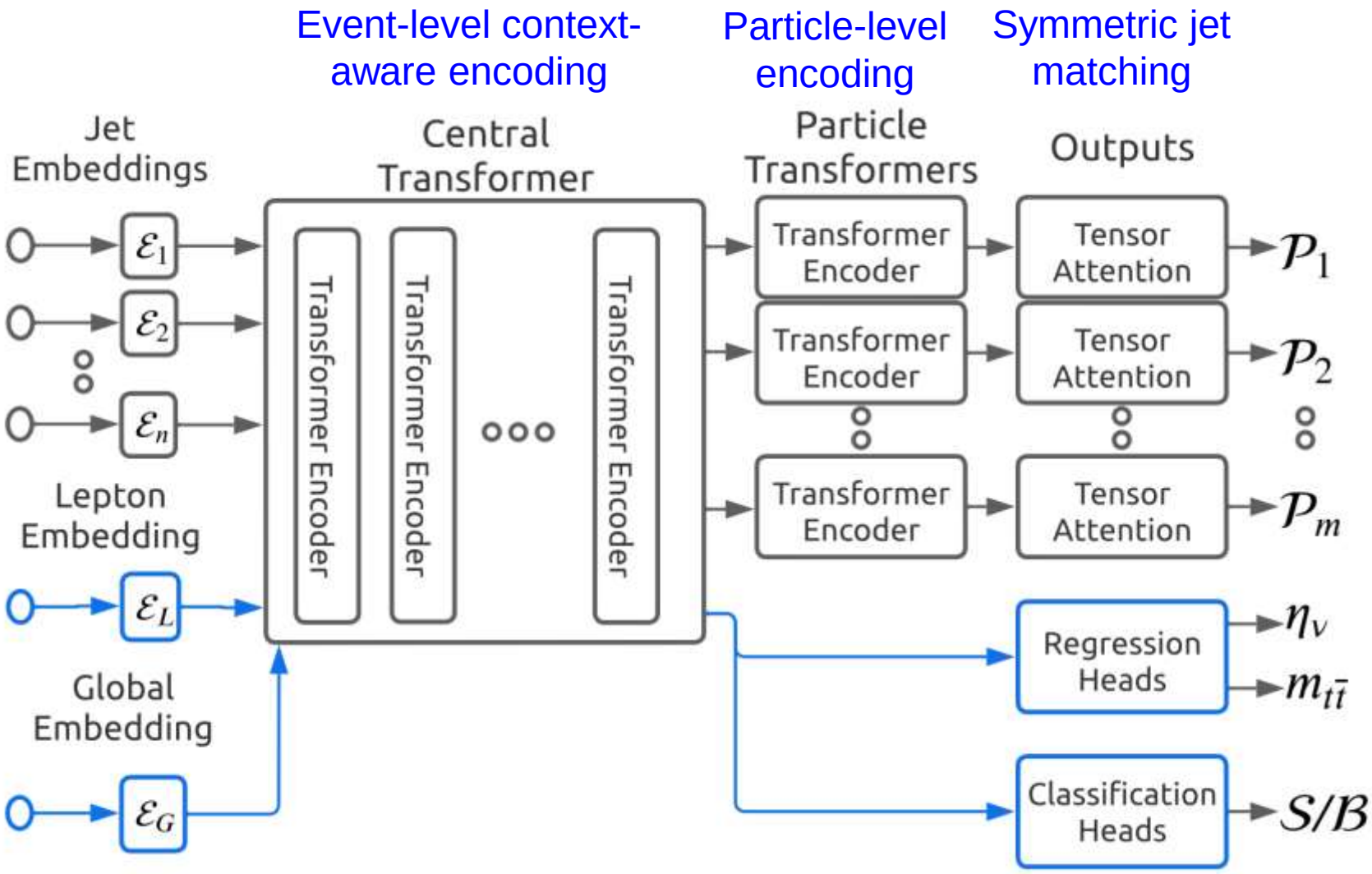
$$O^{ijk} = X^i_n X^j_m X^k_l S^{nml}.$$

$i\leftrightarrow j$ symmetry

- Allow us to test every possible permutation in a single pass.

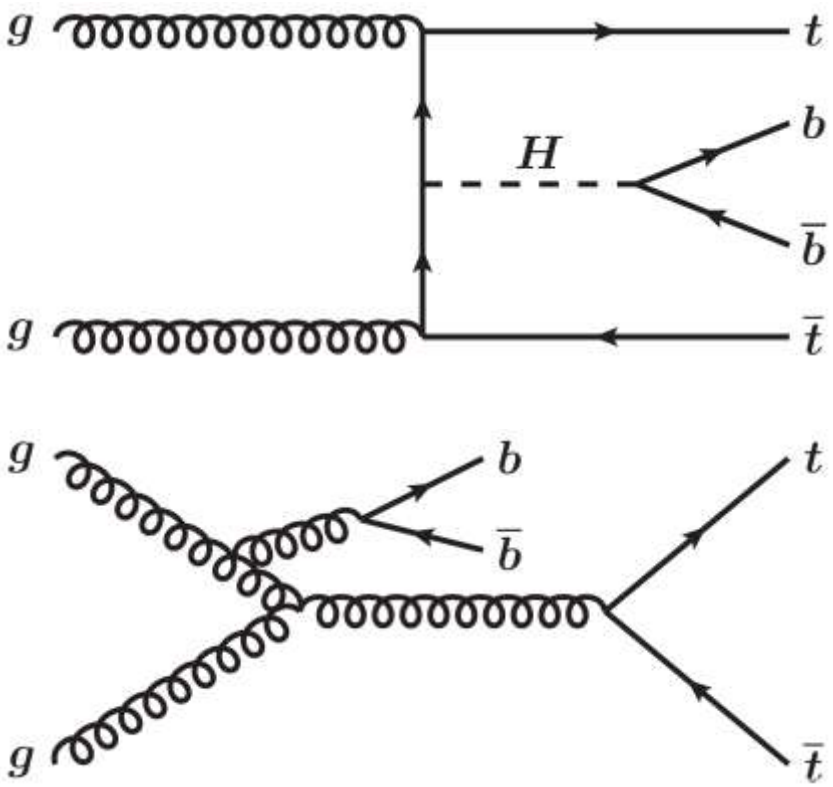
Symmetry Preserving Attention Networks (SPA-Net)

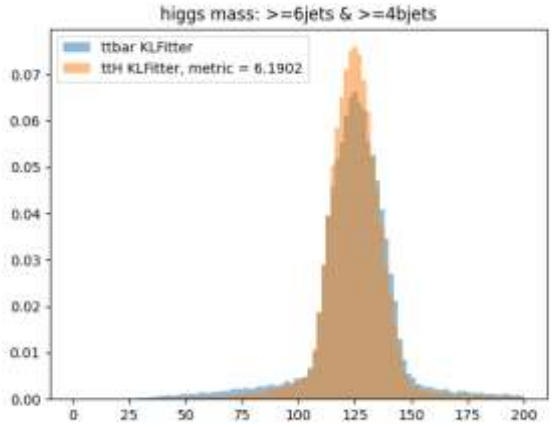
Unordered list of object four-momenta + additional info (e.g. btag) & event-level variables (e.g. MET)

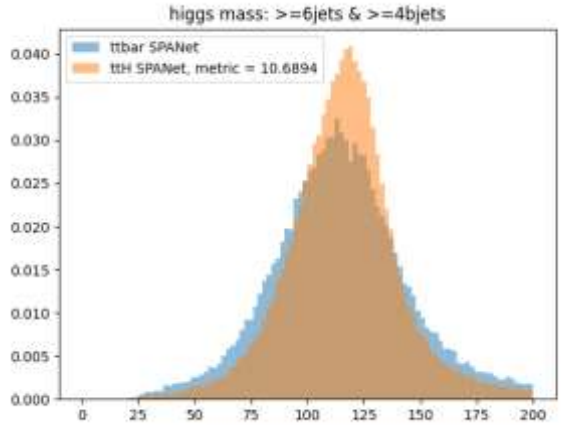


Full jet/doublet/triplet assignment distributions for every particle targe (e.g. t, H)

$t\bar{t}$H(→$b\bar{b}$) semi-leptonic



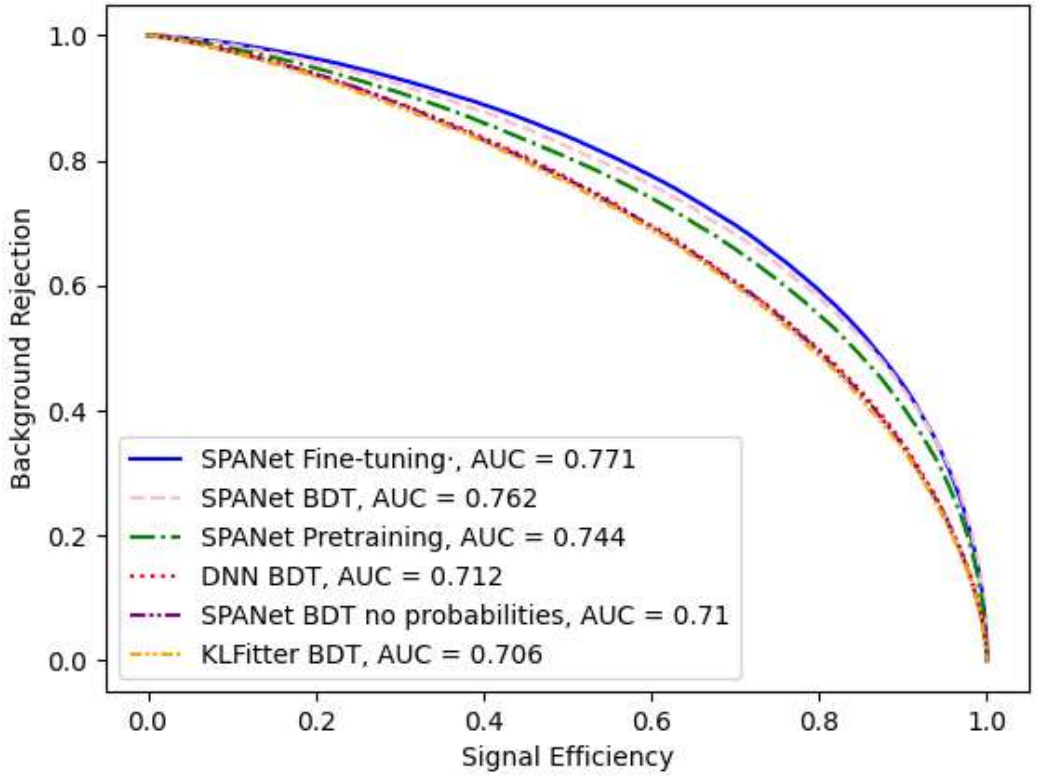




- t & H kinematics are main inputs to the BDT.
  - **Reco. efficiency is significantly improved w/ SPA-Net: 42.6%** in 7jet events (permutation DNN: 36.4%, KLFitter: 17.7%)
- However, the fraction of reconstructable events is only 35% in $t\bar{t}$H semi-lep. events.
- **"Goodness" of the jet-parton assignment is also important to remove unreconstructable events.** → i.e. likelihood for KLFitter, a score for permutation DNN

New Features: Signal/BG Discrimination

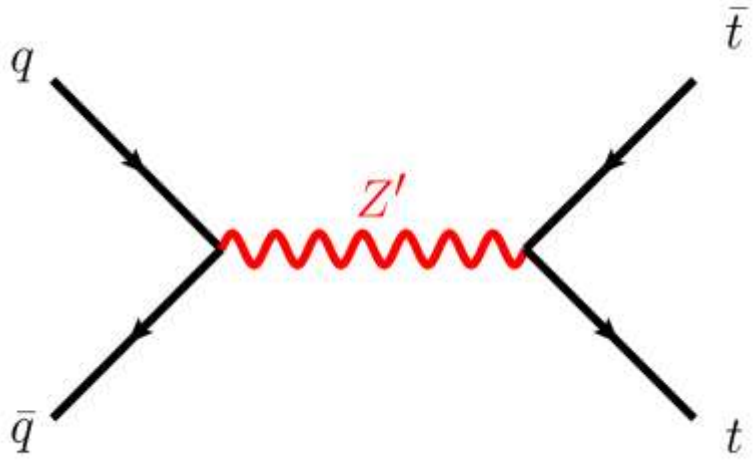
- Using SPA-Net jet assignment & running the traditional kinematics-based BDT analysis gives the 2nd best result.
- Fully using SPA-Net: jet-assignment & BG/signal discrimination with the fine tuning performs the best.
  - SPA-Net can also learn the kinematics!!
- SPA-Net significantly outperforms the traditional method (KLFitter) & even permutation DNN.

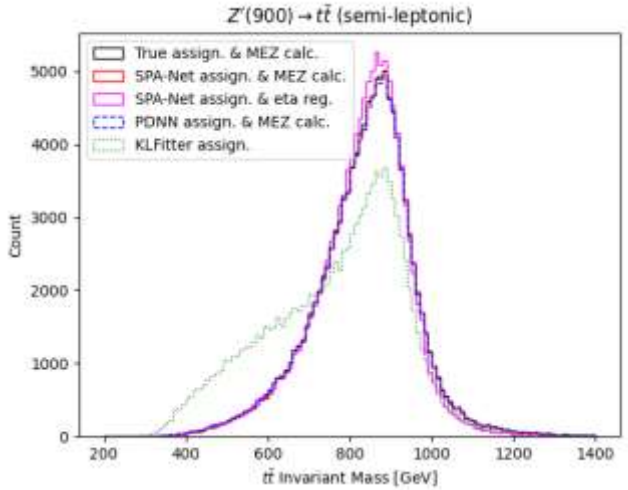


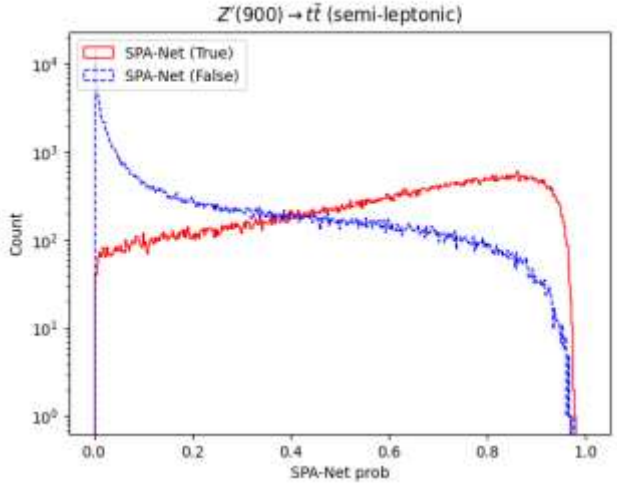
Transformer architecture provides us with meaningful embeddings for every jet, particle, and event: a big benefit over permutation-based models

Z'→$t\bar{t}$ Searches

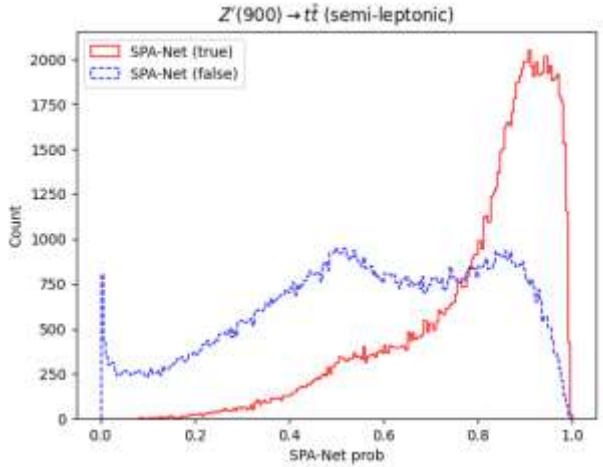
Reco eff.: SPA-Net: 75.6%, PDNN: 64.9%, KLFitter: 52.1%



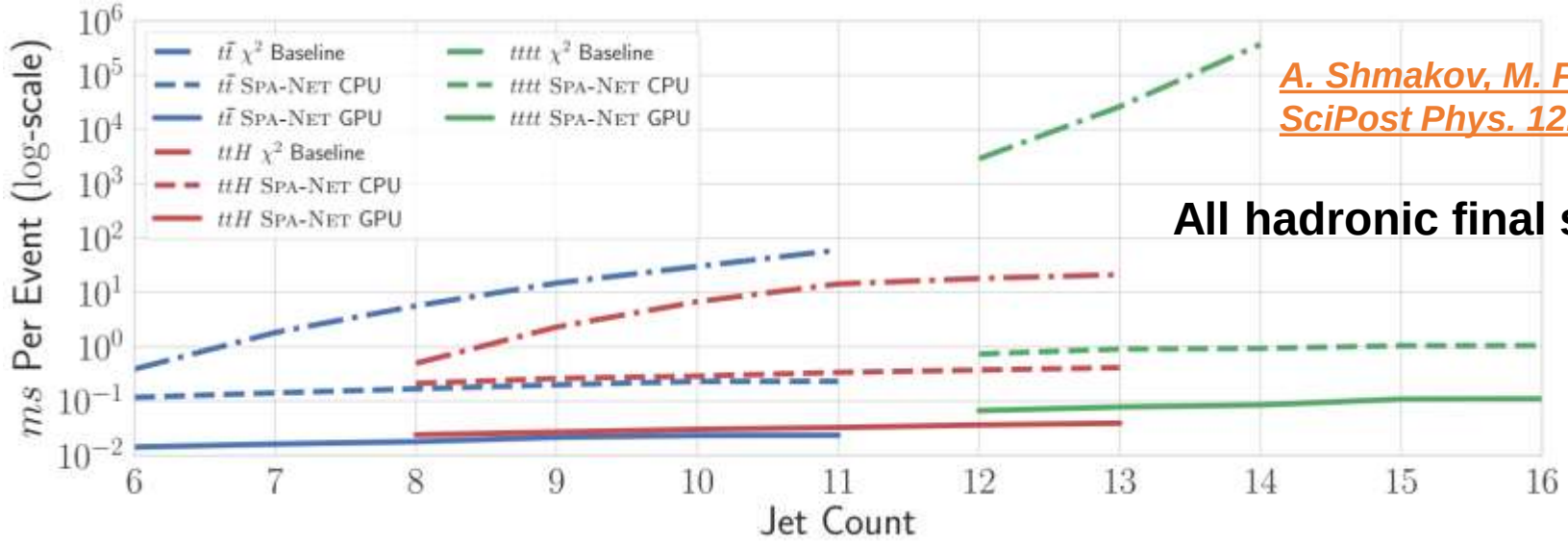




- $t\bar{t}$ resonance searches in LHC Run 2 are already systematics dominated **→ simply adding more data does not help!**
- SPA-Net provides excellent mass reconstruction, compatible w/ truth assignment.
- SPA-Net probabilities will significantly enhance BG rejection.
- Preliminary global significance for 140 fb^{-1} (full LHC Run 2 stat):
  - Z' 500 GeV: 1.2σ (KLFitter) → 1.8σ (PDNN) → 3.3σ (SPA-Net)
  - Z' 900 GeV: 2.6σ (KLFitter) → 3.0σ (PDNN) → 5.0σ (SPA-Net)



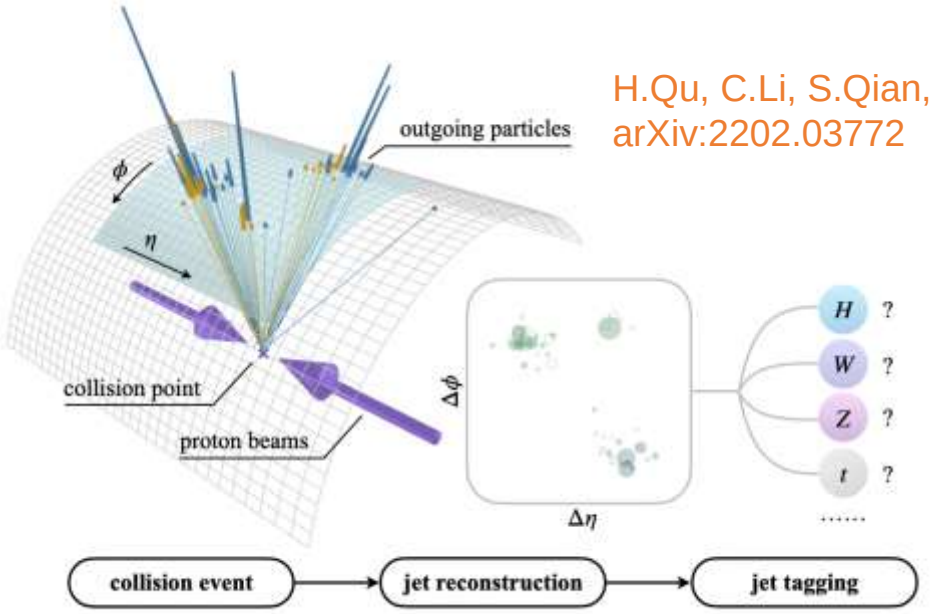
SPA-Net CPU/GPU Time



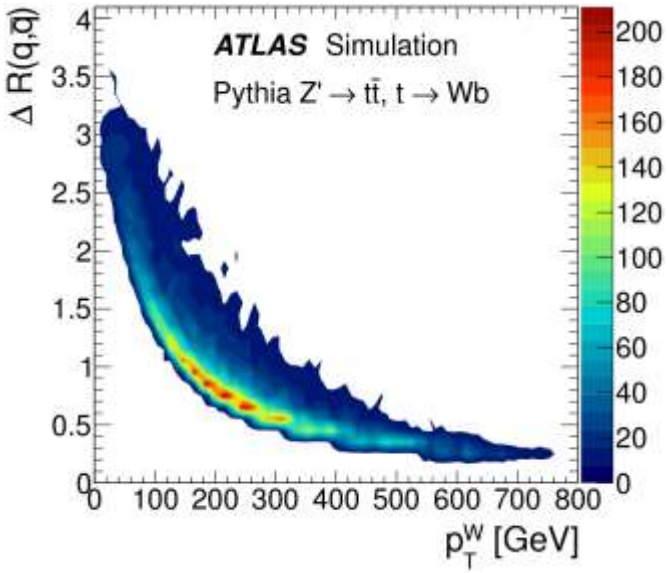
- **A few orders of magnitude improvement** w/ SPA-Net compared to χ^2 or KLFitter. A further acceleration w/ GPU.
- One order of magnitude faster than permutation DNN for ttH (i.e. high multiplicity events)!

	ttH semilep	Z'→ttbar semilep
SPA-Net	3534 events/s [GPU] 852 events/s [CPU]	4407 events/s [GPU] 705 events/s [CPU]
Perm. DNN	101 events/s [GPU] 51.4 events/s [CPU]	3034 events/s [GPU] 2626 events/s [CPU]
KLFitter	1.95 events/s	24.4 events/s

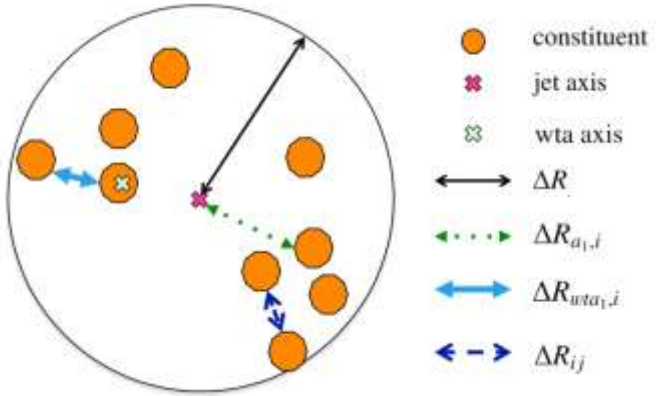
Boosted jet tagging (W)



H.Qu, C.Li, S.Qian, arXiv:2202.03772

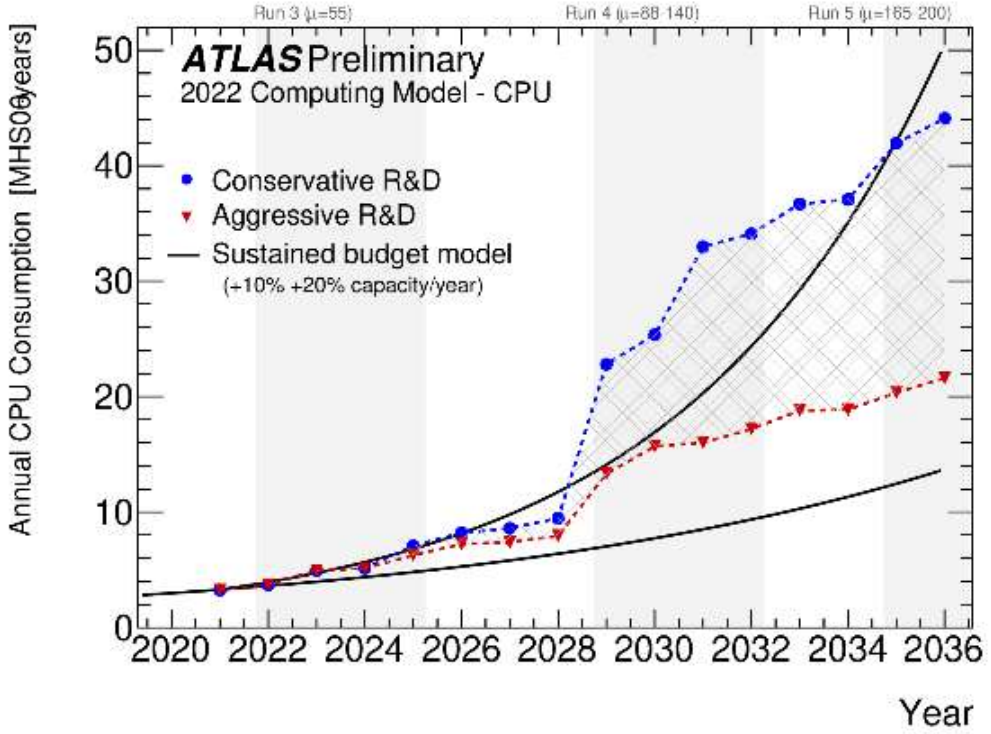


ATLAS Collab., Eur. Phys. J. C 76 (2016) 154



- Hadronically decaying high-p_T bosons and top quarks begin to merge & end up in single jets. Using large-R jets and their substructure allow us to identify such jets and reject multijet BG.
- Crucial component for boosted analyses. Often has dominant impact on the sensitivity.
- IHEP team is leading the newest implementation of the W-jet tagging!

High Luminosity LHC & Beyond



- At the HL-LHC, **we will enter the "Exa-byte" era. Annual computing cost will increase by a factor of 10-20**
- **<u>Without various innovations, the experiment will not be able to operate</u>.** GPUs & other state-of-the-art technologies will be the baseline at the HL-LHC.
- **Quantum computing will also likely bring another "leap".**

- Two of the highly CPU consuming components: **(1) track reconstruction for both data/simulation & (2) simulation of shower development in the calorimeter.**
- **We have agreed to collaborate with DESY on these two topics.**

大川英希 & Federico Meloni et al. (DESY)

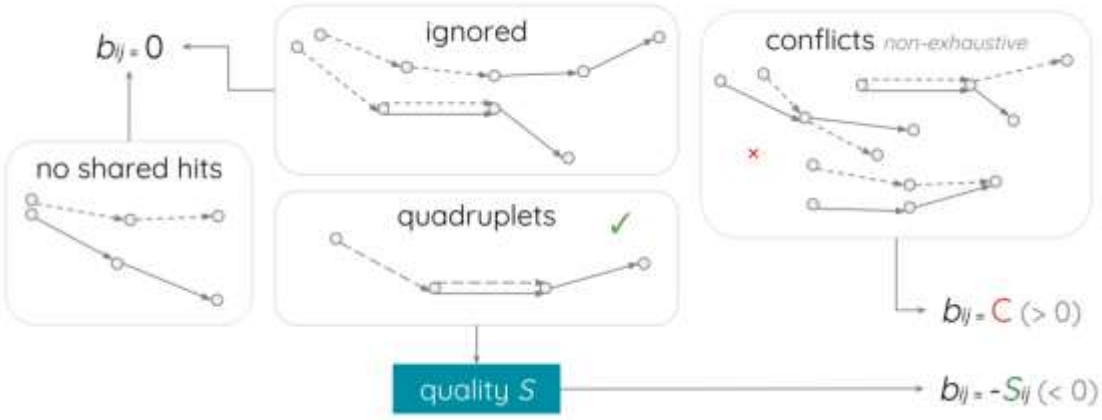
Quantum Tracking

F. Bapst et al. Comp. Soft. Big Sci. 4 (2019) 1.

$$O(a,b,T) = \sum_{i=1}^{N} a_i T_i + \sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j$$

Quality of triplets

Compatibility b/w triplet pairs

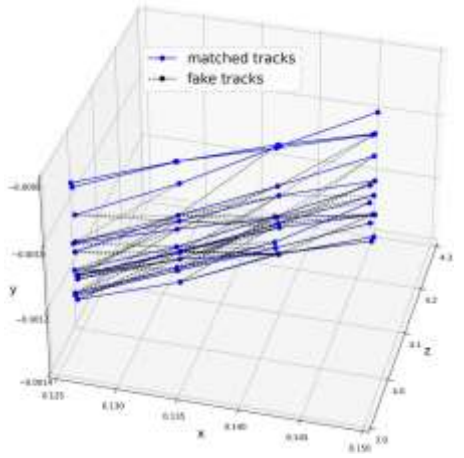


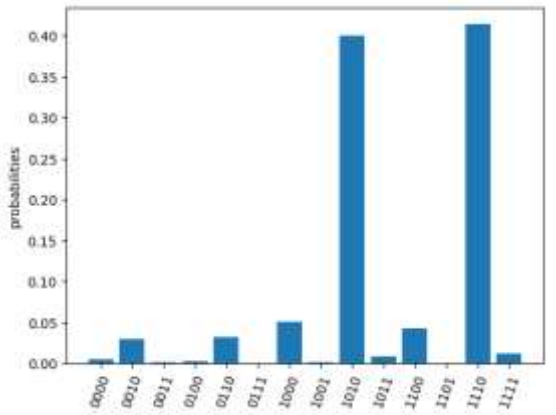
b_{ij} = 0 (if no shared hit)
= 1 (if conflict)
= $-S_{ij}$ (if two hits are shared)

- **Quantum tracking is equivalent to searching for the ground state of Ising Hamiltonian.**
- Triplets (segments w/ 3 hits) are formed from doublets (segments w/ 2 hits).
- Triplets are used to reconstruct tracks & can be regarded as a **quadratic unconstrained binary optimization (QUBO)** problem.

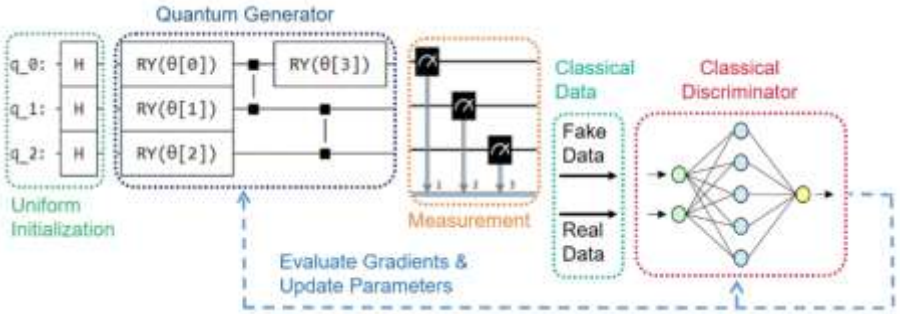
QUBO Studies w/ Quafu

- Tracking is a high multiplicity task & requires **access to high qubit machines.**
- DESY provided test QUBO that meets quafu condition (136 qubit machine) to check the precision.
  - “True” answer & D-wave annealers’ results are available for comparison
- Simple first test with small qubits successfully ran. Currently modifying Hamiltonian & establishing circuits for 136 qubits.



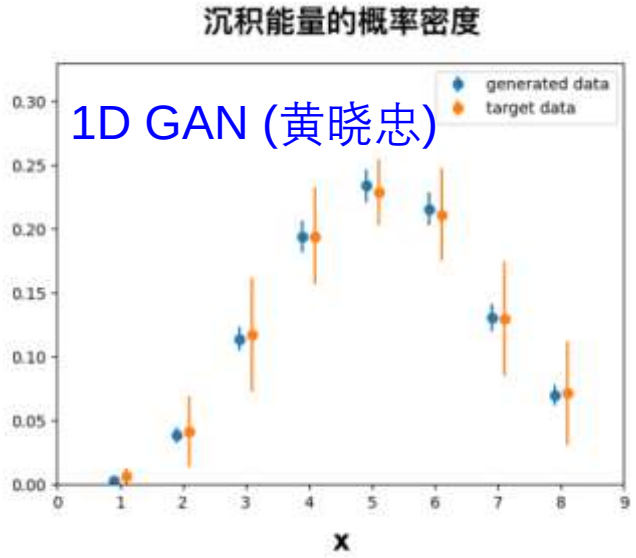


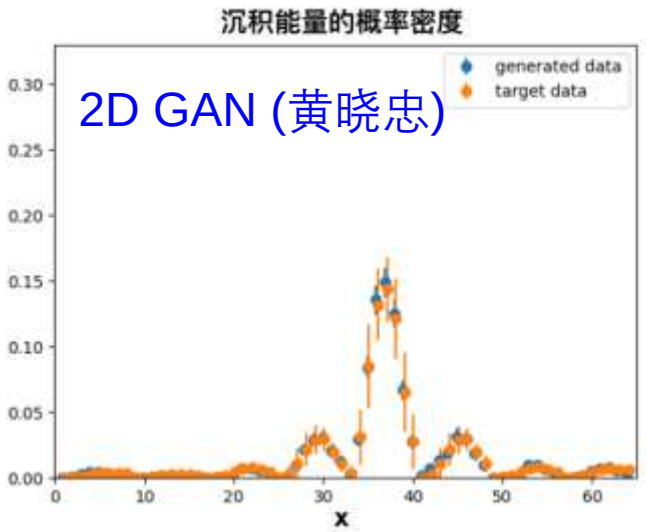
Quantum GAN

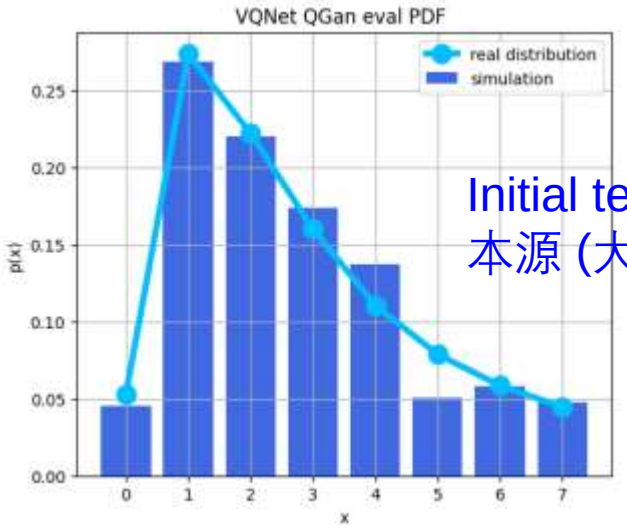


黄晓忠，大川英希，李卫东 & Kerstin Borras et al. (DESY)

- Classical GAN is partially used in fast sim (Atlfast3), but is still time consuming → Quantum GAN may be able to reduce the training time & improve the accuracy.
- DESY & IHEP are using a common CLIC dataset to pursue the QGAN studies.
  - Establishing 1D/2D QGAN & checking noise impact on quantum simulator (黄晓忠)
  - Running QGAN on domestic quantum computers [本源，夸父] (大川英希)







Initial tests w/ 本源 (大川英希)

Summary

- State-of-the-art ML technologies are introducing paradigm shifts in society as well as in high energy physics including LHC experiments.
- Presented two ongoing studies in ATLAS using state-of-the-art ML technologies. Both utilize attention & transformer in some ways.
  - SPA-Net is actively adopted in ATLAS, but studies themselves do not rely on internal data & are collaboration-independent. Paper under preparation.
  - W-tagger studies are aiming for an ATLAS PUB note.
- In addition to classical ML, quantum ML may bring in another phase of innovation for the future colliders.
  - Two collaborative projects with DESY are ramping up.

Stay tuned! 谢谢大家！