Energy Flow and Jet Substructure

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> Harvard Particle Lunch Talk 11/28/2018

Based on work with Eric Metodiev and Jesse Thaler

<u>1712.07124</u> <u>1810.05165</u>





Jets from the Standard Model

++ = Mass from QCD Radiation

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Slide by Jesse Thaler

≈ 70%

≈ 60%

W/Z

≈ 70%

b

C

g

u,d,s

+



Boosted Event Topologies at the LHC





Machine Learning in High Energy Physics

Machine Learning for Jet Physics 2018

indico.cern.ch/event/ml4jets2018



Organizing Committee: Pushpa Bhat (Fermilab) Kyle Cranmer (NYU) Sergei Gleyzer (U Florida) Ben Nachman (LBNL) Tilman Plehn (Heidelberg) Local Organizing Committee: Gabriele Benelli (Brown U), Javier Duarte (Fermilab) Benjamin Kreis (Fermilab) Nhan Tran (Fermilab) Justin Pilot (UC Davis)



Images: J. Lin, B. Nachman, L. de Oliveira

November 14-16, 2018

LPC Coordinators: Cecilia Gerber (UIC) Sergo Jindariani (Fermilab)





Machine Learning for Jets Activity



Exponential increase in ML4Jets papers!

[Nachman, Boost 2018 Talk, July 18, 2018]

A Cartoon of Machine Learning

For fully-supervised jet classification

$$\ell_{\rm MSE} = \left\langle \left(h(\vec{x}) - 1 \right)^2 \right\rangle_{\rm signal} + \left\langle \left(h(\vec{x}) - 0 \right)^2 \right\rangle_{\rm background}$$

Classifier Inputs



Minimize Loss Function

(assuming infinite training sets, and flexible enough functional form)

$$h(\vec{x}) = \frac{p_{\text{sig}}(\vec{x})}{p_{\text{sig}}(\vec{x}) + p_{\text{bkgd}}(\vec{x})}$$

Optimal Classifier (Neyman–Pearson)

Jet Classification Studies Mix and match



[Lönnblad, Peterson, Rögnvaldsson, 1990, ..., Cogan, Kagan, Strauss, Schwartzman, 1407.5675; Almeida, Backović, Cliche, Lee, Perelstein, 1501.05968; de Oliveira, Kagan, Mackey, Nachman, Schwartzman, 1511.05190; Baldi, Bauer, Eng, Sadowski, Whiteson, 1603.09349; Conway, Bhaskar, Erbacher, Pilot, 1606.06859; Guest, Collado, Baldi, Hsu, Urban, Whiteson, 1607.08633; Barnard, Dawe, Dolan, Rajcic, 1609.00607; Komiske, Metodiev, Schwartz, 1612.01551; Kasieczka, Plehn, Russell, Schell, 1701.08784; Louppe, Cho, Becot, Cranmer, 1702.00748; Pearkes, Fedorko, Lister, Gay, 1704.02124; Datta, Larkoski, 1704.08249, 1710.01305; Butter, Kasieczka, Plehn, Russell, 1707.08966; Fernández Madrazo, Heredia Cacha, Lloret Iglesias, Marco de Lucas, 1708.07034; Aguilar Saavedra, Collin, Mishra, 1709.01087; Cheng, 1711.02633; Luo, Luo, Wang, Xu, Zhu, 1712.03634; Komiske, Metodiev, JDT, 1712.07124; Macaluso, Shih, 1803.00107; Fraser, Schwartz, 1803.08066; Choi, Lee, Perelstein, 1806.01263; Lim, Nojiri, 1807.03312; Dreyer, Salam, Soyez, 1807.04758; Moore, Nordström, Varma, Fairbairn, 1807.04769; plus my friends who will scold me for forgetting their paper (and not updating this after July 23, 2018); plus many ATLAS/CMS performance studies]

Slide by Jesse Thaler





Energy Flow Moments



Energy Flow Polynomials



Patrick Komiske – Energy Flow and Jet Substructure





Energy Flow Moments



Energy Flow Polynomials

Patrick Komiske – Energy Flow and Jet Substructure



An unordered, variable length collection of particles

Due to quantum-mechanical indistinguishability Due to probabilistic nature of jet formation

$$J(\{p_1^{\mu},\ldots,p_M^{\mu}\}) = J(\{p_{\pi(1)}^{\mu},\ldots,p_{\pi(M)}^{\mu}\}),$$

$$\underbrace{M \ge 1}_{\text{Multiplicity}},$$



Permutations

p_i^{μ} represents *all* the particle properties:

- Four-momentum $(E, p_x, p_y, p_z)_i^{\mu}$
- Other quantum numbers (e.g. particle id, charge)
- Experimental information (e.g. vertex info, quality criteria, PUPPI weights)



Point cloud: "A set of data points in space" – Wikipedia

LIDAR data from self-driving car sensor







Particle Collision Events as Point Clouds



Multi-jet event at CMS

Processing Point Clouds

Methods for processing point clouds/jets should respect the appropriate symmetries

Variable constituent multiplicity requires at least one of: Preprocessing to another representation (jet images, N-subjettiness, etc.) Truncation to an (arbitrary) fixed size Recurrent NN structure

Particle permutation symmetry requires:

Permutation symmetric observables Permutation symmetric architectures

Two key choices when analyzing jets

How to represent the jet

- Single expert observable
- A few expert observables
- Many expert observables
- Jet images
- List of particles
- Clustering tree
- N-subjettiness basis
- Energy flow polynomials
- Set of particles

How to analyze that representation

- Threshold cut
- Multidimensional likelihood
- Boosted decision tree (BDT), shallow neural network (NN)
- Convolutional NN (CNN)
- Recurrent/Recursive NN (RNN)
- Fancy RNN
- Dense neural network (DNN)
- Linear classification
- Energy flow network

Jet Representations +---- Analysis Tools

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Deep Sets

Namespace for symmetric function parametrization

A general permutation-symmetric function is *additive* in a latent space

Deep Sets

[1703.06114]

Manzil Zaheer^{1,2}, Satwik Kottur¹, Siamak Ravanbhakhsh¹, Barnabás Póczos¹, Ruslan Salakhutdinov¹, Alexander J Smola^{1,2} ¹ Carnegie Mellon University ² Amazon Web Services

Deep Sets Theorem [63]. Let $\mathfrak{X} \subset \mathbb{R}^d$ be compact, $X \subset 2^{\mathfrak{X}}$ be the space of sets with bounded cardinality of elements in \mathfrak{X} , and $Y \subset \mathbb{R}$ be a bounded interval. Consider a continuous function $f: X \to Y$ that is invariant under permutations of its inputs, i.e. $f(x_1, \ldots, x_M) =$ $f(x_{\pi(1)}, \ldots, x_{\pi(M)})$ for all $x_i \in \mathfrak{X}$ and $\pi \in S_M$. Then there exists a sufficiently large integer ℓ and continuous functions $\Phi: \mathfrak{X} \to \mathbb{R}^{\ell}$, $F: \mathbb{R}^{\ell} \to Y$ such that the following holds to an arbitrarily good approximation:¹

$$f(\{x_1,\ldots,x_M\}) = F\left(\sum_{i=1}^M \Phi(x_i)\right)$$

Deep Sets

Namespace for symmetric function parametrization

A general permutation-symmetric function is *additive* in a latent space



General parametrization for a function of sets

Deep Sets for Particle Jets

[PTK, Metodiev, Thaler, 1810.05165]

IRC-safe latent space

Energy Flow Network (EFN)

 $\operatorname{EFN}(\{p_1^{\mu},\ldots,p_M^{\mu}\}) = F\left(\sum_{i=1}^M z_i \Phi(\hat{p}_i)\right)$

Particle Flow Network (PFN)

$$\operatorname{PFN}(\{p_1^{\mu},\ldots,p_M^{\mu}\}) = F\left(\sum_{i=1}^{M} \Phi(p_i^{\mu})\right)$$

Fully general latent space

Particles

Observable



Latent Space IRC Safety

Latent space defines new physics observables

IRC safety is a key theoretical and experimental property of observables

QCD has soft and collinear divergences associated with gluon radiation

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

$$C_q = C_A = 3$$

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

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

Collinear (C) safety – observable is unchanged under a collinear splitting of a particle $S(\{p_1^{\mu}, \dots, p_M^{\mu}\}) = S(\{p_1^{\mu}, \dots, (1-\lambda)p_M^{\mu}, \lambda p_{M+1}^{\mu}\}), \quad \forall \lambda \in [0, 1]$

Latent Space IRC Safety



Approximating Φ and F with Neural Networks

Employ neural networks as arbitrary function approximators

Use fully-connected networks for simplicity Default sizes $-\Phi$: (100, 100, ℓ), F: (100, 100, 100) Φ Particles Observable Per-Particle Representation **Event Representation** Latent Space Φ F╋ Φ Φ Energy/Particle Flow Network

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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.

Other formats possible, e.g. $(\varepsilon_s, 1/(1-\varepsilon_b)), (\varepsilon_s, \varepsilon_s/\sqrt{1-\varepsilon_b})$

Classification Performance



EFPs are comparable to EFN

PFN: No particle type info, arbitrary energy dependence

EFN: IRC-safe latent space



PFN-ID slightly better than RNN-ID

EFN Latent Dimension Sweep

PFN-ID: Full particle flavor info $(\gamma, \pi^{\pm}, K^{\pm}, K_L, p, \bar{p}, n, \bar{n}, e^{\pm}, \mu^{\pm})$ PFN-Ex: Experimentally accessible info $(\gamma, h^{\pm,0}, e^{\pm}, \mu^{\pm})$ PFN-Ch: Particle charge info (+, 0, -)

PFN: No particle type info, arbitrary energy dependence

EFN: IRC-safe latent space



Energy Flow Network Visualization

EFN observables are two-dimensional geometric functions

Visualize EFN observables as *filters* in the translated rapidity-azimuth plane



Jet images as EFN filters

[Cogan, Kagan, Strauss, Schwartzman, 2014] [de Oliviera, Kagan, Mackey, Nachman, Schwartzman, 2015]

Moments as EFN filters



[Donoghue, Low, Pi, 1979] [Gur-Ari, Papucci, Perez, 2011]

Filter 1 Filter 2 Filter 3 Filter 4 ٠ Translated Azimuthal Angle ϕ <u>Filte</u>r 5 Filter 6 Filter 7 Filter 8 , Filter 9 Filter 10 Filter 12 Filter 11 Filter 13 Fil<u>ter 16</u> Filter 14 Filter 15

Translated Rapidity y

Generally see blobs of all scales

Local nature of activated region lends interpretation as "pixels"

EFN seems to have learned a dynamically sized jet image









l = 8



ℓ = I6



ℓ = 32



ℓ = 64



ℓ = 128



Measuring Q/G EFN Filters

Power-law dependence between filter size and distance from center is observed



Emission plane area element

Non-perturbative physics, axis recoil, higher order effects cause deviations from slope of 2



Visualizing Q/G EFN Filters in the Emission Plane



Extracting New Analytic Observables



EFN ($\ell = 2$) has approximately radially symmetric filters

Fit functions of the forms:

$$A_{r_0} = \sum_{i=1}^{M} z_i \, e^{-\theta_i^2/r_0^2}, \qquad B_{r_1,\beta} = \sum_{i=1}^{M} z_i \, \ln(1 + \beta(\theta_i - r_1))\Theta(\theta_i - r_1)$$

Separate soft and collinear phase space regions

Extracting New Analytic Observables

Can visualize F in the two dimensional $(\mathcal{O}_1, \mathcal{O}_2)$ phase space



Benchmarking New Analytic Observables

Individually, extracted observables are comparable to other angularities

Extracted C(A, B) performs nearly as well as EFN (ℓ = 2)

Meanwhile, multivariate combination (BDT) of three other angularities does not show improvement



Top Jet Samples and Other Methods

Common top and QCD dijet samples for standardized benchmarking

 $p_T \in [550, 650]$ GeV, AK8 jets, fully-merged, Delphes simulation, 2m jets total

Approach	AUC	Acc.	1/eB @ (eS=0.3)	Contact	Comments
LoLa	0.979	0.928		G. Kasieczka S. Leiss	Preliminary number, based on LoLa
LBN	0.981	0.931	863	M. Rieger	Preliminary number
CNN	0.981	0.93	780	D. Shih	Model from (1803.00107)
P-CNN (1D CNN)	0.980	0.930	782	H. Qu, L. Gouskos	Preliminary, use kinematic info only
6-body N-subs. (+mass and pT) NN	0.979	0.922	856	K. Nordstrom	Based on 1807.04769
8-body N-subs. (+mass and pT) NN	0.980	0.928	795	K. Nordstrom	Based on 1807.04769
Linear EFPs	0.980	0.932	380	PTK, E. Metodiev	d<= 7, chi <= 3 EFPs with FLD. Based on 1712.07124
Particle Flow Network (PFN)	0.982	0.932	888	PTK, E. Metodiev	Median over ten trainings. Based on Table 5 in 1810.05165
Energy Flow Network (EFN)	0.979	0.927	619	PTK, E. Metodiev	Median over ten trainings. Based on Table 5 in 1810.05165

Classification Performance



Latent space dimension ℓ = 256

EFN/PFN rotation and reflection preprocessing helpful

EFPs are comparable to EFN and even better at high signal efficiency

EFN Latent Dimension Sweep





l = 8

Without rotation/reflection preprocessing



 $\ell = 16$

 $\ell = 4$



ℓ = 32



ℓ = 64



ℓ = I28



With rotation/reflection preprocessing





ℓ = I6





ℓ = 32



ℓ = 64



ℓ = 128







Energy Flow Moments



Energy Flow Polynomials

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Energy Flow Networks

Energy Flow Moments



Energy Flow Polynomials

Energy Flow Polynomials (EFPs)

[PTK, Metodiev, Thaler, 1712.07124]



Generalizes many well-known and studied classes of energy correlators observables

A family of energy correlators with angular structures determined by multigraphs

$$\mathbf{Multigraph \ correspondence}$$

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Linear Basis of IRC-Safe Observables

One can show via the Stone-Weierstrass approximation theorem that any IRC-safe observable is a linear combination of EFPs

$$\mathcal{S} \simeq \sum_{G \in \mathcal{G}} s_G \text{EFP}_G, \quad \mathcal{G} \text{ a set of multigraphs}$$

$$\bigwedge$$

$$Multivariate \ combinations \ of \ EFPs \ only \ require linear \ methods \ to \ achieve \ full \ generality$$

$$\bigwedge$$

$$Strategy: \text{Learn coefficients } s_G \text{ via linear regression or classification}$$

Fun with the Stone-Weierstrass Theorem

Weierstrass function – continuous everywhere, differentiable on a measure zero set of points ∞



Familiar Observables as EFPs



Even angularities are exact linear combinations of EFPs

EFPs organized by degree d – number of edges



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EFPs for Quark vs. Gluon Jets



EFPs for Boosted Tops







Energy Flow Networks

Jet symmetries, point clouds, Deep Sets, performance, versatility, simplicity, visualization, new analytic observables

Energy Flow Moments

Linear in M computation of EFPs, additivity, algebraic identities



Energy Flow Polynomials

Linear basis of IRC-safe observables

EnergyFlow Python Package

Implements variable elimination for efficient EFP computation

Contains EFN and PFN implementations in Keras

CNN, DNN architectures included for easy model comparison

Several detailed examples demonstrating how to train models and make visualizations



EnergyFlow Python Package

Contains EFN and PFN implementations in Keras

CNN, DNN architectures included for easy model comparison

Includes quark/gluon jet samples used in [1810.01565]

Several detailed examples demonstrating how to train models and make visualizations



Thank You!

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Computation Complexity of EFPs – Variable Elimination

Naive computation complexity of an energy correlator is $\mathcal{O}(M^N)$

For ~100 particles this becomes intractable for N > 4

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EnergyCorrelator fjcontrib package gives up in this case



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Variable elimination (VE) algorithm can speedup EFPs by finding efficient elimination ordering

$$\frac{2}{1 \cdot 3 \cdot 5} = \left(\sum_{i_1=1}^{M} \sum_{i_2=1}^{M} \sum_{i_3=1}^{M} z_{i_1} z_{i_2} z_{i_3} \theta_{i_1 i_2}^2 \theta_{i_2 i_3} \right) \left(\sum_{i_4=1}^{M} \sum_{i_5=1}^{M} z_{i_4} z_{i_5} \theta_{i_4 i_5}^4 \right) \quad \text{Disconnected is product} \\
= \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} \sum_{i_3=1}^{M} \sum_{i_4=1}^{M} \sum_{i_5=1}^{M} \sum_{i_6=1}^{M} \sum_{i_6=1}^{M} \sum_{i_7=1}^{M} \sum_{i_8=1}^{M} z_{i_1} z_{i_2} z_{i_3} z_{i_4} z_{i_5} z_{i_6} z_{i_7} z_{i_8} \prod_{j=2}^{T} \theta_{i_1 i_j} \\
= \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} \sum_{i_3=1}^{M} \sum_{i_4=1}^{M} \sum_{i_5=1}^{M} \sum_{i_6=1}^{M} \sum_{i_7=1}^{M} \sum_{i_8=1}^{M} z_{i_1} z_{i_2} z_{i_3} z_{i_4} z_{i_5} z_{i_6} z_{i_7} z_{i_8} \prod_{j=2}^{T} \theta_{i_1 i_j} \\
= \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} z_{i_1} \left(\sum_{i_2=1}^{M} z_{i_2} \theta_{i_1 i_2} \right)^{T} \quad \mathcal{O}(M^8) \\
= \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} z_{i_1} \left(\sum_{i_2=1}^{M} z_{i_2} \theta_{i_1 i_2} \right)^{T} \quad \mathcal{O}(M^8) \\
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= \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} \sum_$$