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## Machine Learning the Top Mass

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- Measuring the Top Mass with Energy Correlators
- 2. Machine Learning Energy Correlator Space
- 3. Shape Optimization





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# Why Energy Correlators?



Studies of jet substructure have been productive, but often rely on (groomed) observables which cannot be precisely computed. Energy correlators offer a precise alternative.

Energy flow operators describe the flux of energy along a particular direction, integrated over time. They provide a theoretical definition of calorimeter cells.

$$\varepsilon(\hat{n}) = \int_{0}^{\infty} dt \lim_{r \to \infty} r^{2} n^{i} T_{0i}(t, r\vec{n})$$

Energy correlators are small angle correlation functions of these operators. They are not defined event wise.

Two point correlation functions obey a definite scaling, while other scales imprint in higher point correlators.



[0803.1467: Hoffman, Maldecena] [Pietarinen, Stirling, PLB 84; 2004.11381: Chen et al] [Image - 2205.03414: Lee et al] Measuring the Top-quark Mass



Since the Top-quark has a three pronged decay, its mass should be embedded in the E3C. The E3C is

$$E3C(\zeta_{12}, \zeta_{23}, \zeta_{31}) = \sum_{i < j < k} \int d\sigma \frac{E_i E_j E_k}{Q^3} \delta_{\text{shape}}(\zeta_{ij}, \zeta_{jk}, \zeta_{ki})$$

in terms of energies (or transverse momenta, for hadron colliders) and pairwise distances  $\zeta_{ij}$ . The pairwise distances are

$$\hat{\zeta}_{ij} = (1 - \cos(\theta_{ij}))/2 \quad (e^+e^-)$$
$$\hat{\zeta}_{ij} = \Delta \eta_{ij}^2 + \Delta \phi_{ij}^2 \qquad \text{(hadron)}$$

[Holguin et al: 2201.08393]

Shape Dependence



In order to compare to precision theory, these are projected onto 1d observables using  $\delta_{shape}$ . The simplest choice is equilateral

$$\delta_{\text{equilateral}} = \delta(3\zeta - \Sigma\zeta_{pair}) \prod \theta(\delta\zeta - |\zeta_{ij} - \zeta_{jk}|)$$

where  $\zeta = (\zeta_{12} + \zeta_{23} + \zeta_{31})/3$ 



Equilateral triangles are not optimal, because a large fraction of triplets are discarded. Nearly isosceles triangles work better. Picking an optimal shape is hard!
[Holguin et al: 2311.02157, 2311.14389, 2407.12900] [Holguin et al: 2201.08393, Xiao et al: 2405.20001]

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Why Add ML? Measuring *m*<sub>t</sub> by comparing to

precision theory calculations requires picking a 1d triangle "shape" to project.

But this choice is arbitrary, and affects the results! Different shapes perform differently. Can we choose the best shape, or avoid picking one all together?



## Yes! With ML, we can:

- Learn the full distribution & avoid shape choice
- Choose an optimal shapes



## A two step process



## Our ML approach follows a two step process:

1. Learn the full EC distribution from simulation using an unsupervised approach

### Dense Network

- Outputs Energy Correlator  $\overline{E} p(\zeta_i, m_t | \text{sim})$  directly
- Trained with energy weighted MLE + explicit integral constraint

### Normalizing Flows (NFs)

- Using NFs for density estimation of joint prob  $p(\zeta_i, E_i, m_t | \text{sim})$
- Integrate to get energy correlators

2. Extract the Top-quark mass from the distribution.

### Fit to Data Histograms

- Goal: Get optimal performance with as much shape info as possible
- Minimize over  $m_t^{fit}$ :  $\sum_{bins} |EEC_{net}(\zeta_i, m_t^{fit}) - EEC_{data}(\zeta_i, m_t)|$

#### Shape Distillation

- Goal: Choose optimal shape which can be precisely computed
- Use neural ratio estimation

# The Dense Net Approach



This is a modified version of maximum likelihood estimation:

$$Loss = \sum_{ij} E_{ij} \ln NN(\zeta_i, m_t)$$
$$= \ln \Pi_{ij} NN(\zeta_i, m_t)^{E_{ij}}$$
$$= \ln \Pi_i NN(\zeta_i, m_t)^{\sum_j E_{ij}}$$

#### **Details:**

- Very sensitive to hyperparameters
- Trained with AdamW with weight decay and gradient clipping
- Need to preprocess inputs to be  $\mathcal{O}(1)$
- Integral computed with gpu Torchquad
- Use stochastic weight averaging after half the epochs

# Dense Net Results



#### The dense net learns the full distribution differential in $\zeta_1$ , $\zeta_2$ , $\zeta_3$ , and $m_t$ .



Getting the 1D projected ECs simply requires integrating the full distribution over a wedge determined by  $\delta_{\rm Shape}$ .



## Normalizing Flows Background

Normalizing flows are an invertible map between a Gaussian distribution and a more complicated one. One direction estimates the density, while the other samples.

The loss is again the negative log likelihood, but normalization is now automatic.



#### Details:

- Spline coupling flow with 3 layers, each followed by a batch norm.
- Trained with Adam for 20 epochs
- Inputs with  $\zeta < 0.005$  masked
- All inputs rescaled using logit

[Papamakarios et al: 1906.04032] [Image - LiLian Wang 2018]

# Normalizing Flows

We learn the 6d joint probability  $p(\zeta_i, E_i)$  with NFs. We are working on the 7d probability  $p(\zeta_i, E_i, m_t)$ .

We multiply by and integrate over  $E_i$  to compute the 3d ECs. 1d correlators are computed by integrating slices over  $\zeta_i$ .

This avoids integration during training, but requires a very precise distribution since energy weighting isn't naturally learned.



0.05



10<sup>3</sup>

10<sup>2</sup>

10<sup>1</sup>

100

 $10^{-1}$ 

 $10^{-2}$ 





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- Goal: to find the best performing energy correlator (projection), even if it can't be compared directly to data, including both the full distribution and lower dimensional marginalizations.
- Compare EC value the network learns for an arbitrary  $m_t^{fit}$  value to a histogram with fixed  $m_t$  value
- True value of  $m_t^{fit}$  should minimize

 $\sum |EEC_{net}(\zeta_i, m_t^{fit}) - EEC_{data}(\zeta_i, m_t)|$ 



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Top Mass Errors:  $\zeta$  fit,  $\delta \zeta \leq 0.02$ : 0.104 GeV  $\zeta$  fit,  $\delta \zeta \leq 0.01$ : 0.45 GeV  $\zeta$  fit,  $\delta \zeta \leq 0.005$ : 0.396 GeV  $\zeta$  fit, 2D: 0.308 GeV

# **Neural Ratio Estimation**



## NRE learns the likelihood to evidence ratio $p(\theta, data)$

 $\frac{1}{p(\theta)p(data)}$ 

via a classifier which distinguishes between samples with true  $m_t$  and samples with fake  $m_t$  drawn from a uniform distribution.

Since we know  $p(\theta)$ , this can be used to extract  $p(\theta | data)$  for a new data sample once the classifier is trained. The true  $m_t$ maximizes the posterior. Posterio  $EEC_{\delta}(\zeta, \zeta, \zeta), \delta = 0.005$ 



[Hermans et al: 1903.04057]

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# Top Mass Results II









ML can be used to learn the full energy correlator distribution.

This distribution can be used to optimize the 1d Energy Correlator projection, and also to directly put a bound on how well the Top Mass can be extracted from the full correlator.







# **Back Up Slides**

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