

# Point Cloud Strategies for Boosted Objects

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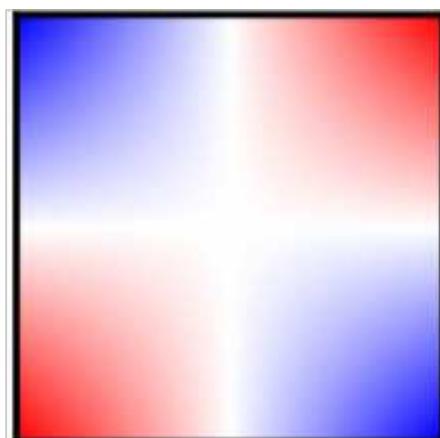
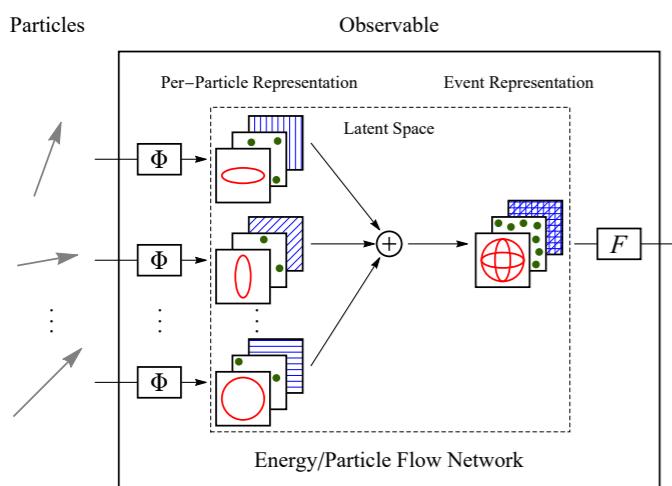
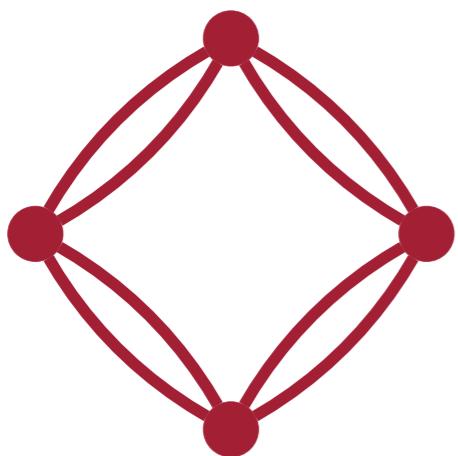
CERN BSM Forum

February 21, 2019

Collaborators: Eric Metodiev and Jesse Thaler

[I7I2.07I24](#)

[I8I0.05I65](#)



# Energy Flow Polynomials

# "Understanding the space of IRC-safe observables"

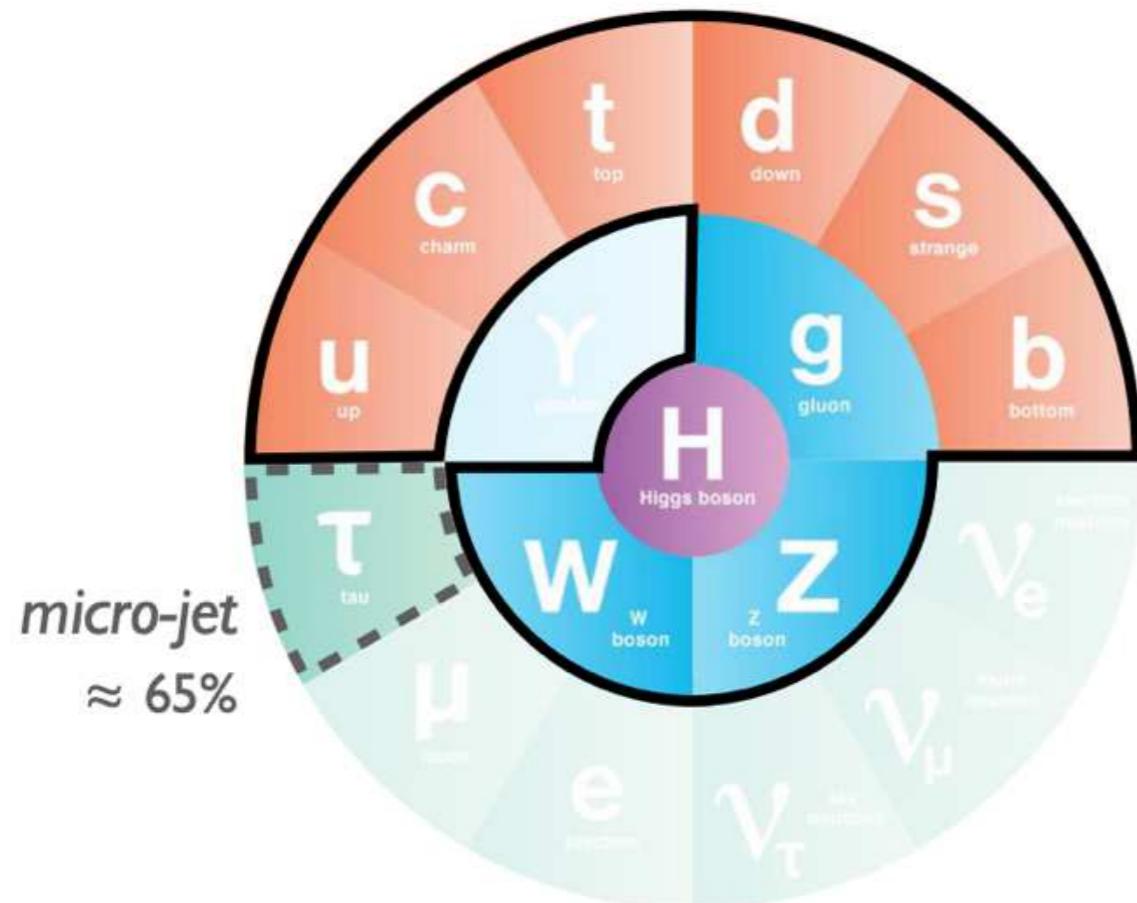
# Energy Flow Networks

# "Power of ML meets IRC-safe physics"

# Energy Flow Moments

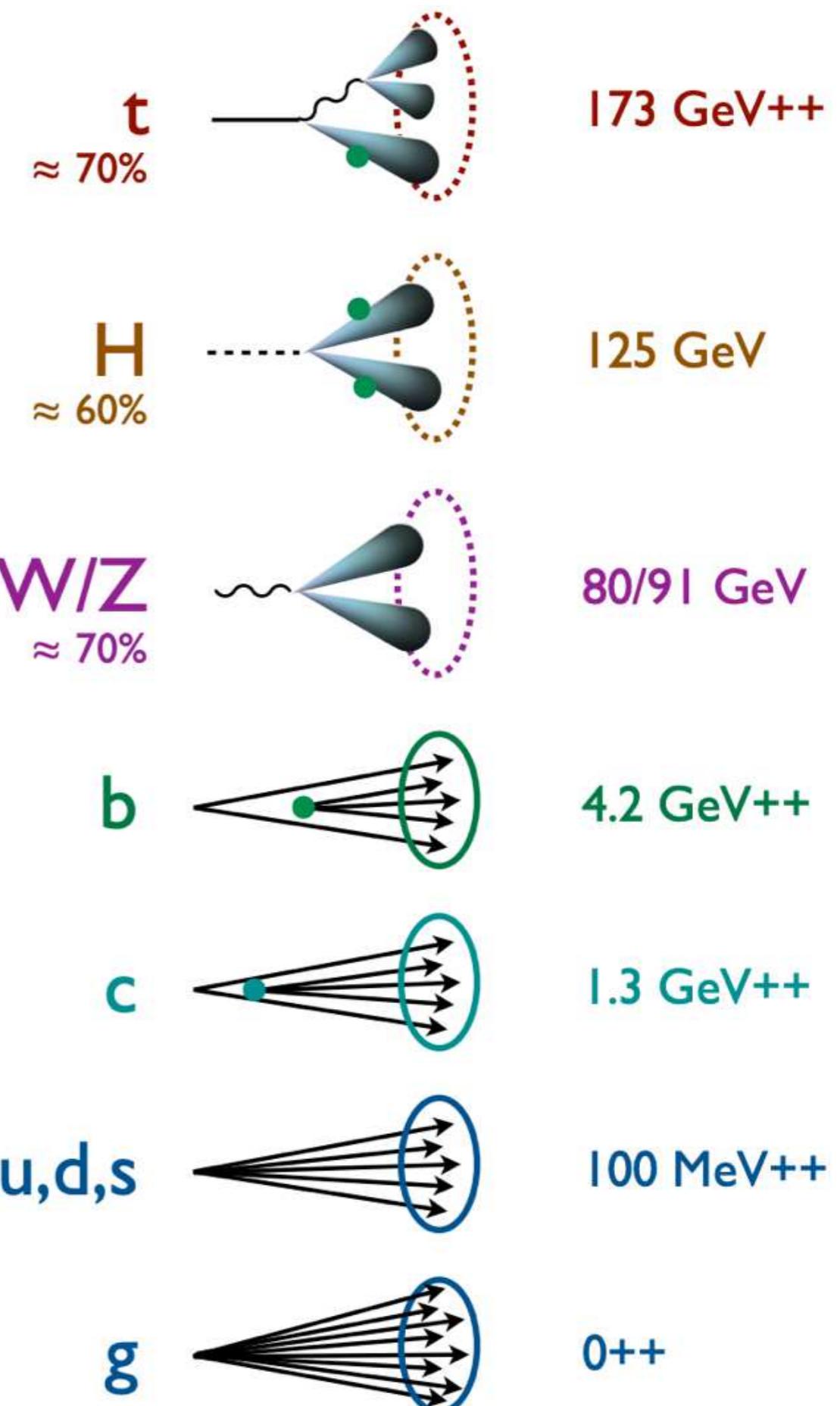
# "A deep connection between EFPs and EFNs"

# Jets in Theory

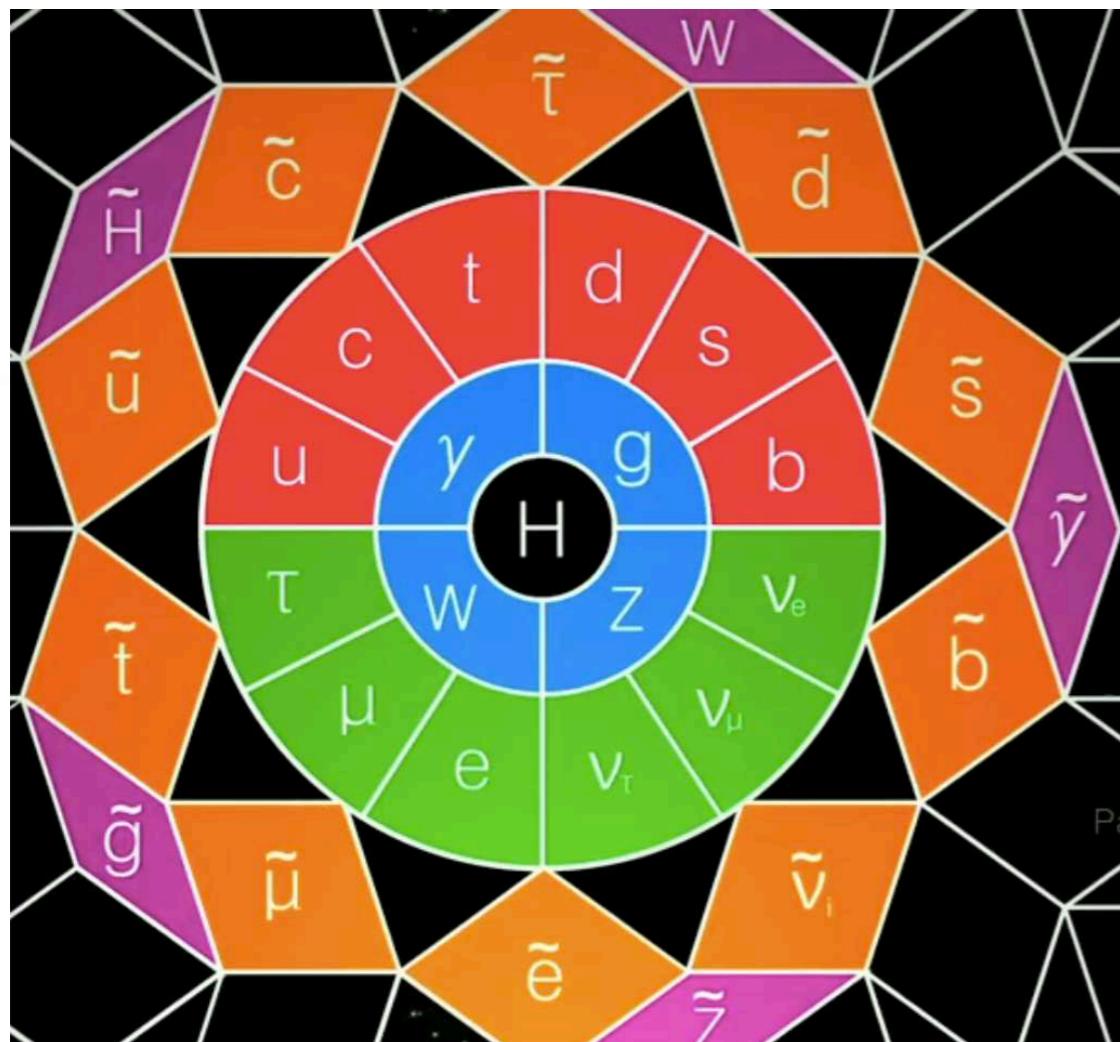


*Jets from the  
Standard Model*

$\text{++} = \text{Mass from QCD Radiation}$



# Jets in Theory



*Jets from Beyond the Standard Model*

++ = Mass from QCD Radiation

$\tilde{t}$   
≈ ?

$\tilde{H}$   
≈ ?

$\tilde{W}/\tilde{Z}$   
≈ ?

$\tilde{b}$   
≈ ?

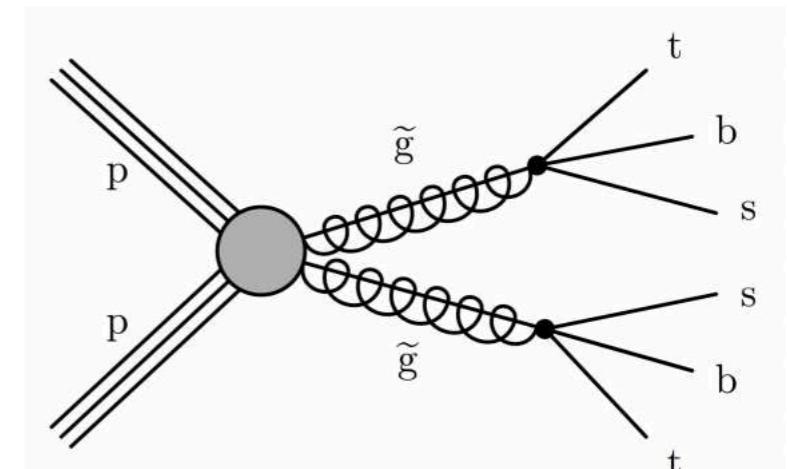
$\tilde{c}$   
≈ ?

$\tilde{u}, \tilde{d}, \tilde{s}$   
≈ ?

$\tilde{g}$   
≈ ?

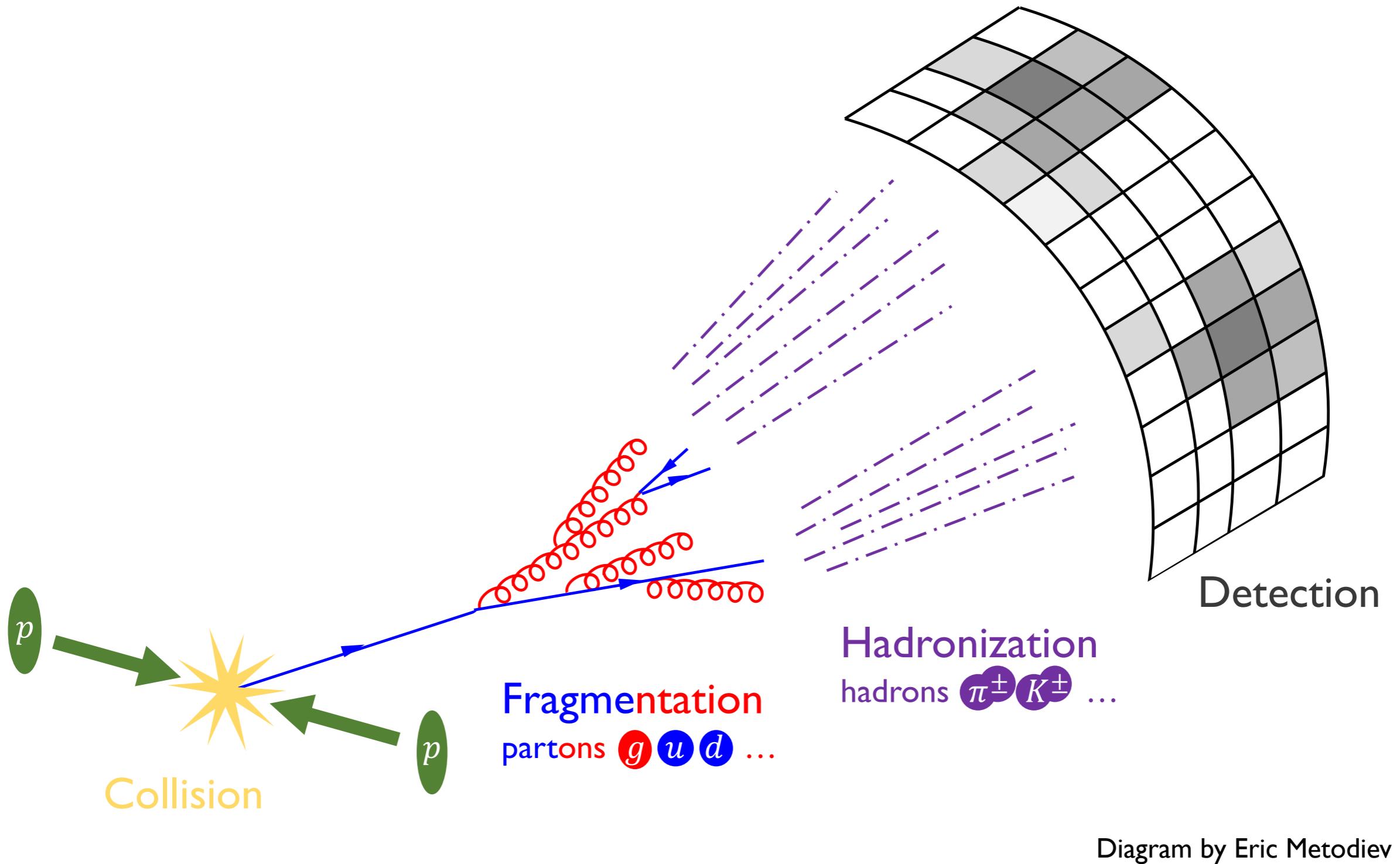
Many models of new physics generate boosted Standard Model hadronic final states

e.g.  $Z' \rightarrow t\bar{t}$ , cascade decays, various SUSY scenarios

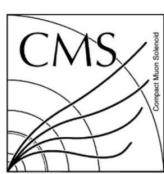


[CMS-SUS-16-040]

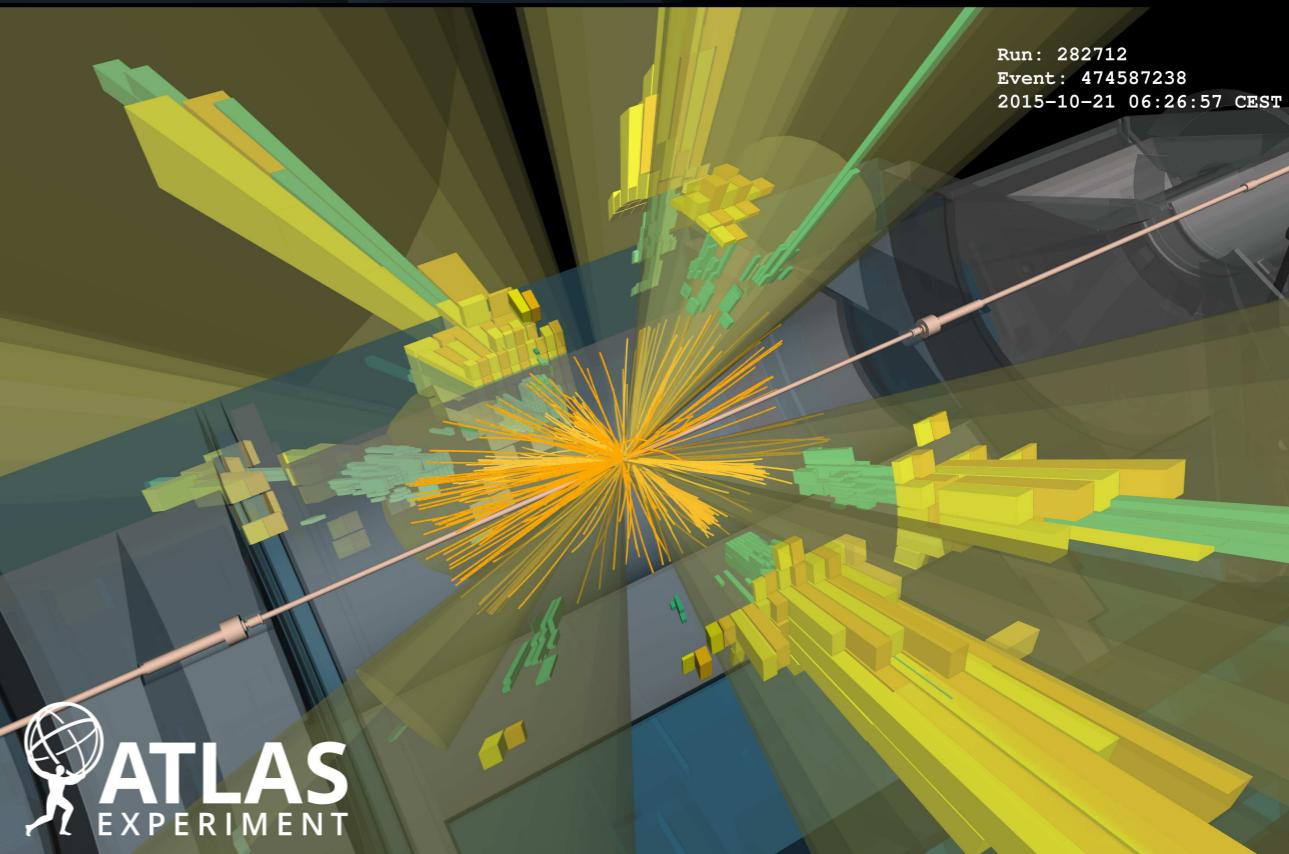
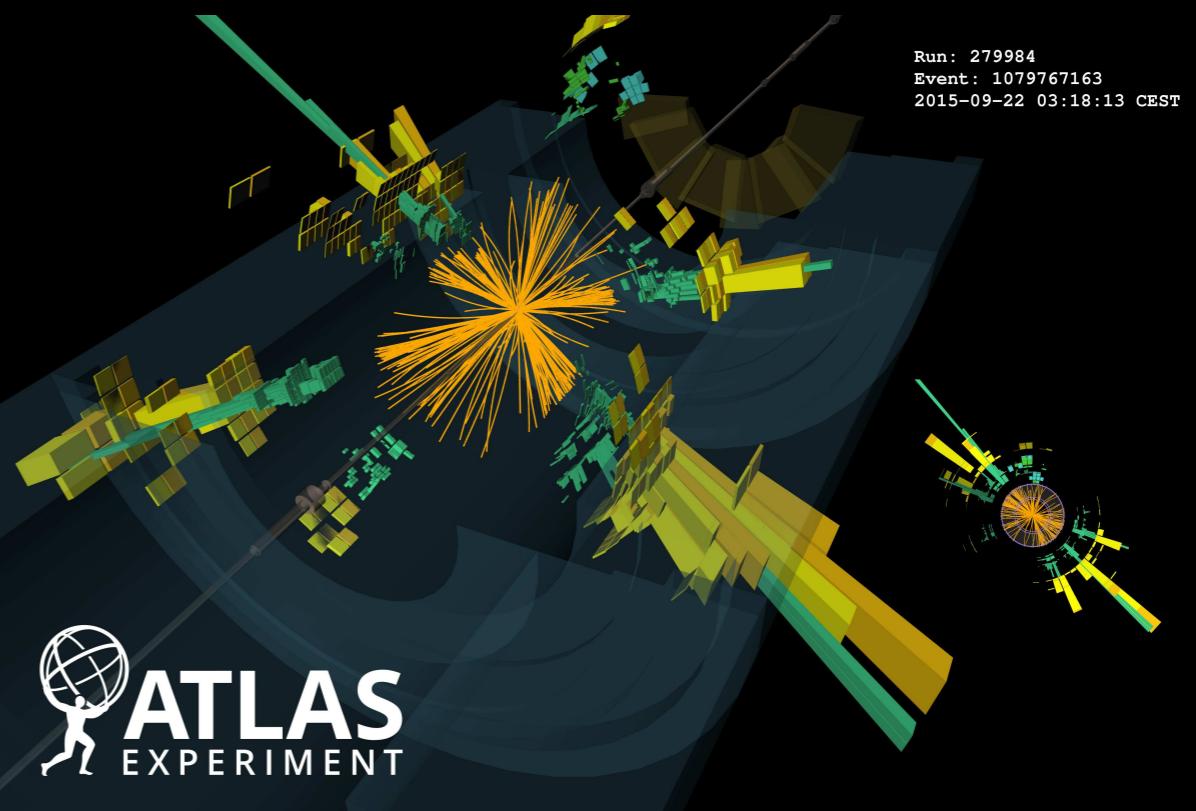
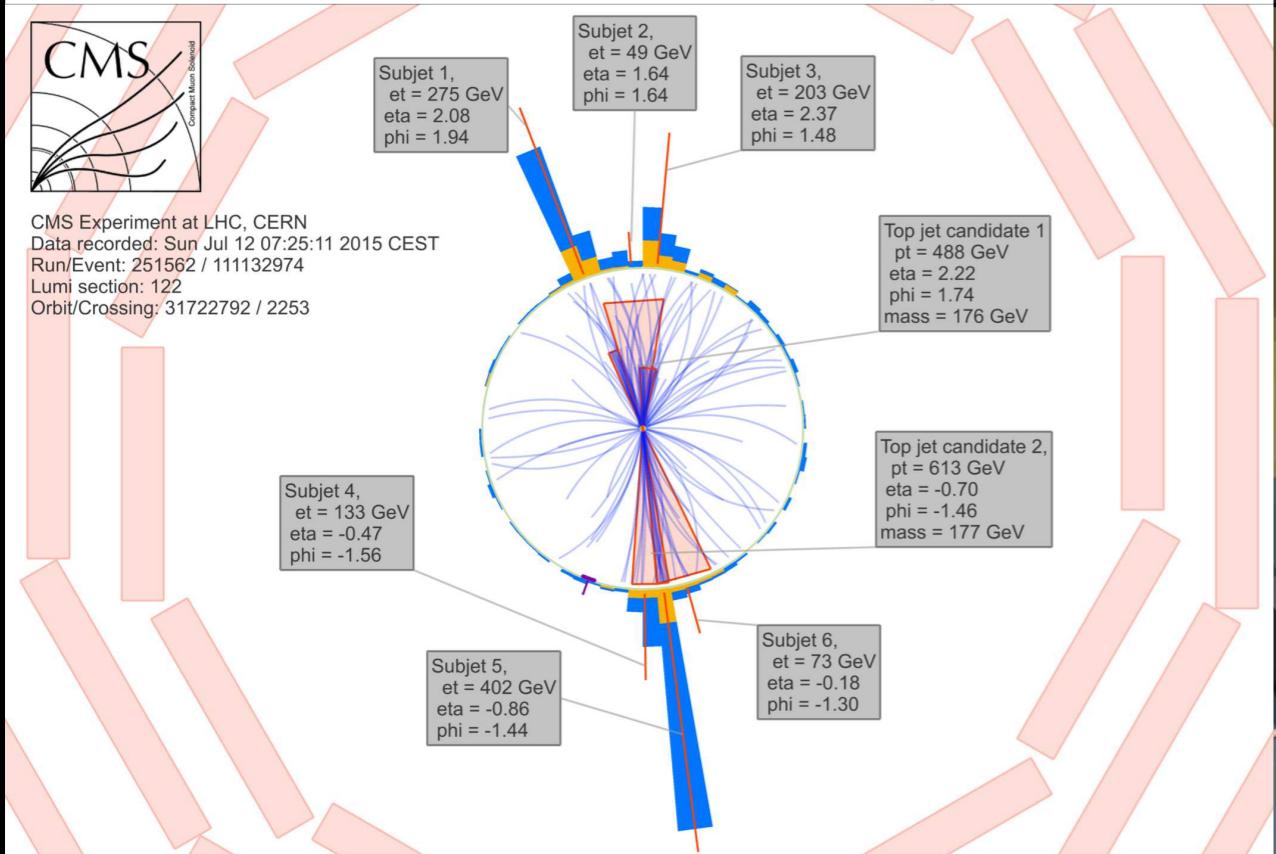
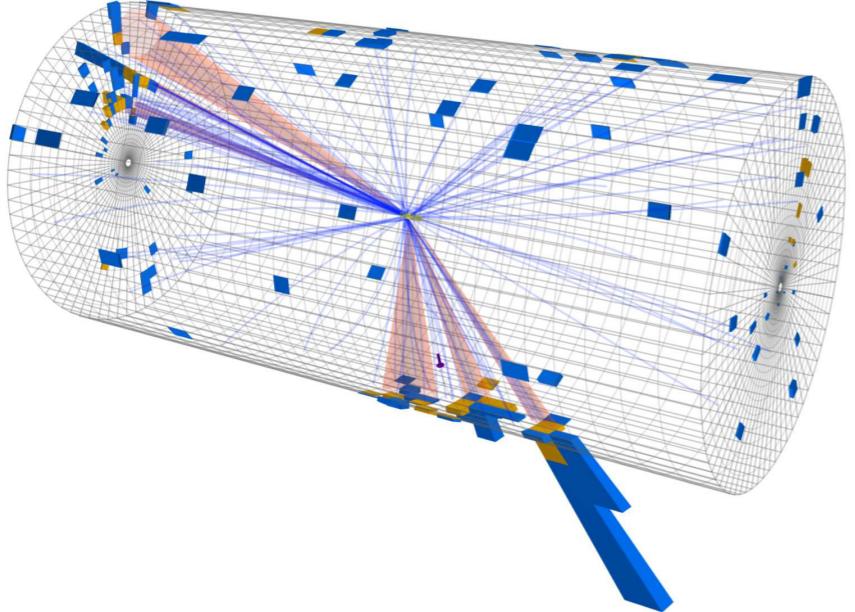
# Cartoon of Jet Formation



# Boosted Event Topologies at the LHC



CMS Experiment at LHC, CERN  
 Data recorded: Sun Jul 12 07:25:11 2015 CEST  
 Run/Event: 251562 / 111132974  
 Lumi section: 122  
 Orbit/Crossing: 31722792 / 2253



# What is a Jet?

An **unordered**, **variable length** collection of particles

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

$$J(\{p_1^\mu, \dots, p_M^\mu\}) = J(\{p_{\pi(1)}^\mu, \dots, p_{\pi(M)}^\mu\}), \quad \underbrace{M \geq 1}_{\text{Multiplicity}}, \quad \underbrace{\forall \pi \in S_M}_{\text{Permutations}}$$

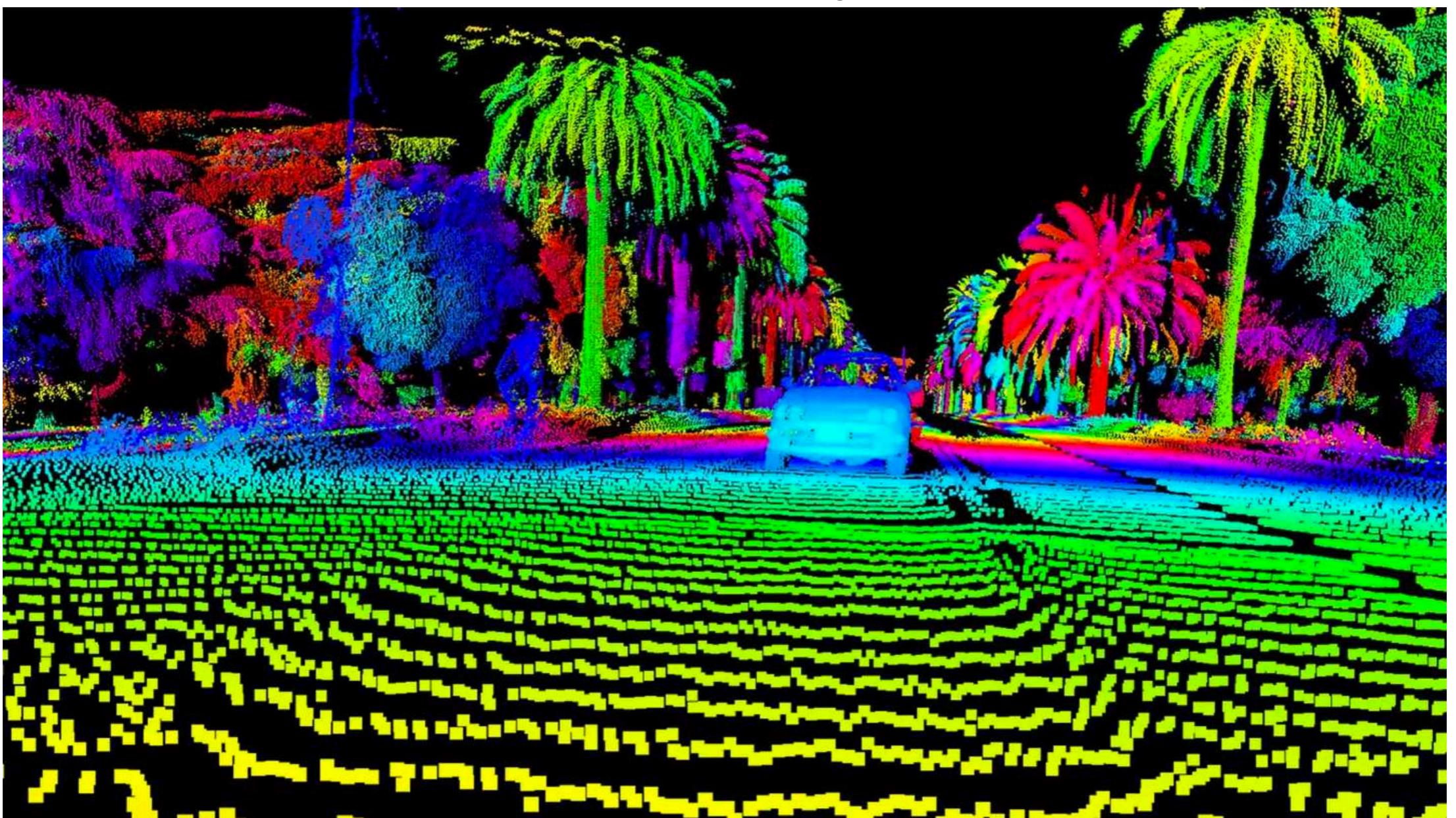
$p_i^\mu$  represents *all* the particle properties:

- 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



# Point Clouds

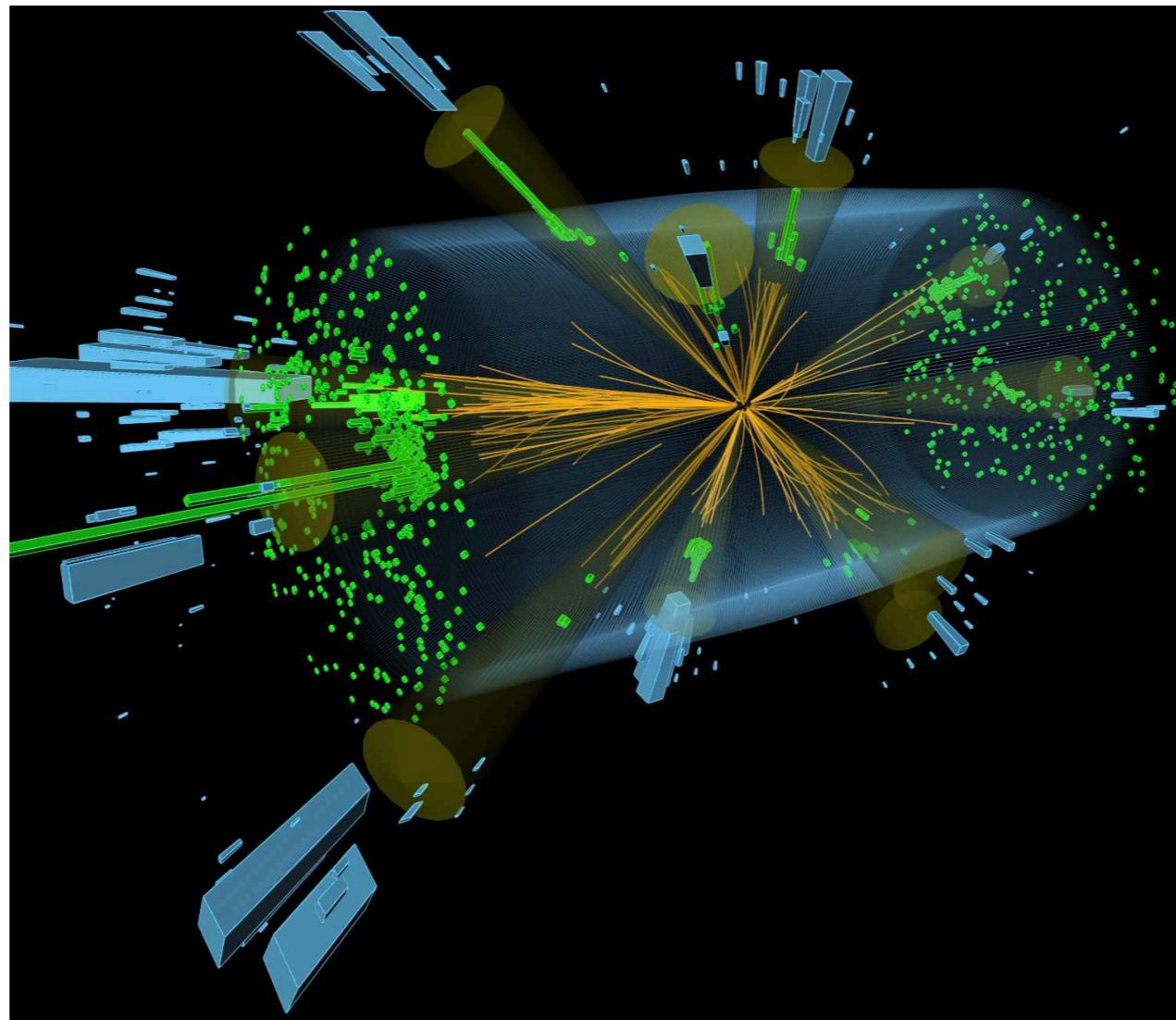
[Popular Science, 2013]



# Particle Collision Events as Point Clouds

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

Jet/event                          Particles                          Feature space

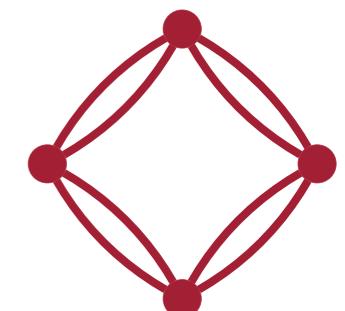


# Processing Point Clouds

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

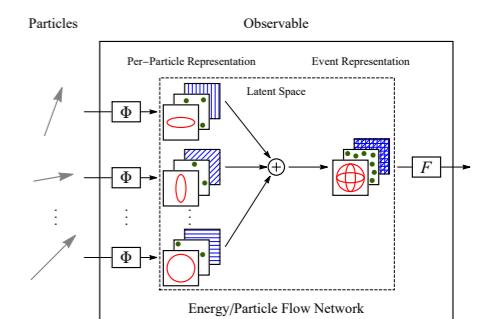
Variable constituent multiplicity requires at least one of:

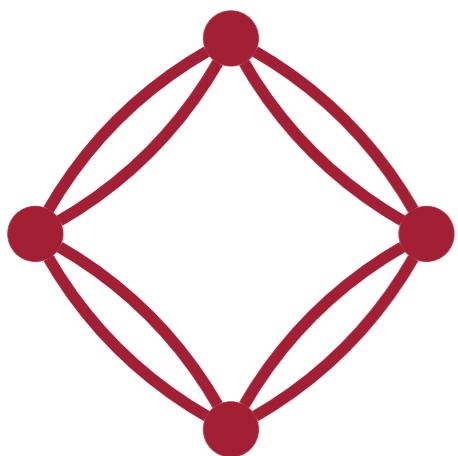
- Preprocessing to another representation (jet images, N-subjettiness, etc.)
- Truncation to an (arbitrary) fixed size
- Recurrent NN structure



Particle permutation symmetry requires:

- Permutation symmetric observables
- Permutation symmetric architectures





# Energy Flow Polynomials

## *Fixed preprocessing of a point cloud*

# Energy Flow Networks

# Energy Flow Moments

# Infrared and Collinear (IRC) Safety

QCD has soft and collinear divergences associated with gluon radiation



$$dP_{i \rightarrow ig} \simeq \frac{2\alpha_s}{\pi} C_a \frac{d\theta}{\theta} \frac{dz}{z}$$

$$\begin{aligned} C_q &= C_F = 4/3 \\ C_g &= C_A = 3 \end{aligned}$$

KLN Theorem: **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

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

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

$$S(\{p_1^\mu, \dots, p_M^\mu\}) = S(\{p_1^\mu, \dots, (1-\lambda)p_M^\mu, \lambda p_{M+1}^\mu\}), \quad \forall \lambda \in [0, 1]$$

**IRC** safety is a key theoretical *and* experimental property of observables

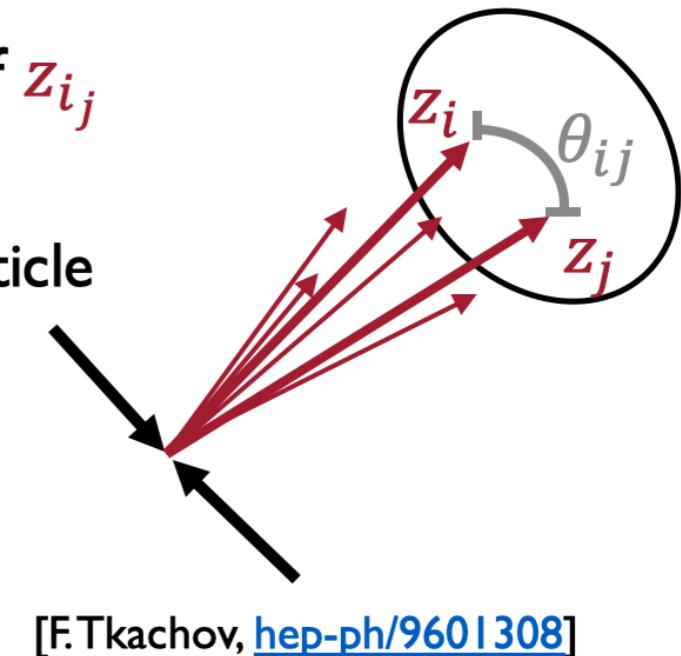
# Derivation of EFP Linear Spanning Basis

Arbitrary **IRC**-safe observable:  $S(p_1^\mu, \dots, p_M^\mu)$

- **Energy expansion\***: Approximate  $S$  with polynomials of  $z_{ij}$ 
  - **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  $f$

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



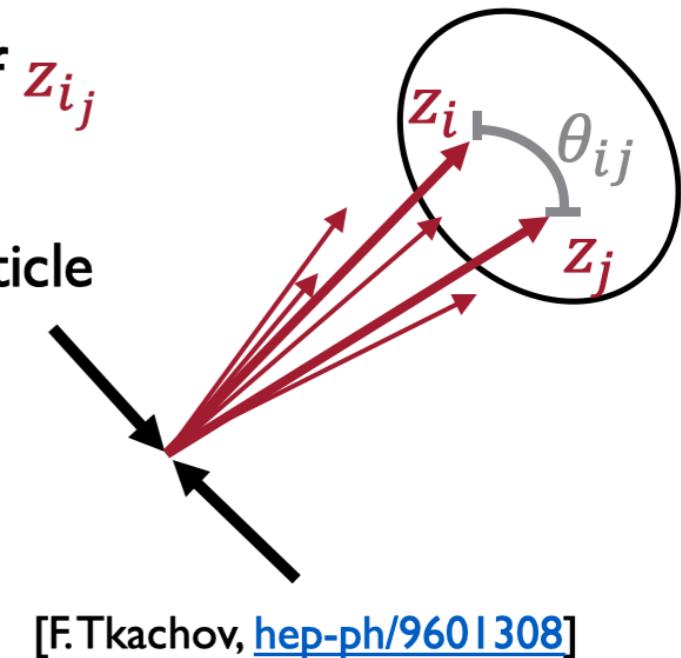
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[F.Tkachov, [hep-ph/9601308](#)]

→ Energy correlators linearly span **IRC**-safe observables

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

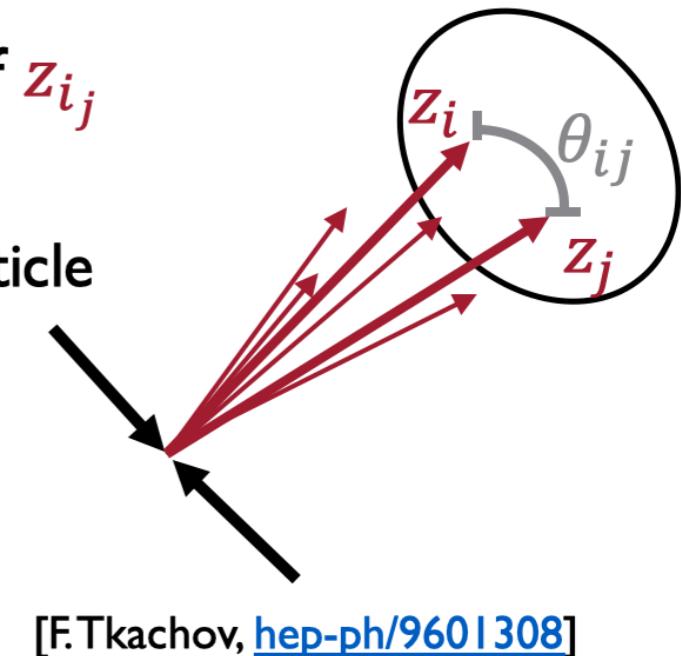
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→ Energy correlators linearly span **IRC**-safe observables

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

→ Linear spanning basis in terms of “EFPs” has been found!

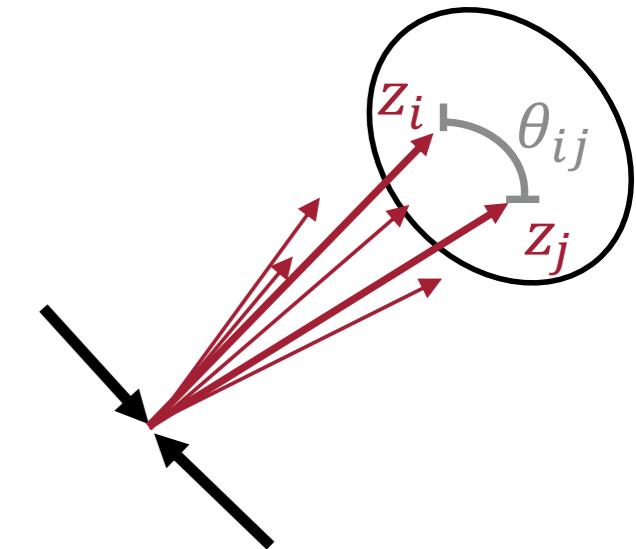
$$S \simeq \sum_{G \in G} s_G \text{EFP}_G, \quad \text{EFP}_G \equiv \sum_{i_1=1}^M \dots \sum_{i_N=1}^M z_{i_1} \dots z_{i_N} \prod_{(k,\ell) \in G} \theta_{i_k i_\ell}$$

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

# Energy Flow Polynomials (EFPs)

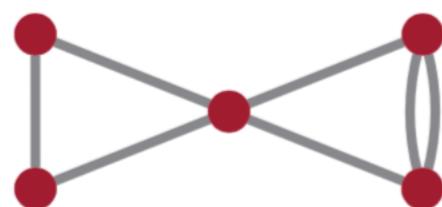
[PTK, Metodiev, Thaler, [1712.07124](#)]

$$\text{EFP}_G = \underbrace{\sum_{i_1=1}^M \cdots \sum_{i_N=1}^M}_{\text{Correlator of Energies}} z_{i_1} \cdots z_{i_N} \underbrace{\prod_{(k,\ell) \in G} \theta_{i_k i_\ell}}_{\text{and Angles}}$$



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

A family of energy correlators with angular structures determined by multigraphs



$$= \sum_{i_1=1}^M \sum_{i_2=1}^M \sum_{i_3=1}^M \sum_{i_4=1}^M \sum_{i_5=1}^M z_{i_1} z_{i_2} z_{i_3} z_{i_4} z_{i_5} \theta_{i_1 i_2} \theta_{i_2 i_3} \theta_{i_1 i_3} \theta_{i_1 i_4} \theta_{i_1 i_5} \theta_{i_4 i_5}^2$$

Multigraph correspondence

$$j \longleftrightarrow z_{i_j} \quad k \longleftrightarrow l \longleftrightarrow \theta_{i_k i_l}$$

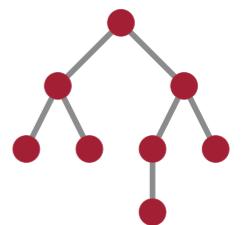
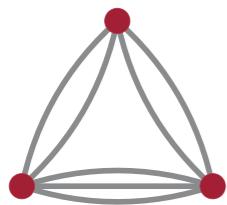
Energy and Angle Measure

Hadronic :  $z_i = \frac{p_{Ti}}{\sum_j p_{Tj}}, \quad \theta_{ij} = (\Delta y_{ij}^2 + \Delta \phi_{ij}^2)^{\beta/2}$

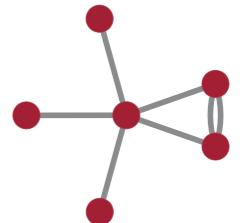
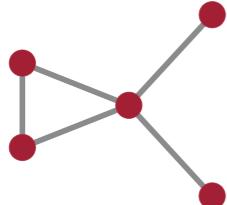
# Linear Basis of **IRC**-Safe Observables

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 linear methods to achieve full generality*



Strategy: Learn coefficients  $s_G$  via linear regression or classification

# Familiar Observables as EFPs

$$m_J^2 = \text{Diagram with two red dots connected by a self-loop edge}$$

[Larkoski, Moult, Neill, 2014]

$$D_2 = \frac{\text{Diagram with three red dots forming a triangle}}{(\text{Diagram with two red dots})^3}$$

[Larkoski, Salam, Thaler, 2013]

Energy correlation functions are complete graphs

Even angularities are exact linear combinations of EFPs

EFPs organized by degree  $d$  – number of edges

Degree	Connected Multigraphs
$d = 1$	
$d = 2$	
$d = 3$	
$d = 4$	
$d = 5$	

# Quantifying a Classifier

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

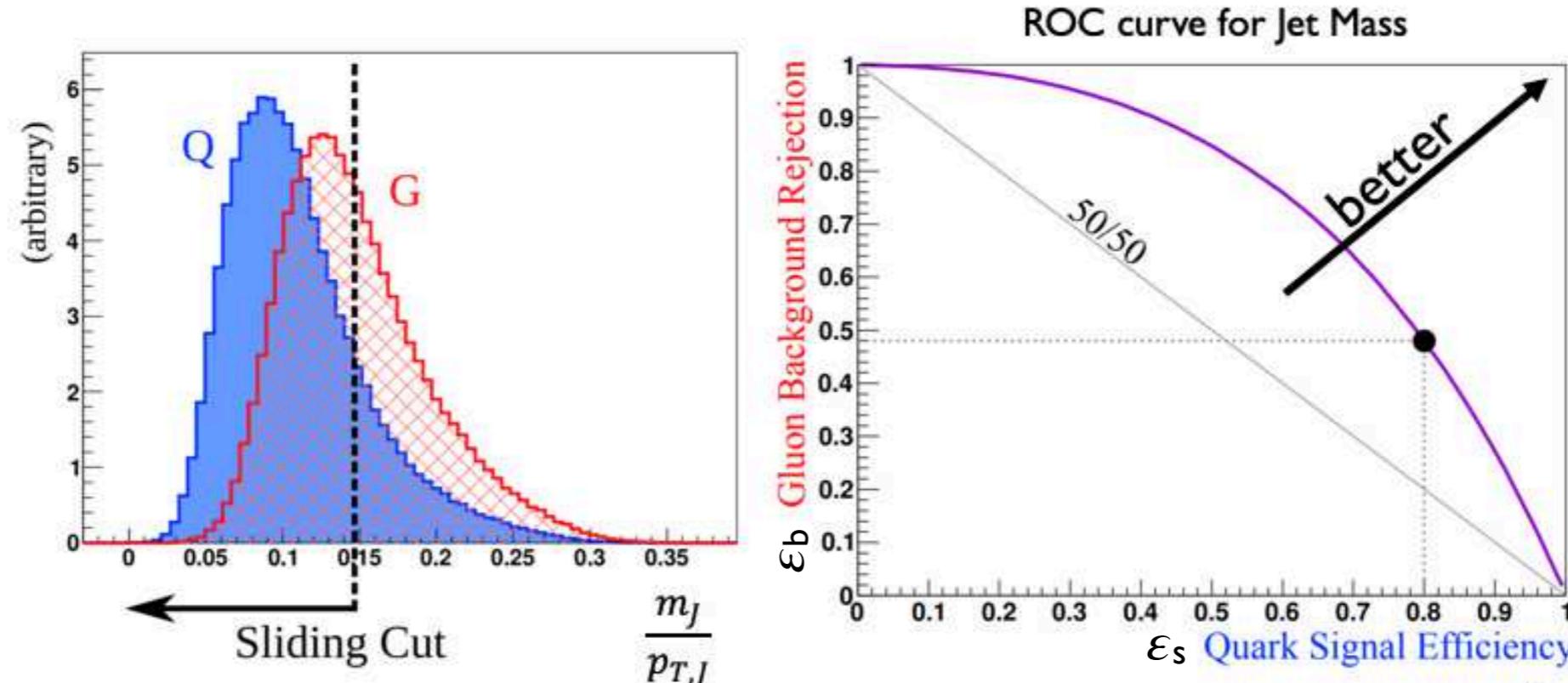
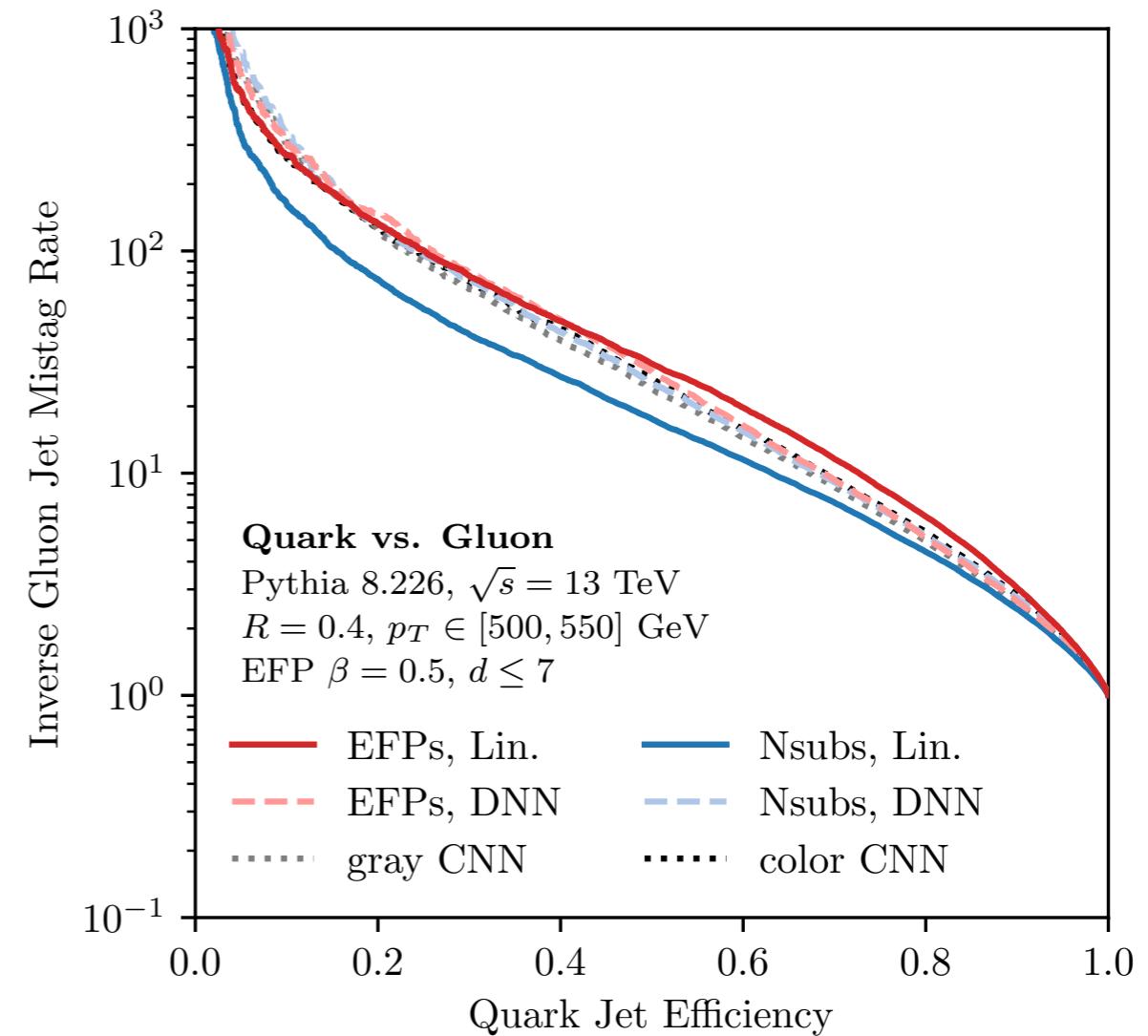
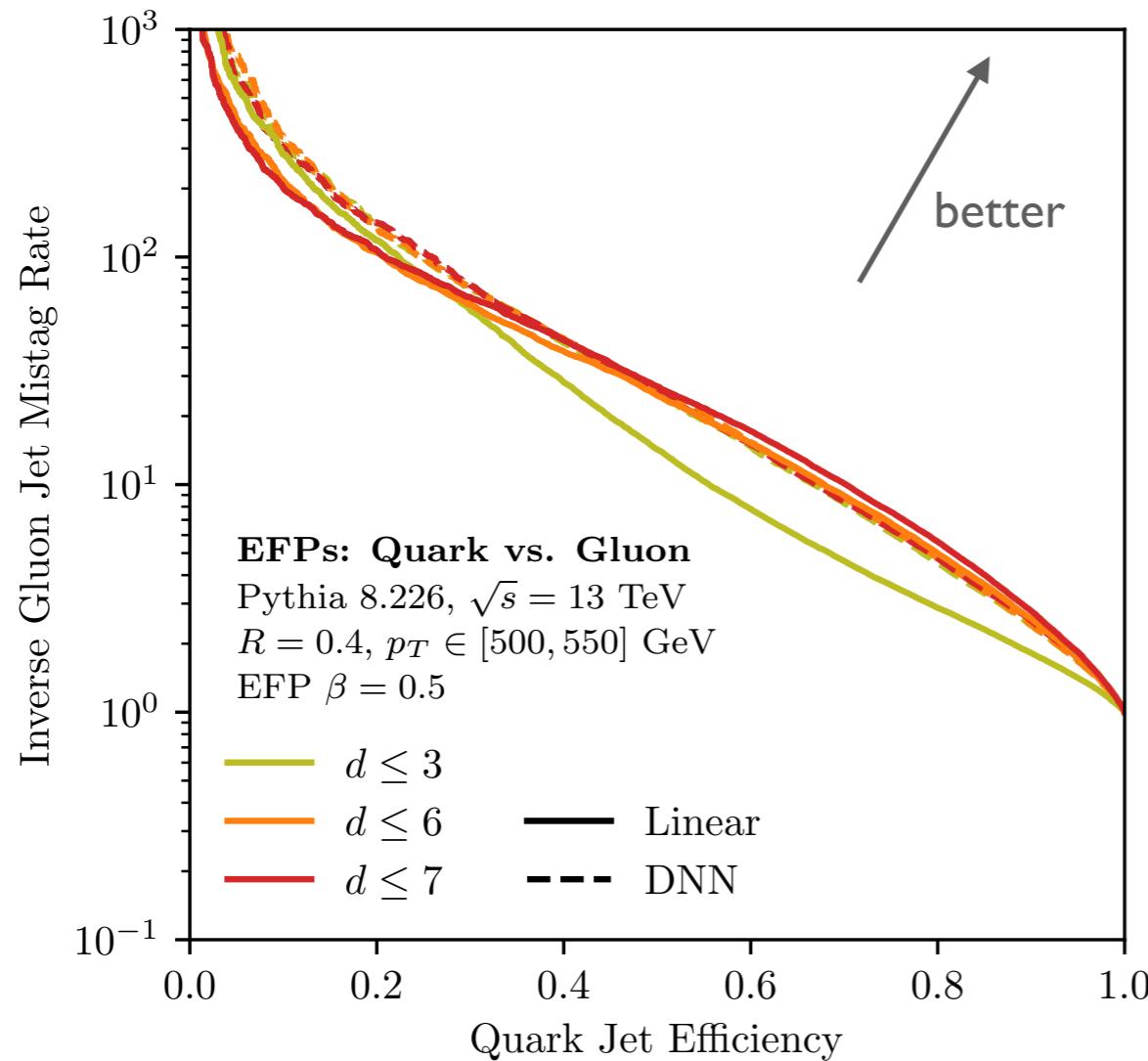


Figure from [1211.7038](#)

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

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

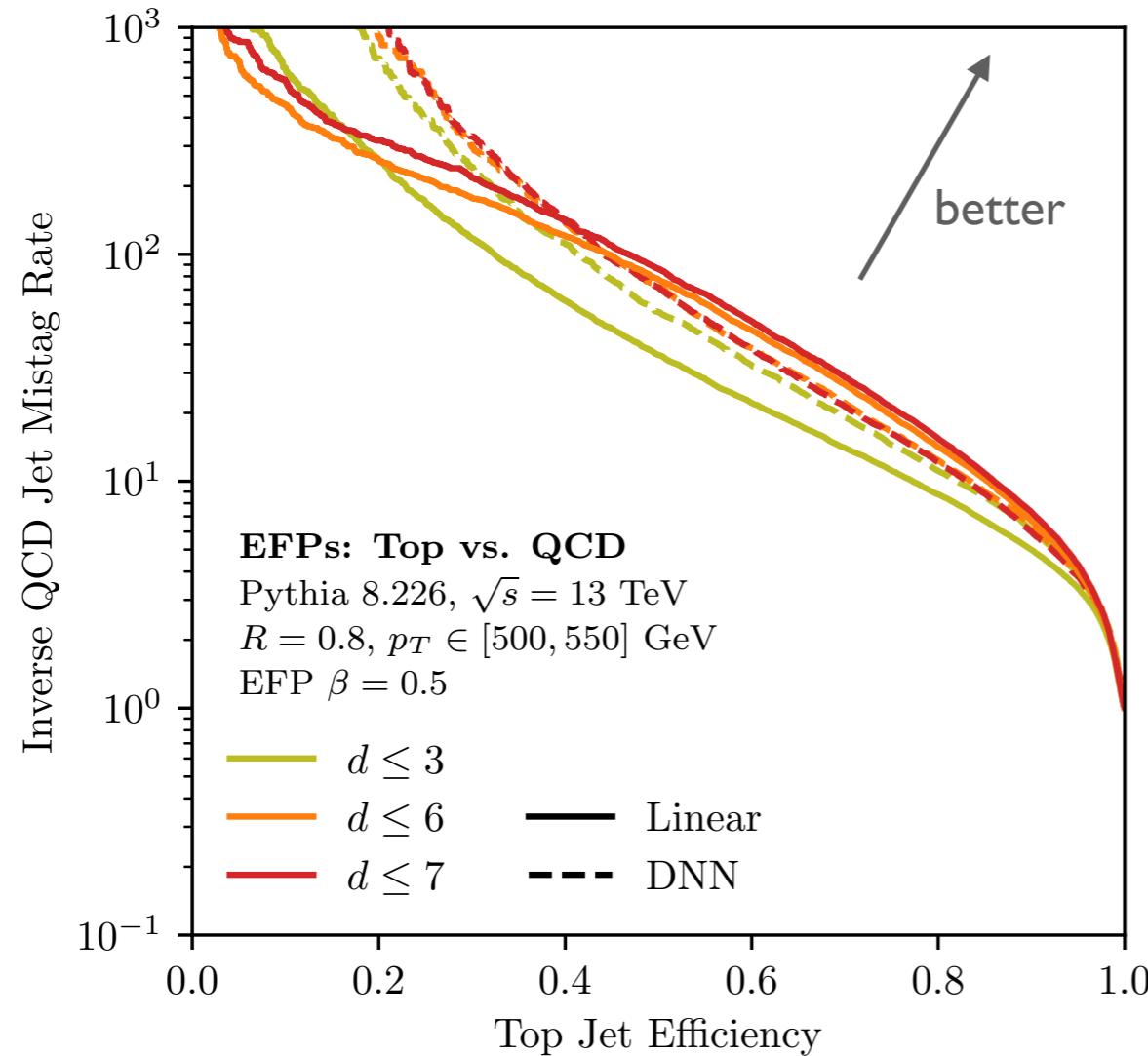
# Quark vs. Gluon: EFP Classification Performance Comparison



Saturation observed with more EFPs

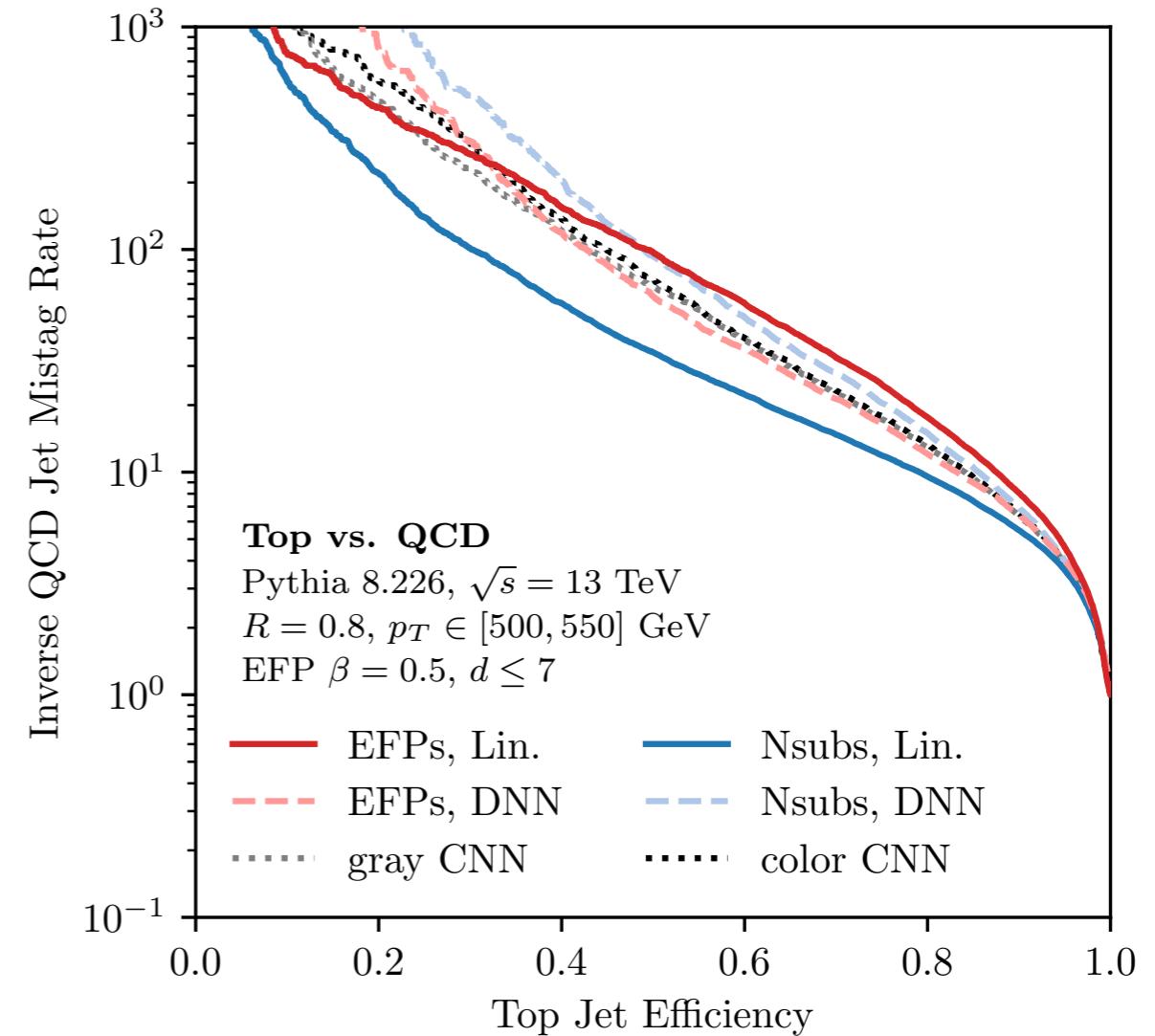
[de Oliveira, Kagan, Mackey, Nachman, Schwartzman, 2015]  
[PTK, Metodiev, Schwartz, 2016]  
[Datta, Larkoski, 2017]

# Boosted Top: EFP Classification Performance Comparison



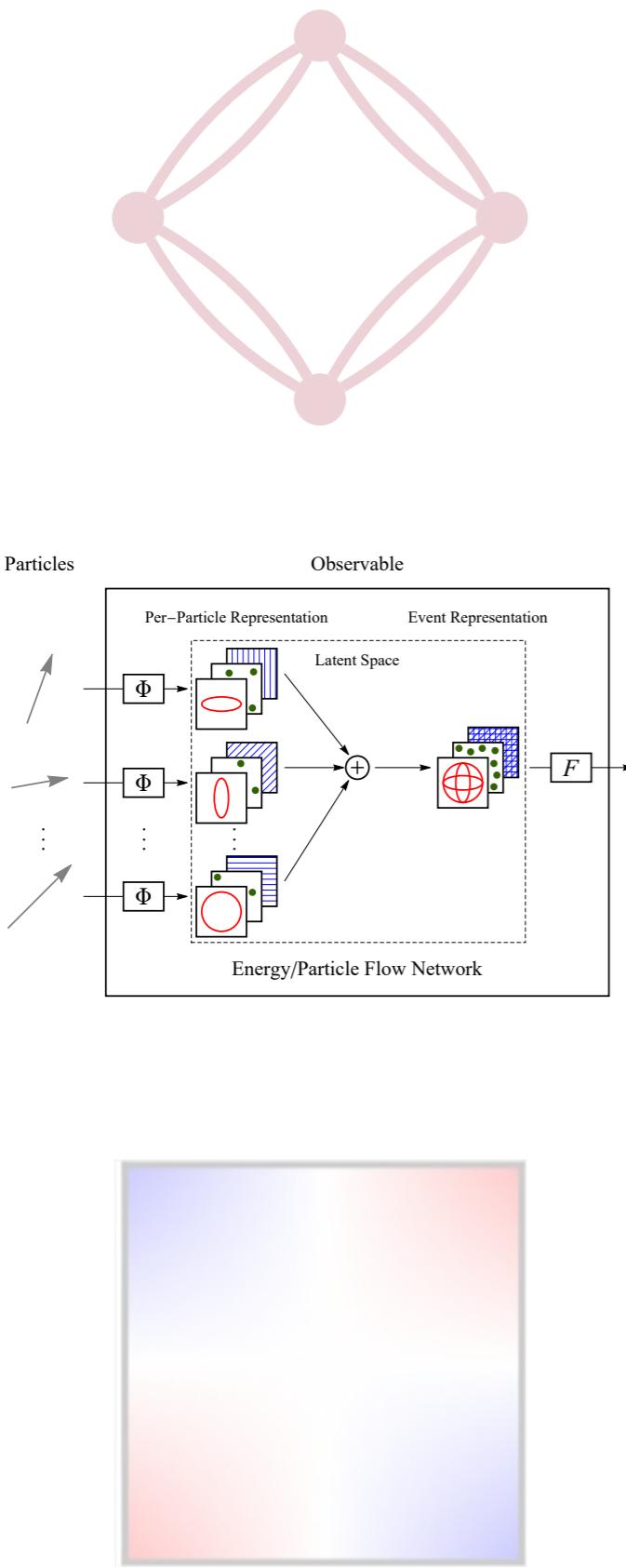
Saturation observed with more EFPs

DNN gets there faster but linear suffices



Linear EFPs excel at high efficiency

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



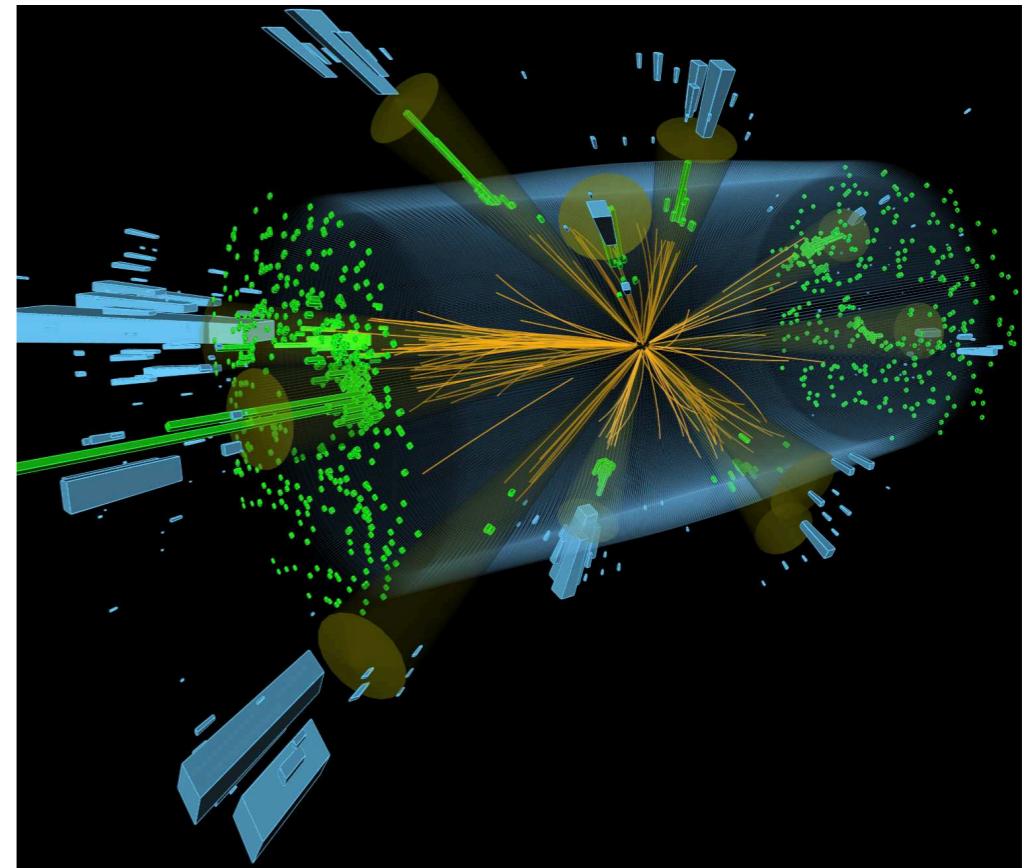
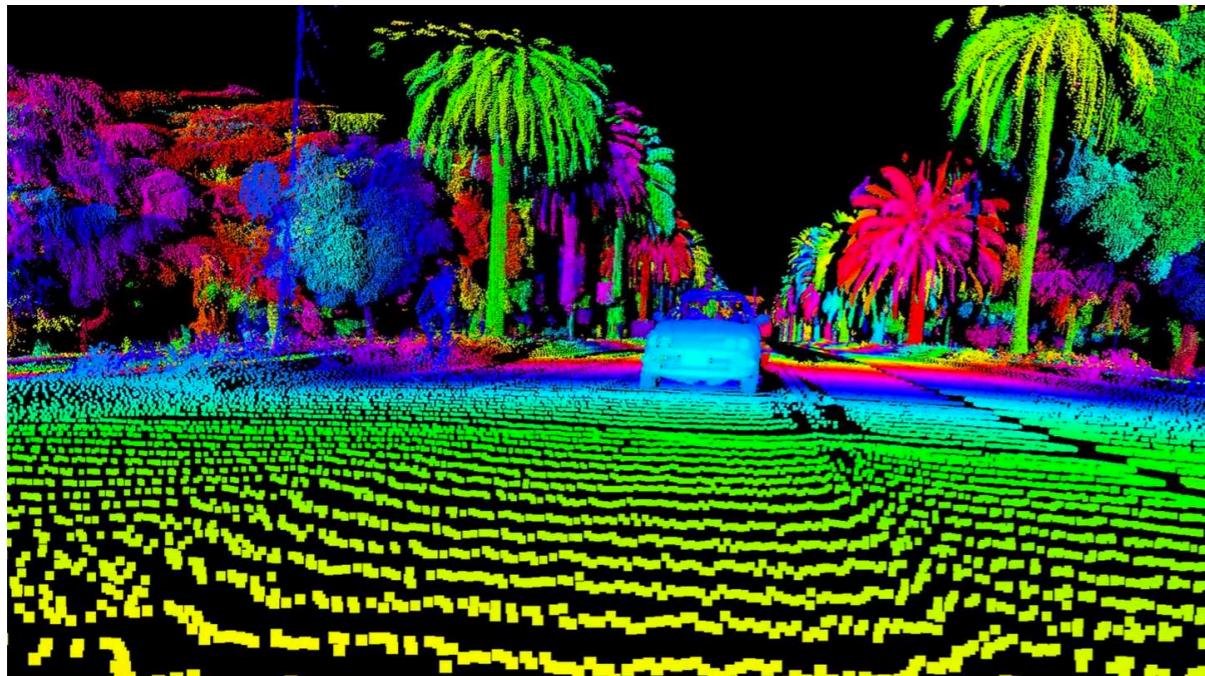
# Energy Flow Polynomials

# Energy Flow Networks

# *Learning to process point clouds into observables*

# Energy Flow Moments

# Point Clouds



How do we make a machine learning architecture to process point clouds?

# Deep Sets

Namespace for symmetric function parametrization

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

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## Deep Sets

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[[1703.06114](#)]

Manzil Zaheer<sup>1,2</sup>, Satwik Kottur<sup>1</sup>, Siamak Ravanbakhsh<sup>1</sup>,  
Barnabás Póczos<sup>1</sup>, Ruslan Salakhutdinov<sup>1</sup>, Alexander J Smola<sup>1,2</sup>  
<sup>1</sup> Carnegie Mellon University      <sup>2</sup> Amazon Web Services

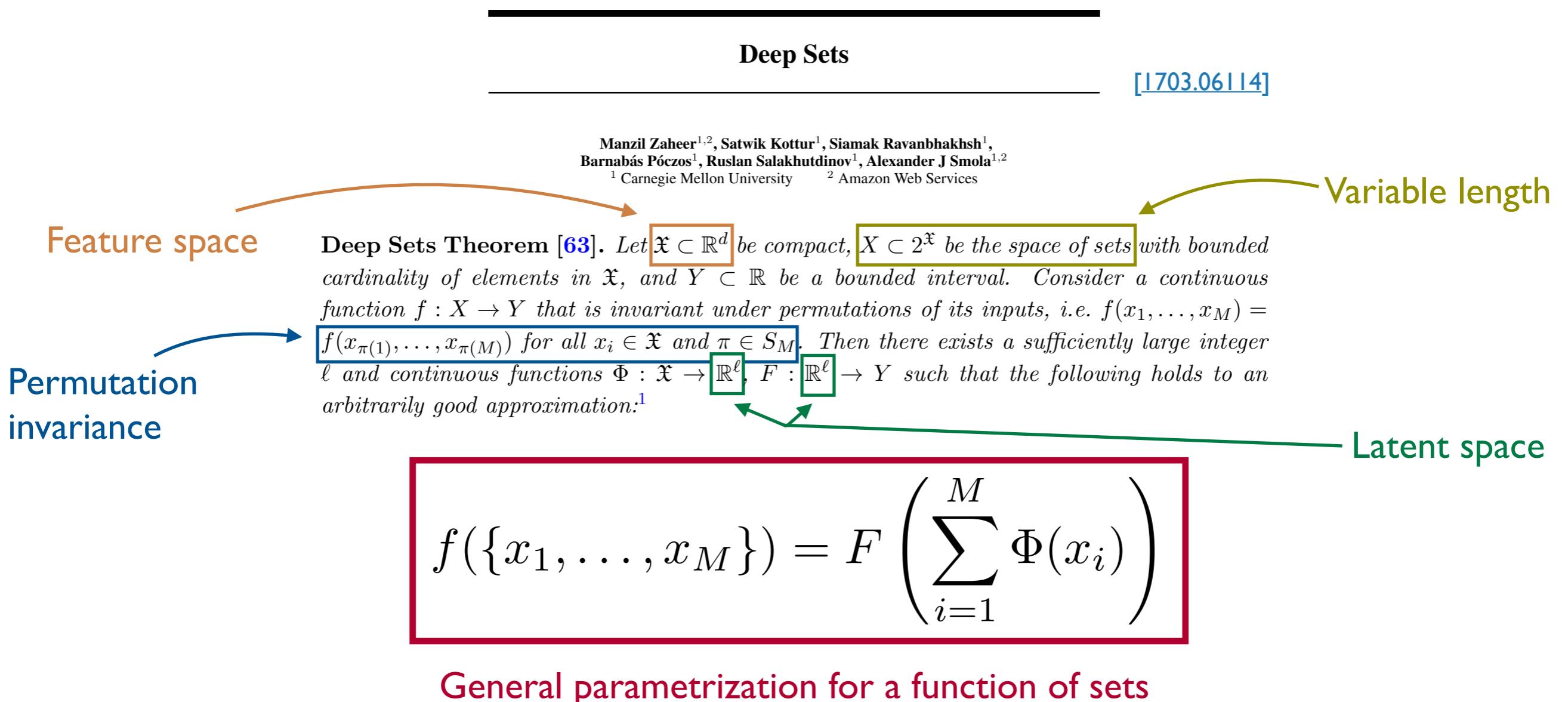
**Deep Sets Theorem [63].** Let  $\mathfrak{X} \subset \mathbb{R}^d$  be compact,  $X \subset 2^{\mathfrak{X}}$  be the space of sets with bounded cardinality of elements in  $\mathfrak{X}$ , and  $Y \subset \mathbb{R}$  be a bounded interval. Consider a continuous function  $f : X \rightarrow Y$  that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

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

# Deep Sets

Namespace for symmetric function parametrization

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



# Infrared and Collinear (IRC) Safety

QCD

**IRC** safety is a statement of *linearity* in energy and  
*continuity* in geometry

KLN T  
diverge

*Theorem:* Any IRC-safe observable can be written in the following form:

Infrared

$$f(\{p_1^\mu, \dots, p_M^\mu\}) = F \left( \sum_{i=1}^M z_i \vec{\Phi}(\hat{p}_i) \right), \quad \hat{p}_i = (y_i, \phi_i).$$

Collinear

*Proof:* In [1810.05165](#).



**IRC** safety is a key theoretical and experimental property of observables

# Deep Sets for Particle Jets

[PTK, Metodiev, Thaler, [1810.05165](#)]

*Particle Flow Network (PFN)*

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

Fully general latent space

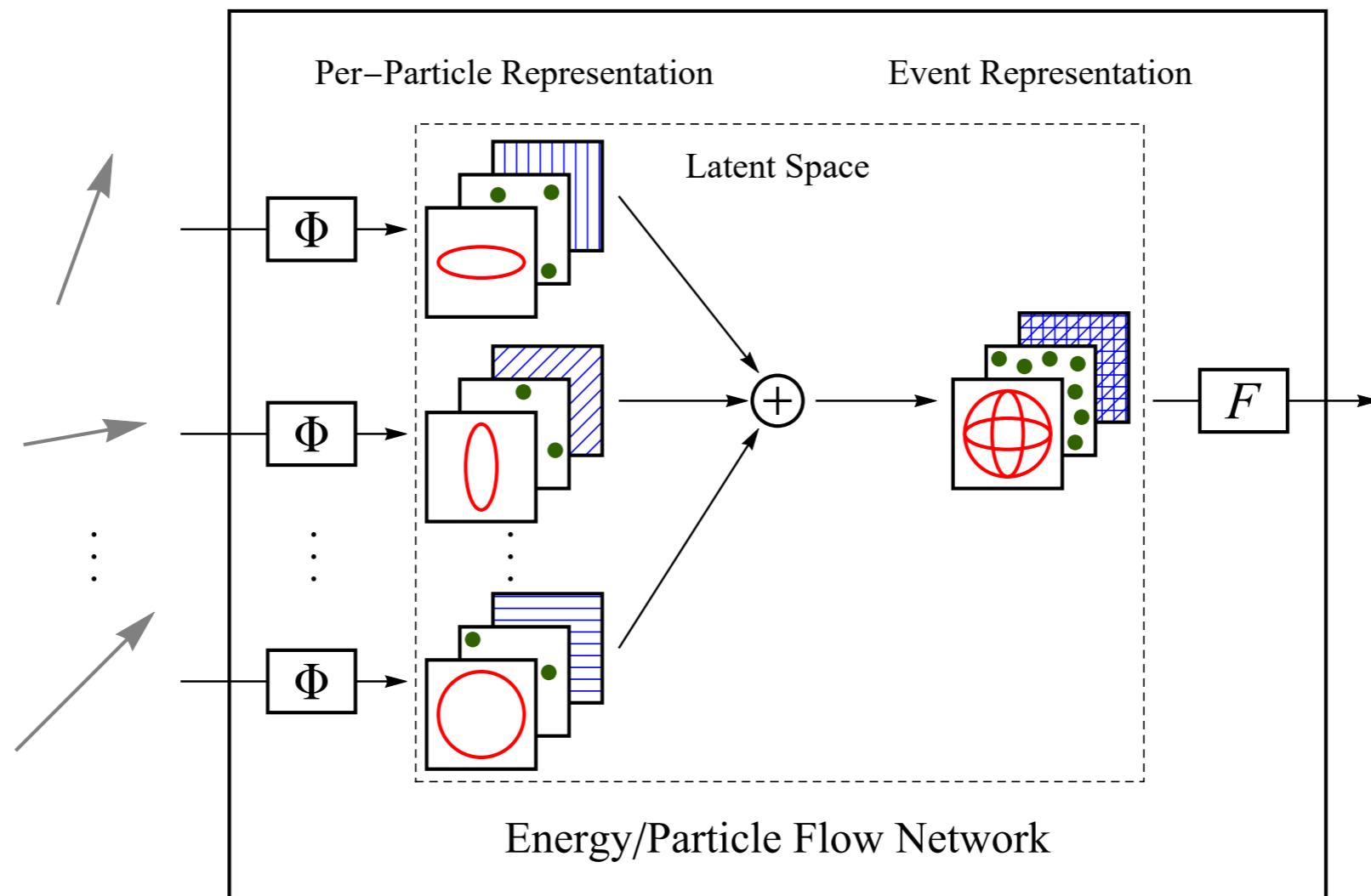
*Energy Flow Network (EFN)*

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

**IRC**-safe latent space

Particles

Observable



# Approximating $\Phi$ and $F$ with Neural Networks

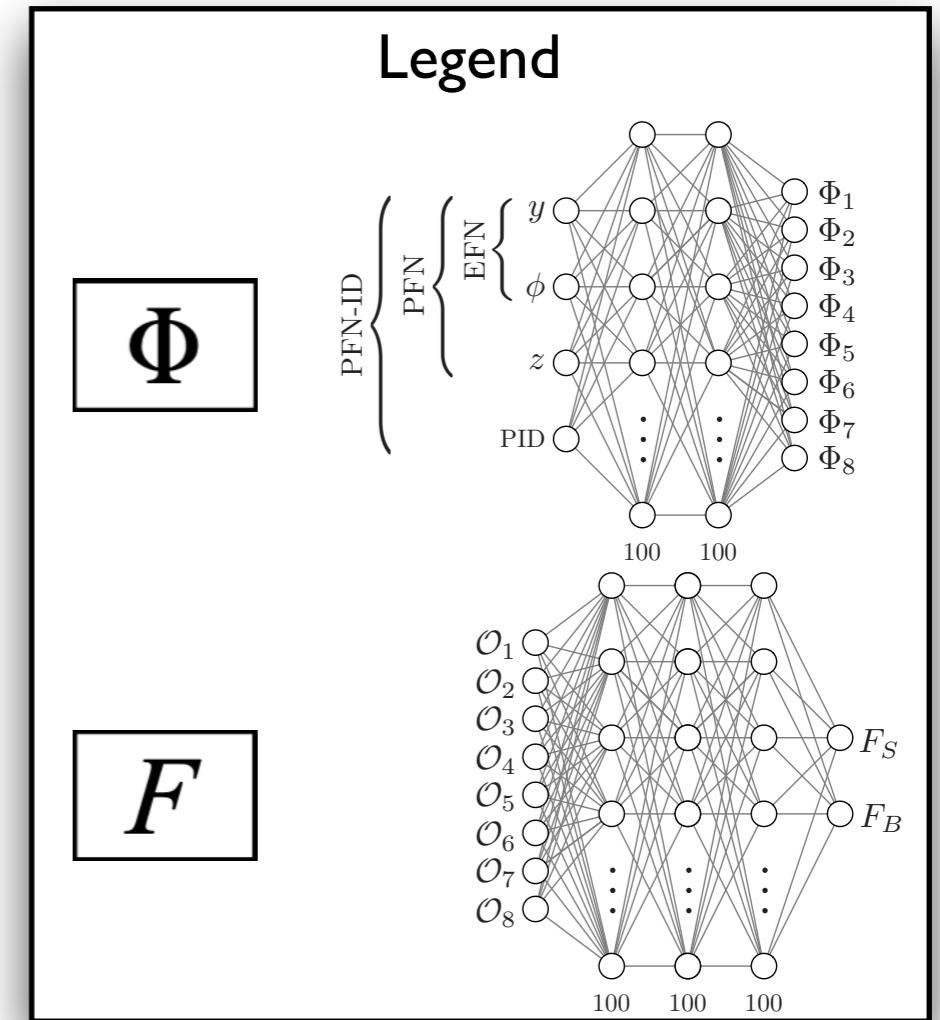
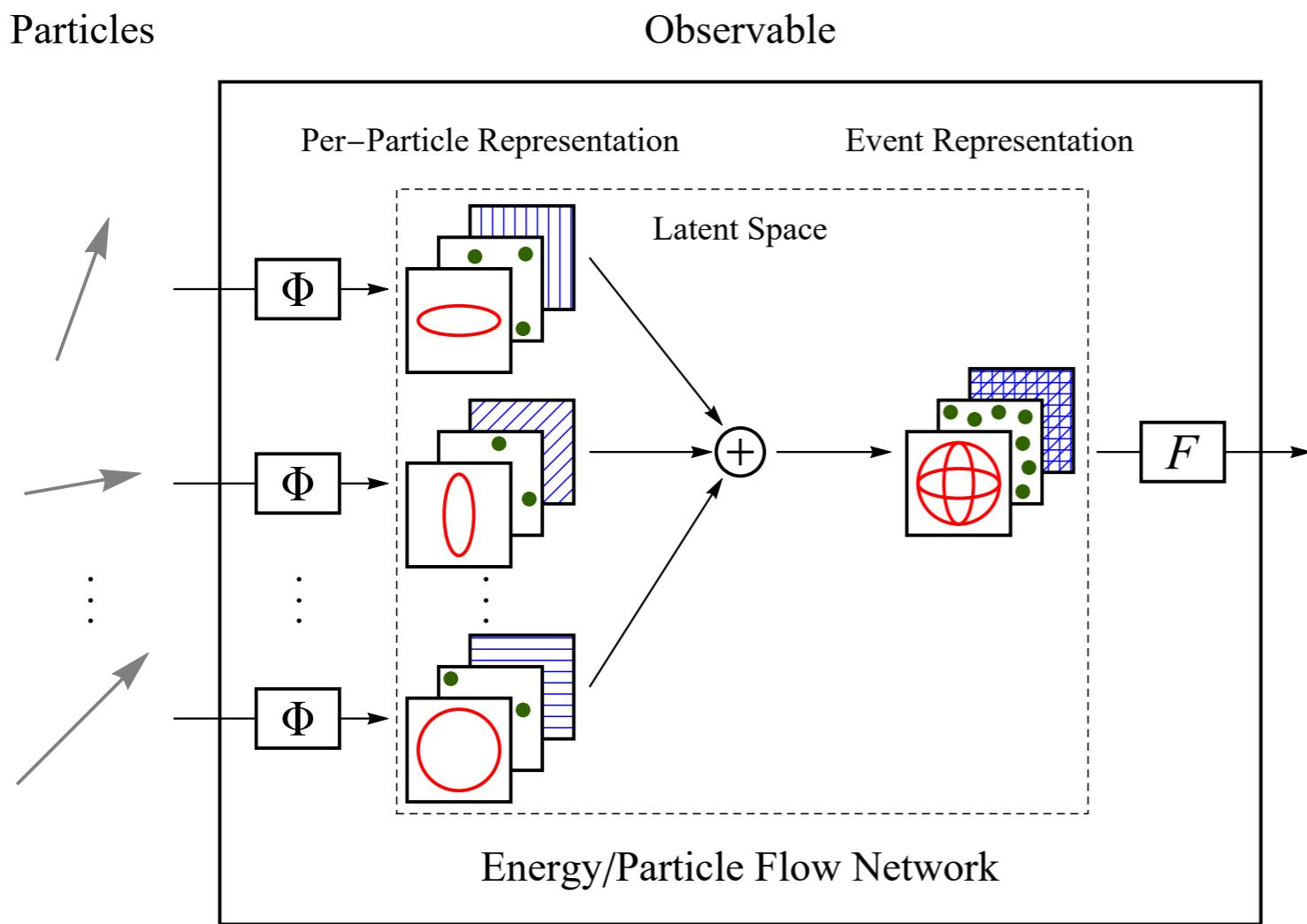
Employ neural networks as arbitrary function approximators

Use fully-connected networks for simplicity

Graph CNNs also interesting (see H. Qu's [talk](#) at ML4Jets)

Default sizes –  $\Phi: (100, 100, \ell)$ ,  $F: (100, 100, 100)$

Particles

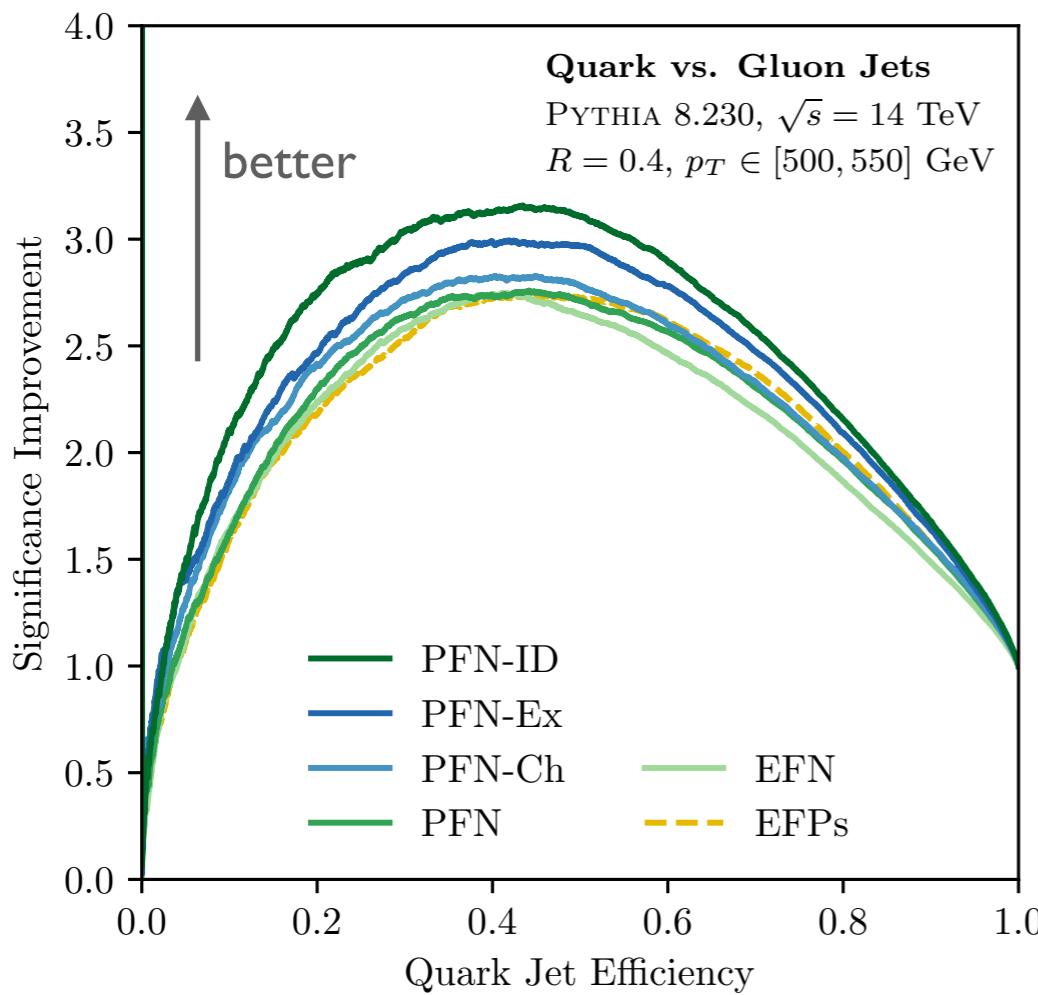


$$\text{EFN} : \mathcal{O}_a = \sum_{i=1}^M z_i \Phi_a(y_i, \phi_i)$$

$$\text{PFN} : \mathcal{O}_a = \sum_{i=1}^M \Phi_a(z_i, y_i, \phi_i, [\text{PID}_i])$$

# Quark vs. Gluon: Classification Performance

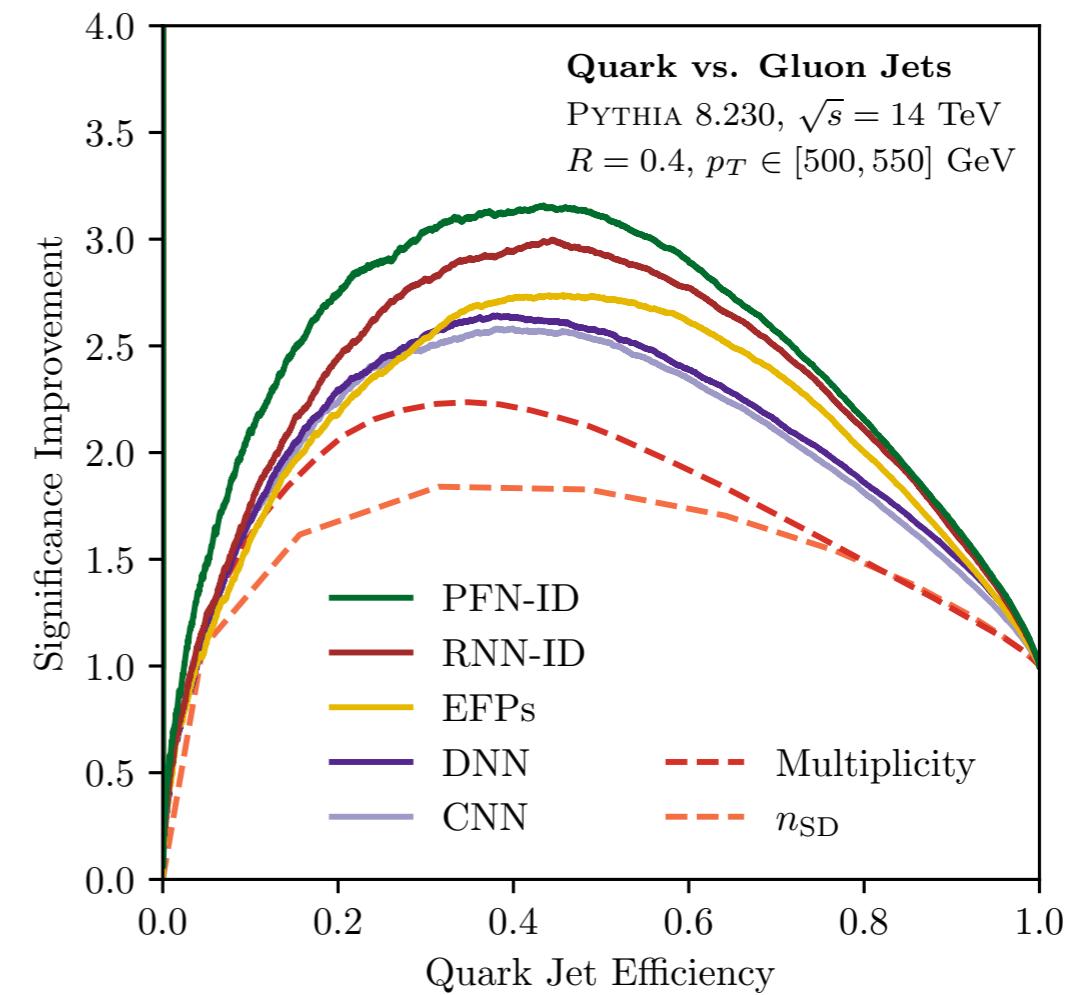
**PFN-ID:** Full particle flavor info  
 $(\gamma, \pi^\pm, K^\pm, K_L, p, \bar{p}, n, \bar{n}, e^\pm, \mu^\pm)$   
**PFN-Ex:** Experimentally accessible info  
 $(\gamma, h^{\pm,0}, e^\pm, \mu^\pm)$   
**PFN-Ch:** Particle charge info  
 $(+, 0, -)$



Latent space dimension  $\ell = 256$

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

# Quark vs. Gluon: EFN Latent Dimension Sweep

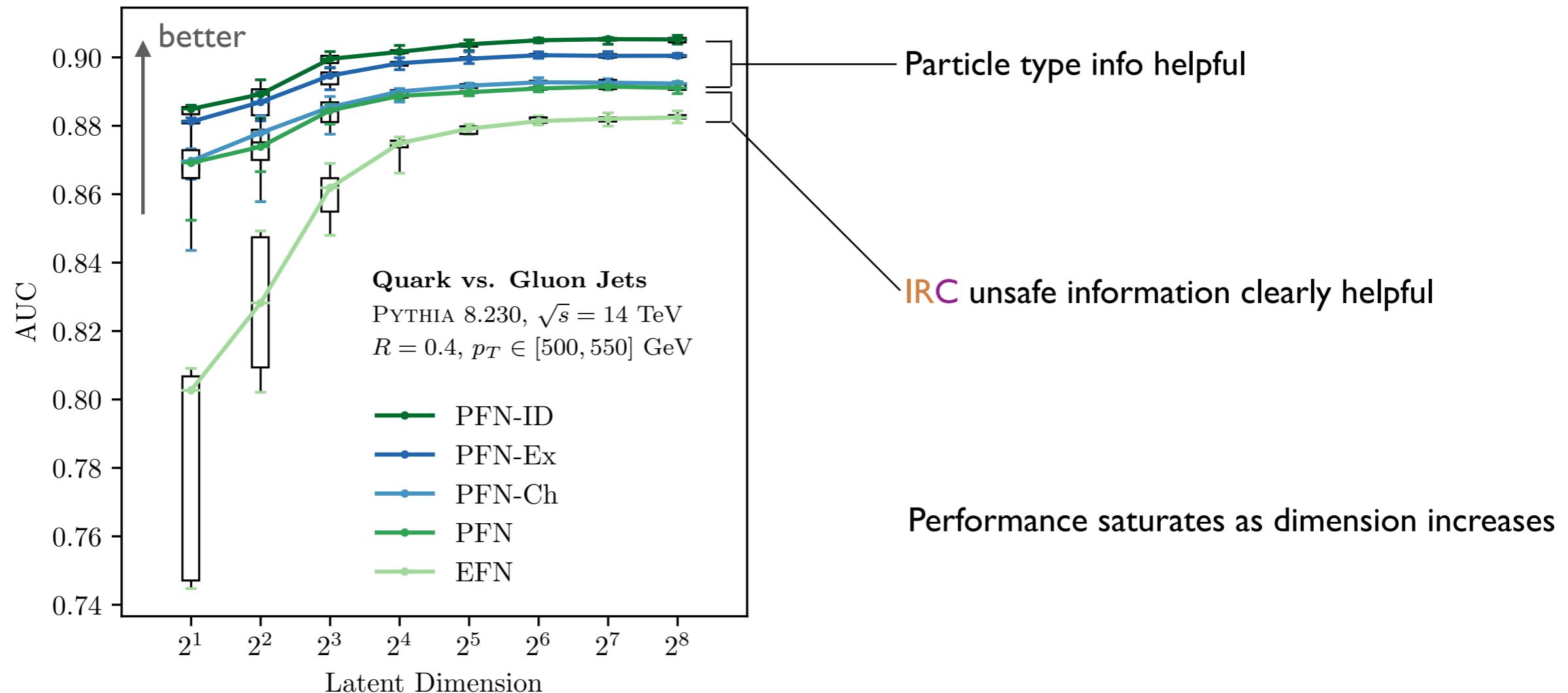
PFN-ID: Full particle flavor info  
 $(\gamma, \pi^\pm, K^\pm, K_L, p, \bar{p}, n, \bar{n}, e^\pm, \mu^\pm)$

PFN-Ex: Experimentally accessible info  
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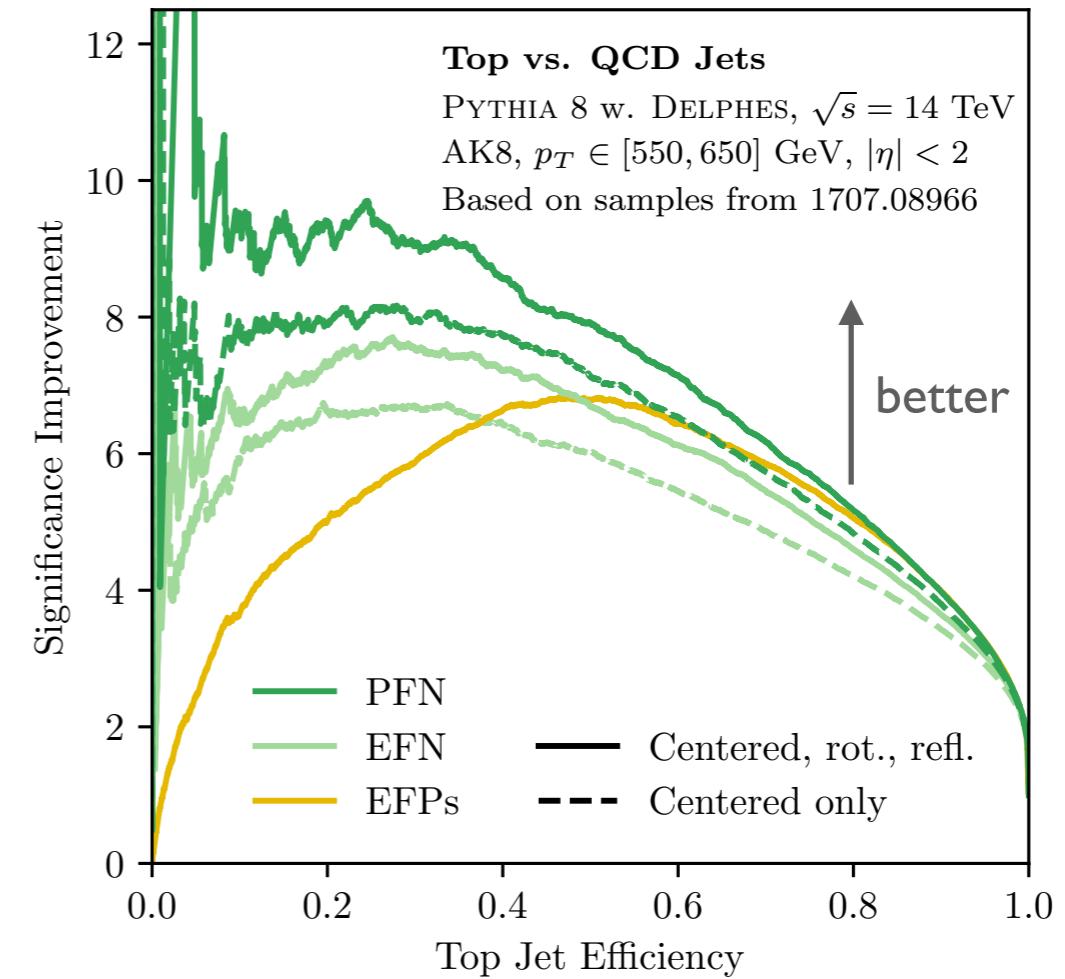
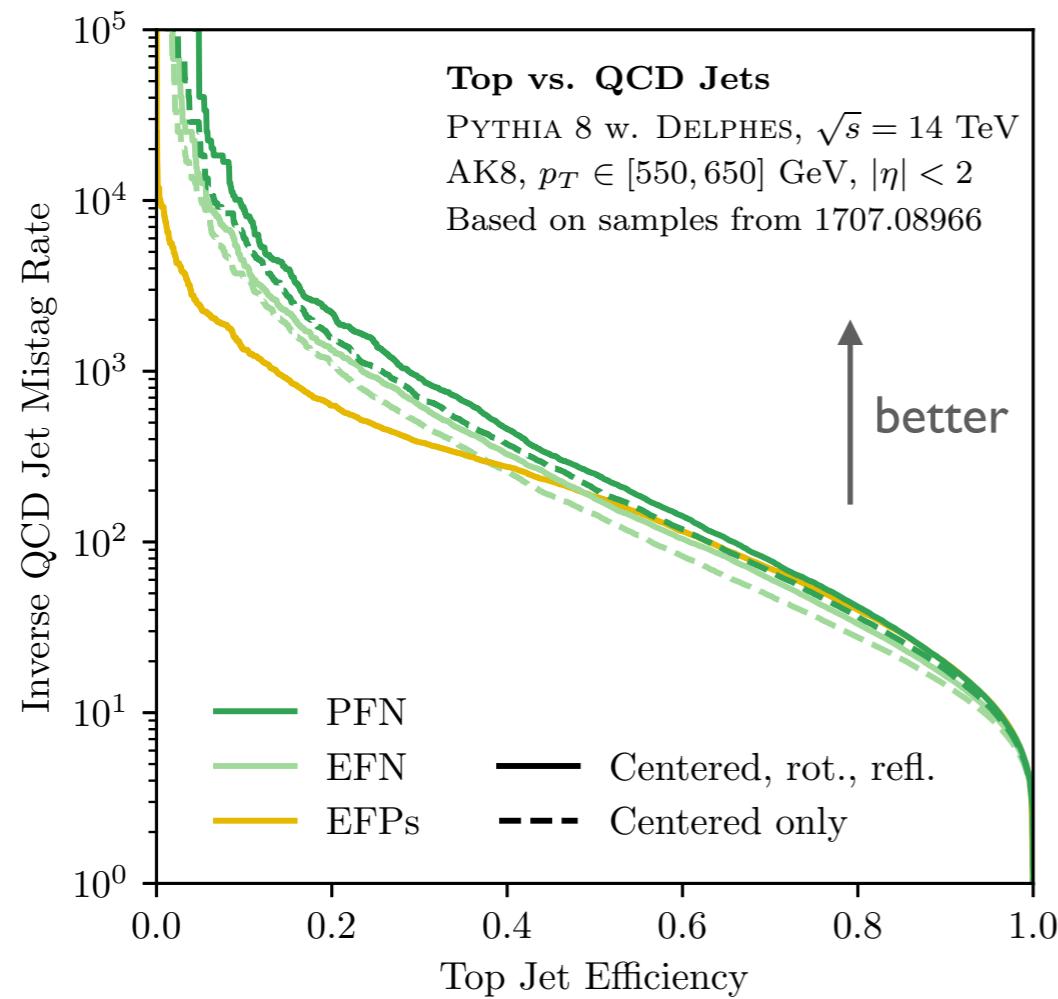
PFN-Ch: Particle charge info  
 $(+, 0, -)$

PFN: No particle type info, arbitrary energy dependence

EFN: **IRC**-safe latent space



# Boosted Top: Classification Performance

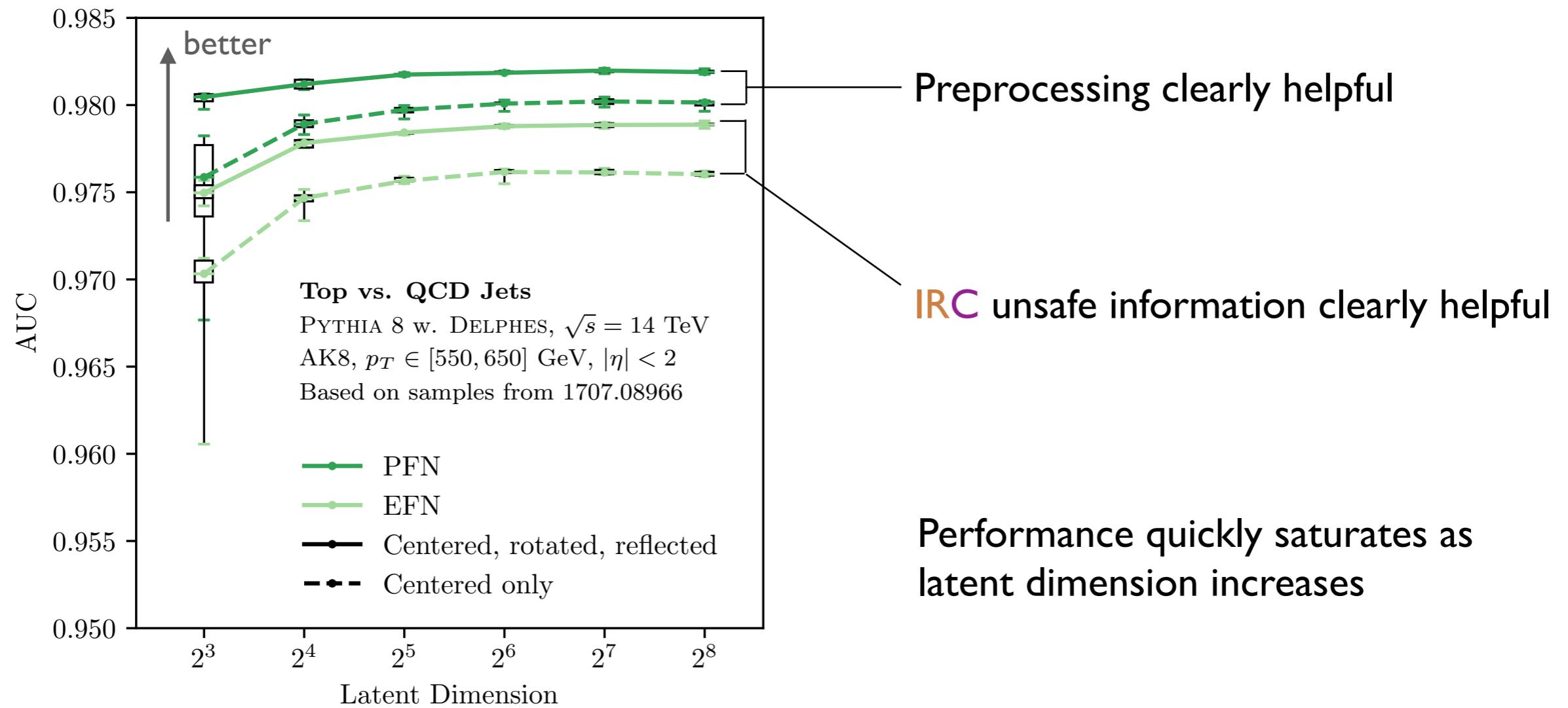


Latent space dimension  $\ell = 256$

EFN/PFN rotation and reflection preprocessing helpful

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

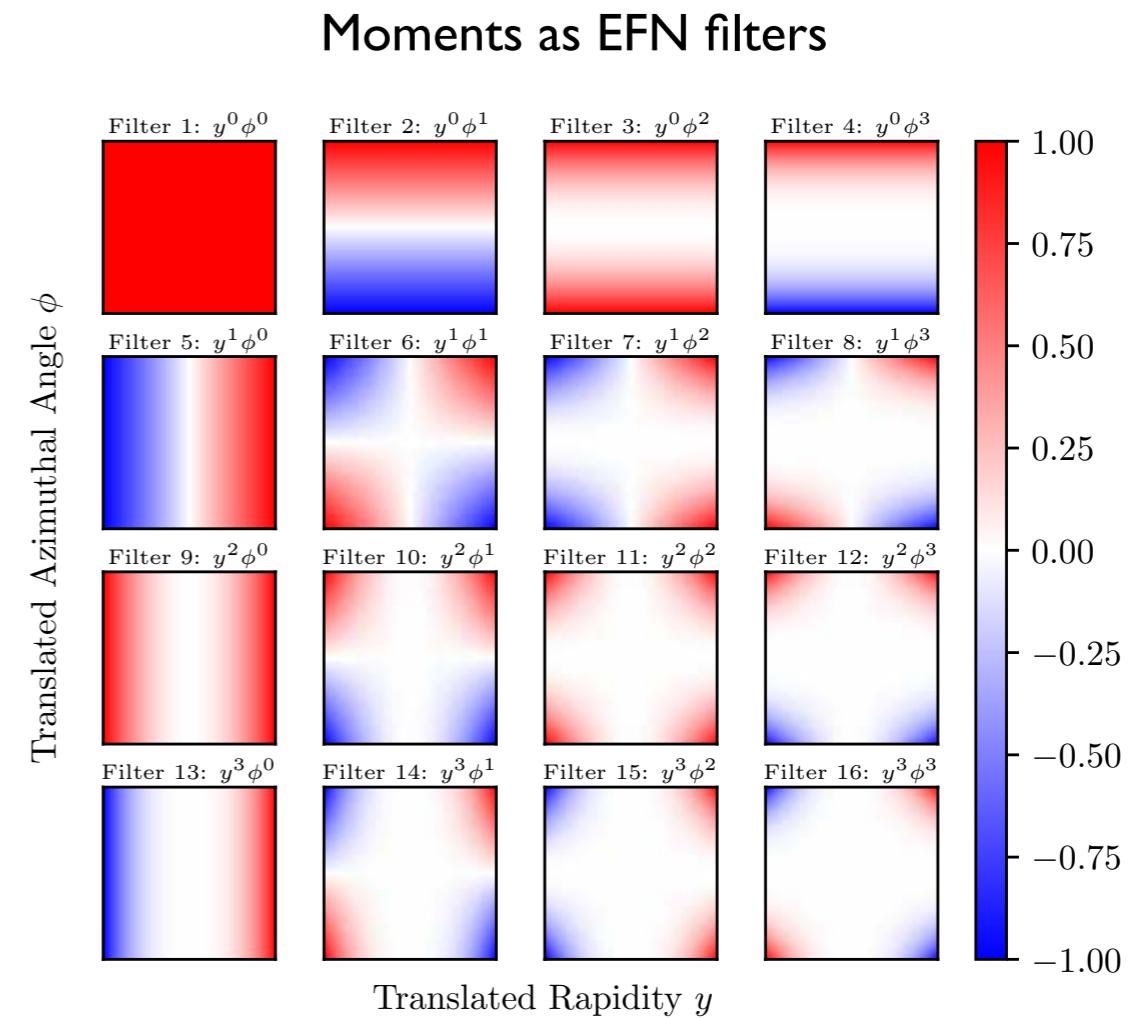
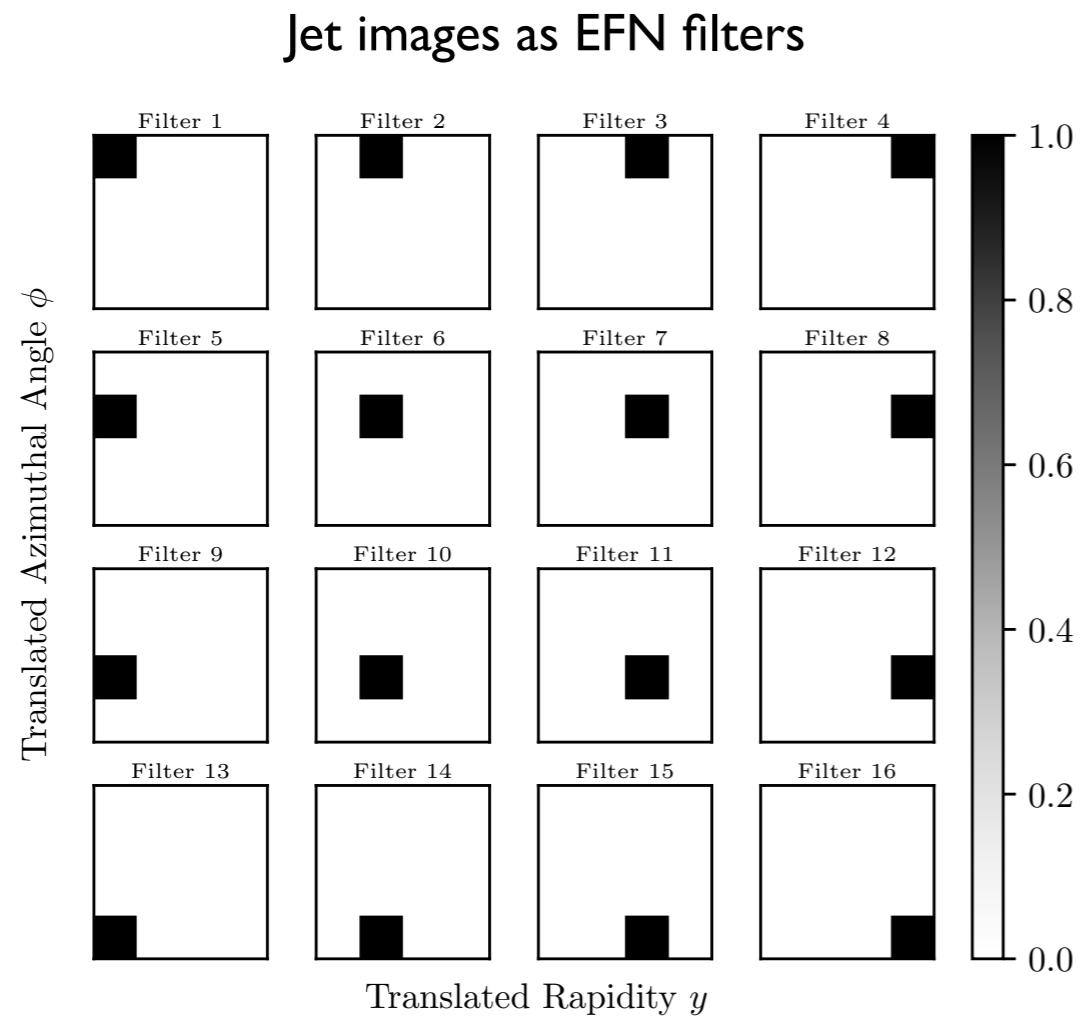
# Boosted Top: EFN Latent Dimension Sweep



# Energy Flow Network Visualization

EFN observables are two-dimensional geometric functions

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



[Cogan, Kagan, Strauss, Schwartzman, 2014]

[de Oliveira, Kagan, Mackey, Nachman, Schwartzman, 2015]

[Donoghue, Low, Pi, 1979]

[Gur-Ari, Papucci, Perez, 2011]

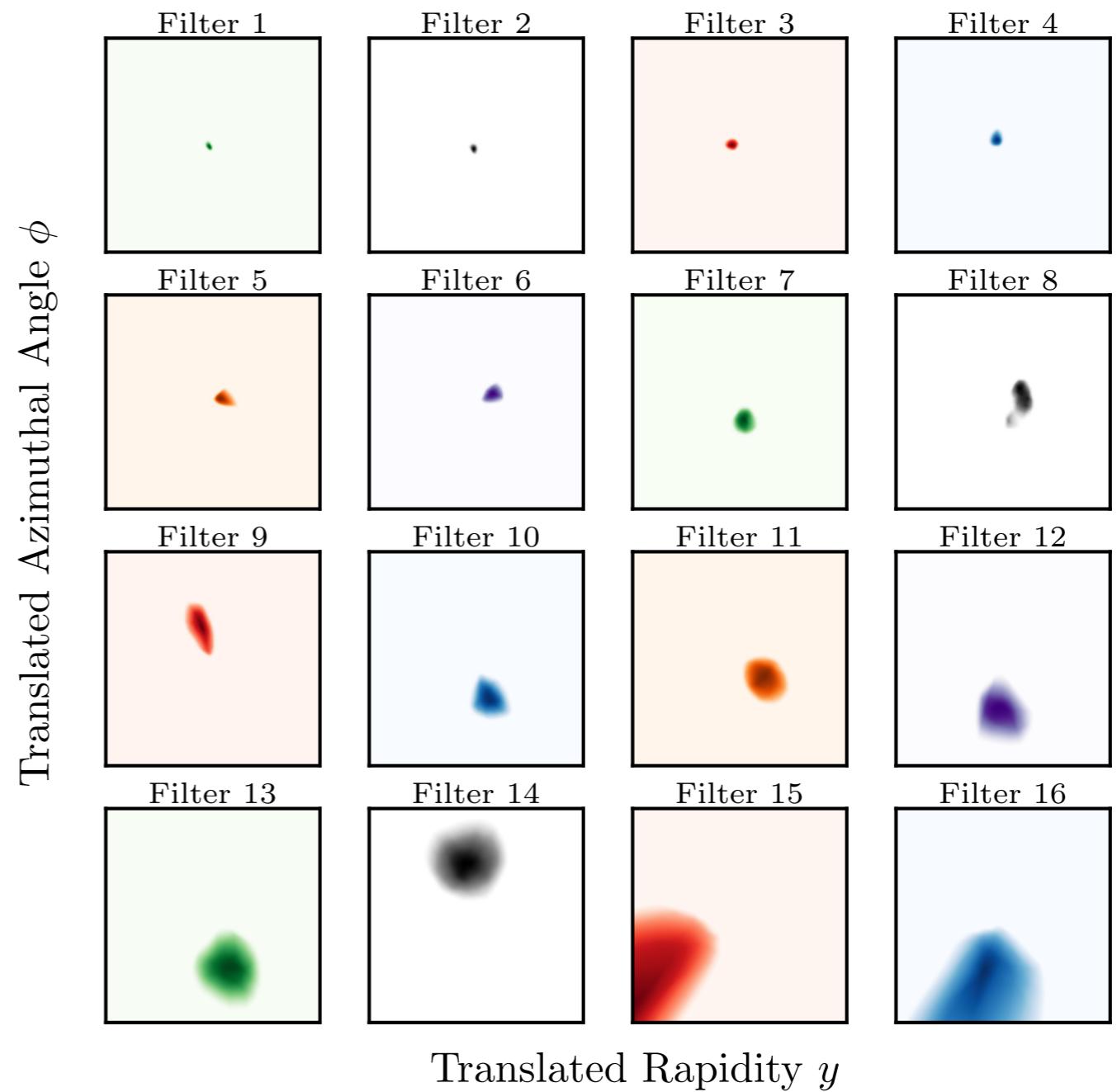
# Quark vs. Gluon: Visualizing EFN Filters

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

EFN ( $\ell = 256$ ) randomly selected filters, sorted by size

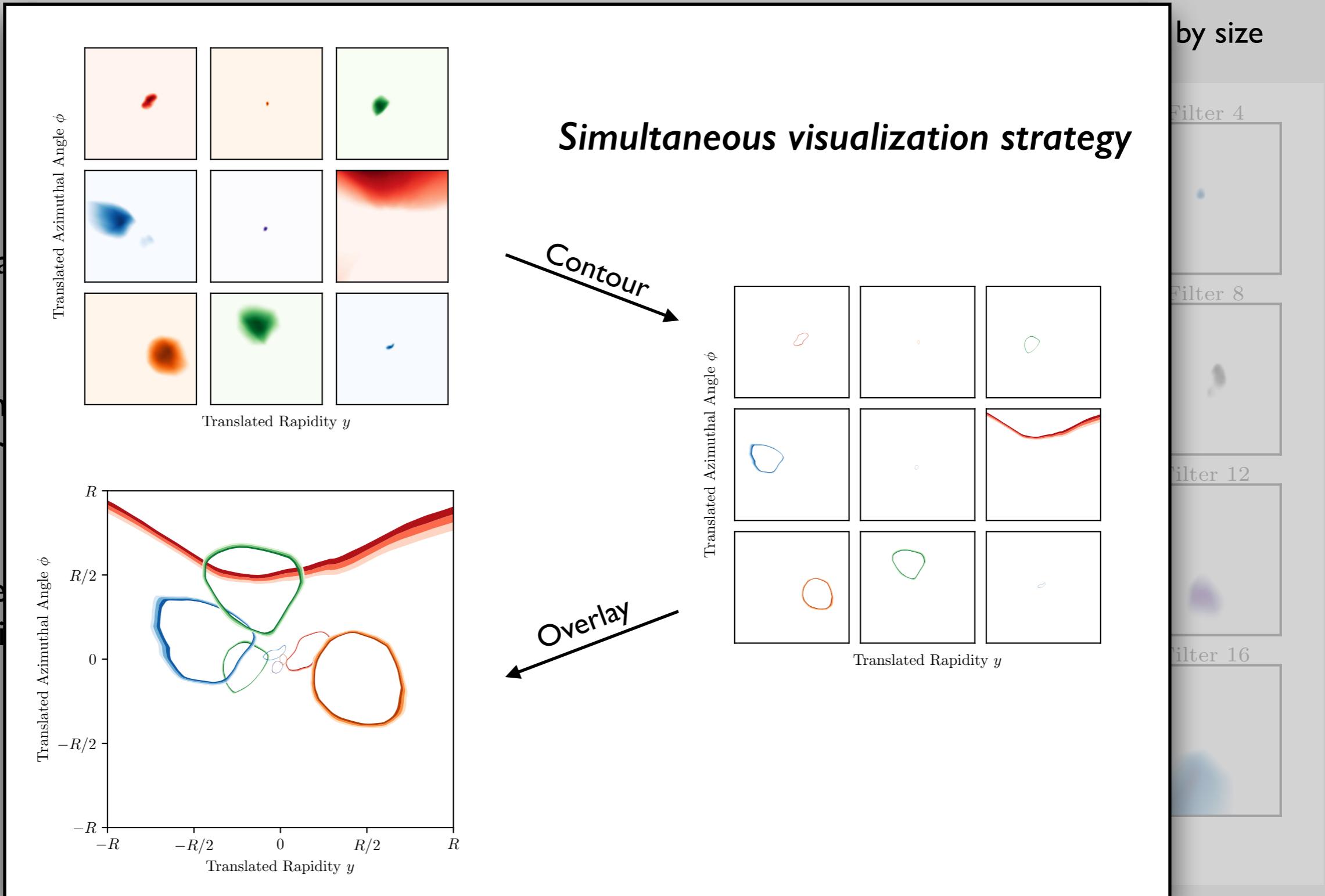


# Quark vs. Gluon: Visualizing EFN Filters

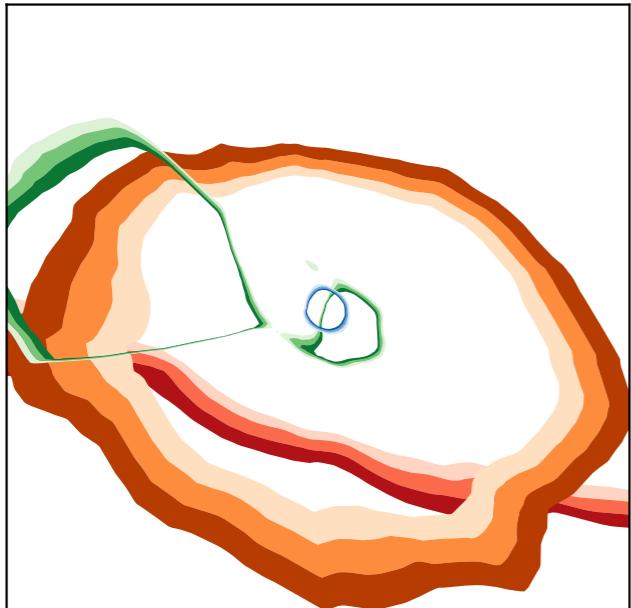
General

Local n  
interpret

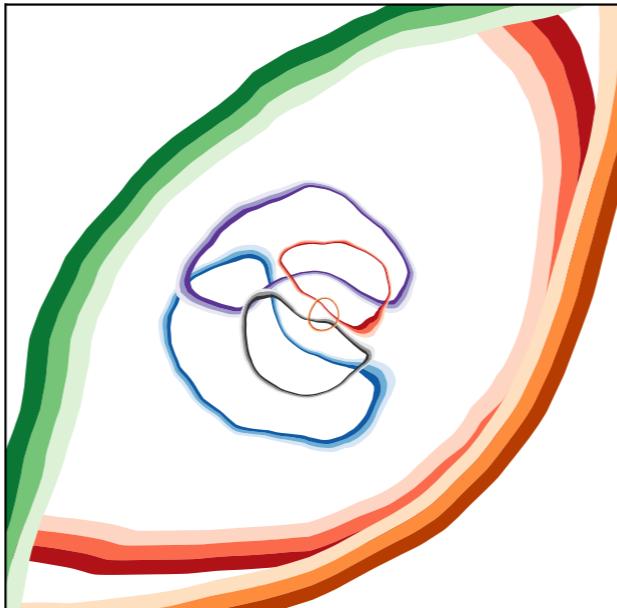
EFN se  
dynam



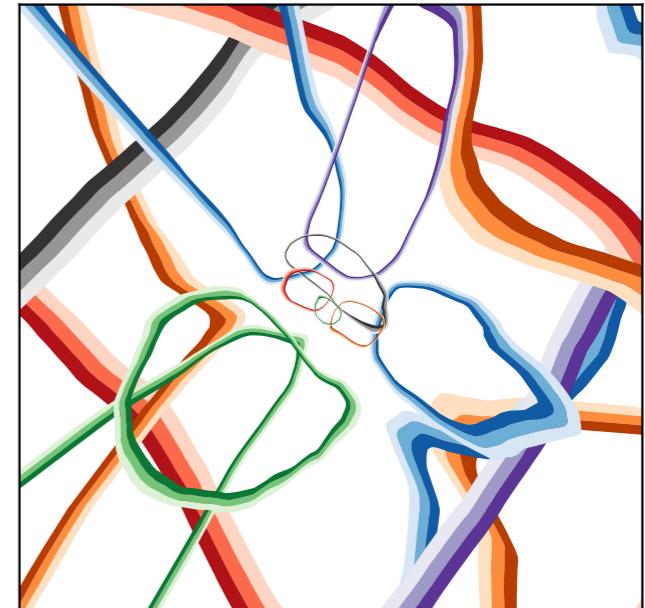
# Quark vs. Gluon: Visualizing EFN Filters



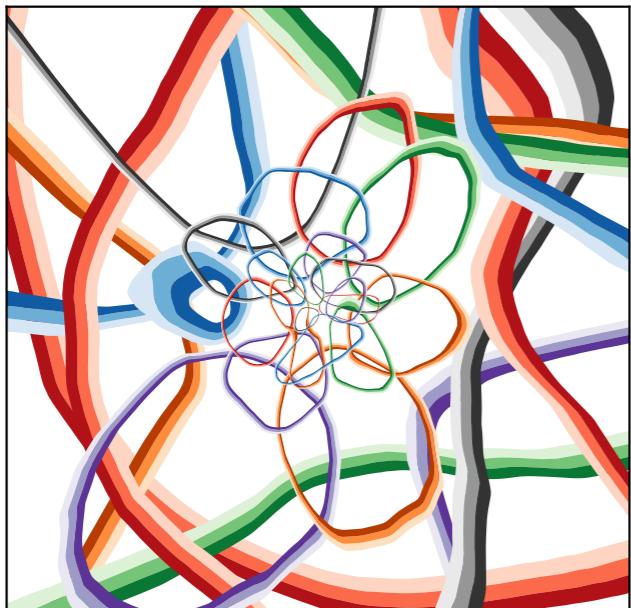
$\ell = 4$



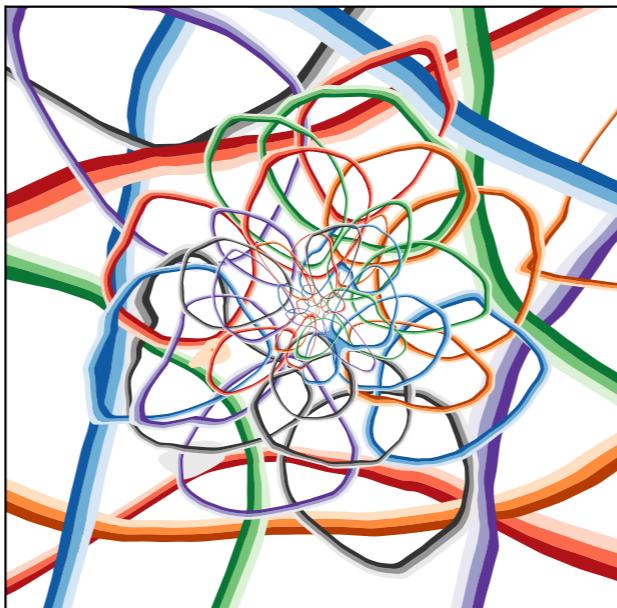
$\ell = 8$



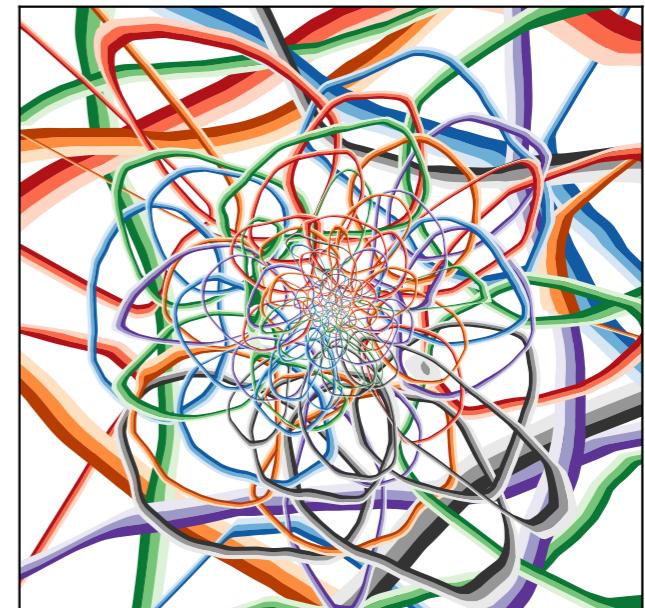
$\ell = 16$



$\ell = 32$

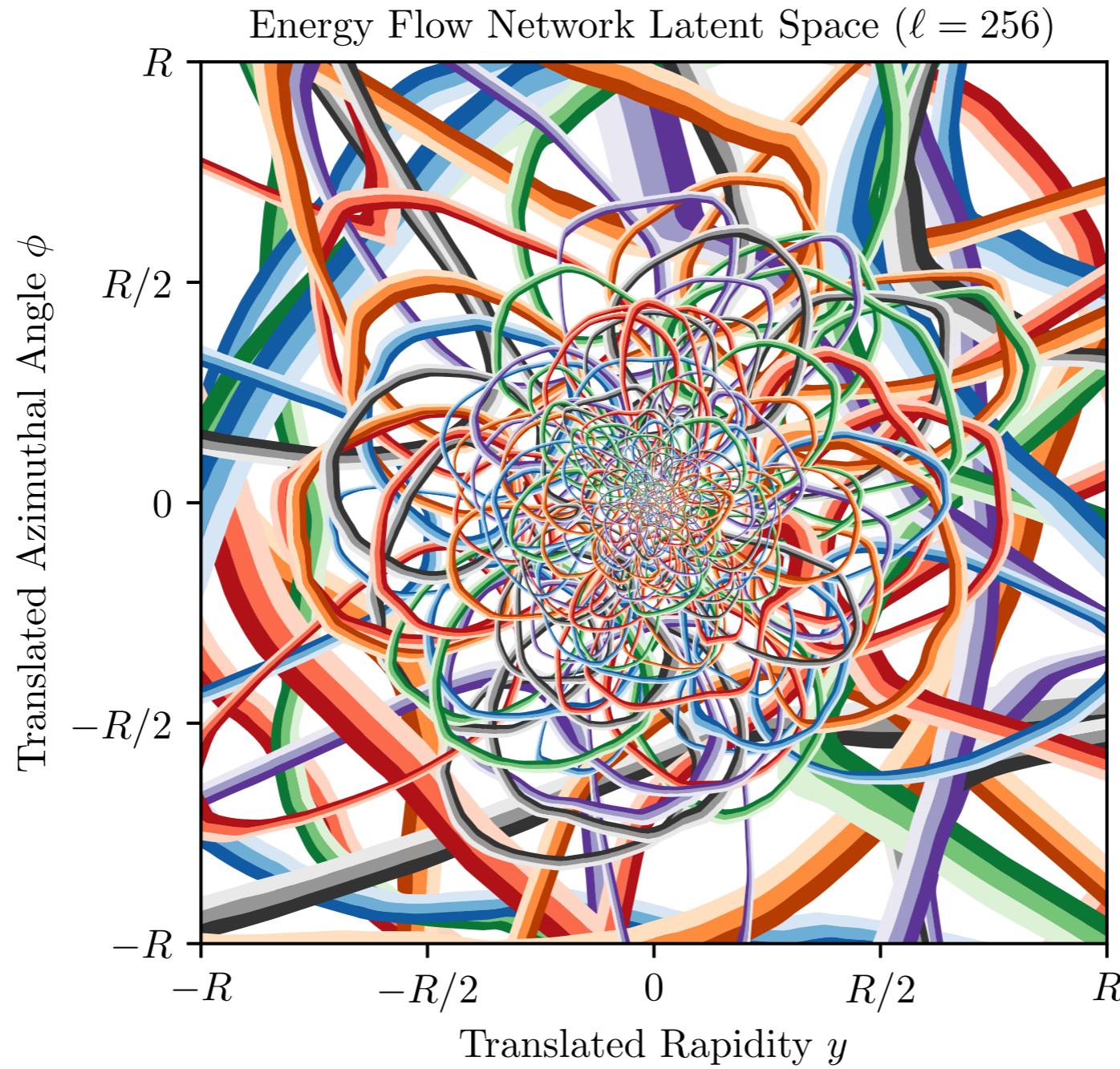


$\ell = 64$

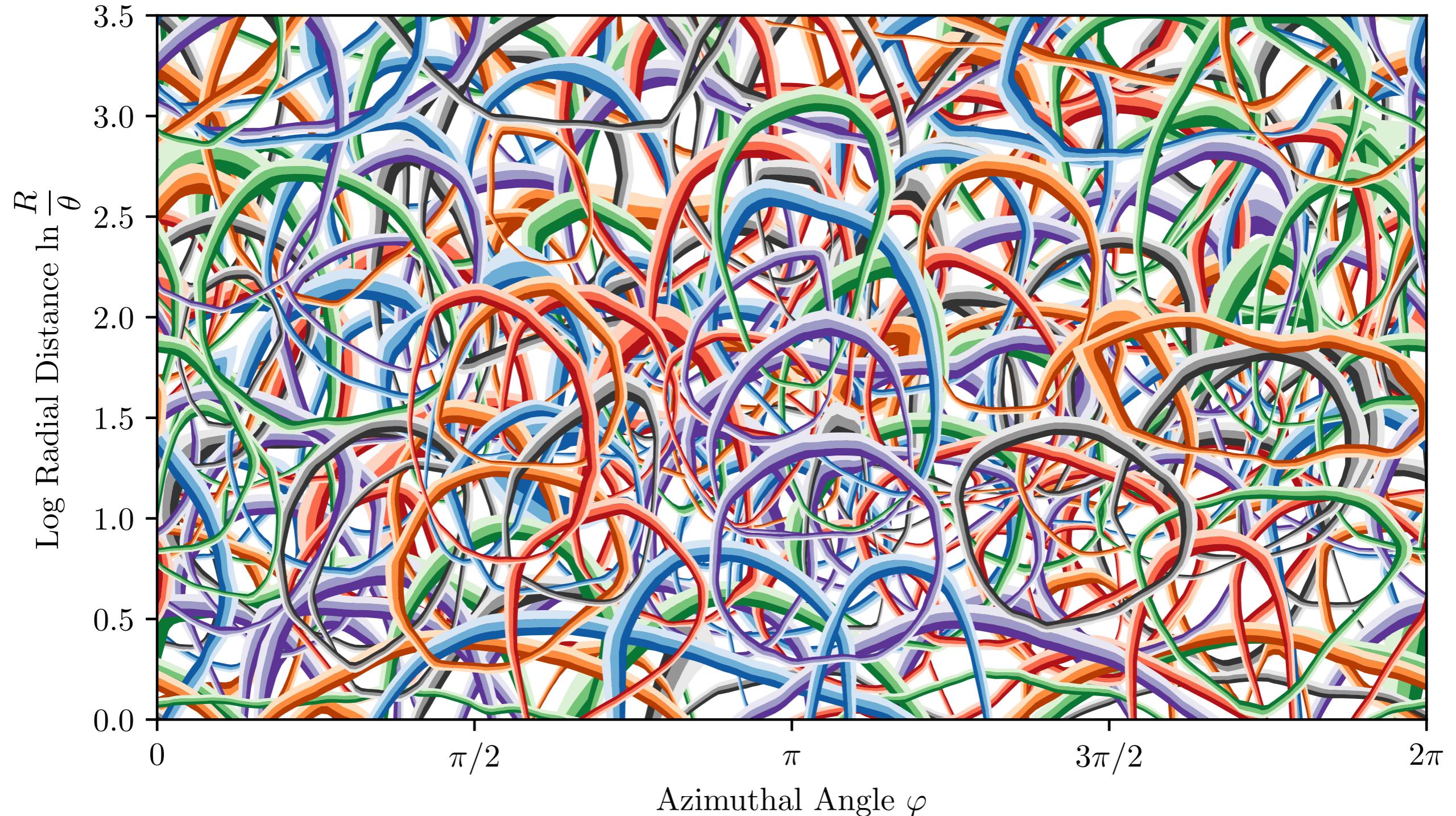


$\ell = 128$

# Quark vs. Gluon: Visualizing EFN Filters



# 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

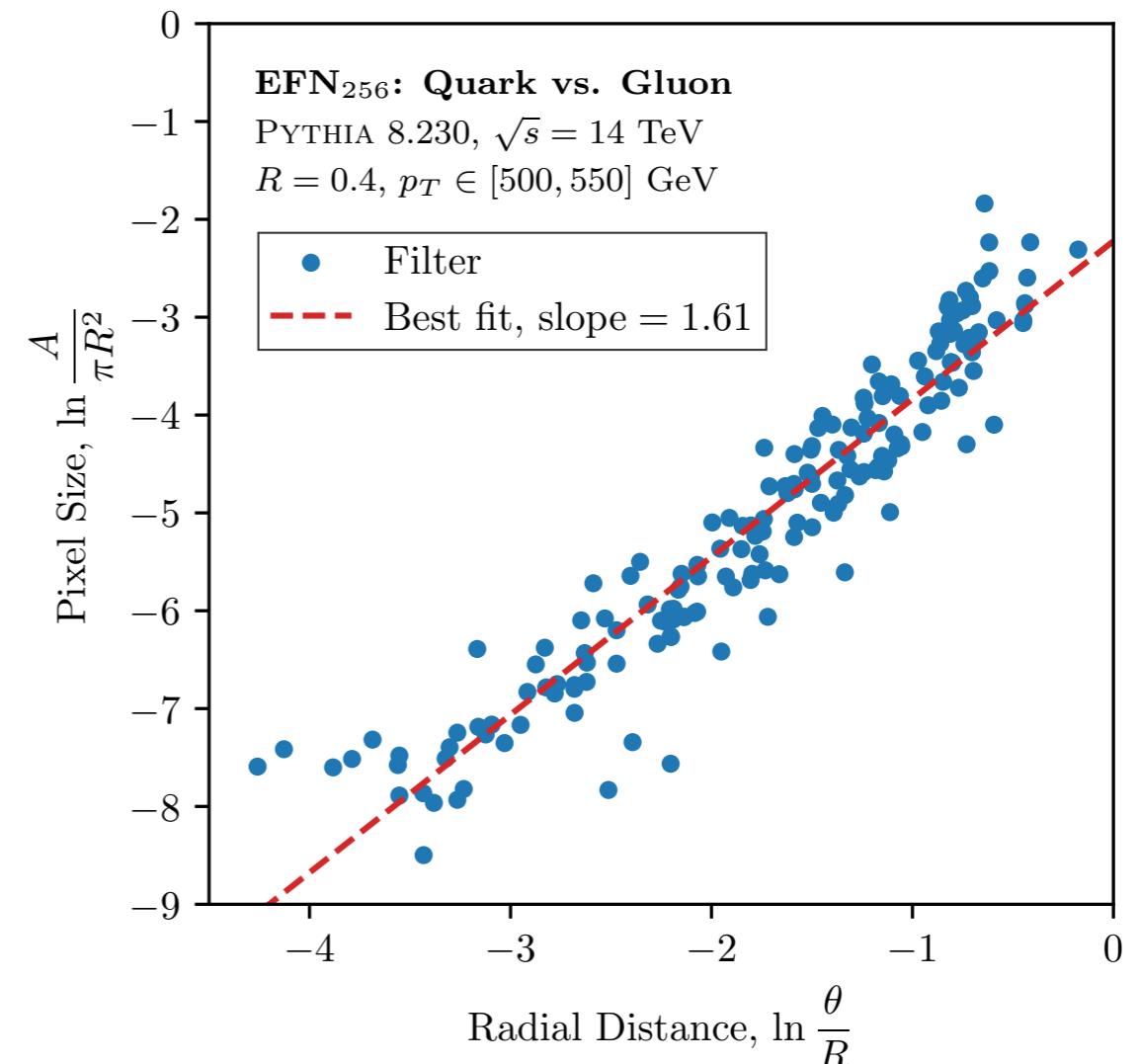
Slope of 2 is predicted at leading log

$$d \ln \frac{\theta}{R} d\varphi = \theta^2 dy d\phi$$

↑  
Emission plane area element

↑  
Area element in rap-phi plane

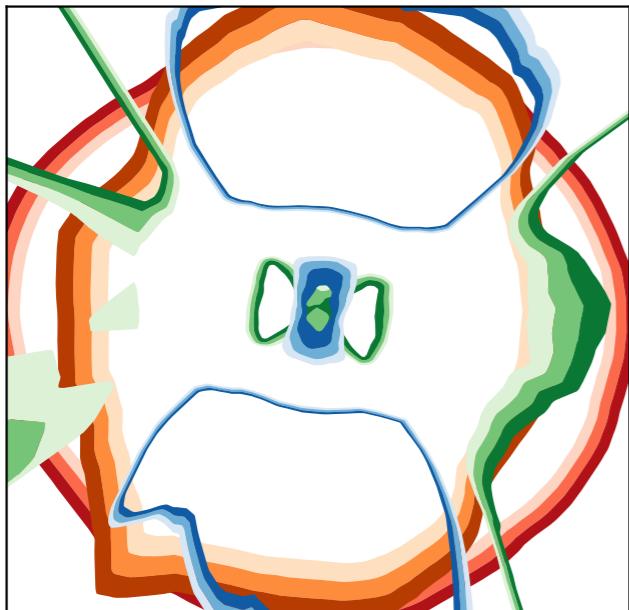
Non-perturbative physics, axis recoil, higher order effects cause deviations from slope of 2



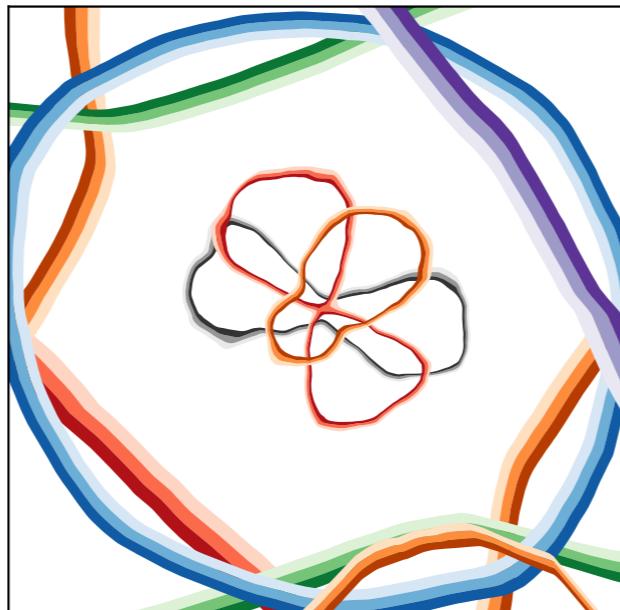
$$dP_{i \rightarrow ig} \sim \frac{2\alpha_s}{\pi} C_a \frac{d\theta}{\theta} \frac{dz}{z}$$

# Boosted Top: Visualizing EFN Filters

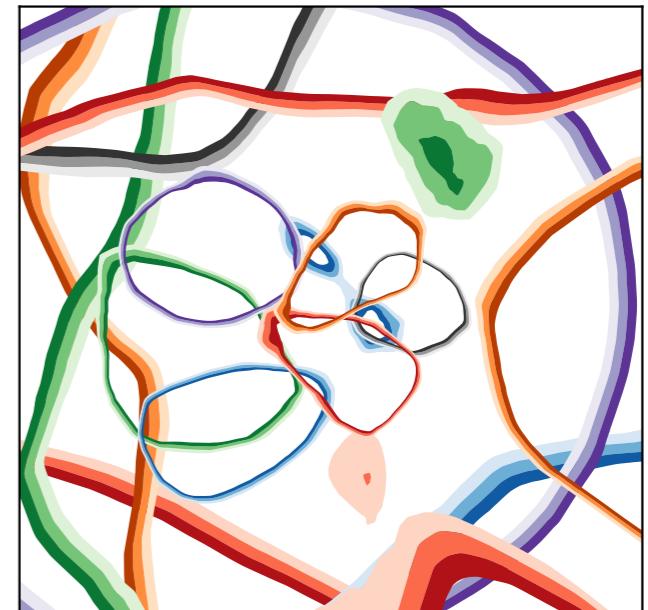
Without rotation/reflection preprocessing



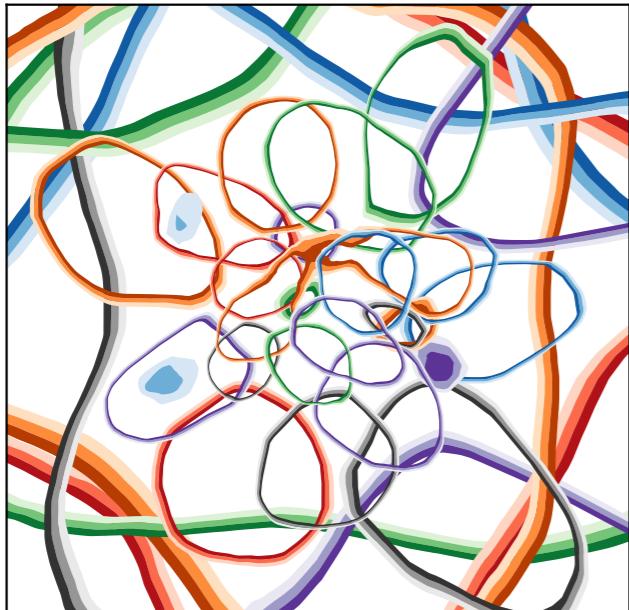
$\ell = 4$



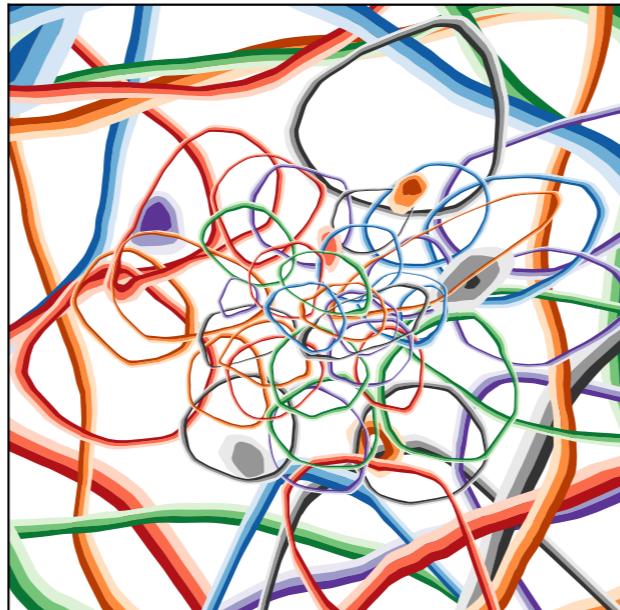
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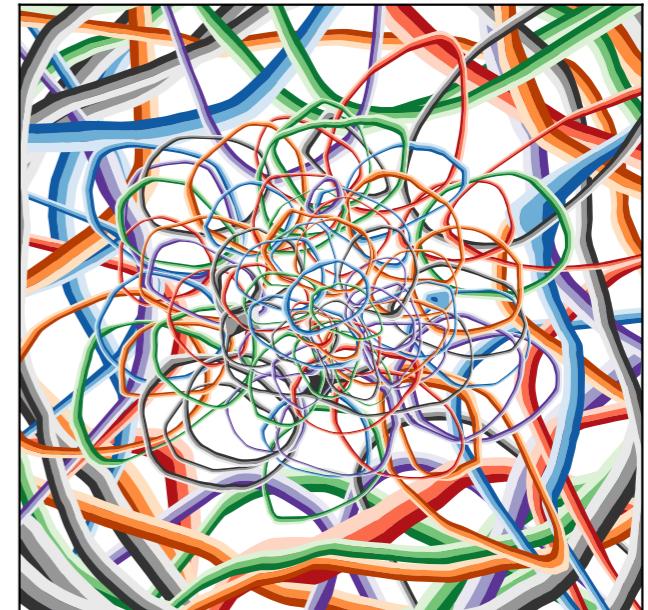
$\ell = 16$



$\ell = 32$



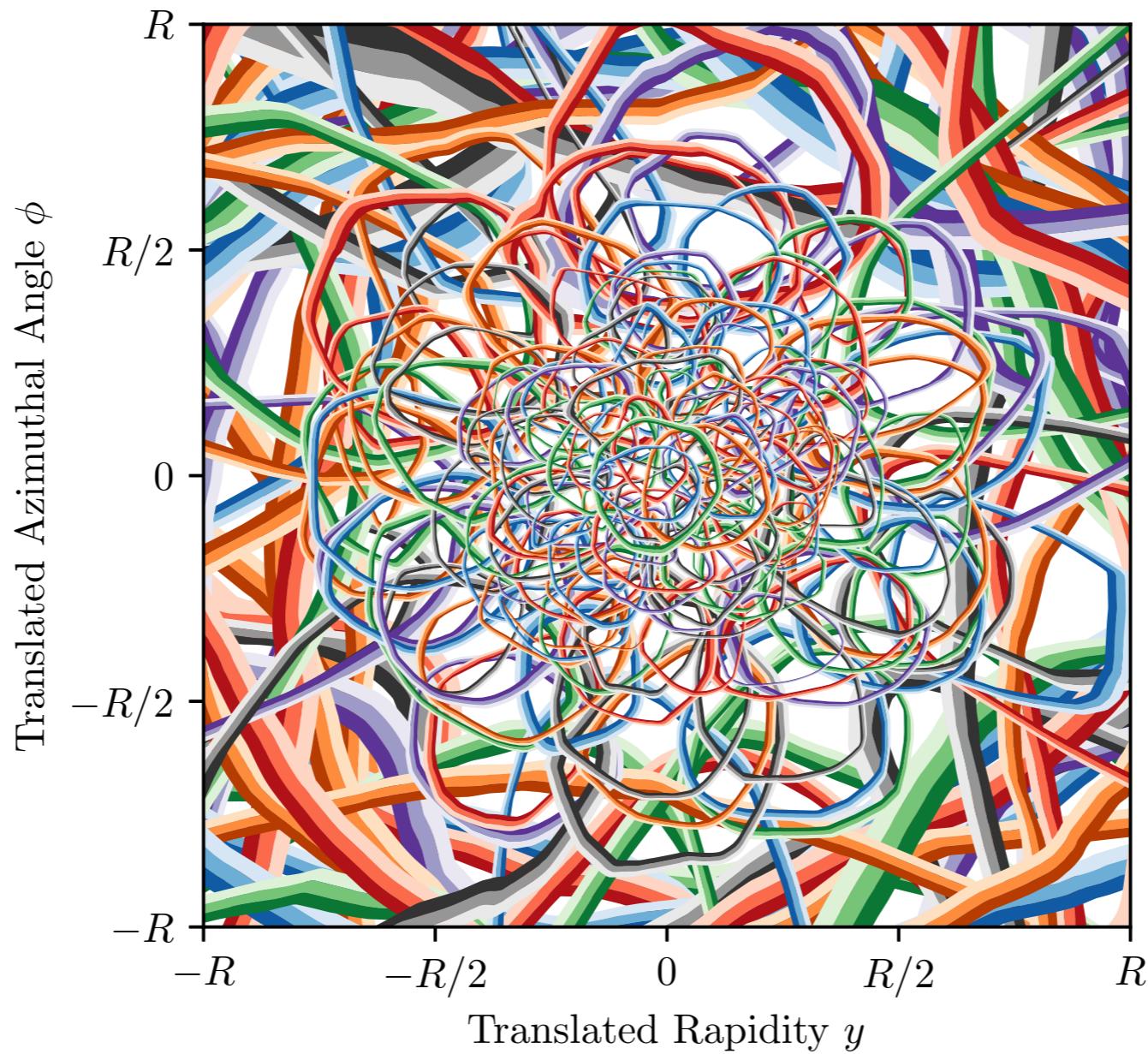
$\ell = 64$



$\ell = 128$

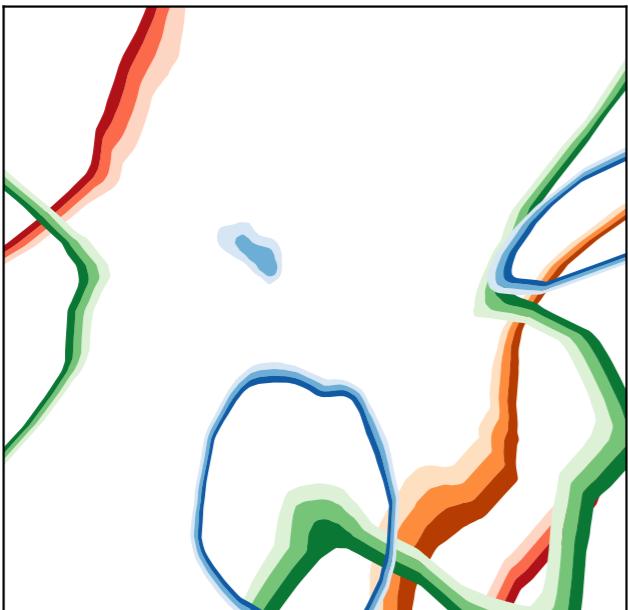
# Boosted Top: Visualizing EFN Filters

Without rotation/reflection preprocessing

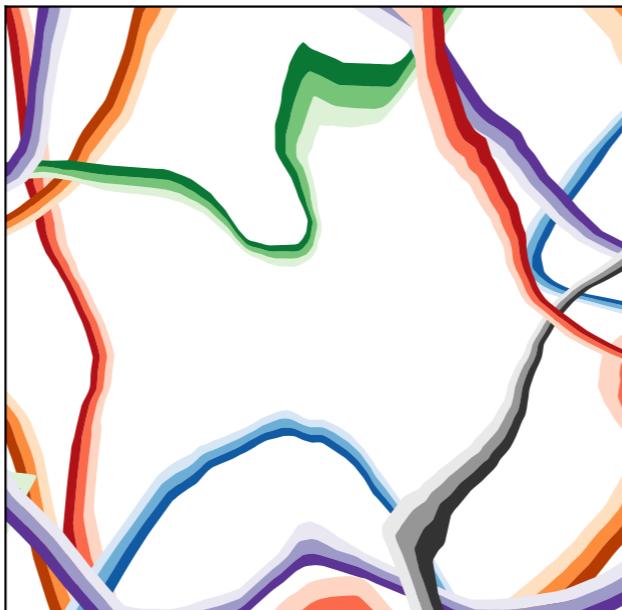


# Boosted Top: Visualizing EFN Filters

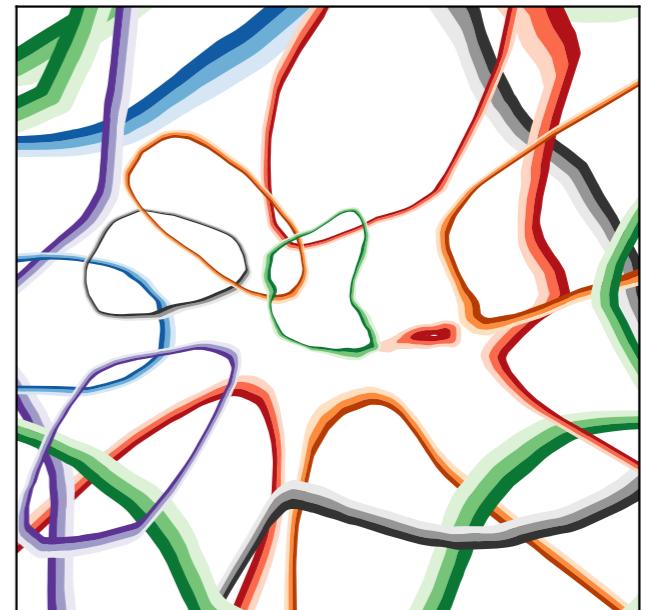
With rotation/reflection preprocessing



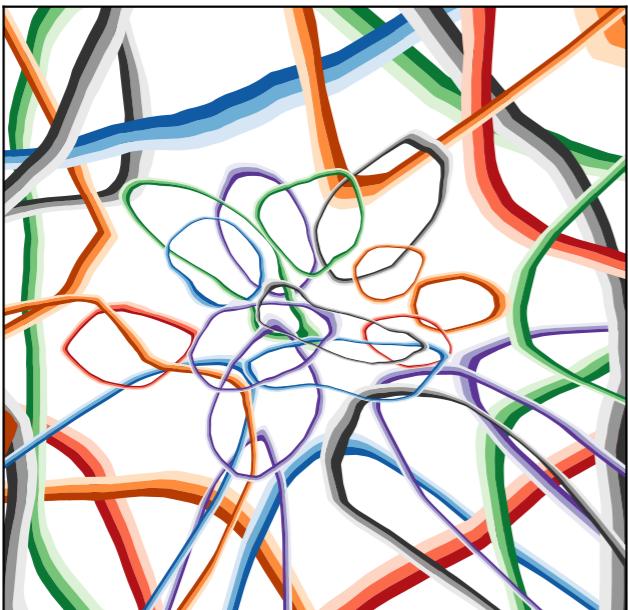
$\ell = 4$



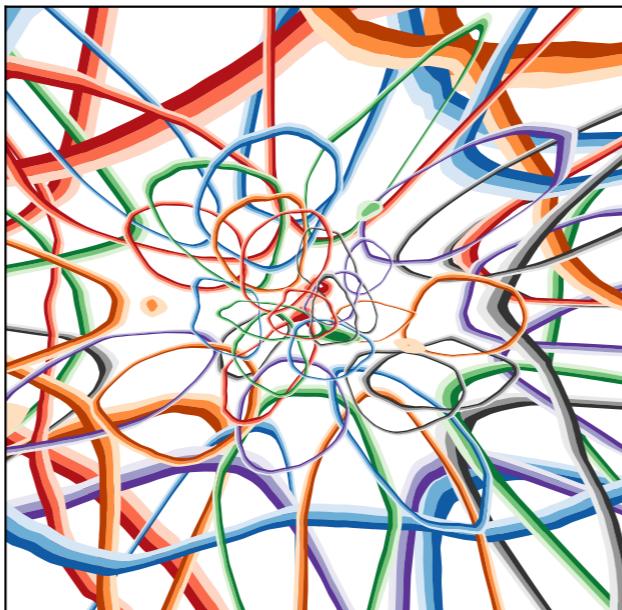
$\ell = 8$



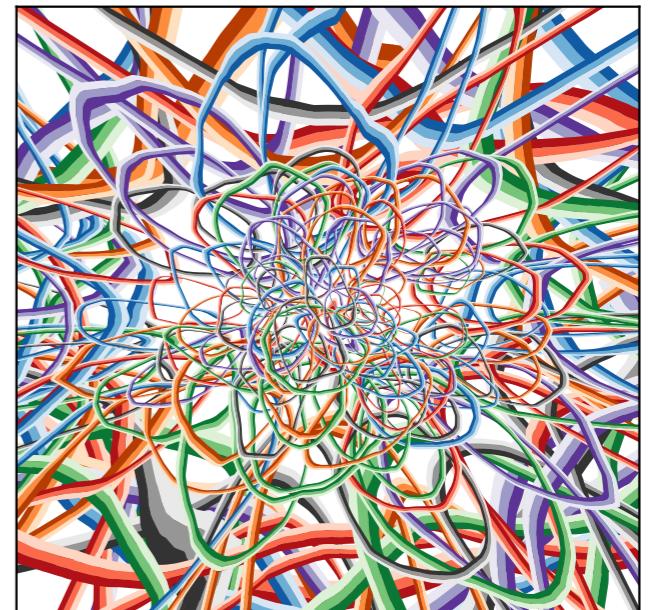
$\ell = 16$



$\ell = 32$



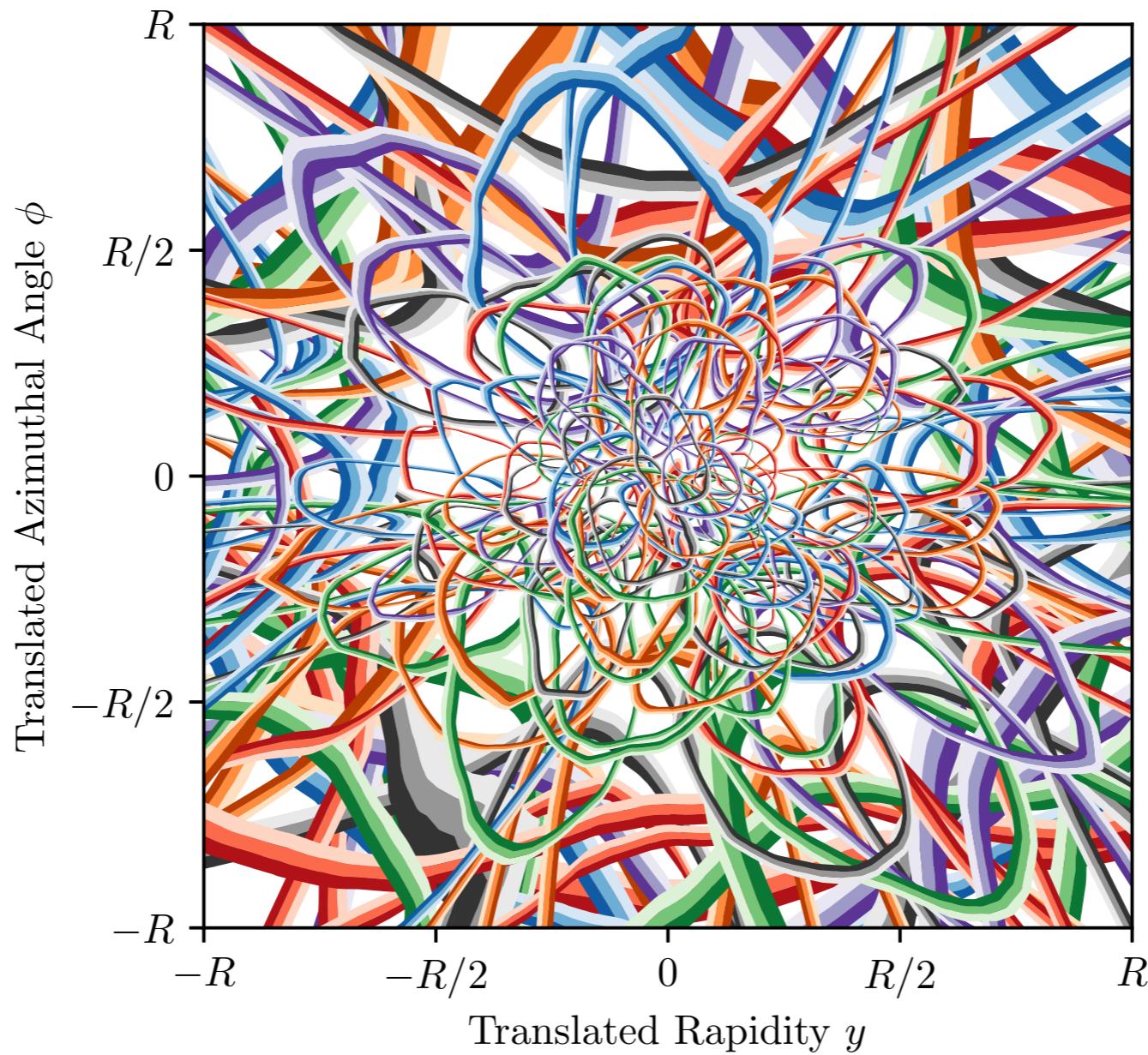
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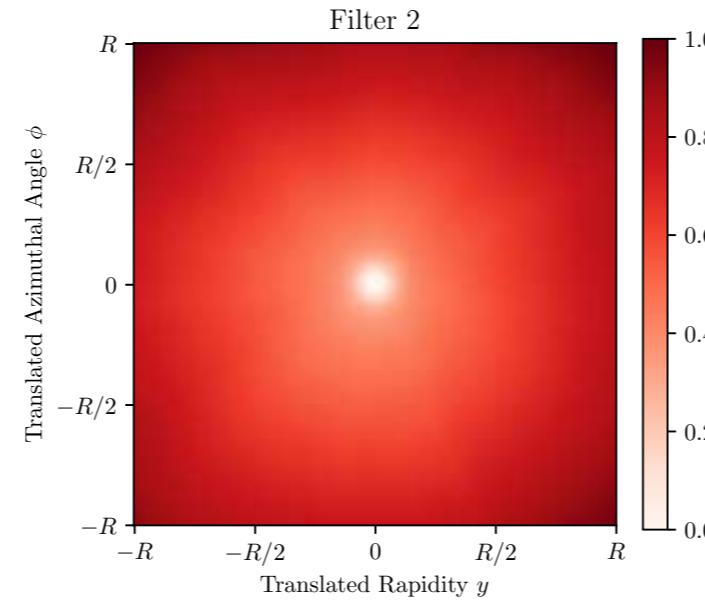
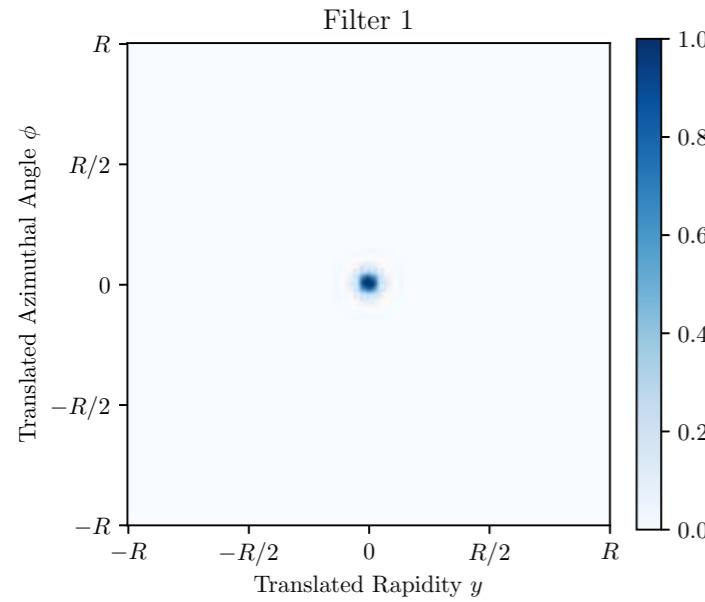
$\ell = 128$

# Boosted Top: Visualizing EFN Filters

Without rotation/reflection preprocessing

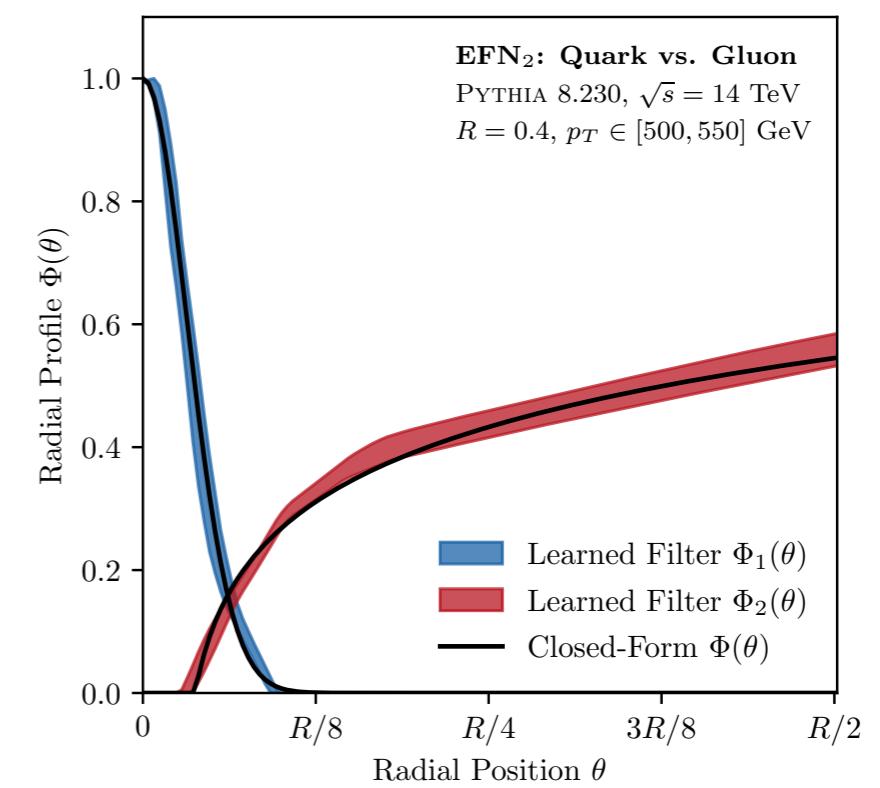


# Quark vs. Gluon: Extracting New Analytic Observables



$$\mathcal{O}_1 = \sum_{i=1}^M z_i \Phi_1(\theta_i)$$

$$\mathcal{O}_2 = \sum_{i=1}^M z_i \Phi_2(\theta_i)$$



Take radial slices to obtain envelope

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

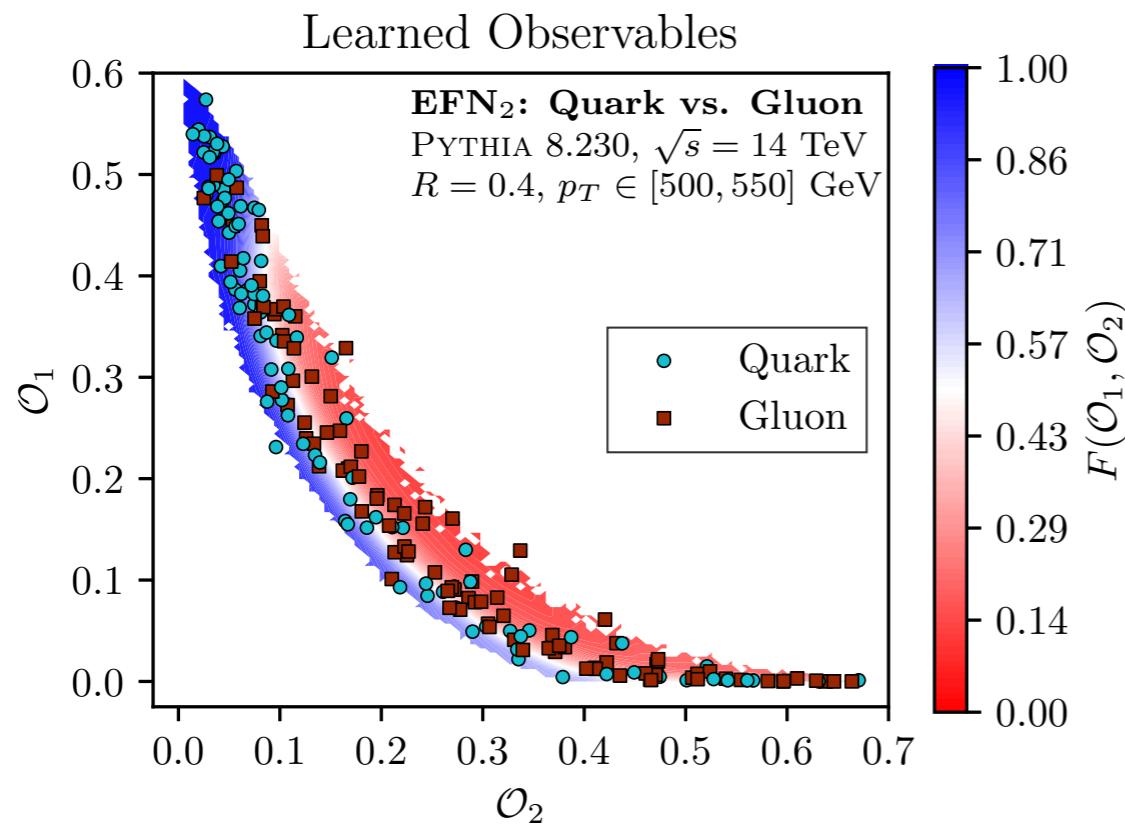
Fit functions of the forms:

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

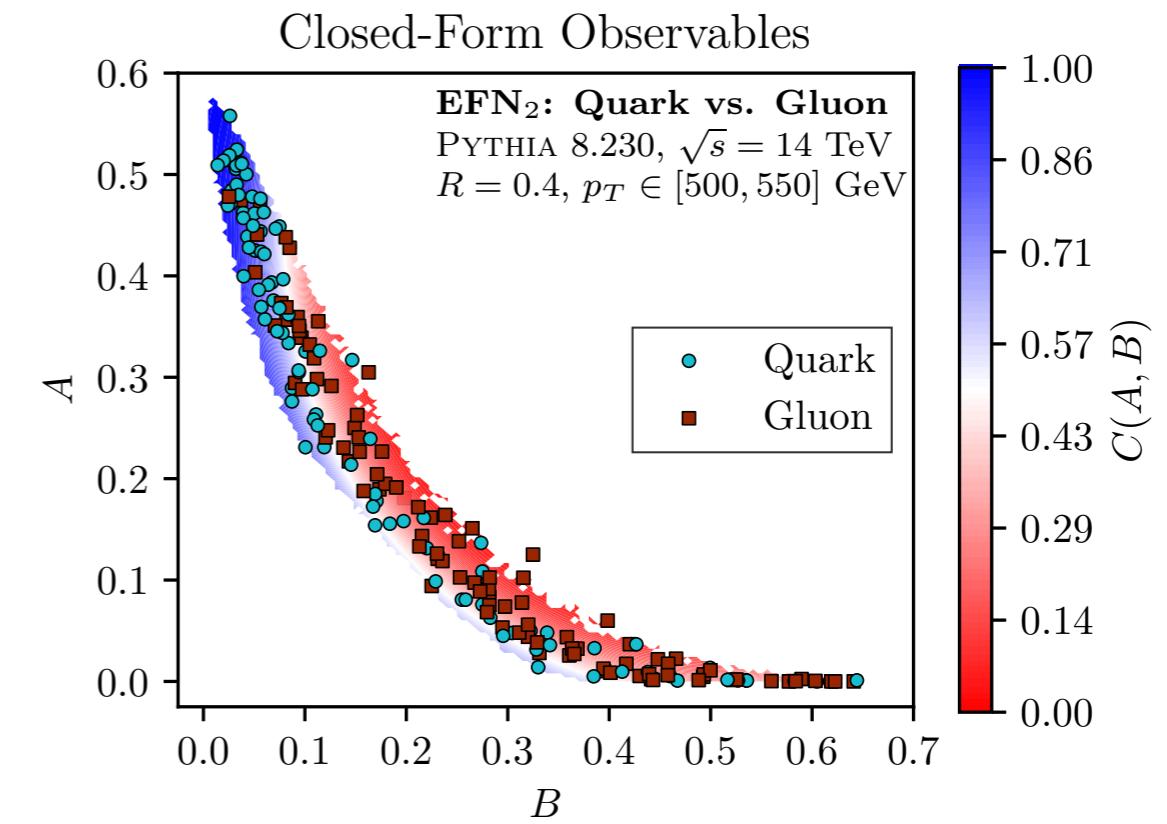
Separate soft and collinear phase space regions

# Quark vs. Gluon: Extracting New Analytic Observables

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



Learned



Extracted

Extract analytic form for  $F$  as (squared) distance from a point:

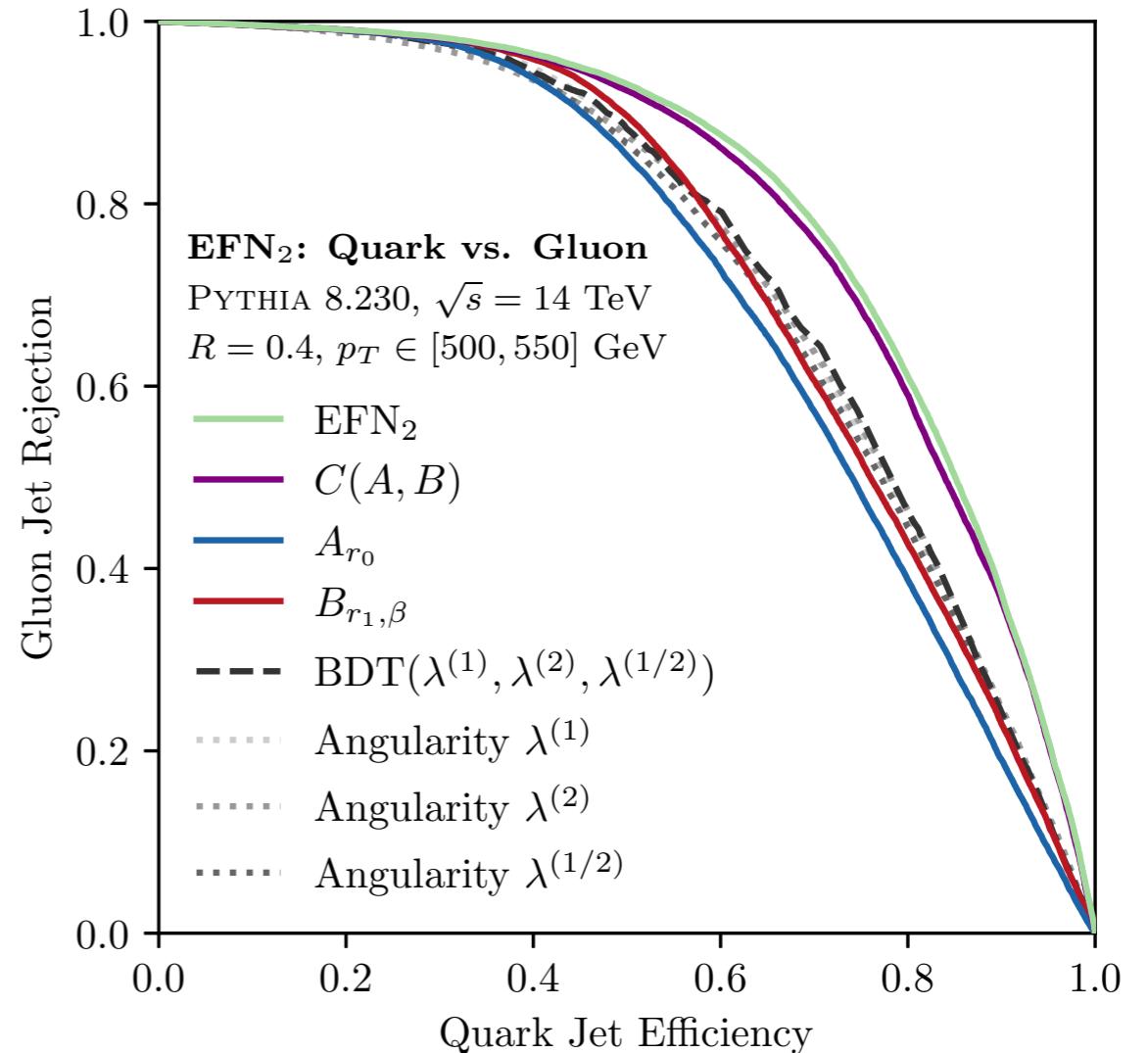
$$C(A, B) = (A - a_0)^2 + (B - b_0)^2$$

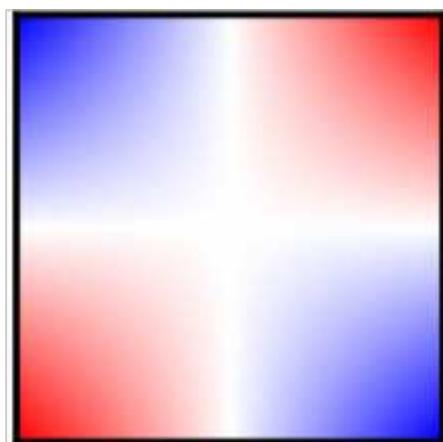
# Quark vs. Gluon: Benchmarking New Analytic Observables

Individually, extracted observables are comparable to other angularities

Extracted  $C(A, B)$  performs nearly as well as EFN ( $\ell = 2$ )

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





# Energy Flow Polynomials

# Energy Flow Networks

# Energy Flow Moments

## Relating EFPs and EFNs via additivity

# 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  $v$ :  $\mathcal{I}^{\mu_1 \dots \mu_v} = \sum_{i=1}^M z_i \hat{p}_i^{\mu_1} \dots \hat{p}_i^{\mu_v}$

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



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

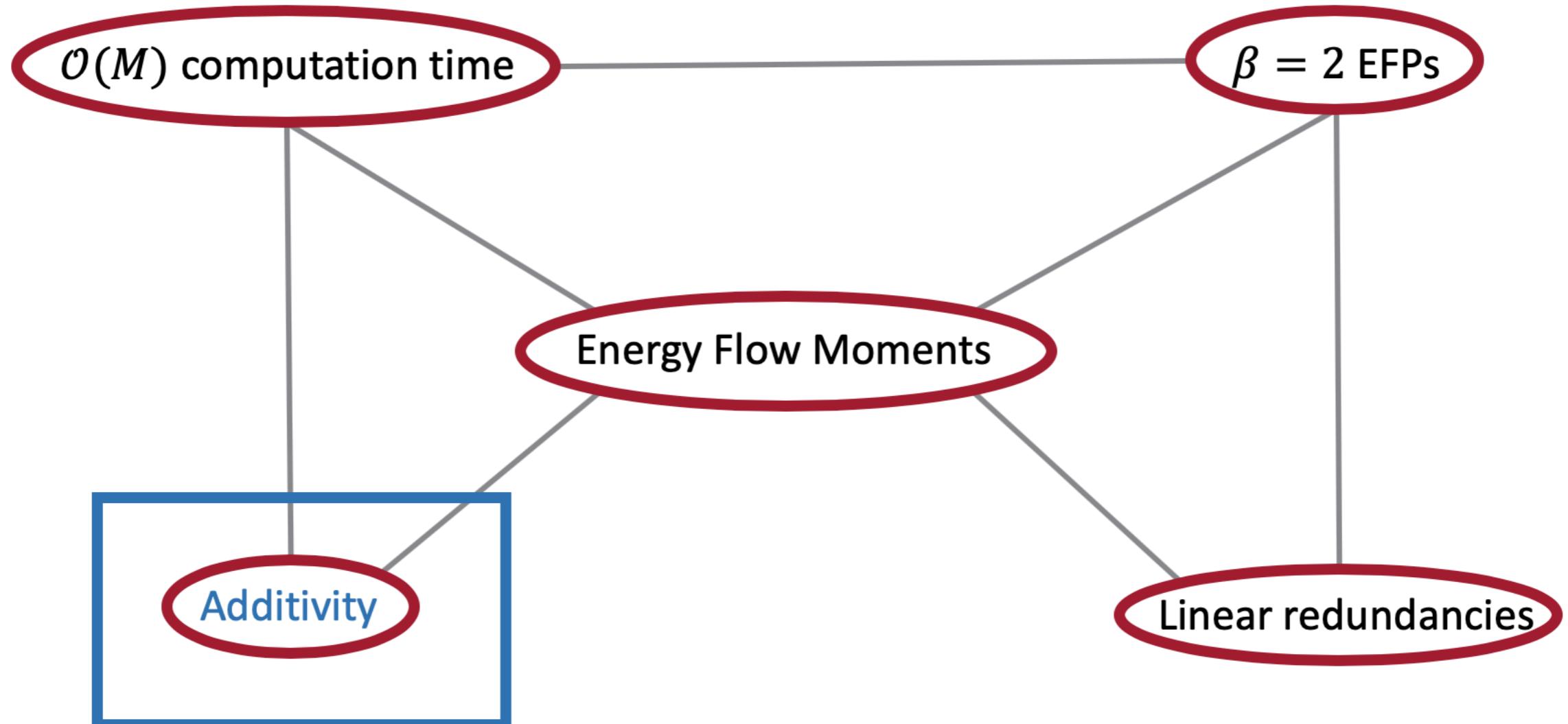
A multigraph correspondence also exists for EFMs:



$$k \longleftrightarrow \mathcal{I}^{\mu_k \dots \mu_\ell}$$

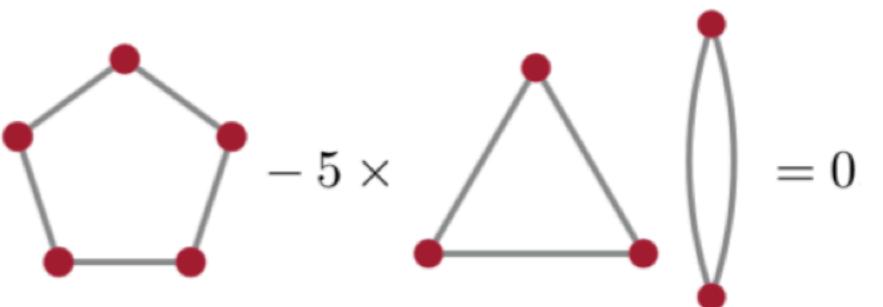
$$i \xrightarrow{} j \iff \eta_{\mu_i \mu_j}$$

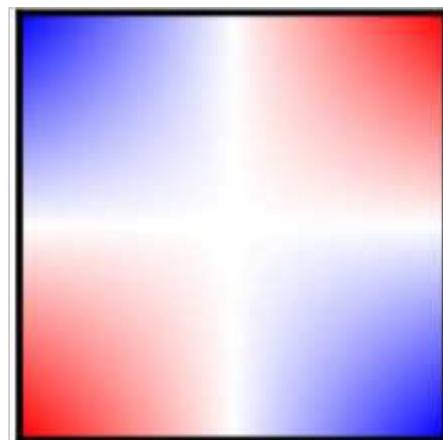
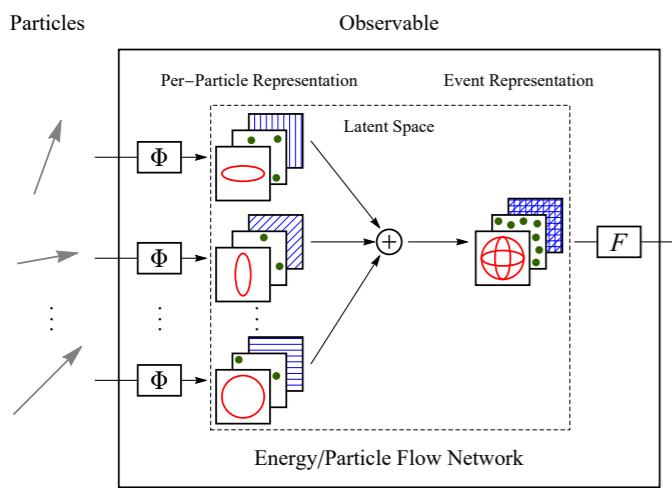
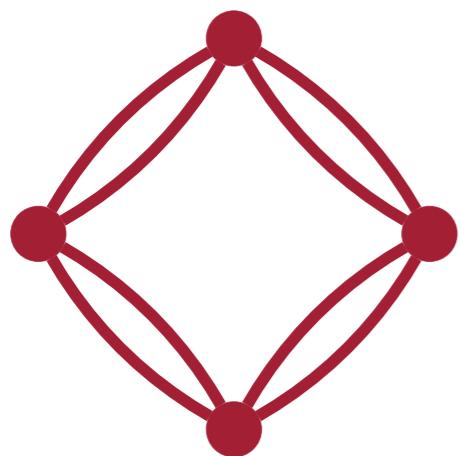
# Energy Flow "Network"



Additivity is the link to the Deep Sets decomposition and EFNs

$$5! \times \mathcal{I}_{[\mu_1 \mu_2 \mu_3 \mu_4 \mu_5]}^{\mu_2} \mathcal{I}_{[\mu_1 \mu_2 \mu_3 \mu_4 \mu_5]}^{\mu_3} \mathcal{I}_{[\mu_1 \mu_2 \mu_3 \mu_4 \mu_5]}^{\mu_4} \mathcal{I}_{[\mu_1 \mu_2 \mu_3 \mu_4 \mu_5]}^{\mu_5} \mathcal{I}_{[\mu_1 \mu_2 \mu_3 \mu_4 \mu_5]}^{\mu_1} = 6 \times \text{(pentagon diagram)} - 5 \times \text{(triangle diagram)} = 0$$





# 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*

# 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

The screenshot shows the EnergyFlow documentation website. The header features a red logo with a diamond-shaped graph icon and the text "EnergyFlow". A search bar labeled "Search docs" is present. The main navigation menu includes "Home", "Welcome to EnergyFlow", "References", "Copyright", "Getting Started" (which is currently selected), "Installation", "Demo", "Examples", "FAQs", "Documentation", "Energy Flow Polynomials", "Architectures", "EMD", "Measures", "Generation", "Utils", and "Datasets". Below the menu, there are GitHub and "Next »" links. The main content area has a "Docs » Home" breadcrumb and a title "Welcome to EnergyFlow". It contains three images: a colorful particle simulation, a diagram of the Energy/Particle Flow Network architecture, and a scatter plot titled "EMD: 125.4 GeV". The text describes the package's history from EFPs to EFNs and PFNs, and lists its main features:

EnergyFlow is a Python package containing a suite of particle physics tools. Originally designed to compute Energy Flow Polynomials (EFPs), as of version 0.10.0 the package expanded to include implementations of Energy Flow Networks (EFNs) and Particle Flow Networks (PFNs). As of version 0.11.0, functions for facilitating the computation of the Energy Mover's Distance (EMD) on particle physics events are included. To summarize the main features:

- **Energy Flow Polynomials:** EFPs are a collection of jet substructure observables which form a complete linear basis of IRC-safe observables. EnergyFlow provides tools to compute EFPs on events for several energy and angular measures as well as custom measures.
- **Energy Flow Networks:** EFNs are infrared- and collinear-safe models designed for learning from collider events as unordered, variable-length sets of particles. EnergyFlow contains customizable Keras implementations of EFNs.
- **Particle Flow Networks:** PFNs are general models designed for learning from collider events as unordered, variable-length sets of particles, based on the Deep Sets framework. EnergyFlow contains customizable Keras implementations of PFNs.
- **Energy Mover's Distance:** The EMD is a common metric between probability distributions that has been adapted for use as a metric between collider events. EnergyFlow contains code to

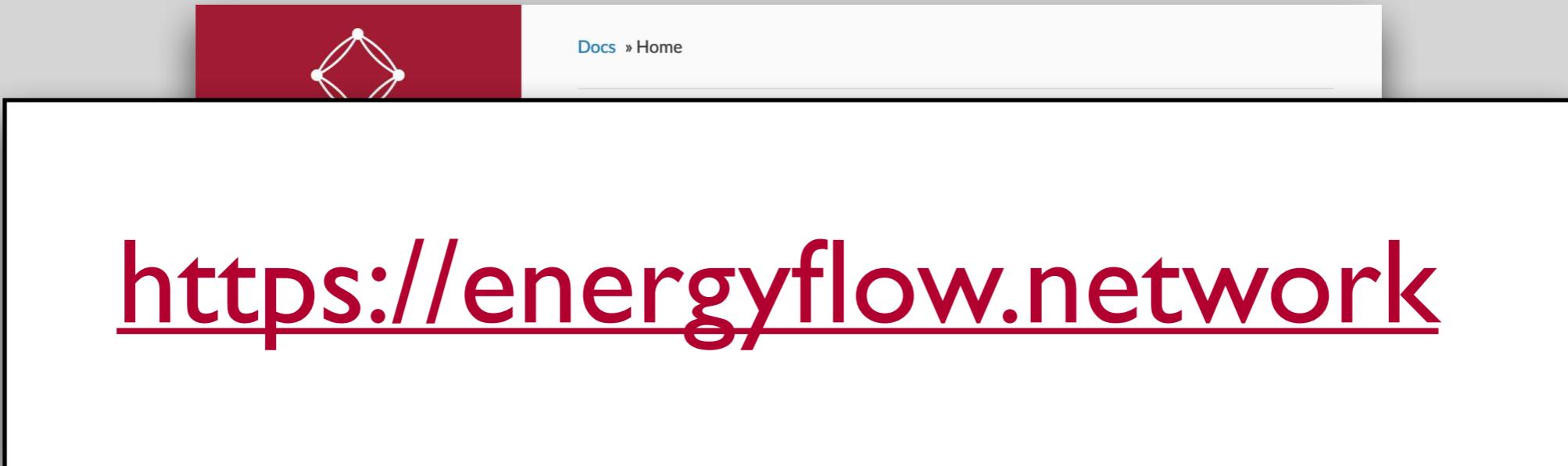
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CNN, DNN architectures included  
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The screenshot shows the homepage of the EnergyFlow network documentation. At the top, there is a red header bar with a white diamond logo and the text "Docs » Home". Below the header, the main title "https://energyflow.network" is displayed in a large, bold, red font. On the left side, there is a dark sidebar with a list of links: Examples, FAQs, Documentation, Energy Flow Polynomials, Architectures, EMD, Measures, Generation, Utils, and Datasets. At the bottom of the sidebar, there are GitHub and Next links. The main content area contains text about the package's features, mentioning Energy Flow Networks (EFNs) and Particle Flow Networks (PFNs), and listing several bullet points about its capabilities.

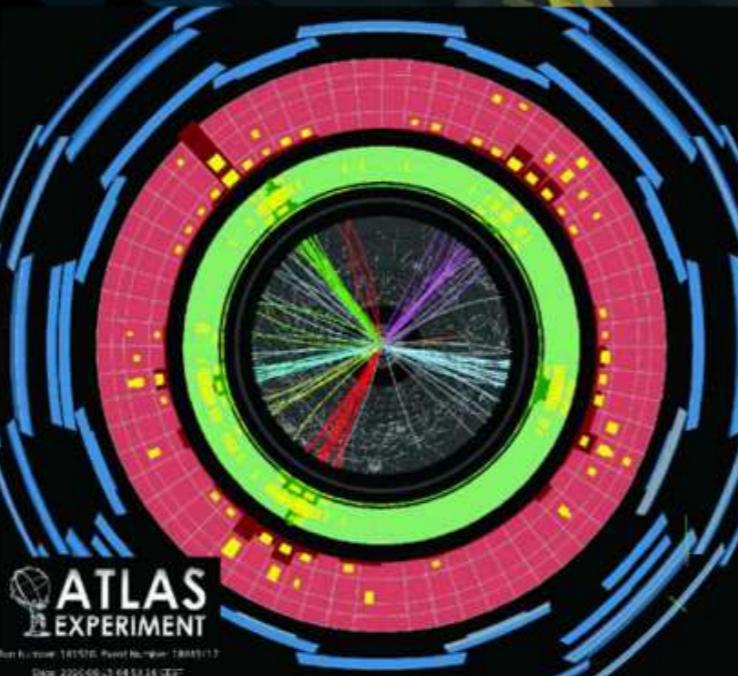
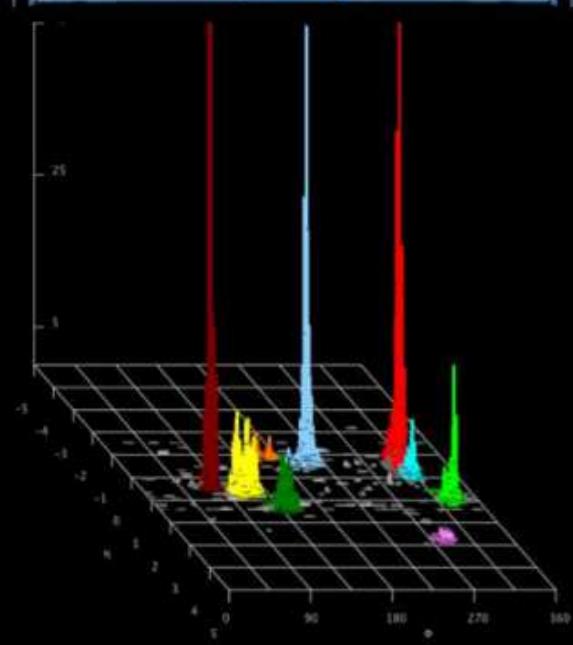
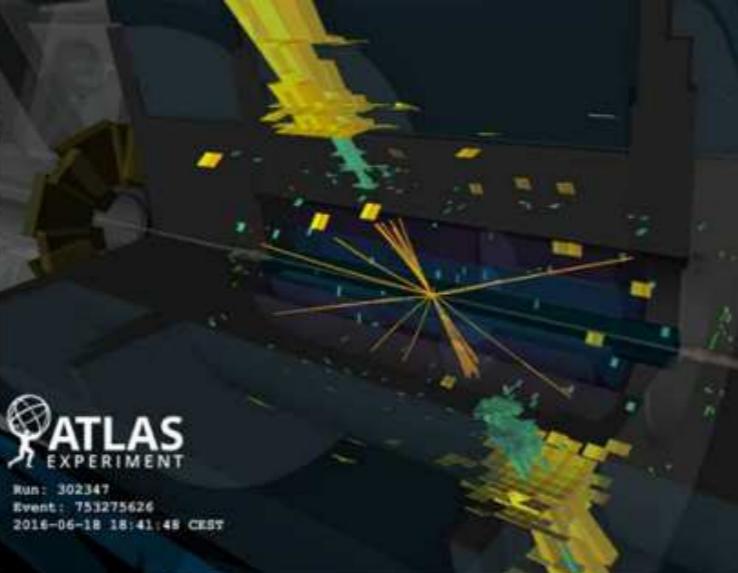
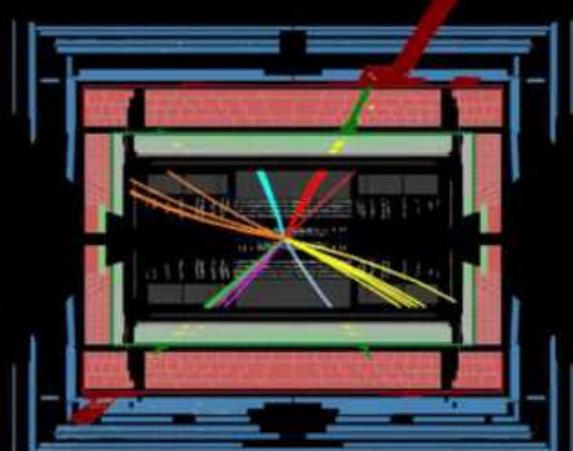
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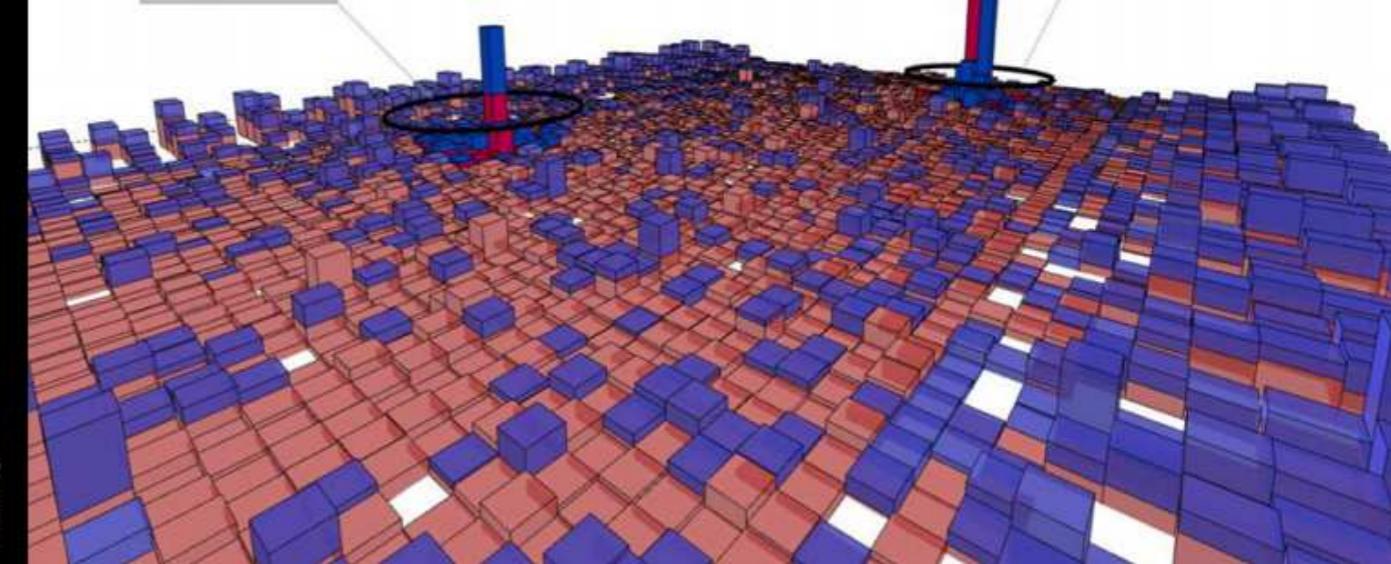
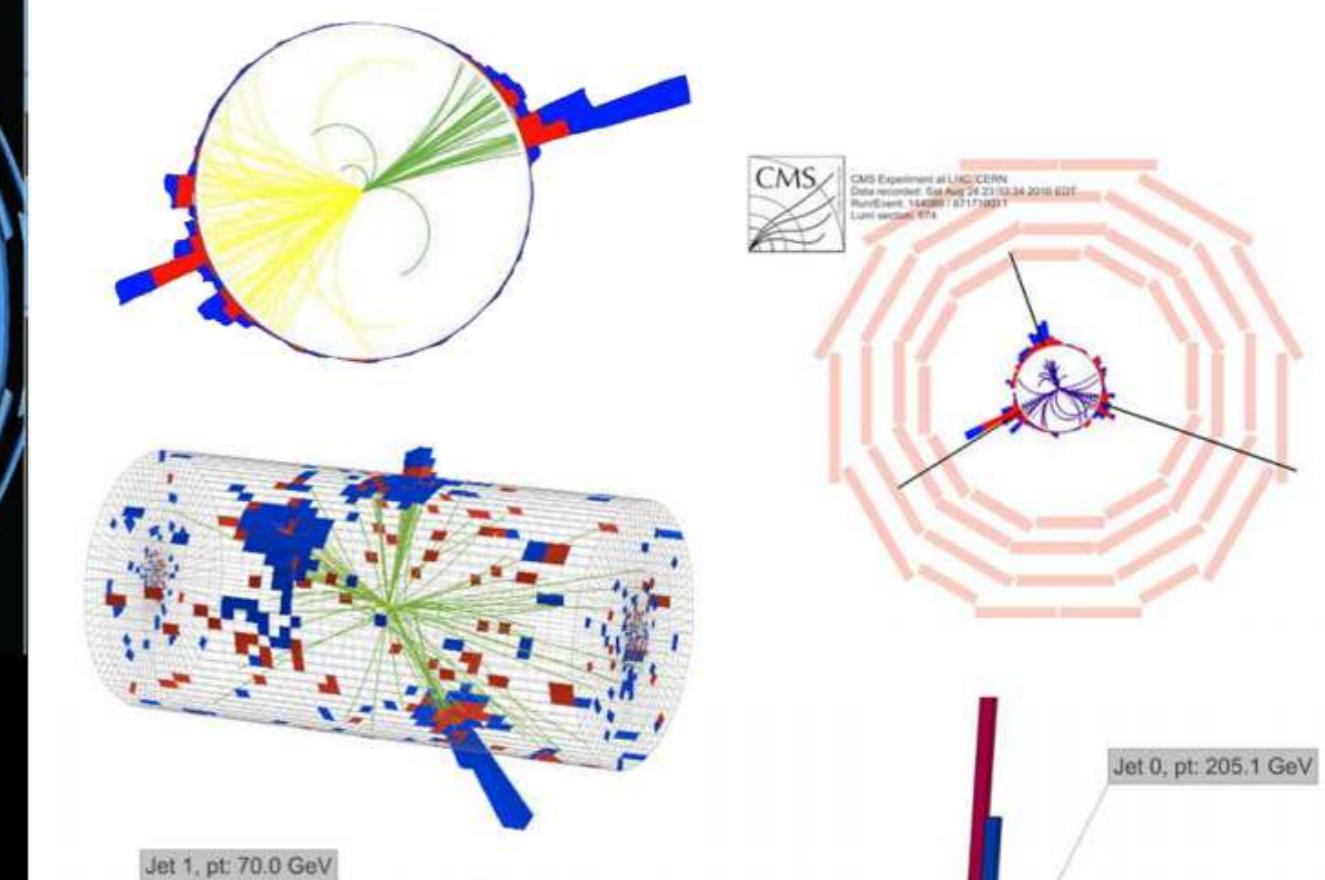
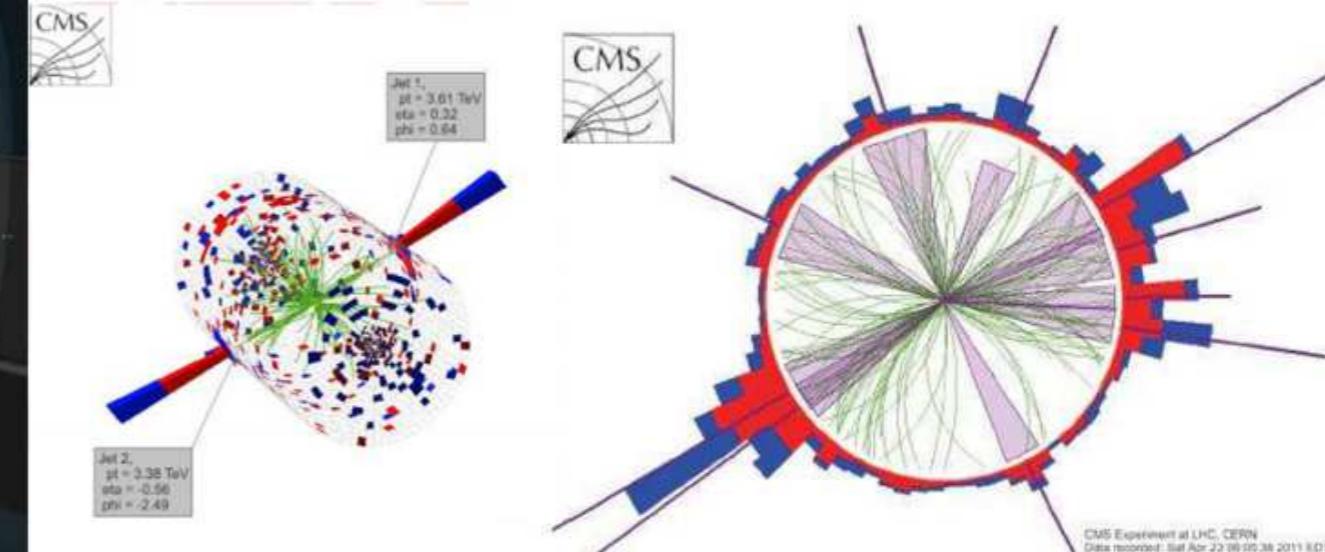
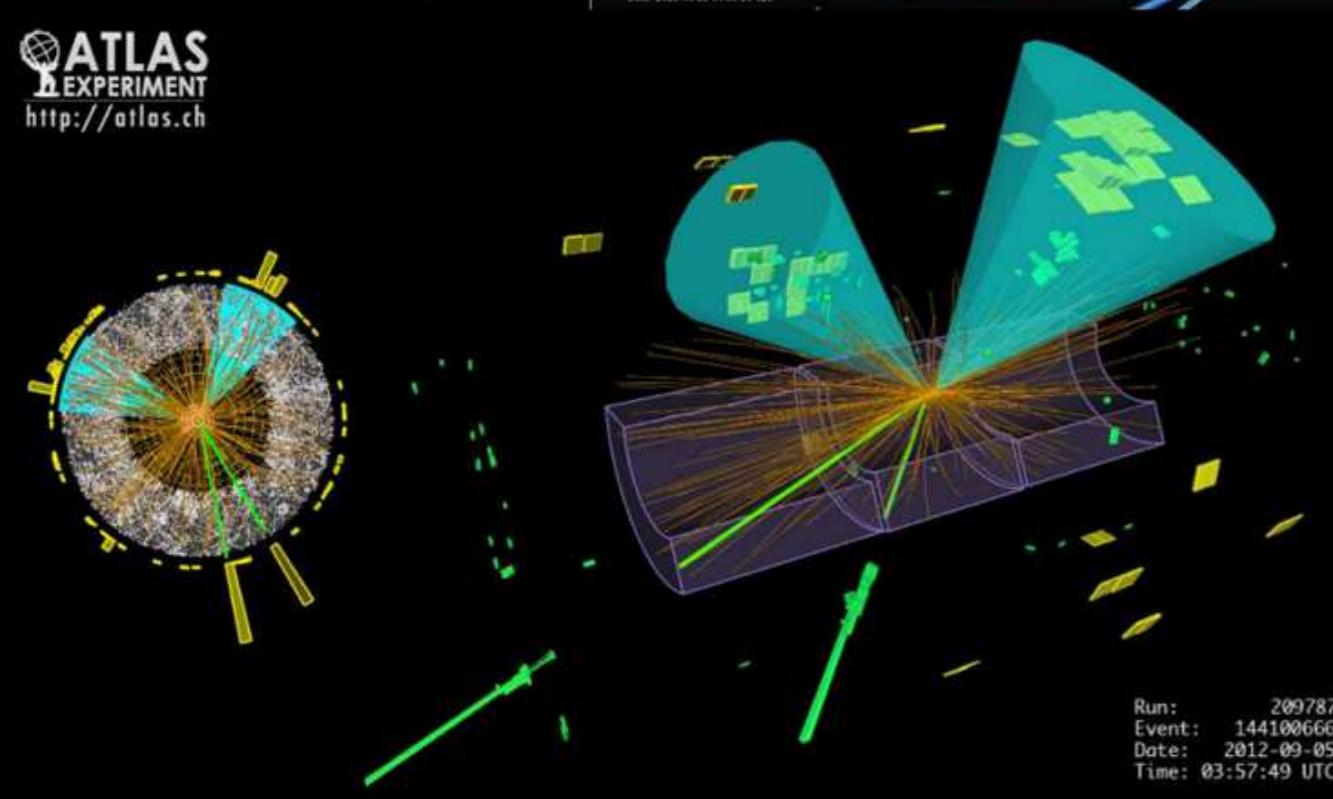
# Thank You!

Run Number: 159224, Event Number: 3533152

Date: 2010-07-18 11:05:54 CEST



**ATLAS**  
EXPERIMENT  
<http://atlas.ch>



# Jet Representations $\longleftrightarrow$ Analysis Tools

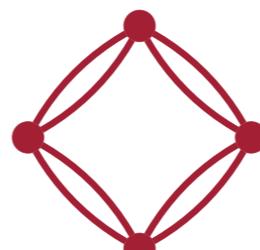
Two key choices when analyzing jets

## 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

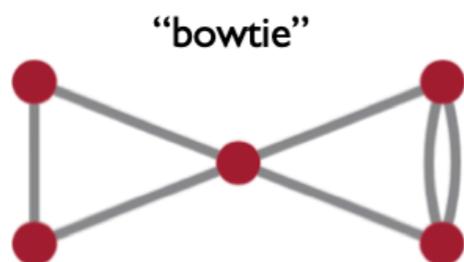
- Threshold cut
- Multidimensional likelihood
- Boosted decision tree (BDT), shallow neural network (NN)
- Convolutional NN (CNN)
- Recurrent/Recursive NN (RNN)
- Fancy RNN
- Dense neural network (DNN)
- Linear classification
- Energy flow network



# Multigraph/EFP Correspondence

Multigraph  $\longleftrightarrow$  EFP

---



$$= \sum_{i_1=1}^M \sum_{i_2=1}^M \sum_{i_3=1}^M \sum_{i_4=1}^M \sum_{i_5=1}^M z_{i_1} z_{i_2} z_{i_3} z_{i_4} z_{i_5} \theta_{i_1 i_2} \theta_{i_2 i_3} \theta_{i_1 i_3} \theta_{i_1 i_4} \theta_{i_1 i_5} \theta_{i_4 i_5}^2$$

---

$$\begin{array}{c} j \\ \text{---} \\ k \quad l \end{array} \longleftrightarrow \begin{array}{c} z_{i_j} \\ \theta_{i_k i_l} \end{array}$$

---

$N$  Number of vertices  $\longleftrightarrow$  N-particle correlator

$d$  Number of edges  $\longleftrightarrow$  Degree of angular monomial

$\chi$  Treewidth + 1  $\longleftrightarrow$  Optimal VE Complexity

---

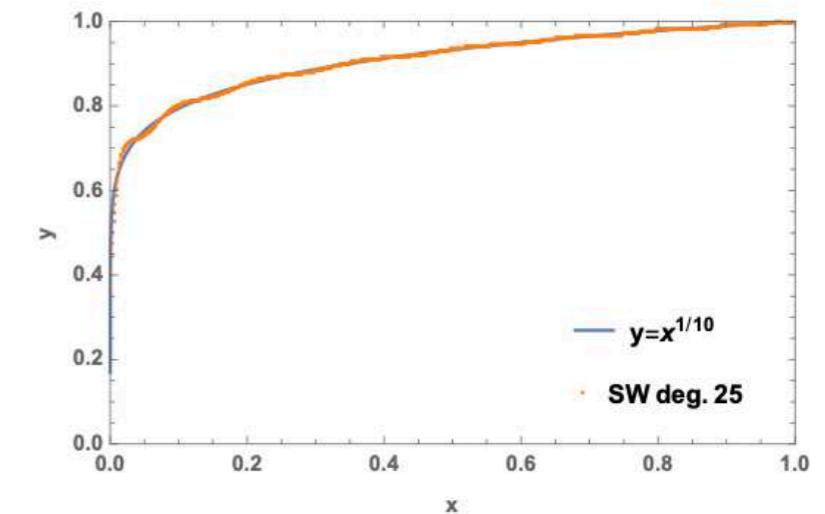
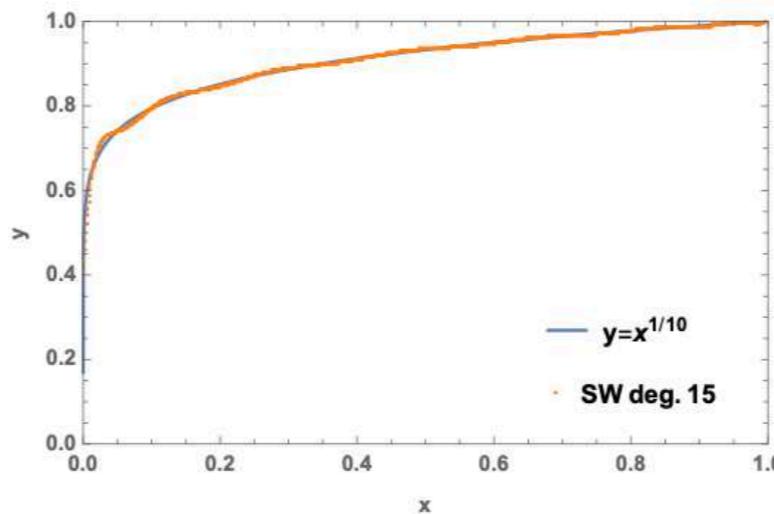
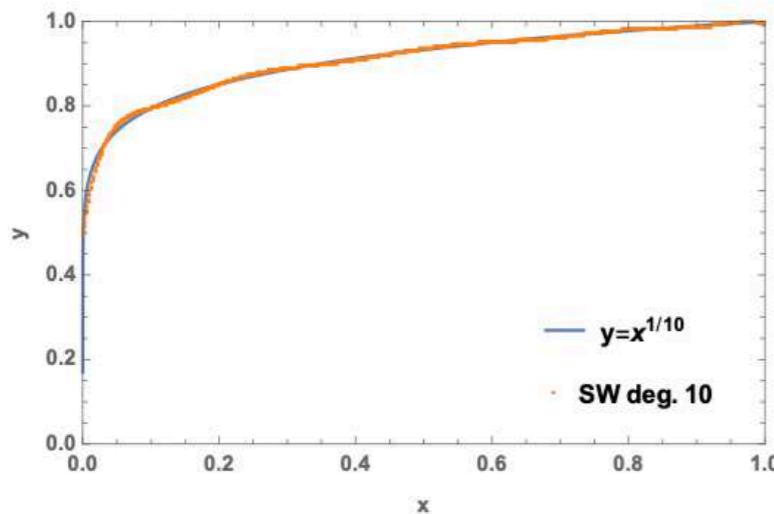
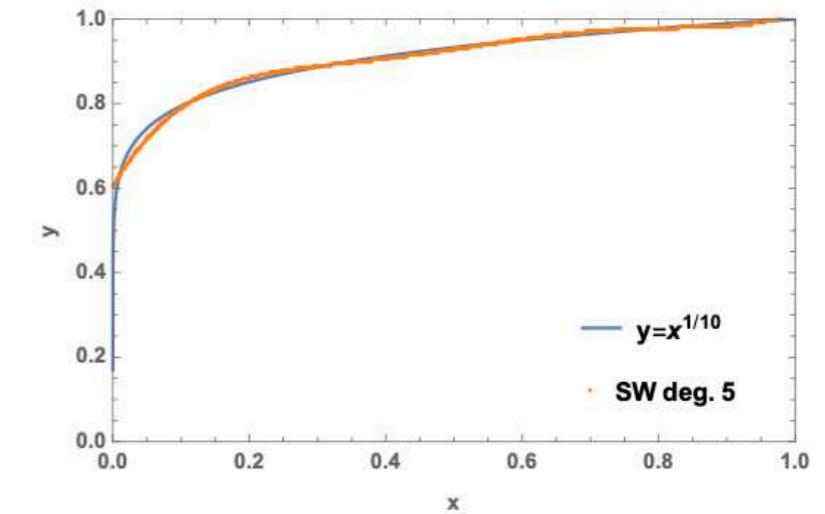
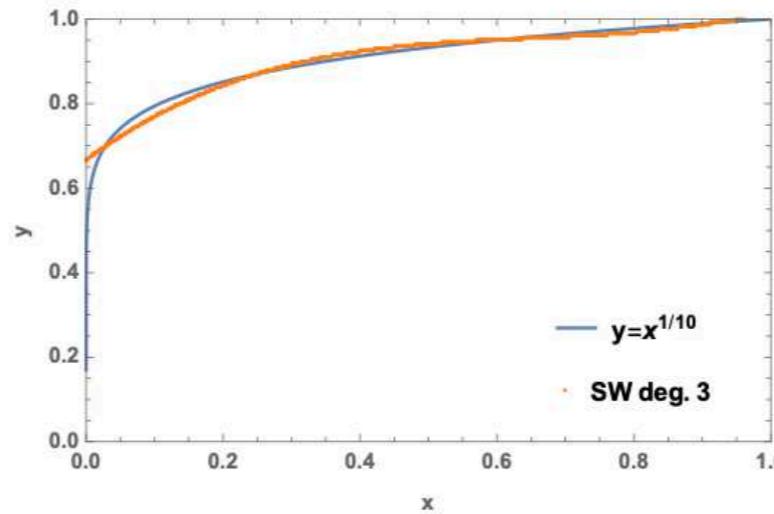
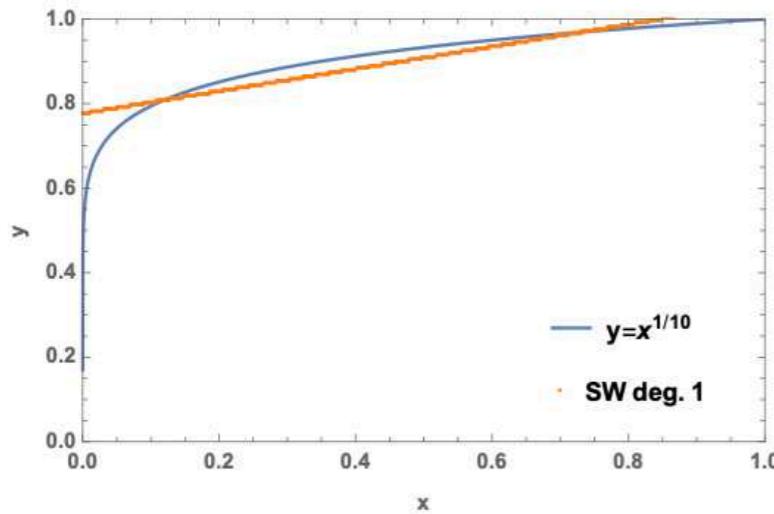
Connected  $\longleftrightarrow$  Prime

Disconnected  $\longleftrightarrow$  Composite

:

# Fun with the Stone-Weierstrass Theorem

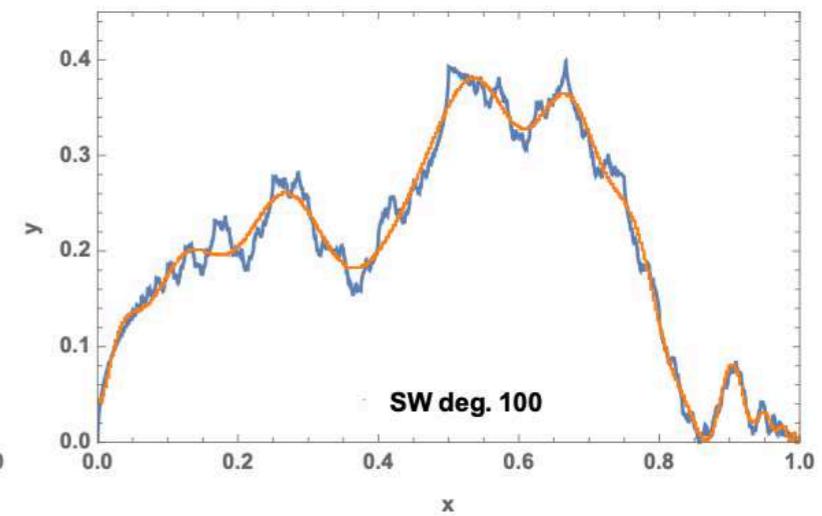
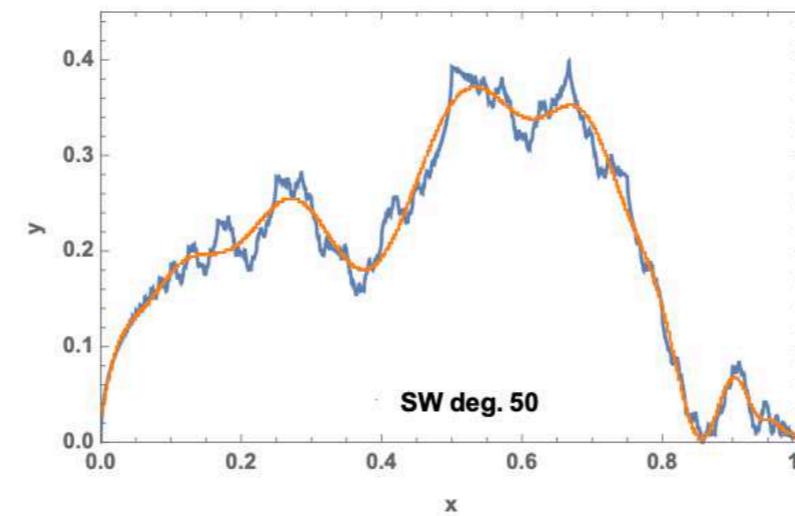
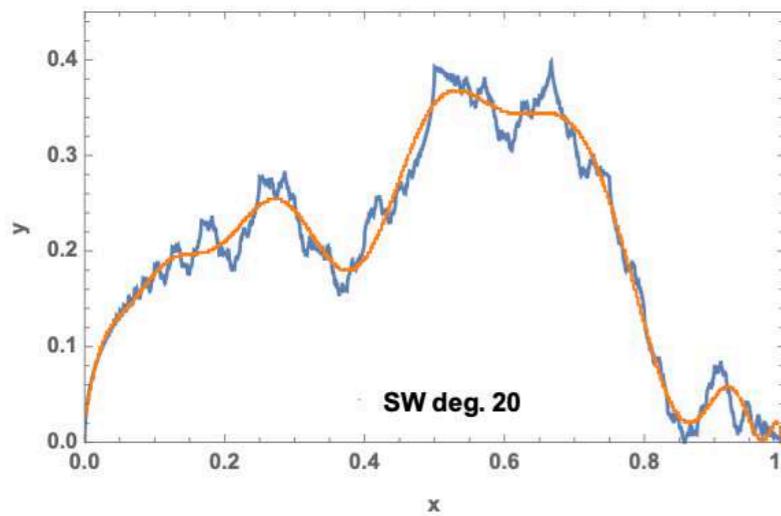
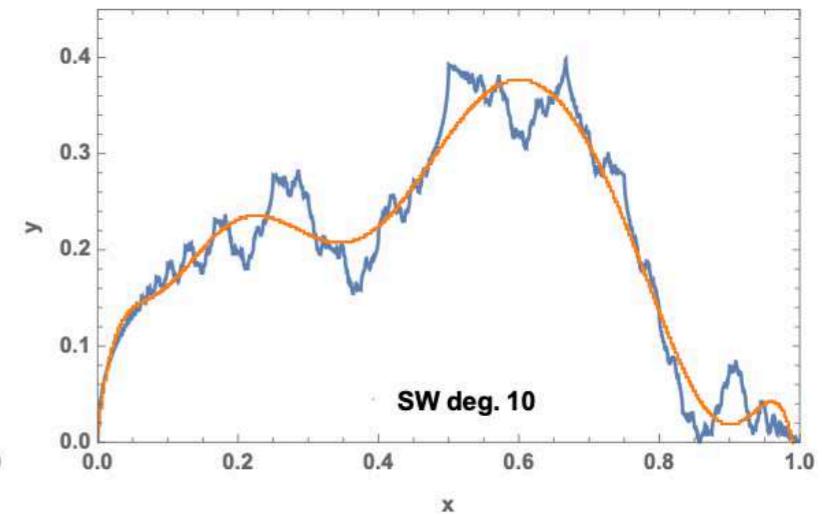
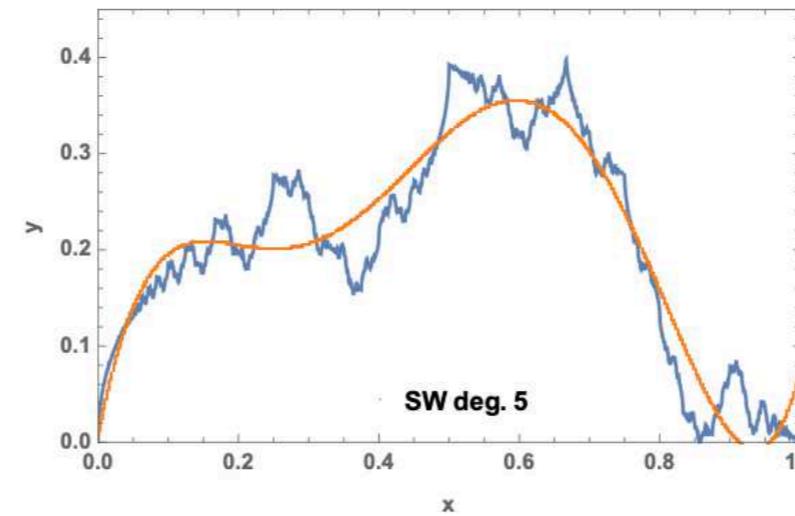
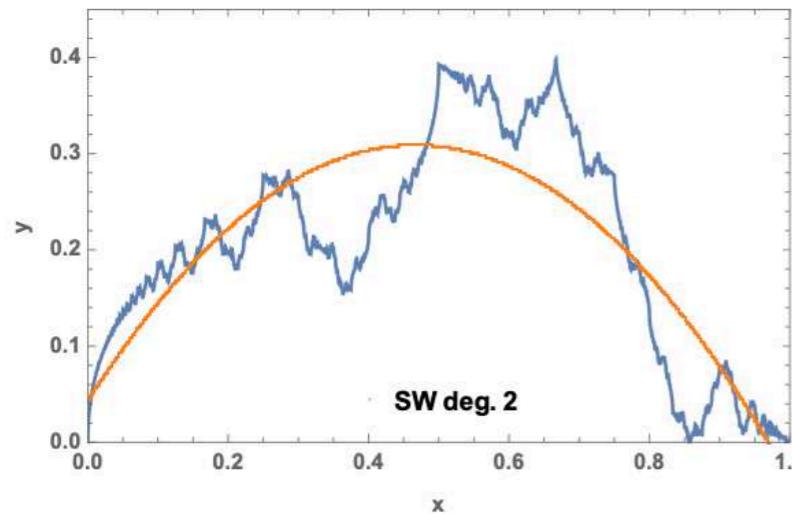
Try to approximate function that has no Taylor expansion around zero



# Fun with the Stone-Weierstrass Theorem

$$y = \sum_{k=1}^{\infty} \frac{\sin(\pi k^2 x)}{\pi k^2}$$

That was too easy, try the Weierstrass function (continuous everywhere, differentiable on a measure zero set of points)



# Computation Complexity of EFPs – Variable Elimination

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

For  $\sim 100$  particles this becomes intractable for  $N > 4$

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if (_N > 5) {
    throw Error("EnergyCorrelator is only hard coded for N = 0,1,2,3,4,5");
}
```

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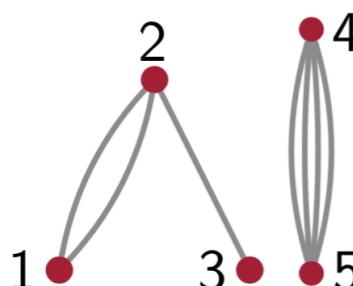
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```

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


$$= \left( \sum_{i_1=1}^M \sum_{i_2=1}^M \sum_{i_3=1}^M z_{i_1} z_{i_2} z_{i_3} \theta_{i_1 i_2}^2 \theta_{i_2 i_3} \right) \left( \sum_{i_4=1}^M \sum_{i_5=1}^M z_{i_4} z_{i_5} \theta_{i_4 i_5}^4 \right)$$

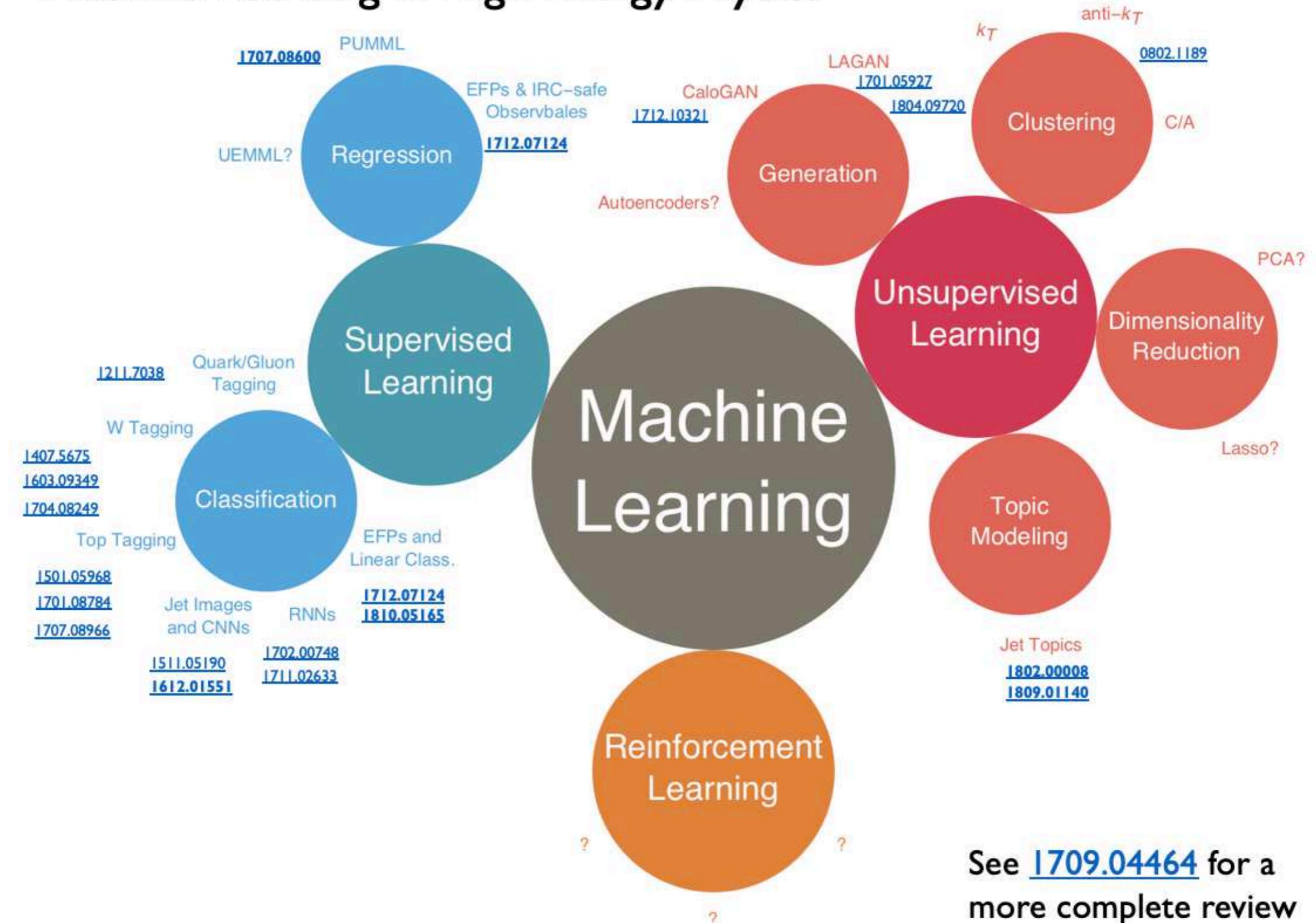
Disconnected is product of connected


$$\begin{aligned} &= \underbrace{\sum_{i_1=1}^M \sum_{i_2=1}^M \sum_{i_3=1}^M \sum_{i_4=1}^M \sum_{i_5=1}^M \sum_{i_6=1}^M \sum_{i_7=1}^M \sum_{i_8=1}^M z_{i_1} z_{i_2} z_{i_3} z_{i_4} z_{i_5} z_{i_6} z_{i_7} z_{i_8}}_{\mathcal{O}(M^8)} \prod_{j=2}^7 \theta_{i_1 i_j} \\ &= \underbrace{\sum_{i_1=1}^M z_{i_1} \left( \sum_{i_2=1}^M z_{i_2} \theta_{i_1 i_2} \right)^7}_{\mathcal{O}(M^2)} \end{aligned}$$

Clever parentheses placement corresponds to good elimination ordering

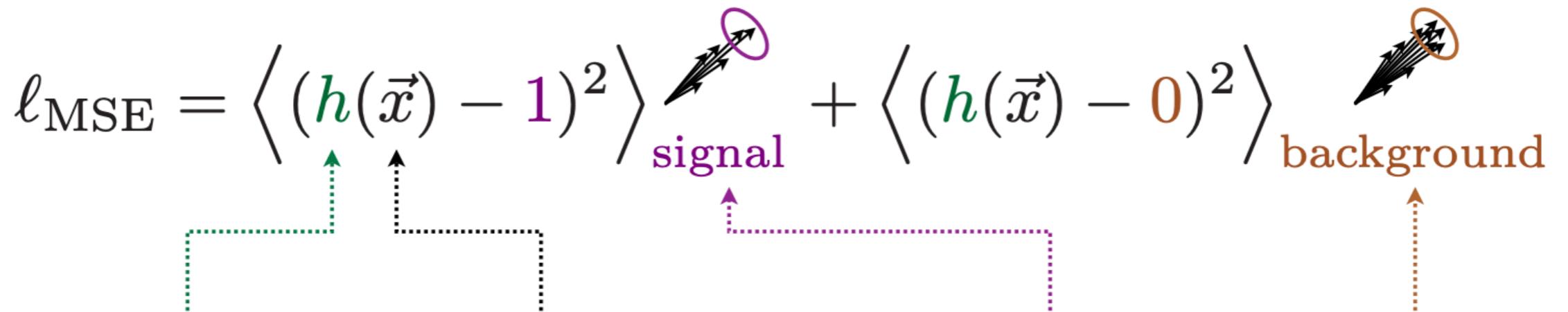
All tree graphs become  $\mathcal{O}(M^2)$

# Machine Learning in High Energy Physics



# Jet Classification Studies

*Mix and match*

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


## Classifier

Boosted Decision Tree  
Fisher Linear Discriminant  
Shallow Neural Network  
Deep Neural Network  
Convolutional Neural Network  
Recurrent Neural Network  
Recursive Neural Network  
Combination/Lorentz Layers  
...

## Inputs

High-Level Features  
Basis of High-Level Features  
Jet Image  
Multi-channel Jet Image  
Abstract Jet Image  
Sorted Four-Vectors  
Clustered Four-Vectors  
Lund Plane Emissions  
Kitchen Sink  
...

## Signal vs. Background

Quark Jets	vs.	Gluon Jets
Up-type Quarks	vs.	Down-type Quarks
W/Z Bosons	vs.	QCD Jets
W Bosons	vs.	Z Bosons
Top Quarks	vs.	QCD Jets
Exotic Boosted Objects	vs.	QCD Jets
CMS Open Data Samples	vs.	Each other
...	vs.	...

[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]

# Top Jet Samples and Other Methods

[Butter, Kasieczka, Plehn, Russell, 2017]

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

Performance saturation?

# Top Jet Samples and Other Methods

Comm

$p_T \in [5$

ehn, Russell, 2017]

*Not yet!*

<b>Particle Flow Network (PFN)</b>	<b>0.982</b>	<b>0.932</b>	<b>888</b>	<b>PTK, E. Metodiev</b>	<b>Median over ten trainings. Based on Table 5 in 1810.05165</b>
<b>2D CNN [ResNeXt50]</b>	<b>0.984</b>	<b>0.936</b>	<b>1086</b>	<b>Huilin Qu, Loukas Gouskos</b>	<b>Preliminary from <a href="https://indico.cern.ch/event/745718/contributions/3202526">indico.cern.ch/event/745718/ contributions/3202526</a></b>
<b>DGCNN</b>	<b>0.984</b>	<b>0.937</b>	<b>1160</b>	<b>Huilin Qu, Loukas Gouskos</b>	<b>Preliminary from <a href="https://indico.cern.ch/event/745718/contributions/3202526">indico.cern.ch/event/745718/ contributions/3202526</a></b>

However, ResNeXt50 has 25m parameters and DGCNN takes 2 days to train

PFN has 40k parameters and takes 1 hour to train