# (Machine) Learning Jet Physics

## CTP Lunch Talk

Patrick T. Komiske

**Center for Theoretical Physics** 

Massachusetts Institute of Technology



Collaborators: Eric Metodiev, Benjamin Nachman, Matthew Schwartz, and Jesse Thaler May 18, 2018



Run: 302347 Event: 753275626 2016-06-18 18:41:48 CEST p

#### Higgs Decays



#### Higgs Decays







#### Higgs Decays



Higgs Decays



Higgs Decays









#### Jets in Theory



#### Jets in Theory



Jets in Theory in Practice



Jets in Theory in Practice in Theory



Jets in Theory in Practice in Theory in Practice



Jets in Theory in Practice in Theory in Practice...  $\otimes$ 



## Jets in Theory in Practice in Theory in Practice.





Slide from overview talk by Matthew Schwartz at 2017 ML for lets workshop at LBNL

0.4

#### Jet Tasks I'll Talk About

Jet Tagging: How can we distinguish a quark jet vs. a gluon jet? A W jet vs. a QCD jet?



Pileup Mitigation: Can we decontaminate the jet radiation from soft, diffuse pileup?



**Data vs. Simulation:** Do we really need simulations to provide labeled training data? Or are there ways to train algorithms directly on the (unlabeled) data?



## Machine Learning





#### Machine Learning in High Energy Physics





Quark color charge:  $C_F = 4/3$  Gluons radiate more than quarks and are "wider" Gluon color charge:  $C_A = 3$ 

Inherently difficult problem for conventional taggers (both are one-pronged jets)

Machine learning to the rescue!



Jet Images

Center on patch of the pseudorapidityazimuth plane containing a jet

Treat energy/transverse momentum deposits in calorimeter as pixel intensities



Additional input channels possible: **Red**:  $p_T$  of charged particles **Green**:  $p_T$  of neutral particles **Blue**: charged particle multiplicity Gluons

Jet images are sparse

Gluons wider than quarks

#### Convolutional Net for QG



### Quantifying a Classifier

Receiver Operating Characteristic (**ROC**) curve: True negative rate of the classifier at different true positive rates



Area Under the ROC Curve (AUC) captures the classifier performance in a number.

#### **Classification Performance**



CNN outperforms expert observables!

Multi-channel images help at high  $p_T$ 



HL-LHC tīt event in ATLAS ITK at <µ>=200



Pileup

#### Pileup Mitigation with Machine Learning (PUMML)

[PTK, E.M. Metodiev, B. Nachman, M.D. Schwartz, 1707.08600]

Pileup comes from additional interaction vertices

Soft and uniform (on average) noise

Want to remove pileup to be sensitive to high energy effects

PUMML is first application of MML regression in particle physics



30



#### Pileup Mitigation with Machine Learning (PUMML)



## Average PUMML Jet Image Inputs



#### **Comparison of Pileup Removal Methods**

PUMML compares favorably to other existing pileup mitigation methods!



#### **Back to Observables**

# TRUST ME

# I'M AN EXPERT

Jet mass Angularities Subjet Count N-subjettiness

Geometric Moments

**Energy Correlation Functions** 

#### What is IRC Safety?

Infrared (IR) safety – observable is unchanged under addition of a soft particle:

$$S(\{p_1^{\mu}, \dots, p_M^{\mu}\}) = \lim_{\epsilon \to 0} S(\{p_1^{\mu}, \dots, p_M^{\mu}, \epsilon p_{M+1}^{\mu}\}), \qquad \forall p_{M+1}^{\mu}$$

Collinear (C) safety – observable is unchanged under collinear splitting of a particle:

$$S(\{p_1^{\mu}, \dots, p_M^{\mu}\}) = \lim_{\epsilon \to 0} S(\{p_1^{\mu}, \dots, (1-\lambda)p_M^{\mu}, \lambda p_M^{\mu}\}), \qquad \forall \lambda \in [0,1]$$

A necessary and sufficient condition for soft/collinear divergences of a QFT to cancel at each order in perturbation theory (KLN theorem)

Divergences can be seen in QCD splitting function:

$$dP_{i \to ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{d\theta}{\theta} \frac{dz}{z} \qquad C_q = C_F = 4/3$$
$$C_g = C_A = 3$$

IRC-safe observables probe high energy structure while being insensitive to low energy modifications



Progress has been made in computing correlations of  $\hat{\mathcal{E}}(\hat{n}, v)$  in conformal field theory [D. Hofman and J. Maldecena, 0803.1467]

IRC-safe observables are built out of energy correlators:

$$C_{f} = \sum_{i_{1}=1}^{M} \sum_{i_{2}=1}^{M} \cdots \sum_{i_{N}=1}^{M} E_{i_{1}} E_{i_{2}} \cdots E_{i_{N}} f(\hat{p}_{i_{1}}, \cdots, \hat{p}_{i_{N}})$$
Rigid energy structure Arbitrary angular function  $f$ 

$$E_{i_{1}}E_{i_{2}} \cdots E_{i_{N}} f(\hat{p}_{i_{1}}, \cdots, \hat{p}_{i_{N}})$$



### Multigraph/EFP Correspondence



#### EFPs linearly span IRC-safe observables



Organization of the basis

EFPs *linearly* span all IRC-safe observables!

EFPs are truncated by angular degree *d*, the order of the angular expansion.

Online Encyclopedia of Integer Sequences (OEIS)

- <u>A050535</u> # of multigraphs with d edges # of EFPs of degree d
- A076864 # of connected multigraphs with d edges # of prime EFPs of degree d



Exactly 1000 EFPs up to degree d=7!

#### Jet Substructure Observables as EFPs

#### Linear Regression and IRC-safety

 $\frac{m_J}{p_{TJ}}$ : IRC safe. No Taylor expansion due to square root.

 $\lambda^{(\alpha=1/2)}$ : IRC safe. No simple analytic relationship.

 $\tau_2$ : IRC safe. Algorithmically defined.

 $\tau_{21}$ : Sudakov safe. Safe for 2-prong jets and higher.

 $au_{32}$ : Sudakov safe. Safe for 3-prong jets and higher.

Multiplicity: IRC unsafe.







Expected to be IRC safe = Solid. Expected to be IRC unsafe = Dashed. A. Larkoski, S. Marzani, and J. Thaler, 1502.01719

## Jet Tagging Comparison

ROC curves for W jet vs. QCD jet tagging



(Linear classification with EFPs)  $\sim$  (MML) for efficiency > 0.5!

N-subjettiness: 1011.2268,

N-subjettiness basis: 1704.08249,



## Jet Tagging Comparison

ROC curves for quark vs. gluon tagging and top tagging



(Linear classification with EFPs)  $\sim$  (MML) for efficiency > 0.5!

## **Escaping the Simulation**

#### Simulation vs. Data

In physics, we usually don't have access to labelled training data.

If we knew which jets were quark and gluon jets... we wouldn't need a tagger!



In collider physics, we usually rely on (imperfect) simulations to provide labelled examples.



Modern machine learning exploits subtle correlations. The simulations do not fully capture all of the complex correlations. Is this a fundamental obstacle to all ML in Physics?

#### Simulation vs. Data



Important differences between simulation and data even for simple observables! 47



### "Physics ML"

This is relatively new territory for Machine Learning.

In "Usual ML": Automate a task that is possible but time consuming for humans (e.g. cat jet vs dog jet).



In "Physics ML": Automate a task that is impossible for humans (e.g. quark jet vs gluon jet)



49

#### **Mixed Samples**

#### Data does not have pure labels, but does have mixed samples!

Some caveats apply. See e.g. P. Gras, et al., arXiv: 1704.03878



$$p_{M_a}(x) = f_a p_S(x) + (1 - f_a) p_B(x)$$



Fractions of quark and gluon jets studied in detail in: J. Gallicchio and M.D. Schwartz, arXiv: 1104.1175

### **Mixed Samples**

### Data does not have pure labels, but does have mixed samples!

Some caveats apply. See e.g. P. Gras, et al., arXiv: 1704.03878



**Different Purities**:  $f_a \neq f_b$  for some *a* and *b*.

(Known Fractions): The fractions  $f_a$  are known.

#### Weak Supervision



#### ML Umbrella term for any classification framework using partial label information.

Collection of	f supervision	models.
---------------	---------------	---------

Model	References	Description	
Full-supervision	[9,24,34,43]	For each example, complete class information is provided.	
Unsupervision	[24]	No class information is provided with the examples.	
Semi-supervision	[5]	Part of the examples are provided fully supervised. The rest are unsupervised.	
Positive-unlabeled	[4,10,21,32]	Part of the examples are provided fully supervised, all of them with the same categorization. The rest are unsupervised.	
Candidate labels	[7,13,16]	For each example, a set of class labels is provided. In this set, the class label(s) that compose the real categorization of the example are included.	
Probabilistic labels	[18]	For each example, the probability of belonging to each class label is provided. This probability distribution is expected to assign high probability to the real label(s).	
Incomplete	[3,33,42]	For each example, a subset of the labels that compose its real categorization is provided (SIML or MIML, Table 1).	
Noisy labels	[2,44]	For each example, complete class information is provided, although its correctness is not guaranteed.	
Crowd	[30,40]	For each example, many different non-expert annotators provide their (noisy) categorization.	
Mutual label constraints	[19,20,31]	For each <b>group</b> of examples, an explicit relationship between their class labels is provided (e.g., all the examples have the same categorization).	
Candidate labeling vectors	[22]	For each <b>group</b> of examples, a set of labeling vectors (including the real one) is provided. A labeling vector provides a class label for each examples of a group.	
Label proportions	[15,25,28]	For each <b>group</b> of examples, the proportion of examples belonging to each class label is provided.	

J. Hernández-González et al. / Pattern Recognition Letters 69 (2016) 49–55

No exact weak supervision framework for the physics (mixture) use-case.

An opportunity to develop new ML tools for the job!

## Learning from Label Proportions (LLP) (LoLiProp)

Try to match the signal fractions in aggregate

[L. Dery, et al., arXiv: 1702.00414]



Classification Without Labels (CWoLa, "koala")

[E.M. Metodiev, B. Nachman, and J. Thaler, arXiv: 1708.02949] Classify [T. Cohen, M. Freytsis, and B. Ostdiek, arXiv: 1706.09451] [PTK, E.M. Metodiev, B. Nachman, and M.D. Schwartz, arXiv: 1801.10158] See also: [G. Blanchard, M. Flaska, G. Handy, S. Pozzi, and C. Scott, arXiv:1303.1208]



No label proportions needed during training!

Smoothly connected to the fully supervised case as  $f_1, f_2 \rightarrow 0, 1$ 

Note: Need small test sets with known signal fractions to determine the ROC.

Classify mixed samples from each other





Classification Without Labels (CWoLa, "koala")

Why does CWoLa work?



#### Neyman-Pearson Lemma:

There is an optimal binary classifier: the likelihood ratio.

 $L_{S/B}(\boldsymbol{x}) = \frac{p_S(\boldsymbol{x})}{p_B(\boldsymbol{x})}.$ 

The mixed-sample likelihood ratio is related to the signal/background likelihood ratio by:

$$L_{M_1/M_2} = \frac{p_{M_1}}{p_{M_2}} = \frac{f_1 p_S + (1 - f_1) p_B}{f_2 p_S + (1 - f_2) p_B} = \frac{f_1 L_{S/B} + (1 - f_1)}{f_2 L_{S/B} + (1 - f_2)}.$$

This is a monotonic rescaling of the signal/background likelihood ratio!

Therefore Mixture 1 vs. Mixture 2 and Signal vs. Background define the same classifier. They have the same ROC curves.



CWoLa and LLP have been shown to work for simple architectures and small inputs.

Can these weak supervision methods be used for real deep learning applications in collider physics? Are they ready for the big leagues?

To answer this question, we did our quark/gluon tagging with jet images using only mixtures of quarks and gluons – no labels.



Short answer: **WOLa** generalizes very well LLP needs tuning, but it works

Potential to train on data!



### Purity and Number of Data







Purity/Data plot can characterize tradeoffs in a weak learning method

CWoLa performs near full supervision if the samples are relatively pure.

LLP lags behind but still achieves good classification performance.





## Batch Size and Training Time

We explored hyperparameters, training times, and other lessons from using the methods in practice.

Batch size As usual for CWoLa

Need large batch size for LLP Batch Size > 1000  $\ell_{\text{LLP}} = \sum_{a} \ell \left( f_{a}, \frac{1}{N_a} \sum_{i=1}^{N_a} h(x) \right)$ 



### Weak Supervision in Summary

We now have two candidate methods to train ML algorithms directly on jet data



Moral of this story: use CWoLa

#### **CWoLa Hunting!**

[]. Collins, K. Howe, B. Nachman, 1805.02664]



Cool way to use CWoLa to incorporate high-dimensional features in bump hunts

Process-agnostic, data-driven new physics search strategy





#### Jet Tasks I Talked About

Jet Tagging: How can we distinguish a quark jet vs. a gluon jet? A W jet vs. a QCD jet?



**Data vs. Simulation:** Do we really need simulations to provide labeled training data? Or are there ways to train algorithms directly on the (unlabeled) data?







#### Weak Supervision

[PTK, E. Metodiev, B. Nachman, and M.D. Schwartz, 1801.10158]

#### Many Interesting Ideas Out There!

A wealth of new ways to directly access physics with machine learning methods!



# Thank you!

#### Robustness of PUMML



Train and test on different amounts of pileup

PUMML more robust than PUPPI and SK across a wide amount of pileup!

#### Train and test on different processes



PUMML demonstrates process independence!

### What is PUMML Learning?

#### Train PUMML on a simplified architecture



Approximately learns linear cleansing!

$$p_T^{N,LV} = p_T^{N,tot} - \left(\frac{1}{\overline{\gamma_0}} - 1\right) p_T^{C,PU}$$

#### Energy Flow (Network) Analysis





### Energy Flow Analysis





67