Automated discovery of jet substructure analyses

Yue Shi Lai

Lawrence Berkeley National Lab, Division of Nuclear Science

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“Why” and “what can you do with it?”

- Jet substructure studied as “on-off switches”, results have not been shown how to probe the medium quantitatively with jet substructure

- E.g. CMS $z_g$: Red-dashed (BDMPS) and orange-dashed (SCET) require 10% accuracy, beyond experimental reach

- State-of-the-art flow analyses look like this:

A. M. Sirunyan et al. (CMS), Phys. Rev. Lett. 120, 142302 (2018)

Ingredient: Neural network (NN)

- Repetition of: linear transform + nonlinear “activation”
- Universal function approximator
- Scalability/throughput for huge datasets (and many “success stories”)
- But learned information is hidden inside 100–10^8 neurons

Ingredient: Symbolic Regression

Genetic algorithm ("mutation" of the equation as a graph) search for the right equation

- Regularize by complexity = number of nodes
- Difficult to apply for high dimension and (HEP/NP-) large data sample
- Schmidt & Lipson criticized for having the exact right phase space for Hamiltonian mechanics as input

Nature of stat. analyses, permutation symmetry

- Analyses are always mathematical functions:
  - Per-event or per-reconstructed object observable
  - Observable is then statistically analyzed (histograms = a series of step-functions, means, ..., correlation, event mixing)

- Key ingredient is permutation symmetry:
  - Regular NN can be made permutation symmetric by symmetric polynomials
  - New even for NN: previously never attempted large-scale and with more than 1 simultaneous variable
  - Training works, and each training step corresponds to $N!$ normal NN training
    $\Rightarrow$ Gigantic speed-up (typically $N \approx 1000$ with a “minimal” analysis)

- See arXiv:1810.00835 for details how to construct them
A NN that simultaneously builds observables and tests, if a legal (permutation symmetric) analysis can be constructed to use it.
Input Monte Carlo

- Jewel and Linearized Boltzmann Transport (LBT) for $\sqrt{s_{NN}} = 5.02$ TeV Pb-Pb 0–10% embedded into HYDJET 1.9 0–10%
- Jet $100 < p_T < 500$ GeV/c selection after UE (UE subtracted) and has the smearing of an actual measurement

- Jewel with $0.16 \leq T_i \leq 0.76$ GeV/$k$, $0.2 \leq \tau_i \leq 0.8$ fm
- 200k events per $T_i$, $\tau_i$, or 3.2M Jewel events total

- LBT with Gubser flow, $0.383 \leq \hat{T} \leq 0.538$ GeV/$k$ (to match Jewel)
- Initial partons + hadronization with PYTHIA 8
- 200k events per $\hat{T}$, or 0.8M LBT events total

- Fully “whitened”: jet spectra are reweighted to have no $T_i$, $\hat{T}$ or $\tau_i$ dependence, Jewel/LBT centrality randomized with HYDJET centrality
Input jet shape/substructure

- Each polynomial corresponds to a multigraph $G = (V, E)$

\[ EFP_G = \sum_{j_1} \cdots \sum_{j_{NV}} \left( z_{j_1} \cdots z_{j_{NV}} \prod_{(k,l) \in E} \theta_{kl} \right) \]

- Set size of $E = \text{degree of polynomial}$
- 490 polynomials up to degree 7, 486 are used (4 remaining takes 6 min per jet to calculate)
- Substructures are not UE subtracted (left for NN)

\[ = \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} \sum_{i_3=1}^{M} \sum_{i_4=1}^{M} z_{i_1} z_{i_2} z_{i_3} z_{i_4} \theta_{i_1i_2} \theta_{i_2i_3} \theta_{i_2i_4} \theta_{i_3i_4} \]

Last ingredient: “Nudge” the NN to simplicity

\[ R(x_1, x_2, x_3) \text{ in 3D} \]

See arXiv:1810.00835

- \( R \) takes the bound \( l_{im} = \frac{\partial \text{out}_l}{\partial \text{in}_m} \) and counts how many variables are in use.
- Adjust the regularization \( R \) until the result is simple enough (LASSO).
- Also new for NN: Interval arithmetic bounds for regularization.
- Regularized NN can then be fed into symbolic regression, with a (weakly) modified FFX [M. Trent, Genetic Programming Theory and Practice IX, Springer (2011)].
N = 2500 jets needed to determine $T_i$

Overall analysis:
\[ d_{1,SR} = 8.99 - 0.176N\langle c_{16} \rangle - 0.175N\langle c_1 \rangle \]

First approximate $c_1$ (Einstein notation):
\[ c_{1,SR} = 0.0112 + 45.5\theta_{ab}\theta_{ac}\theta_{bc}\theta_{ad}\theta_{bd}\theta_{ae}\theta_{de}\theta_{za} \cdots \theta_{ze} + 
+ 20.9\theta_{ab}\theta_{ac}\theta_{bd}\theta_{ad}\theta_{be}\theta_{ze} \cdots \theta_{ze} + 
+ 17.7\theta_{ab}\theta_{ac}\theta_{bd}\theta_{cd}\theta_{ae}\theta_{de}\theta_{za} \cdots \theta_{ze} + 
+ 8.63\theta_{ab}\theta_{ac}\theta_{bd}\theta_{ad}\theta_{ae}\theta_{de}\theta_{ze} \cdots \theta_{ze} - 
- 3.08\theta_{ab}\theta_{ac}\theta_{ad}\theta_{ae}\theta_{de}\theta_{za} \cdots \theta_{ze} - 
- 1.08\theta_{ab}\theta_{ac}\theta_{ad}\theta_{de}\theta_{za} \cdots \theta_{ze} + 0.769\theta_{ab}\theta_{ac}\theta_{ad}\theta_{ae}\theta_{af}\theta_{ag}\theta_{ah}\theta_{za} \cdots \theta_{zh} - 
- 0.233\theta_{ab}\theta_{ac}\theta_{ad}\theta_{de}\theta_{za} \cdots \theta_{ze} - 0.0377\theta_{ab}\theta_{ac}\theta_{ad}\theta_{de}\theta_{za} \cdots \theta_{ze} - 
- 0.00483\theta_{ab}\theta_{ac}\theta_{ad}\theta_{de}\theta_{za} \cdots \theta_{ze} - 0.00508\theta_{ab}\theta_{ac}\theta_{ad}\theta_{de}\theta_{za} \cdots \theta_{ze} - 
- 4.51 \times 10^{-5}\theta_{ab}\theta_{ac}\theta_{ad}\theta_{de}\theta_{za} \cdots \theta_{ze} \]

$c_{1,SR}$ uses 5th and 7th order (“prongs”) correlation

$c_{1,SR} < 0$ becomes depopulated with lower temperature

A feature of Jewel recoil

The NN never saw any non-recoil events, yet it found out something similar to the groomed jet mass (CMS-HIN-16-024, arXiv:1805.05145)!

100 < $p_T$ < 300 GeV/c plotted
Result for Jewel

- **Approximate** $c_{16}$:

$$c_{16,SR} = 0.0362 + 0.594 \theta_{ab}^3 \theta_{ac} \theta_{ad} \theta_{ae} z_a \cdots z_e + 0.575 \theta_{ab}^2 \theta_{ac} \theta_{ad}^2 z_a \cdots z_e + 0.420 \theta_{ab} \theta_{ac} \theta_{ad}^4 z_a \cdots z_e + 0.187 \theta_{ab} \theta_{ac} \theta_{ad} \theta_{ae} z_a \cdots z_e - 0.0465 \theta_{ab}^3 z_a z_b - 0.0453 \theta_{ab}^4 z_a z_b - 0.0333 \theta_{ab}^5 z_a z_b - 0.0328 \theta_{ab}^2 z_a z_b - 0.0196 \theta_{ab}^6 z_a z_b - 0.0146 \theta_{ab} z_a z_b - 0.00963 \theta_{ab}^7 z_a z_b$$

- **A gradual, shifting distribution**

- **Expression contains simple 2-particle correlations, with a nonlinearity $\Rightarrow$ subtraction for average jet expectation**

- **100 $< p_T < 300$ GeV/$c$ plotted**
How does it work?

- Jewel was modified to produce (infinitesimal momentum) splitting tags that are clustered into jets.
- Count inside each jet the number of splittings in the same area.
- $c_{1,SR}$ and $c_{16,SR}$ both tagger for the number of internal splittings.
- Most of the regions tag few (1–4) splittings.
- The $c_{1,SR} < 0$ is used to tag very high $> 4$ splittings.
- You can also see how $c_{1,SR} < 0$ tags jets that are rarely produced from PYTHIA 8 (.235, CUETP8M1) and Herwig 7 (.1.1, H7.1-Default).
Result for LBT

- $N = 1200$ jets needed to determine $\hat{T}$
- $d_{1,SR} = 4.49 - 0.318N\langle c_{13} \rangle - 0.00653(N\langle c_{13} \rangle)^2$
- Approximate $c_{13}$:
  
  $c_{13,SR} = 0.0453 - 0.00109 \log_{10}(p_1)(\log_{10}(p_2) + \log_{10}(p_3)) - 0.000829 \log_{10}(p_2) \log_{10}(p_3)$

  $p_1 = \theta_{ab}\theta_{ac}\theta_{bc}\theta_{ad}\theta_{bd}\theta_{ae}\theta_{be}z_a \cdots z_e$

  $p_2 = \theta_{ab}\theta_{ac}\theta_{bd}\theta_{cd}\theta_{ae}\theta_{de}z_a \cdots z_e$

  $p_3 = \theta_{ab}\theta_{ac}\theta_{bd}\theta_{cd}\theta_{ae}\theta_{de}^2z_a \cdots z_e$

- Demonstrates the system generating non-linear observables
- Possibly $\log$ being function of convenience to handle the otherwise long tail (some simplification by hand)
- $100 < p_T < 300 \text{ GeV/c}$ plotted
Summary

- First time an end-to-end system is constructed to:
  - Test if jet substructure can be used to independently extract properties of the medium, with realistic no. of events
  - Discover new observables
- NN with properties that are also new for comp. science
- Observables indeed found to extract temperature for Jewel and LBT from purely observing $N = 1200–2500$ jets
- The presented system discovers the effect of Jewel recoil
  - a system probing models at a detail comparable to the current field of human experts
- Many applications beyond the immediate Pb-Pb and jet substructure studies
Part I

Backup
Jewel with no recoil
Expressibility of permutation symmetry gives the Galois theory of polynomials.

Two well-known types of polynomial:

A. Elementary symmetric polynomials:
   - $e_0(x_1, \ldots, x_n) = 1$
   - $e_1(x_1, \ldots, x_n) = \sum_{1 \leq i \leq n} x_i$
   - $e_2(x_1, \ldots, x_n) = \sum_{1 \leq i < j \leq n} x_i x_j$
   - $\vdots$
   - $e_n(x_1, \ldots, x_n) = \prod_{1 \leq i \leq n} x_i$

B. Power sum symmetric polynomials:
   - $p_k(x_1, \ldots, x_n) = \sum_{1 \leq i \leq n} x_i^k$

Both are equivalent (Newton’s identities), though not equally simple as computational graphs.
Permutation symmetry vs. algebra vs. statistics

- This still does not help with multivariate functions (where two variables cannot have a mutually different permutation)

- Solution:

\[ s_j(x) = \sum_{k=1}^{N} x_{j\pi(k)}^{m-l} x_{(j+1) \mod M, \pi(k)}^l, \quad l \in \{1, \ldots, m-1\} \]

for \( N M \)-dimensional variables (with a special case for \( M = 2 \))

- Can check using all \( M \)-dimensional symmetric polynomials, that \( s_j \) is complete (analogous to Newton’s identities)
$p_T$ dependence

$\frac{N_J}{N_J(T_i=0.36 \text{ GeV}/k)}$ for $100 < p_T < 150 \text{ GeV}/c$

$\frac{N_J}{N_J(T_i=0.36 \text{ GeV}/k)}$ for $200 < p_T < 300 \text{ GeV}/c$
$p_T$ dependence

\begin{align*}
n_{J} & \propto \frac{N_J}{N_J(T_i = 0.36 \, \text{GeV/k})} \\
\end{align*}

$100 < p_T < 150 \, \text{GeV/c}$

$200 < p_T < 300 \, \text{GeV/c}$
$p_T$ dependence

100 < $p_T$ < 150 GeV/c

200 < $p_T$ < 300 GeV/c