



# Automated discovery of jet substructure analyses

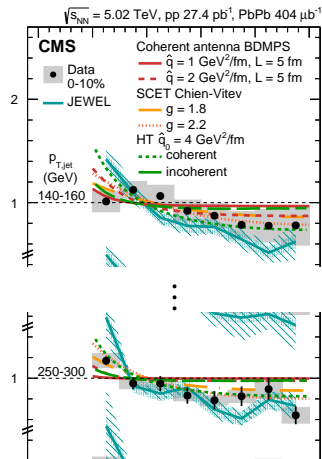
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High- $p_T$  Physics in the RHIC/LHC Era

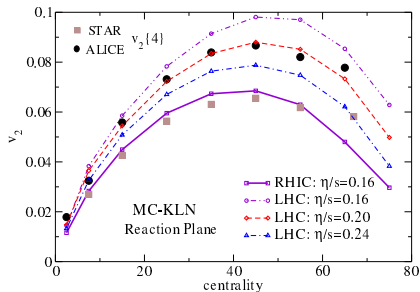
# “Why” and “what can you do with it?”

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



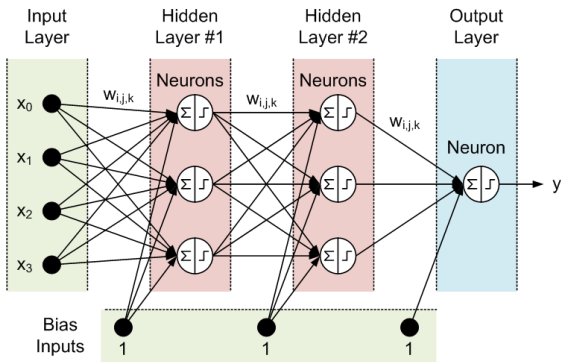
A. M. Sirunyan et al. (CMS), Phys. Rev. Lett. 120, 142302 (2018)

- 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:



H.-c. Song, S. A. Bass, U. Heinz, Phys. Rev. C 83, 054912 (2011)

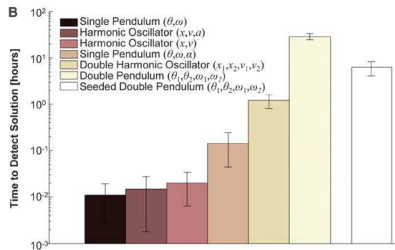
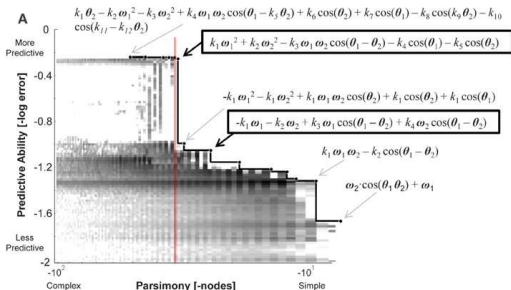
# Ingredient: Neural network (NN)



<https://www.mq15.com/en/code/9002>

- 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

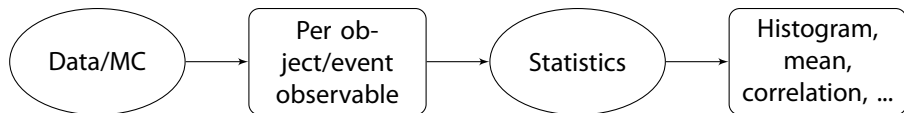
# Ingredient: Symbolic Regression



M. Schmidt & H. Lipson, Science. 324(5923), 81 (2009)

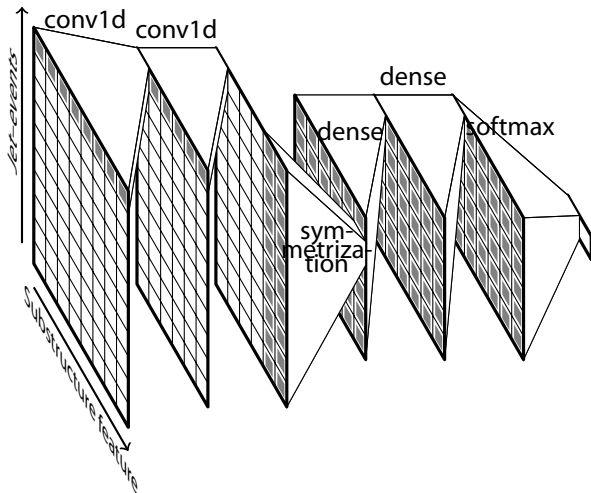
- Genetic algorithm (“mutation” of the equation as a graph) search for the right equation
- Regularize by complexity = number of nodes
- Difficult to apply for high dimension and (HEP/NP-) large data sample
- Schmidt & Lipson criticized for having the exact right phase space for Hamiltonian mechanics 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  
⇒ Gigantic speed-up (typically  $N \approx 1000$  with a “minimal” analysis)
- See arXiv:1810.00835 for details how to construct them

# Layout of the NN that approximates all possible analyses



- conv1d: Per jet/event analysis expressed as 1D convolution
- dense: Fully connected NN layer
- softmax: Transform into probability-like  $[0, 1]$

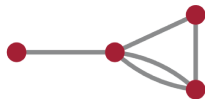
- A NN that simultaneously builds observables and tests, if a legal (permutation symmetric) analysis can be constructed to use it

# 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

- Energy flow polynomial (EFP) by Komiske, Metodiev, Thaler [J. High Energy Phys. 04 (2018): 13]
- Each polynomial corresponds to a multigraph  $G = (V, E)$
- $$\text{EFP}_G = \sum_{j_1} \cdots \sum_{j_{N_V}} \left( z_{j_1} \cdots z_{j_{N_V}} \prod_{(k,l) \in E} \theta_{kl} \right)$$
- Set size of  $E =$  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)

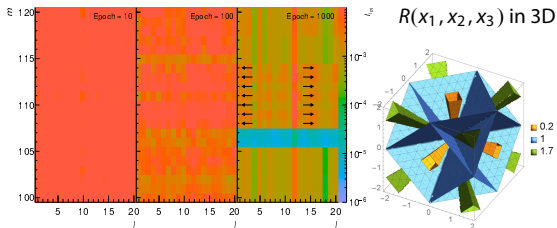
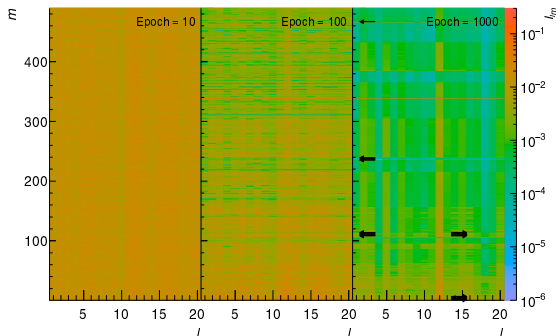


$$= \sum_{i_1=1}^M \sum_{i_2=1}^M \sum_{i_3=1}^M \sum_{i_4=1}^M z_{i_1} z_{i_2} z_{i_3} z_{i_4} \theta_{i_1 i_2} \theta_{i_2 i_3} \theta_{i_2 i_4}^2 \theta_{i_3 i_4}$$

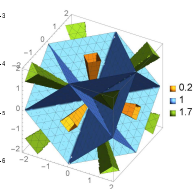
from P. T. Komiske, E. M. Metodiev, J. Thaler, J. High Energy Phys. 04 (2018): 13



# Last ingredient: "Nudge" the NN to simplicity



$R(x_1, x_2, x_3)$  in 3D



See arXiv:1810.00835

- $R$  takes the bound  $l_{lm} = \frac{\partial \text{out}_l}{\partial \text{in}_m}$  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)]

# Result for Jewel

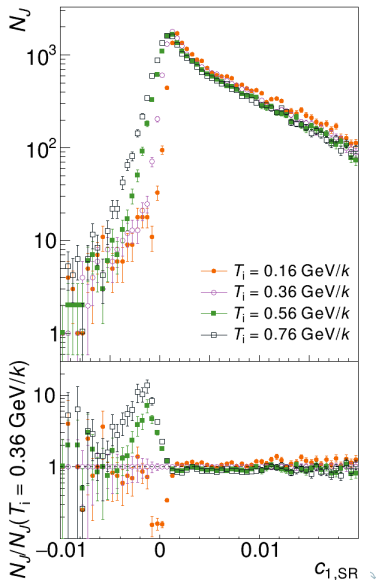
- $N = 2500$  jets needed to determine  $T_i$
- Overall analysis:  
 $d_{1,SR} = 8.99 - 0.176N\langle c_{16} \rangle - 0.175N\langle c_1 \rangle$
- First approximate  $c_1$  (Einstein notation):  

$$c_{1,SR} = 0.0112 + 45.5 \theta_{ab} \theta_{ac} \theta_{bc} \theta_{ad} \theta_{bd} \theta_{ae} \theta_{ce} z_a \cdots z_e +$$

$$+ 20.9 \theta_{ab} \theta_{ac} \theta_{bc} \theta_{ad} \theta_{bd} \theta_{ae} \theta_{be} z_a \cdots z_e +$$

$$+ 26.33 \theta_{ab} \theta_{ac} \theta_{bd} \theta_{cd} \theta_{ae} \theta_{de} z_a \cdots z_e -$$

$$- 4.16 \theta_{ab} \theta_{ac} \theta_{ad} \theta_{ae} z_a \cdots z_e$$
- $c_{1,SR}$  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

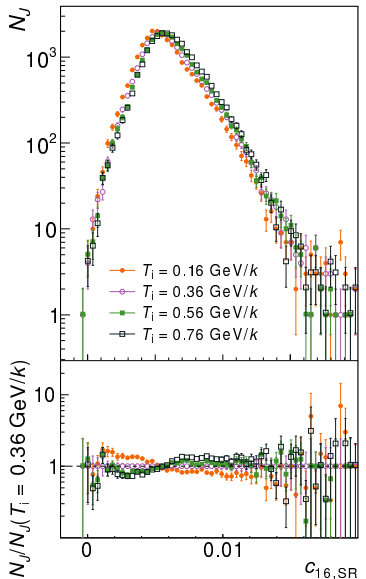


# Result for Jewel

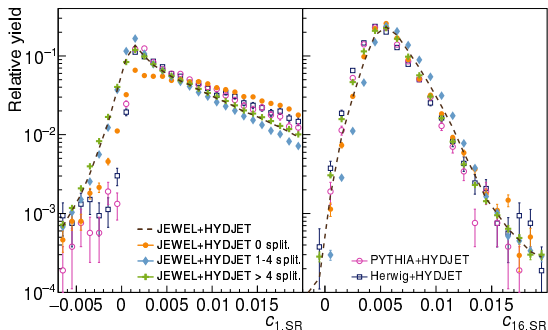
- Approximate  $c_{16}$ :

$$c_{16,SR} = 0.0362 + 2.563 \theta_{ab} \theta_{ac} \theta_{ad} \theta_{ae} z_a \cdots z_e - 0.2017 \theta_{ab} z_a z_b$$

- 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
- Difference in expression to arXiv is due to powers in EFP not generated (mistakenly), update coming

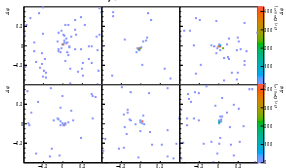


# How does it work?

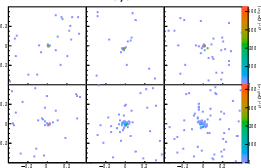


- Jewel was modified to produce (infinitesimal momentum) splitting that are clustered into jets
- Count inside each jet the number of splittings in the same area
- $c_{1,SR}$  and  $c_{16,SR}$  both tagger for no. of internal splittings
- Most of the regions tag few (1–4) splittings
- The  $c_{1,SR} < 0$  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)

$c_{1,SR} < 0.0012$



$0.008 < c_{16,SR} < 0.012$



Hard event only (for clarity)

# Result for LBT

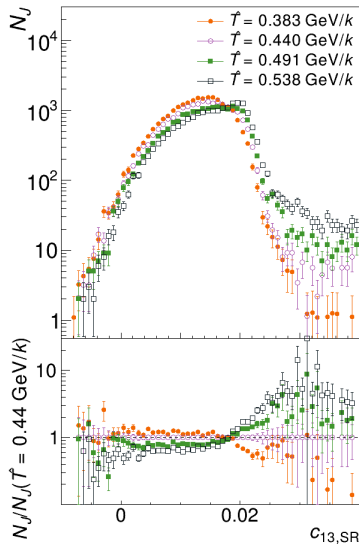
- $N = 1200$  jets needed to determine  $\hat{T}$
- $d_{1,SR} = 4.49 - 0.318N\langle c_{13} \rangle - 0.00653(N\langle c_{13} \rangle)^2$
- Approximate  $c_{13}$ :  

$$c_{13,SR} = 0.0453 - 0.00109 \log_{10}(p_1)(\log_{10}(p_2) + \log_{10}(p_3)) - 0.000829 \log_{10}(p_2) \log_{10}(p_3)$$

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

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

$$p_3 = \theta_{ab}\theta_{ac}\theta_{bd}\theta_{cd}\theta_{ae}\theta_{de}z_a \cdots z_e$$
- Demonstrates the system generating non-linear observables
- Possibly log being function of convenience to handle the otherwise long tail (some simplification by hand)
- $100 < p_T < 300$  GeV/c plotted



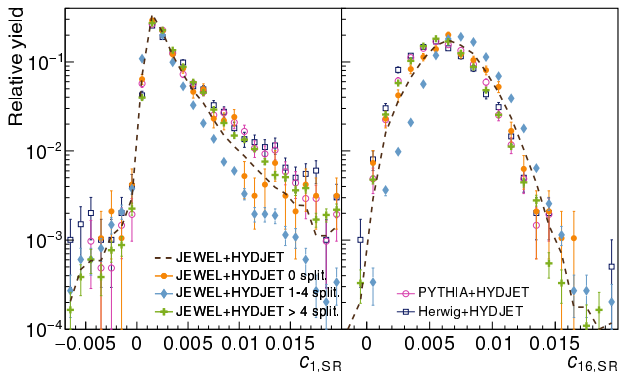
# Summary

- 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  $N = 1200\text{--}2500$  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





# Permutation symmetry vs. algebra vs. statistics

- Expressibility of permutation symmetry gives the Galois theory of polynomials
- Two well-known types of polynomial:

**A** Elementary symmetric polynomials:

$$e_0(x_1, \dots, x_n) = 1$$

$$e_1(x_1, \dots, x_n) = \sum_{1 \leq i \leq n} x_i$$

$$e_2(x_1, \dots, x_n) = \sum_{1 \leq i < j \leq n} x_i x_j$$

⋮

$$e_n(x_1, \dots, x_n) = \prod_{1 \leq i \leq n} x_i$$

**B** Power sum symmetric polynomials:

$$p_k(x_1, \dots, x_n) = \sum_{1 \leq i \leq n} x_i^k$$

- 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)

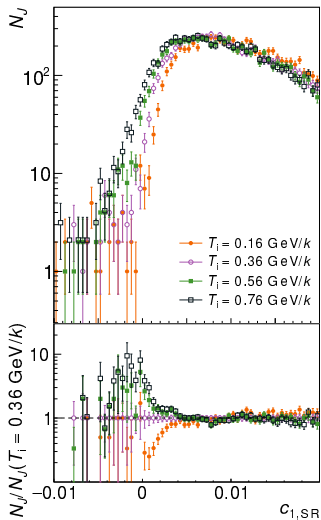
- Solution:

$$s_j(x) = \sum_{k=1}^N x_{j\pi(k)}^{m-l} x_{(j+1)\bmod M, \pi(k)}^l, \quad l \in \{1, \dots, m-1\}$$

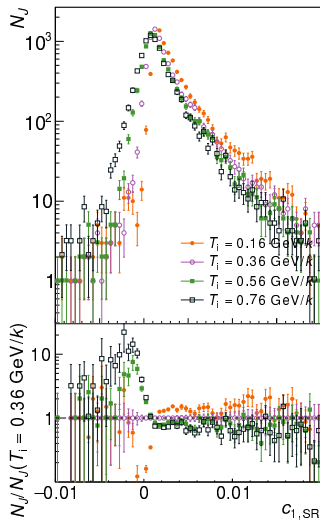
for  $N$   $M$ -dimensional variables (with a special case for  $M = 2$ )

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

# $p_T$ dependence

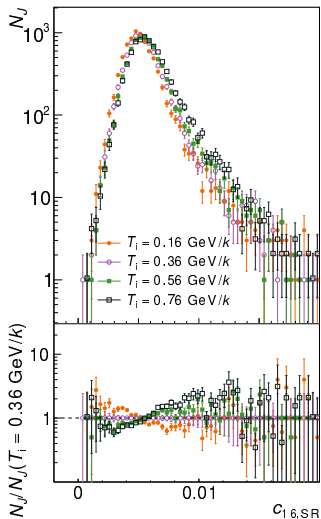


$100 < p_T < 150 \text{ GeV}/c$

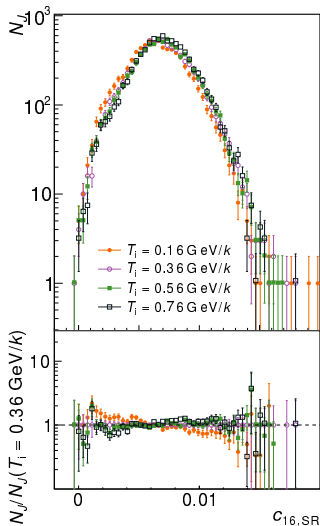


$200 < p_T < 300 \text{ GeV}/c$

# $p_T$ dependence

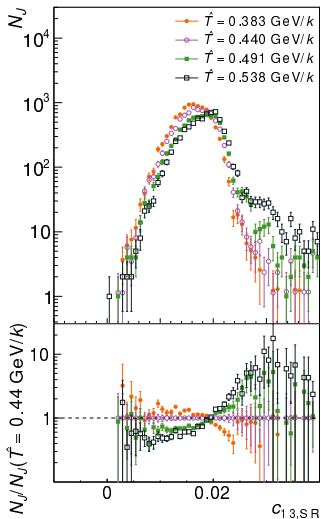


$100 < p_T < 150$  GeV/c

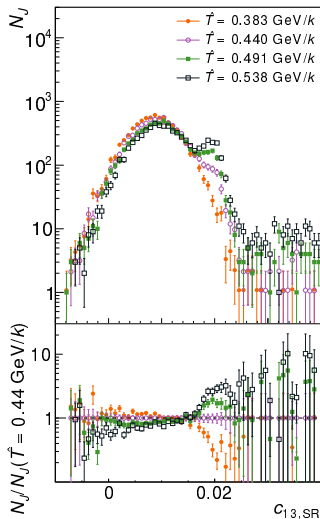


$200 < p_T < 300$  GeV/c

# $p_T$ dependence



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



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