Point Cloud Strategies for Boosted Objects

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Jets in Particle Physics

Point Clouds

Energy Flow Networks







Jets in Particle Physics

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Jets at the LHC

New physics searches and standard model measurements involve jets (collimated sprays of hadrons)



CMS hadronic $t\overline{t}$ event

ATLAS high jet multiplicity events

Jets in Data



Jets in Theory

Hard collision

Good understanding via perturbation theory

Fragmentation

Semi-classical parton shower, effective field theory

Hadronization

Poorly understood (non-perturbative), modeled empirically

Fragmentation partons Ø @ d ...

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Cartoon of jet formation as a multi-scale process

Hadronization

hadrons $\pi^{\pm}K^{\pm}$...

Collision

Detection



Patrick Komiske – Point Cloud Strategies for Boosted Objects Slide by Jesse Thaler







Jets in Particle Physics

Point Clouds

Energy Flow Networks

What is a Jet?

An unordered, variable length collection of particles

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

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

)),
$$\underbrace{M \ge 1}_{\text{Multiplicity}}$$
, $\underbrace{\forall \pi \in S_M}_{\text{Permutations}}$



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 Clouds

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



Processing Point Clouds









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Deep Sets

Namespace for symmetric function parametrization

A general permutation-symmetric function is *additive* in a latent space (piece of math)

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

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A general permutation-symmetric function is *additive* in a latent space (piece of math)



General parametrization for a function of sets

Deep Sets for Particle Jets

[PTK, Metodiev, Thaler, <u>1810.05165</u>]

Energy Flow Network (EFN)

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

Energy-weighted (safe) latent space

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



Approximating Φ and F with Neural Networks

Employ neural networks as arbitrary function approximators

Use fully-connected networks for simplicity

Graph CNNs also interesting (see H. Qu's <u>talk</u> at ML4Jets)

Default sizes $-\Phi$: (100, 100, ℓ), F: (100, 100, 100)







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. $(\varepsilon_s, 1/(1-\varepsilon_b)), (\varepsilon_s, \varepsilon_s/\sqrt{1-\varepsilon_b})$

Quark vs. Gluon: Classification Performance



PFN: No particle type info, arbitrary energy dependence

EFN: Energy-weighted latent space



PFN-ID slightly better than RNN-ID

Quark vs. Gluon: 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: Energy-weighted latent space





Boosted Top: 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

Boosted Top: EFN Latent Dimension Sweep



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 Filter 14 Filter 15 Filter 16

EFN (ℓ = 256) randomly selected filters, sorted by size

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

Translated Rapidity y







ℓ = 8



ℓ = I6



l = 32



l = 64



ℓ = 128



Quark vs. Gluon: Visualizing EFN Filters in the Emission Plane



Quark vs. Gluon: Measuring 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



Without rotation/reflection preprocessing





ℓ = 8



 $\ell = 16$



ℓ = 32



ℓ = 64



l = 128

Without rotation/reflection preprocessing



With rotation/reflection preprocessing





l = 16

l = 4





ℓ = 64



ℓ = 128



Boosted Top: Measuring EFN Filters



Power law behavior not as clear, slope further away from 2







Jets in Particle Physics

Ubiquitous standard model signature, likely BSM final state

Point Clouds

Same structure as jets/events at colliders

Energy Flow Networks

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

EnergyFlow Python Package

https://energyflow.network

Keras implementations of EFNs, PFNs, DNNs, CNNs, efficient EFP computation

Parallelized EMD calculations via the Python Optimal Transport library

Several detailed <u>examples</u> and <u>demos</u> for common use cases and visualization procedures



BOSTON 2019

[BOOST 2019, July 22-26, MIT]

Phenomenology | Reconstruction | Searches | Algorithms | Measurements | Calculations Modeling | Machine Learning | Pileup Mitigation | Heavy-Ion Collisions | Future Colliders

Additional Slides

Quark vs. Gluon: Extracting New Analytic Observables



EFN (ℓ = 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

Quark vs. Gluon: Extracting New Analytic Observables

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



Quark vs. Gluon: 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









Energy Flow Polynomials

Linear basis of IRC-safe observables, fixed processing of point cloud, identify many common observables as combinations

Energy Flow Networks

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

Energy Flow Moments

Connects multiparticle correlators to additive structures, linear in M computation of EFPs, algebraic identities

Infrared and Collinear (IRC) Safety

QCD has soft and collinear divergences associated with gluon radiation



<u>KLN Theorem</u>: IRC safety of an observable is sufficient to guarantee that soft/collinear divergences cancel at each order in perturbation theory

Infrared (IR) safety – observable is unchanged under addition of a soft particle $S(\{p_1^{\mu}, \dots, p_M^{\mu}\}) = S(\{p_1^{\mu}, \dots, (1-\lambda)p_M^{\mu}, \lambda p_M^{\mu}\}), \quad \forall \lambda \in [0, 1]$

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

IRC safety is a key theoretical and experimental property of observables

Derivation of EFP Linear Spanning Basis

Arbitrary IRC-safe observable: $S(p_1^{\mu}, ..., p_M^{\mu})$

- Energy expansion*: Approximate S with polynomials of z_{i_i}
 - IR safety: S is unchanged under addition of soft particle
 - C safety: S is unchanged under collinear splitting of a particle
 - Relabeling symmetry: Particle index is arbitrary

Energy correlator parametrized by angular function f

$$\sum_{i_1=1}^{M} \dots \sum_{i_N=1}^{M} z_{i_1} \dots z_{i_N} f(\hat{p}_{i_1}, \dots, \hat{p}_{i_N})$$

[F. Tkachov, <u>hep-ph/9601308</u>]

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Energy correlators linearly span IRC-safe observables

- Angular expansion*: Approximate f with polynomials in θ_{ij}
- Simplify: Identify unique analytic structure that emerge

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- Angular expansion*: Approximate f with polynomials in θ_{ij}
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Linear spanning basis in terms of "EFPs" has been found!

$$S \simeq \sum_{g \in G} s_G \text{EFP}_G, \qquad \text{EFP}_G \equiv \sum_{i_1=1}^M \dots \sum_{i_N=1}^M Z_{i_1} \dots Z_{i_N} \prod_{(k,\ell) \in G} \theta_{i_k i_\ell}$$

**Generically, approximations exist by the Stone-Weierstrass theorem

Energy Flow Polynomials (EFPs)

[PTK, Metodiev, Thaler, <u>1712.07124</u>]

$$EFP_{G} = \underbrace{\sum_{i_{1}=1}^{M} \cdots \sum_{i_{N}=1}^{M} z_{i_{1}} \cdots z_{i_{N}}}_{Correlator of Energies and Angles} \theta_{i_{k}i_{\ell}}$$

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

A family of energy correlators with angular structures determined by multigraphs

$$\underbrace{\sum_{i_{1}=1}^{M} \sum_{i_{2}=1}^{M} \sum_{i_{3}=1}^{M} \sum_{i_{4}=1}^{M} \sum_{i_{5}=1}^{M} \sum_{i_{4}=1}^{M} \sum_{i_{5}=1}^{M} z_{i_{1}} z_{i_{2}} z_{i_{3}} z_{i_{4}} z_{i_{5}} \theta_{i_{1}i_{2}} \theta_{i_{2}i_{3}} \theta_{i_{1}i_{3}} \theta_{i_{1}i_{4}} \theta_{i_{1}i_{5}} \theta_{i_{4}i_{5}}^{2} }}_{ \underbrace{\text{Multigraph correspondence}}_{k} \underbrace{\text{Energy and Angle Measure}}_{\text{Hadronic}: z_{i} = \frac{p_{Ti}}{\sum_{j} p_{Tj}}, \quad \theta_{ij} = \left(\Delta y_{ij}^{2} + \Delta \phi_{ij}^{2}\right)^{\beta/2} }$$

Patrick Komiske – Point Cloud Strategies for Boosted Objects

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

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

Multivariate combinations of EFPs only require <u>linear</u> <u>methods</u> to achieve full generality

Strategy: Learn coefficients s_G via linear regression or classification

Familiar Observables as EFPs



Even angularities are exact linear combinations of EFPs

EFPs organized by degree d – number of edges



Quark vs. Gluon: EFP Classification Performance Comparison



Saturation observed with more EFPs

[de Oliviera, Kagan, Mackey, Nachman, Schwartzman, 2015] [PTK, Metodiev, Schwartz, 2016] [Datta, Larkoski, 2017]

Boosted Top: EFP Classification Performance Comparison



Energy Flow Moments

Consider a slightly different hadronic angular measure, $\theta_{ij} = (2\hat{p}_i^{\mu}\hat{p}_{j\mu})^{\frac{\beta}{2}}, \ \hat{p}_i^{\mu} = \frac{p_i^{\mu}}{p_{Ti}}$ Agrees with previous hadronic measure in the limit of narrow, central jets When $\beta = 2$, angular measure can be factored, which motivates defining:

Energy Flow Moment (EFM) of valency v:

$$\mathcal{I}^{\mu_1\cdots\mu_v} = \sum_{i=1}^M \mathbf{z}_i \hat{p}_i^{\mu_1}\cdots\hat{p}_i^{\mu_v}$$

 $\beta = 2$ EFPs can be rewritten in terms of EFMs, which are linear in M to compute!

$$\begin{split} & \bigwedge_{i_1=1}^M \sum_{i_2=1}^M \sum_{i_3=1}^M z_{i_1} z_{i_2} z_{i_3} \theta_{i_1 i_2}^2 \theta_{i_1 i_3}^2 \theta_{i_2 i_3} \\ & = 2^5 \underbrace{\left(\sum_{i_1=1}^M z_{i_1} \hat{p}_{i_1}^\alpha \hat{p}_{i_1}^\beta \hat{p}_{i_1}^\gamma \hat{p}_{i_1}^\delta\right)}_{\mathcal{I}^{\alpha\beta\gamma\delta}} \underbrace{\left(\sum_{i_2=1}^M z_{i_2} \hat{p}_{i_2\alpha} \hat{p}_{i_2\beta} \hat{p}_{i_2}^\epsilon\right)}_{\mathcal{I}_{\alpha\beta}\epsilon} \underbrace{\left(\sum_{i_3=1}^M z_{i_3} \hat{p}_{i_3\gamma} \hat{p}_{i_3\delta} \hat{p}_{i_3\epsilon}\right)}_{\mathcal{I}_{\gamma\delta\epsilon}} \end{split}$$

A multigraph correspondence also exists for EFMs:



Energy Flow "Network"



The Energy Mover's Distance

EMD between energy flows defines a metric on the space of events







The Earth Mover's Distance

A metric on normalized distributions in a space with a ground distance measure

symmetric, non-negative, triangle inequality, zero iff identical

The minimum "work" (stuff x distance) required to transport supply to demand





Related to optimal transport theory – commonly used as a metric on the space of images

[Peleg, Werman, Rom, IEEE 1989; Rubner, Tomasi, Guibas, ICCV 1998, ICJV 2000; Pele, Werman, ECCV 2008; Pele, Taskar, GSI 2013]

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Manifold Dimensions of Event Space

Correlation dimension: how does the # of elements within a ball of size Q change?

$$\dim(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i} \sum_{j} \Theta(\text{EMD}(\mathcal{E}_{i}, \mathcal{E}'_{j}) < Q)$$

