Energy Flow and Jet Substructure

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BOOST 2018
Paris, France – July 18, 2018

Based on work with Eric M. Metodiev and Jesse Thaler
1712.07124 EnergyFlow

Program

Overture

Act I

- IRC Safe Jet Observables
- Energy Flow Polynomials
- Linear Classification Performance

Intermission

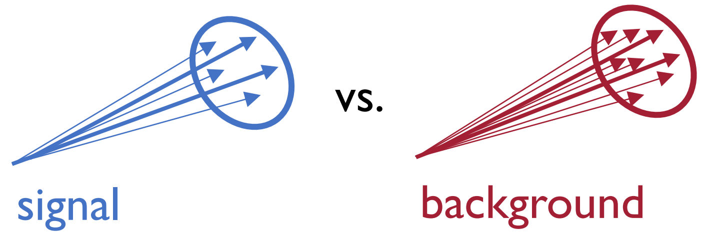
Act II

- Intrinsic Jet Symmetries
- Energy Flow Networks
- Opening the Box

Epilogue

Program

Overture



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Jet Representations ⟷ Analysis Tools

Two key choices when tagging jets

How to represent the jet

- Single expert variable
- A few expert variables
- Many expert variables

- 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
- Deep neural network (DNN)
- Linear classification
- Energy flow network

See Ben Nachman's intro talk for more

Jet Representations ⟷ Analysis Tools

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How to represent the jet		How to analyze that representation
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• Many expert variables		• Boosted decision tree (BDT), shallow neural network (NN)
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• Clustering tree		• Fancy RNN
• *N*-subjettiness basis		• Deep neural network (DNN)
• Energy flow polynomials	**Act I**	• Linear classification
• Set of particles	**Act II**	• Energy flow network

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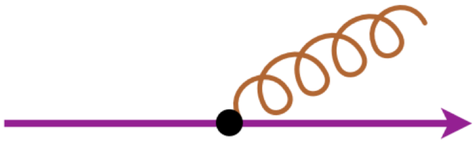

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Expanding an Arbitrary IRC-safe Observable

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

- Energy expansion*: Approximate S with polynomials of z_{i_j}
  - 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

More about IRC safety in backup

Energy correlator parametrized by angular function f

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

[F. Tkachov, hep-ph/9601308]

Energy correlators linearly span IRC-safe observables

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

Linear spanning basis in terms of "EFPs" has been found!

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

**Generically these expansions exist by the Stone-Weierstrass theorem

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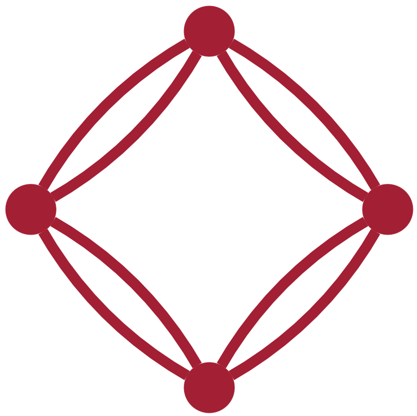
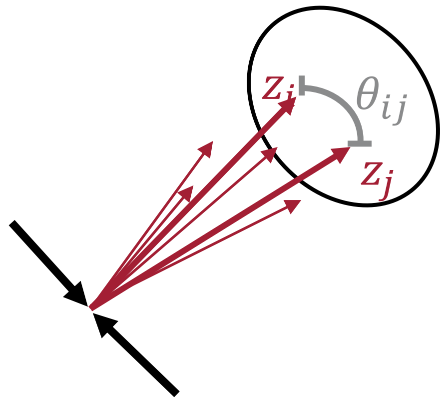


Energy Flow Polynomials (EFPs)

[**PTK**, E. Metodiev, J. Thaler, 1712.07124]



Energy Fraction | Pairwise Angular Distance

$$e^+e^-: \; z_i = \frac{E_j}{\sum_k E_k}, \quad \theta_{ij} = \left(\frac{2p_i^\mu p_{j\mu}}{E_i E_j}\right)^{\frac{\beta}{2}}$$

$$\text{Hadronic:} \; z_i = \frac{p_{Tj}}{\sum_k p_{Tk}}, \quad \theta_{ij} = \left(\Delta y_{ij}^2 + \Delta\phi_{ij}^2\right)^{\frac{\beta}{2}}$$

In equations:

$$\mathrm{EFP}_G = \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} \cdots \sum_{i_N=1}^{M} z_{i_1} z_{i_2} \cdots z_{i_N} \prod_{(k,l)\in G} \theta_{i_k i_l}$$

multigraph

In words:

Correlator of **Energies** and **Angles**

Correlator: Sum over all N-tuples of particle in the event

Energies: Product of the N energy fractions

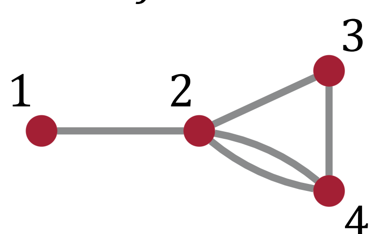
Angles: One $\theta_{i_k i_l}$ for each edge in $(k,l) \in G$

In pictures:

$\longleftrightarrow \; z_{i_j}$

$\longleftrightarrow \; \theta_{i_k i_l}$

(e.g. "fly swatter")



(any index labelling works)

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

See backup for explicit EFP/multigraph mapping

Organizing the Basis

EFPs are most naturally truncated by the degree *d*, the order of the angular expansion (other truncations possible)

Online Encyclopedia of Integer Sequences (OEIS)

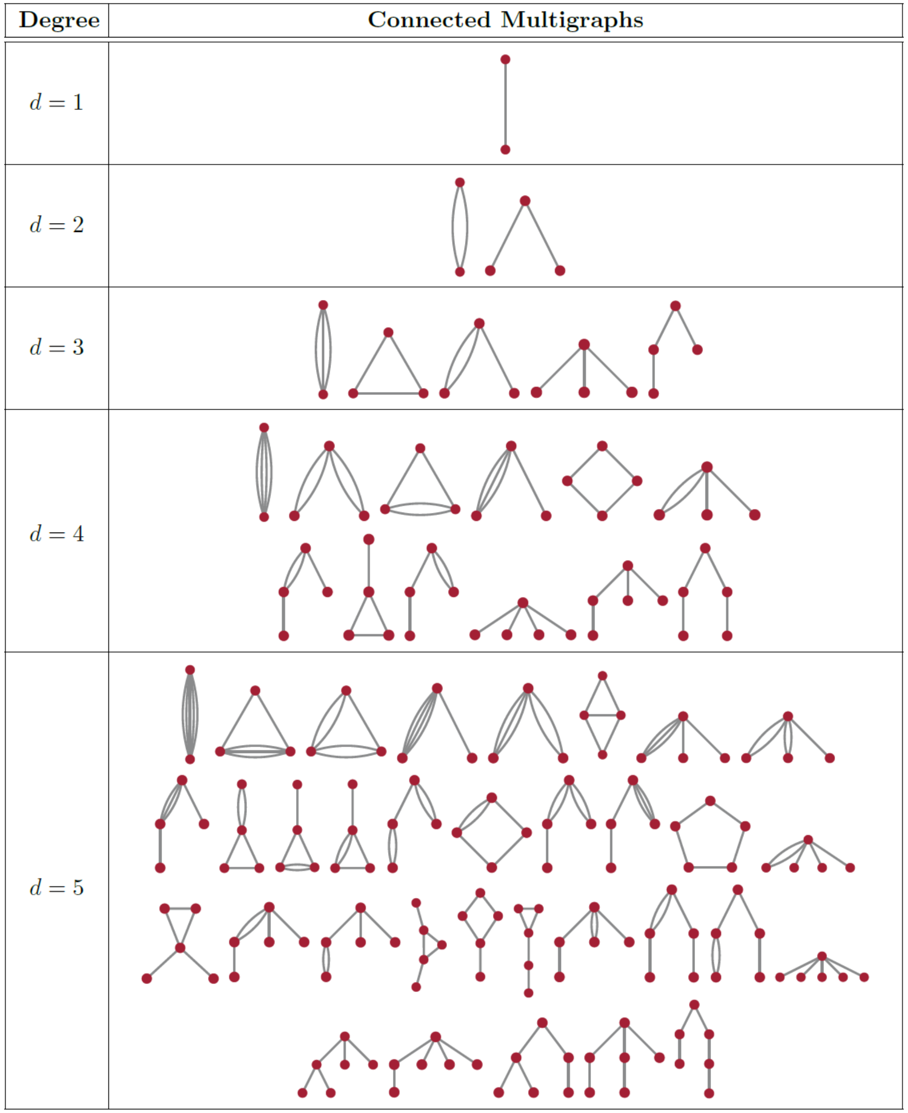
[A050535](A050535) # of multigraphs with *d* edges
# of EFPs of degree *d*

[A076864](A076864) # of connected multigraphs with *d* edges
# of prime EFPs of degree *d*

↓

Exactly 1000 EFPs up to degree *d*=7!

There exist many linear redundancies of several types in the set of EFPs



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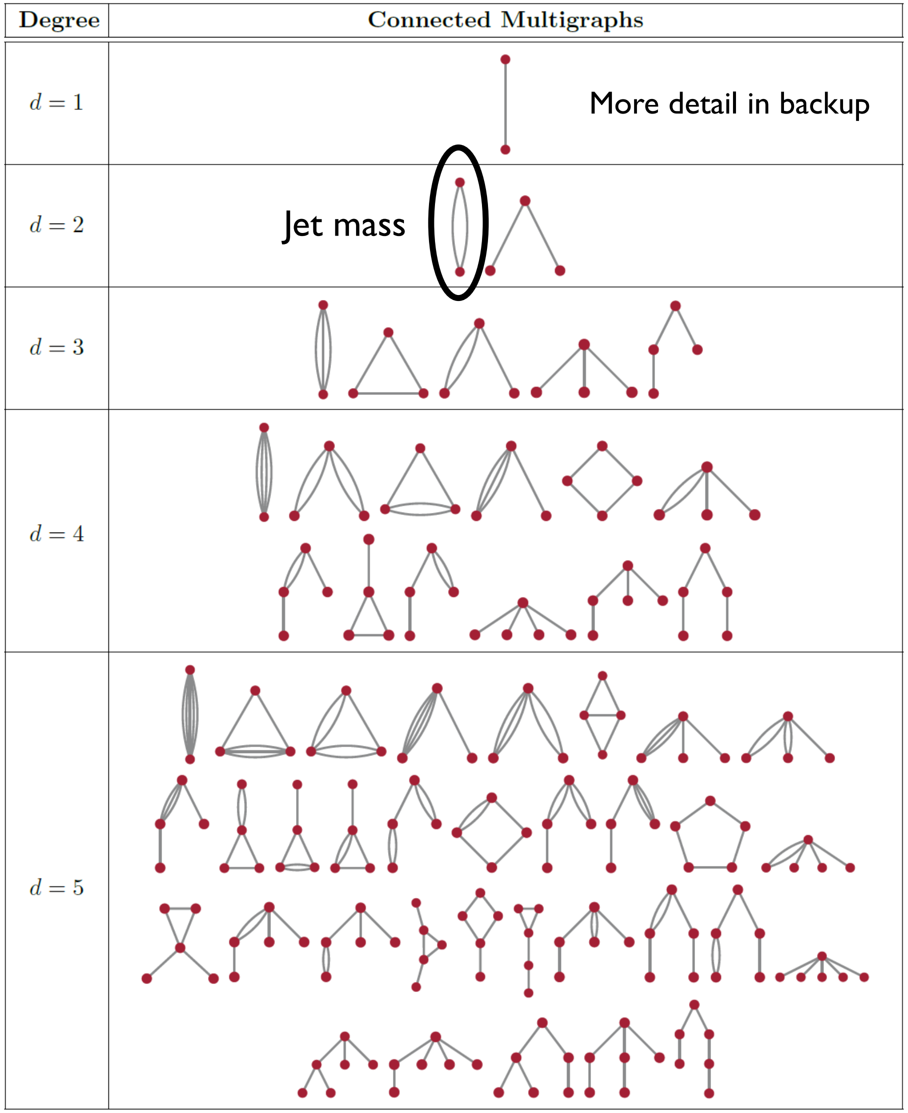

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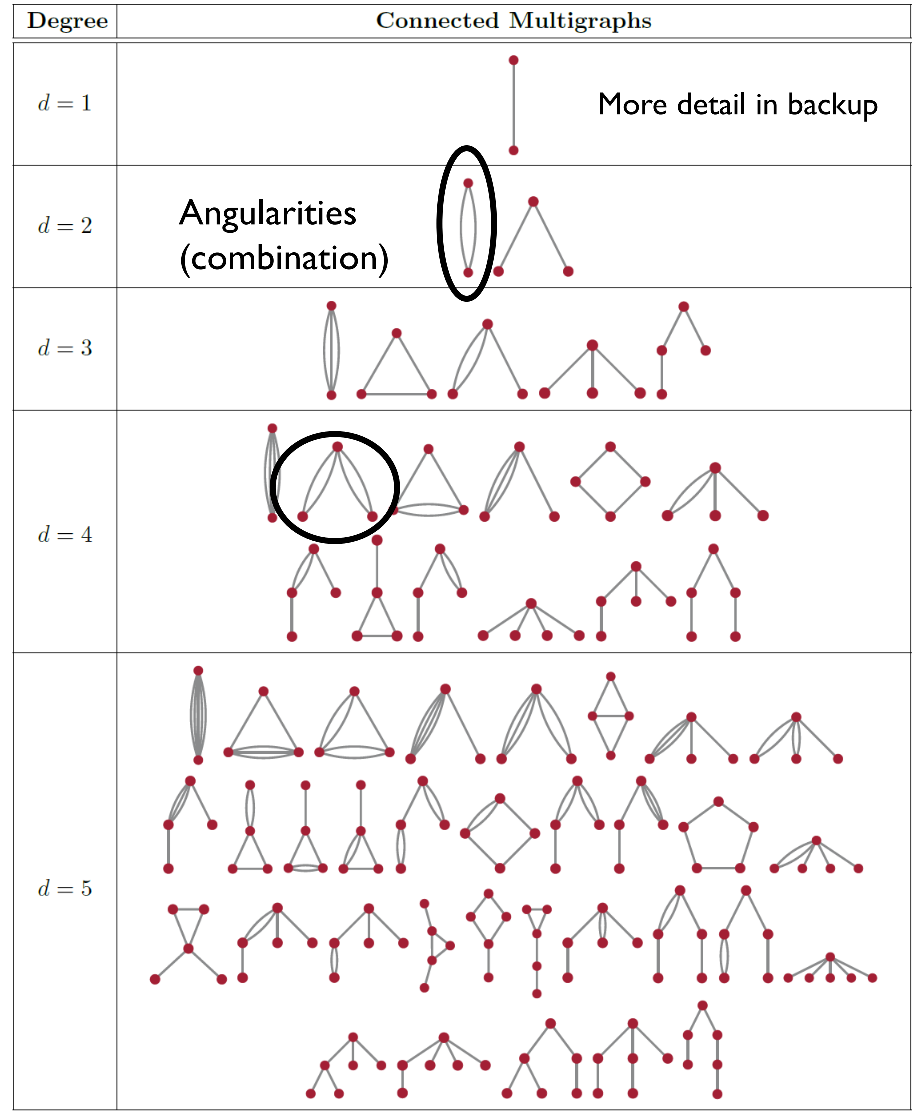

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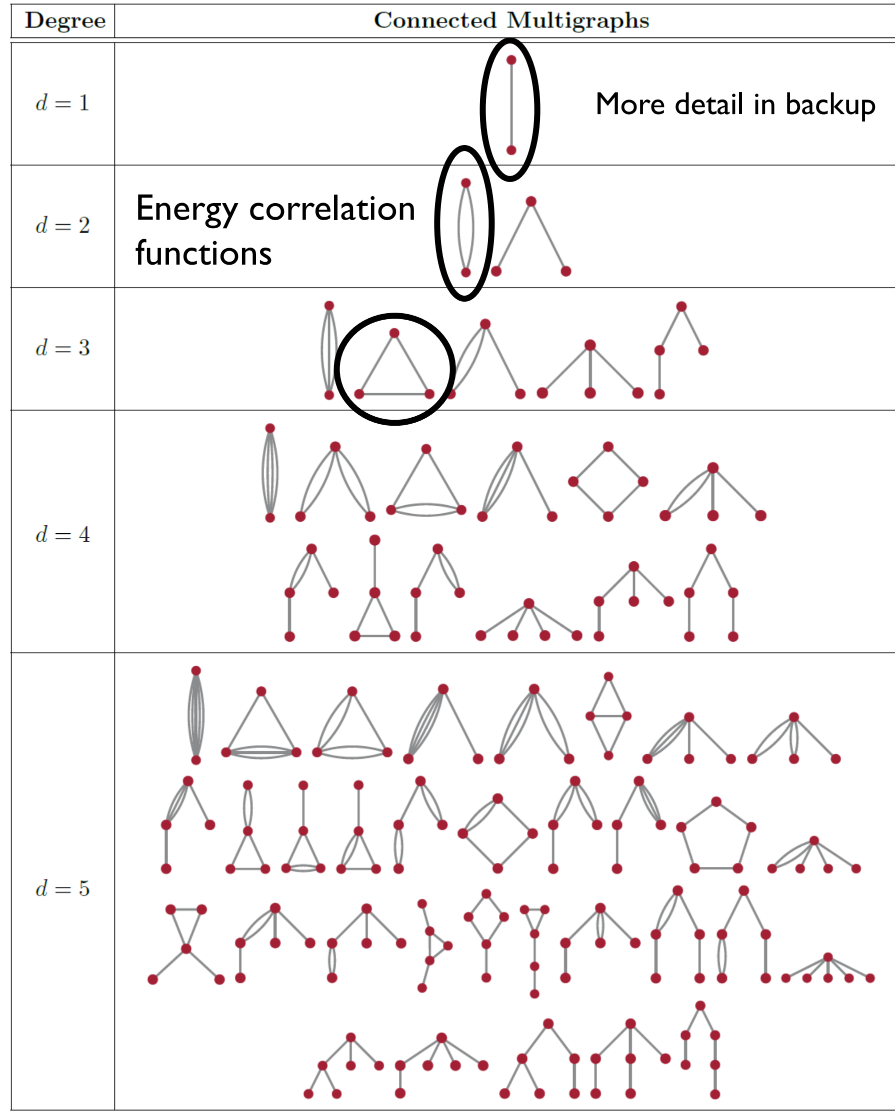

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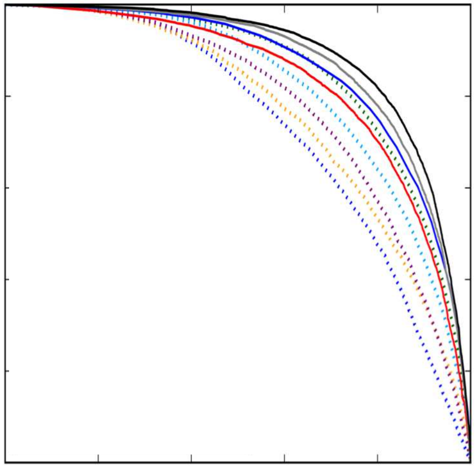

Intermission

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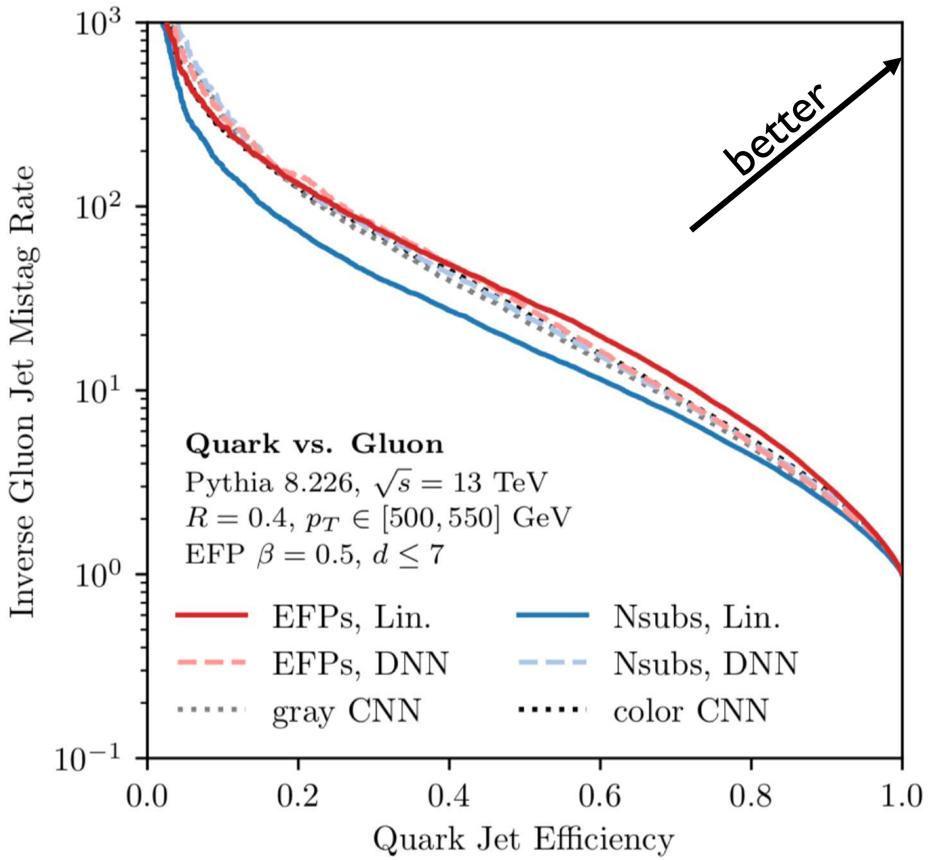
Epilogue

Jet Tagging Performance – Quark vs. Gluon Jets

ROC curves for quark vs. gluon jet tagging



W vs. QCD and top vs. QCD jet tagging in backup

N-subjettiness:
[J. Thaler, K. Van Tilburg, 1011.2268, 1108.2701]

N-subjettiness basis:
[K. Datta, A. Larkoski, 1704.08249]

QG CNNs:
[**PTK**, E. Metodiev, M. Schwartz, 1612.01551]

ML/NN review:
[A. Larkoski, I. Moult, B. Nachman, 1709.04464]

(Linear classification with EFPs) ~ (MML) for efficiency > 0.25!

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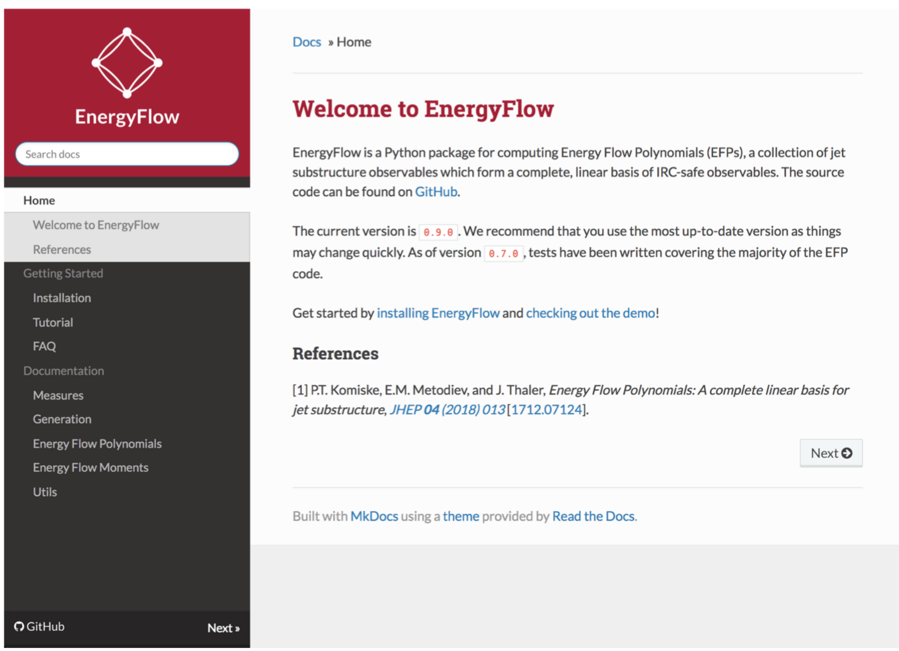
EnergyFlow Python Package

EnergyFlow package is available for python 2 and python 3

Automatically applies variable elimination algorithm to speed up computation

Simple to select combinations of EFPs to compute on various kinds of inputs (pp, e+e-, Euclidean four-momenta, detector coordinates, etc.)



Come to the software demo on Friday to hear more about EnergyFlow and try it for yourself!

https://pkomiske.github.io/EnergyFlow/

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What are Jets?

(See Eric Metodiev's talk tomorrow)

Jets are variable length, **unordered** collections of particles

$$J(\{p_1^\mu, \dots, p_M^\mu\}) = J\left(\{p_{\pi(1)}^\mu, \dots, p_{\pi(M)}^\mu\}\right), \qquad \forall\, \pi \in S_M$$

M is multiplicity of the jet

Permutation group on M elements

Particle properties:

- Four-momenta p_i^μ
- Other quantum numbers (e.g. particle id)
- Experimental information (e.g. vertex info)

Variable jet length requires at least one of:

- Preprocessing into another representation (jet images, EFPs, N-subs, etc.)
- Truncation to an (arbitrary) fixed size
- Recurrent NN structure – induces a dependence on the particle order!

Particle relabeling symmetry requires a new architecture

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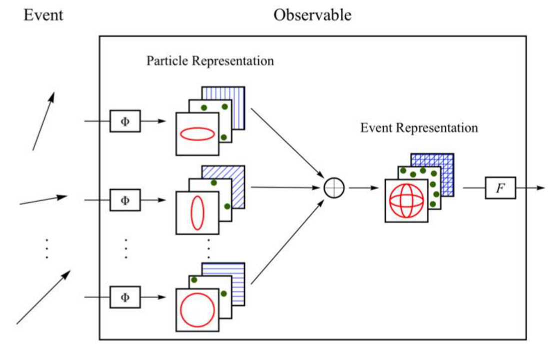


Epilogue

Energy Flow Network (EFN)

[**PTK**, E. Metodiev, J. Thaler, to appear soon]

Desire a manifest relabeling symmetry of model

Embed each particle into a learnable latent space

Combine latent observables with manifestly permutation invariant function (the sum)

Deep Sets

Manzil Zaheer[1,2], Satwik Kottur[1], Siamak Ravanbhakhsh[1], Barnabás Póczos[1], Ruslan Salakhutdinov[1], Alexander J Smola[1,2]
[1] Carnegie Mellon University [2] Amazon Web Services

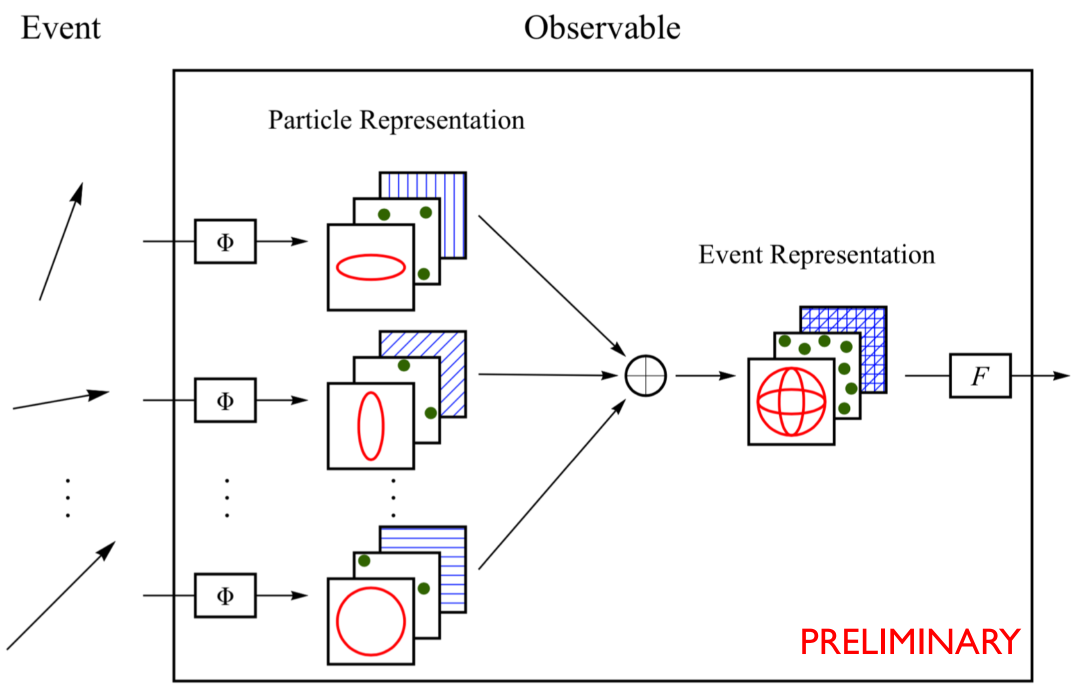
1703.06114

Theorem 7 *Let $f : [0,1]^M \to \mathbb{R}$ be a permutation invariant continuous function iff it has the representation*

$$f(x_1, ..., x_M) = \rho\left(\sum_{m=1}^{M} \phi(x_m)\right) \tag{18}$$

for some continuous outer and inner function $\rho : \mathbb{R}^{M+1} \to \mathbb{R}$ and $\phi : \mathbb{R} \to \mathbb{R}^{M+1}$ respectively.

Key ingredient: Kolmogorov-Arnold representation theorem



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

Manifestly IRC-safe latent space

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

Fully general latent space

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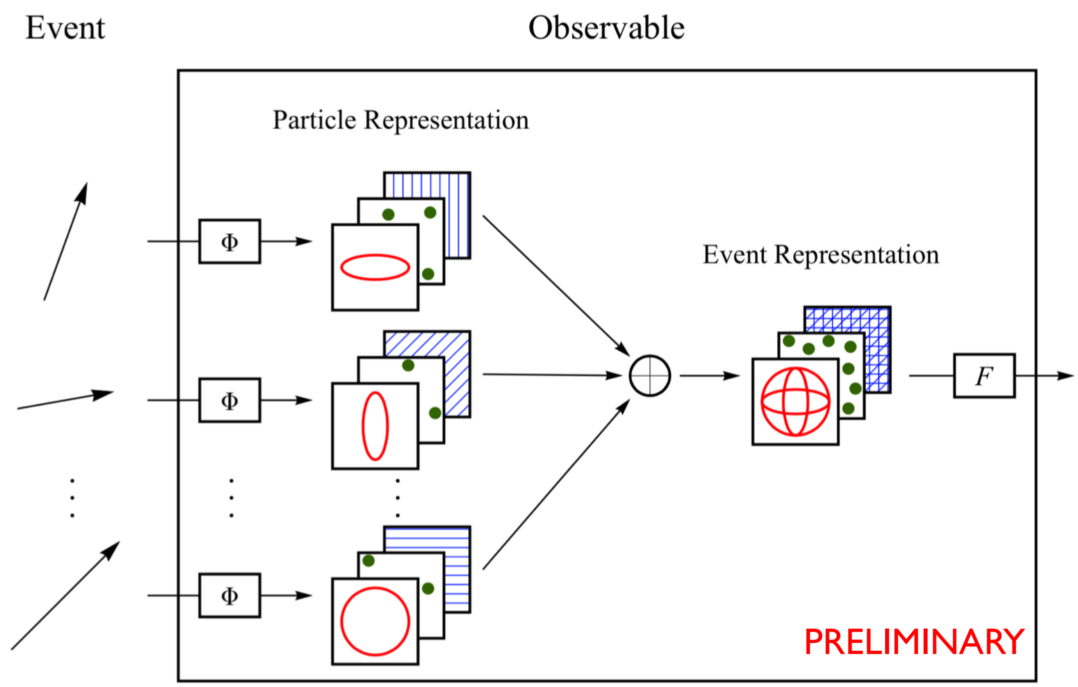

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Fully general latent space

Familiar Jet Substructure Observables as EFNs

PRELIMINARY

Observable		Map $\Phi(q)$	Function F
Mass	m	p^μ	$F(x^\mu) = \sqrt{x^\mu x_\mu}$
Multiplicity	M	1	$F(x) = x$
Track Mass	m_{track}	$p^\mu \mathbb{I}_{\text{track}}$	$F(x^\mu) = \sqrt{x^\mu x_\mu}$
Track Multiplicity	M_{track}	$\mathbb{I}_{\text{track}}$	$F(x) = x$
Momentum Dispersion	p_T^D	(p_T, p_T^2)	$F(x, y) = \sqrt{y/x^2}$
Jet Charge	$\mathcal{Q}_\kappa$	$(p_T, Q\, p_T^\kappa)$	$F(x, y) = y/x^\kappa$
Eventropy	$z \ln z$	$(p_T, p_T \ln p_T)$	$F(x, y) = y/x - \ln x$

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

Many observables are easily interpreted in EFN language

Some observables not as easily handled (e.g. *N*-subjettiness) Iterated EFN structure could address this

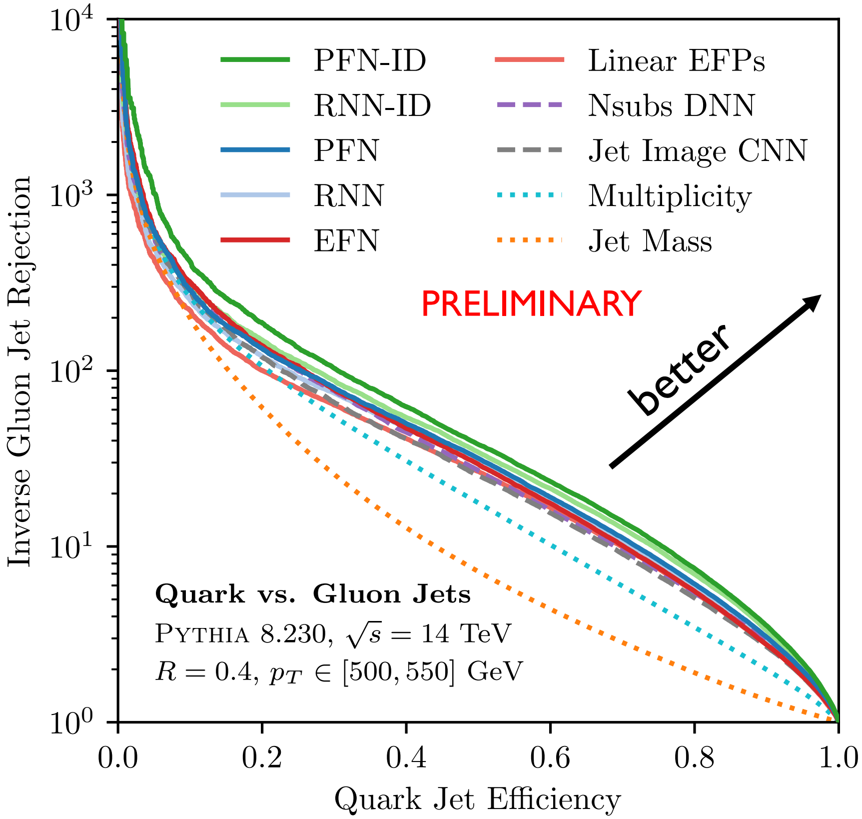
$$\mathrm{PFN}\left(\{p_1^\mu, \ldots, p_M^\mu\}\right) = F\left(\sum_{i=1}^{M} \boldsymbol{\Phi}(p_i^\mu)\right)$$

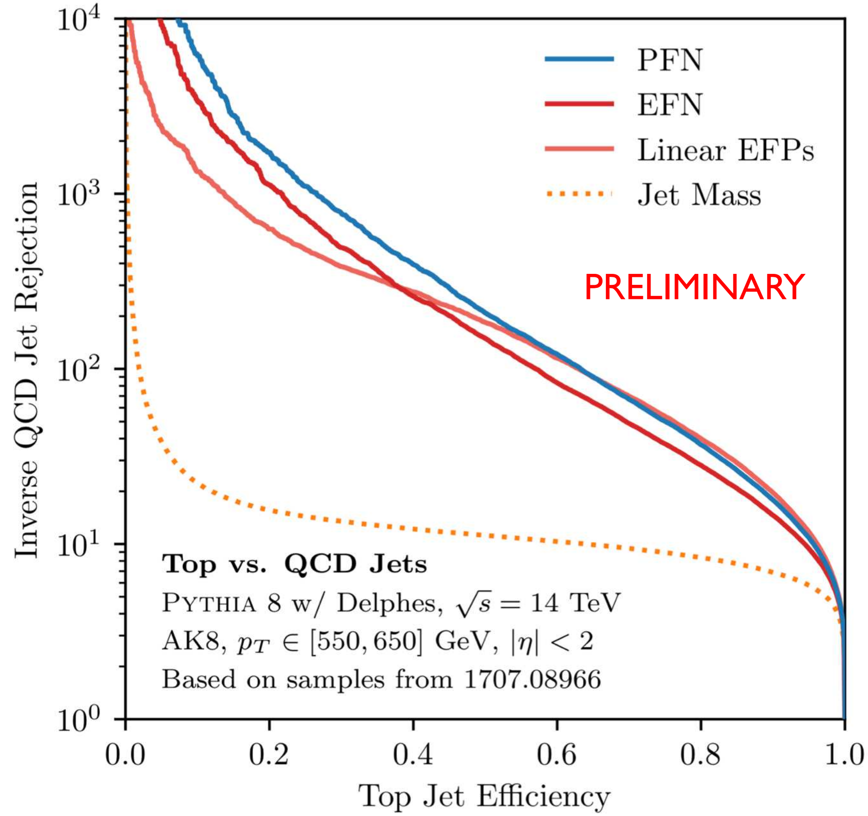
EFPs are also included, albeit opaquely via Energy Flow Moments (EFMs)

$$\mathrm{EFM}^{\mu_1 \cdots \mu_v} = \sum_{i=1}^{M} z_i\, \hat{p}_i^{\mu_1} \ldots \hat{p}_i^{\mu_v}$$

[**PTK**, E. Metodiev, J. Thaler, to appear soon]

Classification Performance



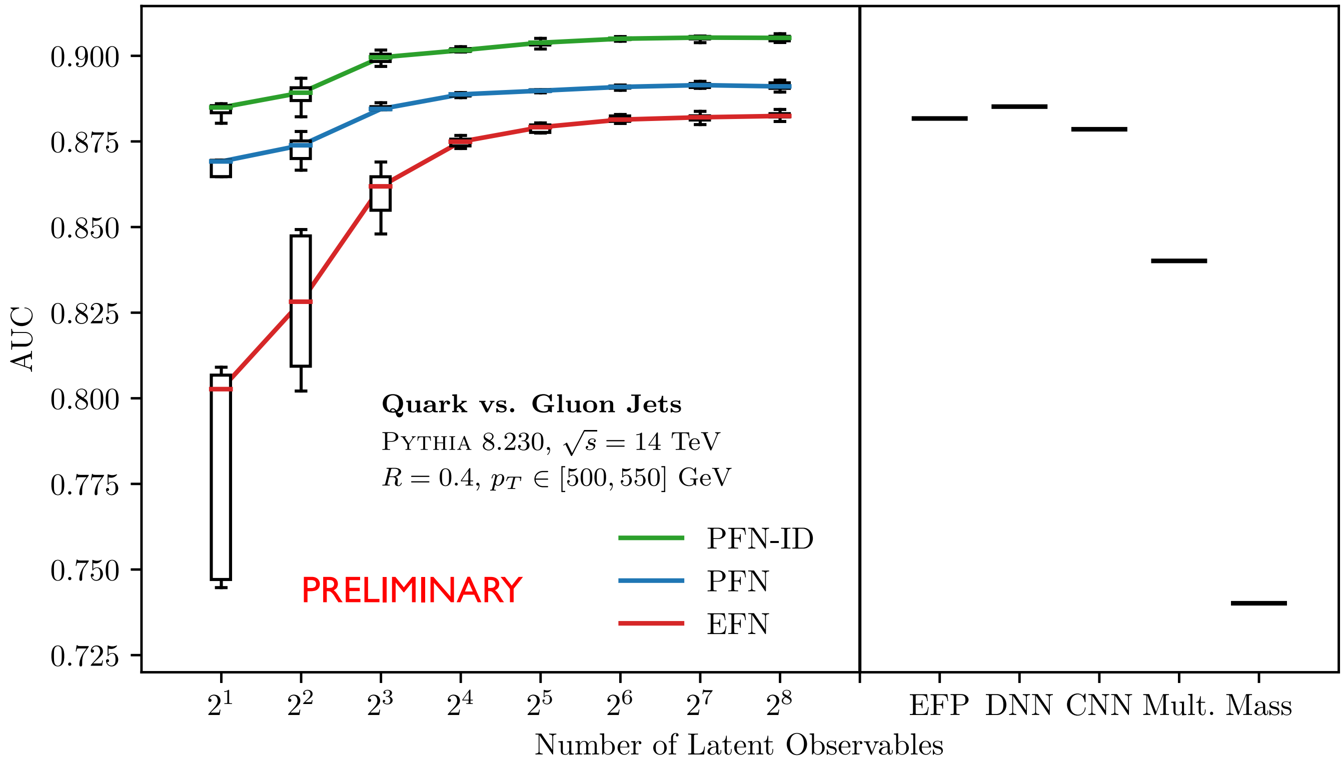


Samples based on and provided by:
[A. Butter, G. Kasieczka, T. Plehn, M. Russell, 1707.08966]

Modern ML models are similar, but PFN-ID is the best

EFPs slightly better than EFN (training neural networks can be challenging)

EFN Latent Dimension Sweep – Quark vs. Gluon Jets

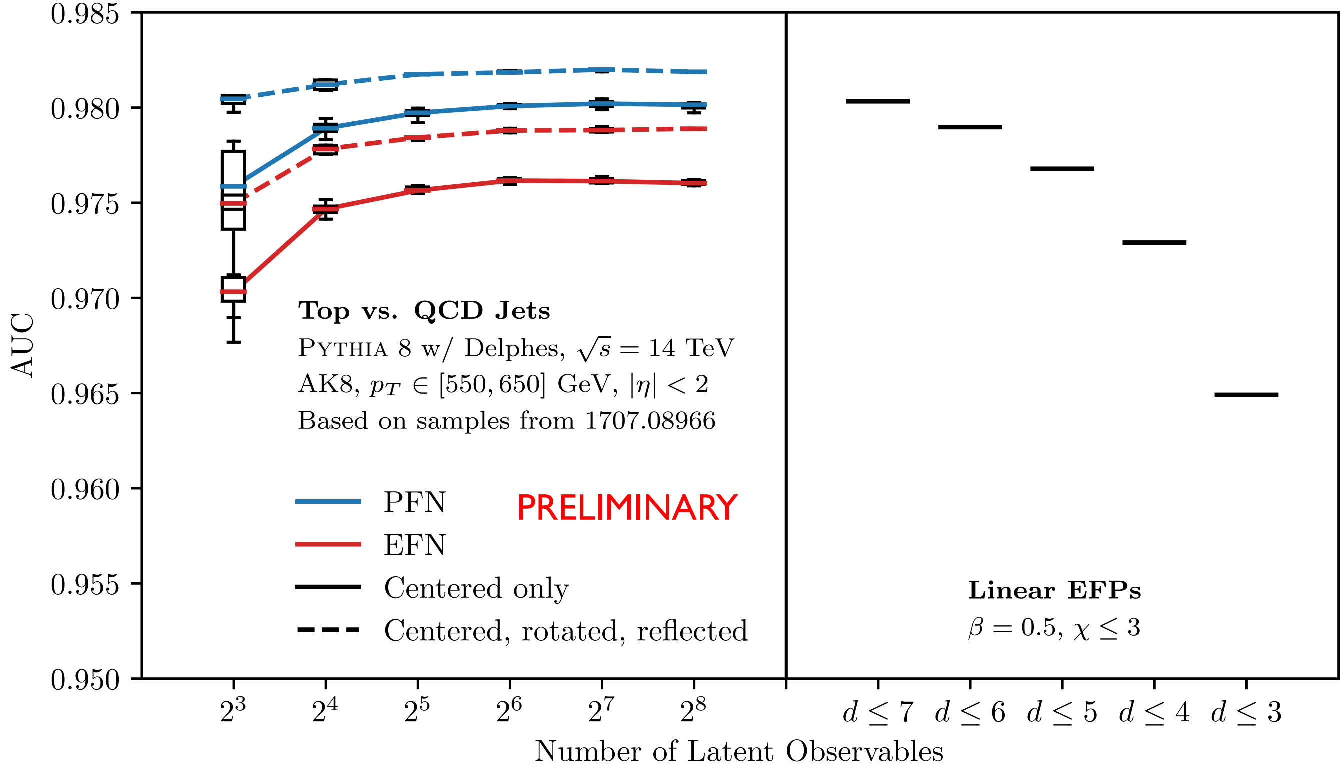


Latent dimension eventually saturates

Comparison models around EFN performance

All models substantially above single best observable (multiplicity)

EFN Latent Dimension Sweep – Top vs. QCD Jets



Latent dimension eventually saturates

EFPs slightly better than EFN (training neural networks can be challenging)

AUC Comparison on Common Top vs. QCD Samples

Approach	AUC	Contact	Comments
LoLa	0.979	GK / SImon Leiss	Preliminary number, based on LoLa
LBN	0.979	Marcel Rieger	Preliminary number
CNN	0.981	David Shih	Model from *Pulling Out All the Tops with Computer Vision and Deep Learning (1803.00107)*
P-CNN (1D CNN)	0.980	Huilin Qu, Loukas Gouskos	Preliminary, use kinematic info only (https://indico.physics.lbl.gov/indico/event/546/contributions/1270/)

Table from this Google Doc

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Table from this Google Doc

EFN	0.976
EFN-rr	0.979
PFN	0.980
EFPs	0.980
PFN-rr	0.982

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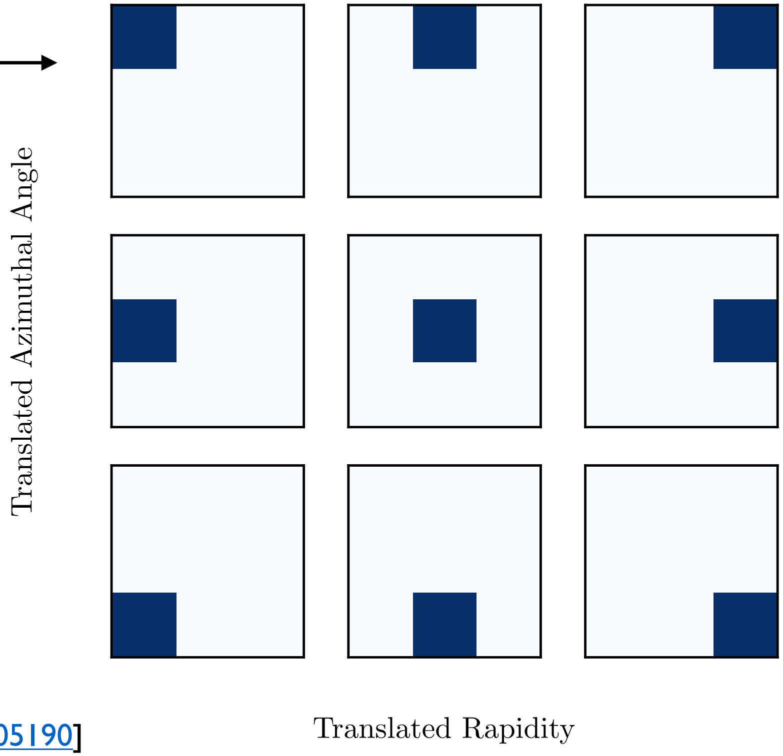
Visualizing the Filters

Given trained model, examine values of latent observables, $\mathbf{\Phi}(\hat{p}) = (\ell_1(\hat{p}), \dots \ell_n(\hat{p}))$

EFN observables are purely geometric functions of (y, ϕ) and can be shown as two-dimensional images (similar to jet images)

EFN structure encompasses many representations, e.g. jet images

Example: Jet images as EFN filters



What will the EFN learn?

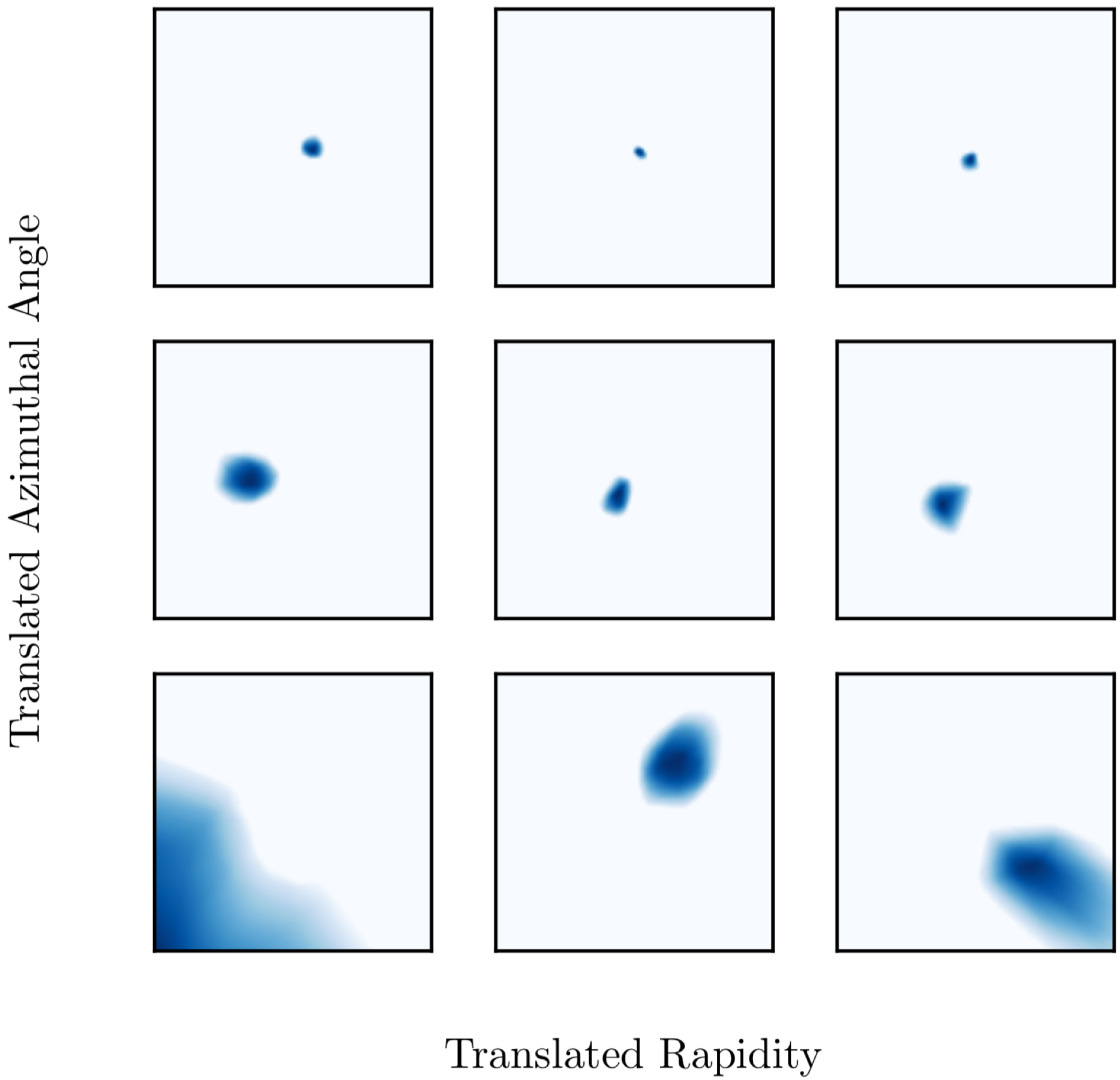
- EFPs (via EFMs)?
- Jet images?
- Something uninterpretable?
- Something interpretable but completely new?

Jet images:

[J. Cogan, M. Kagan, E. Strauss, A. Schwartzman, 1407.5675]

[L. de Oliviera, M. Kagan, L. Mackey, B. Nachman, A. Schwartzman, 1511.05190]

Visualizing the Filters – Quark vs. Gluon Jets



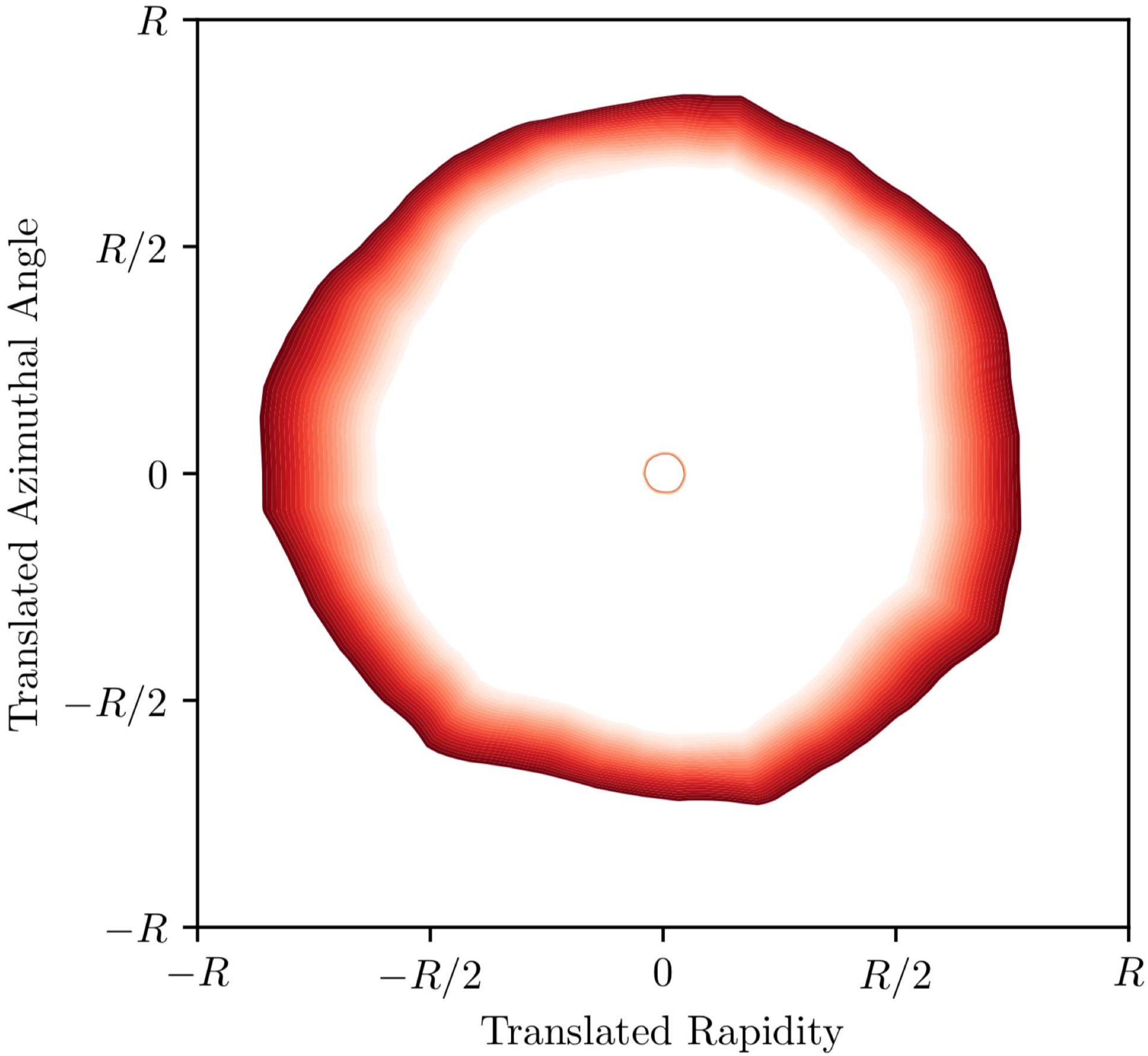
PRELIMINARY

Generally see "peanuts" and "lobes"

EFN_{256} randomly selected filters, sorted by active filter size

Local nature of activated pixel regions is fascinating!

Visualizing the Filters – Quark vs. Gluon Jets

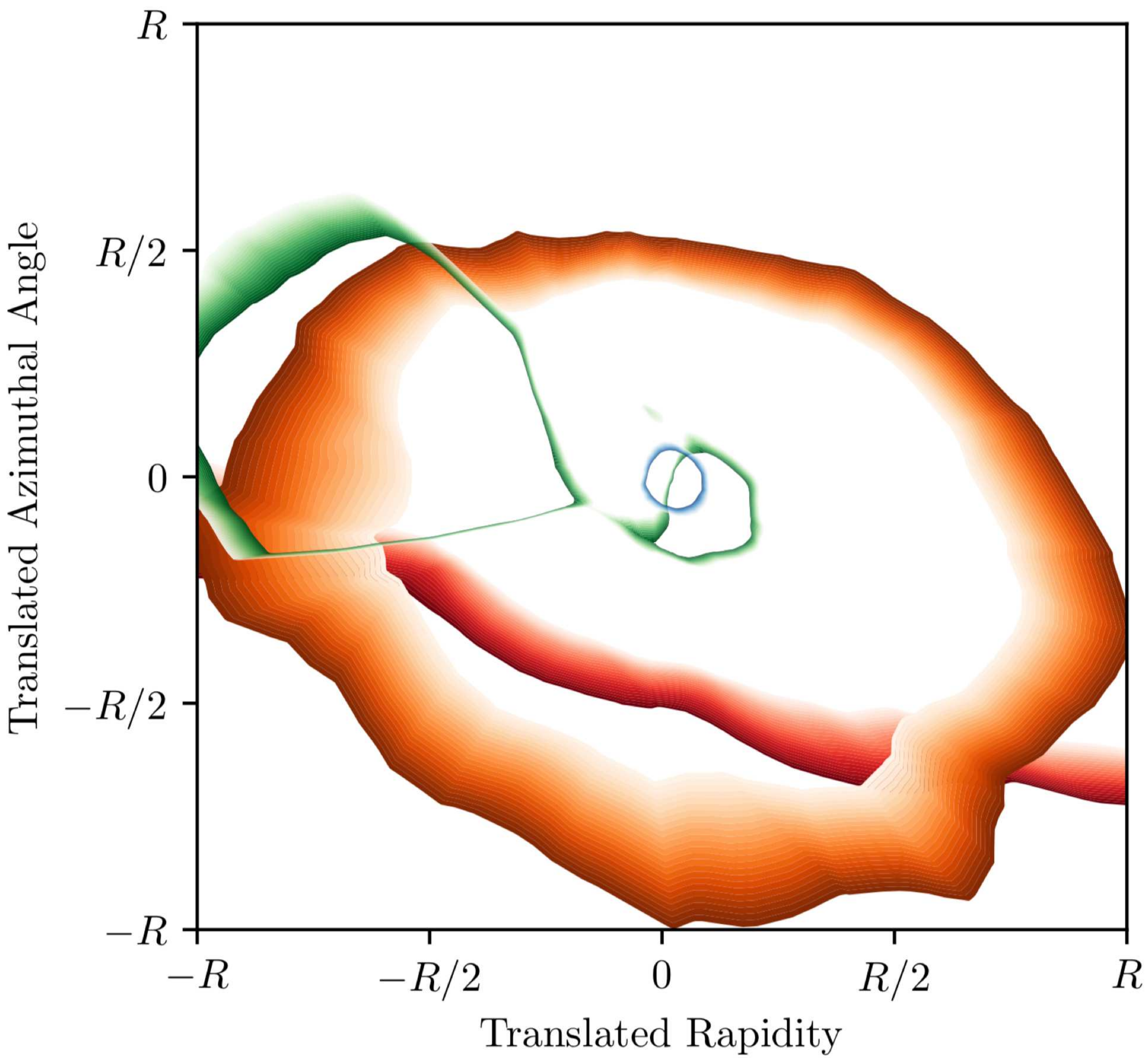


PRELIMINARY

Quark vs. Gluon
2 filters

Colored region is 10% around median

Visualizing the Filters – Quark vs. Gluon Jets

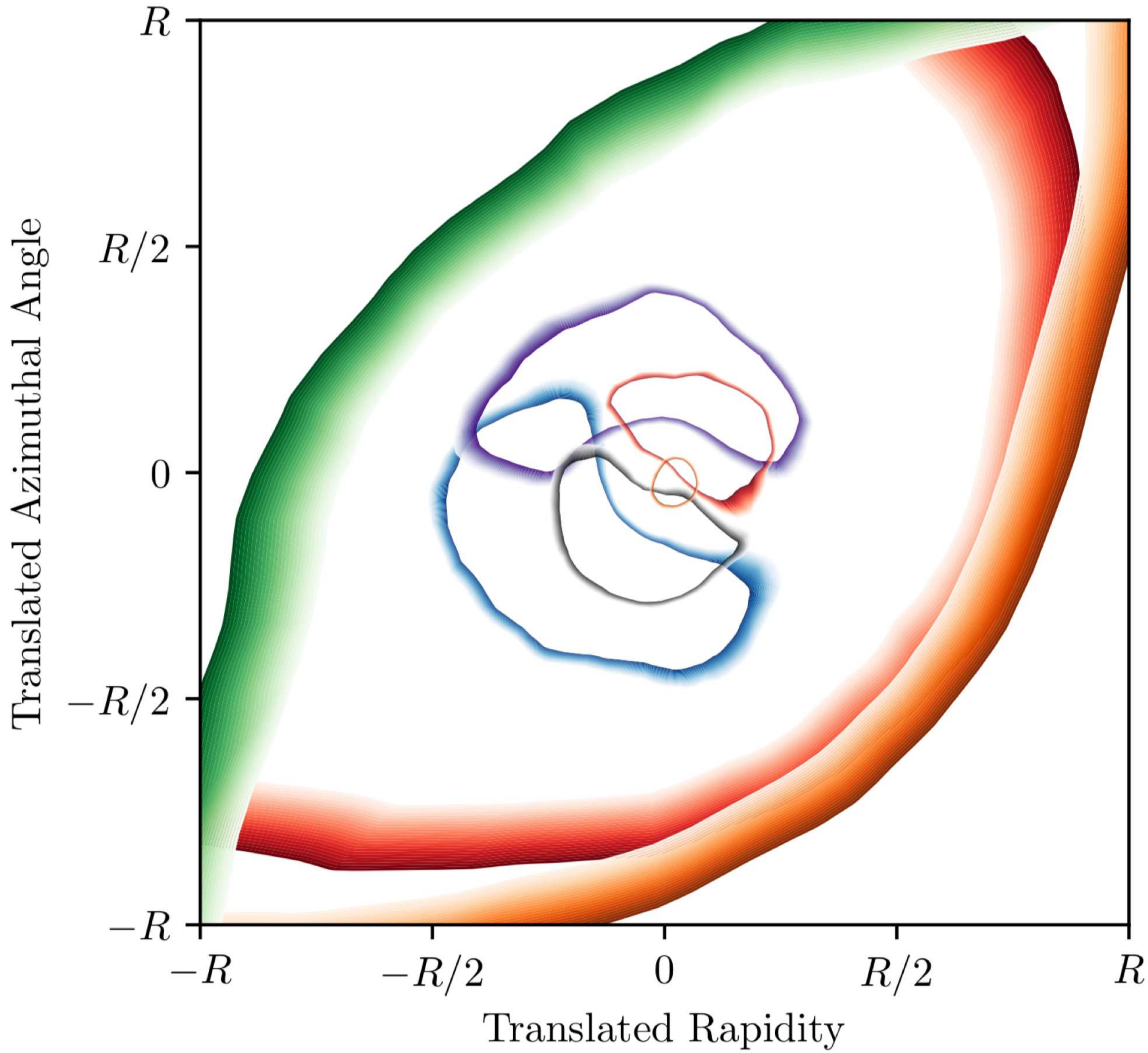


PRELIMINARY

Quark vs. Gluon
4 filters

Colored region is 10% around median

Visualizing the Filters – Quark vs. Gluon Jets

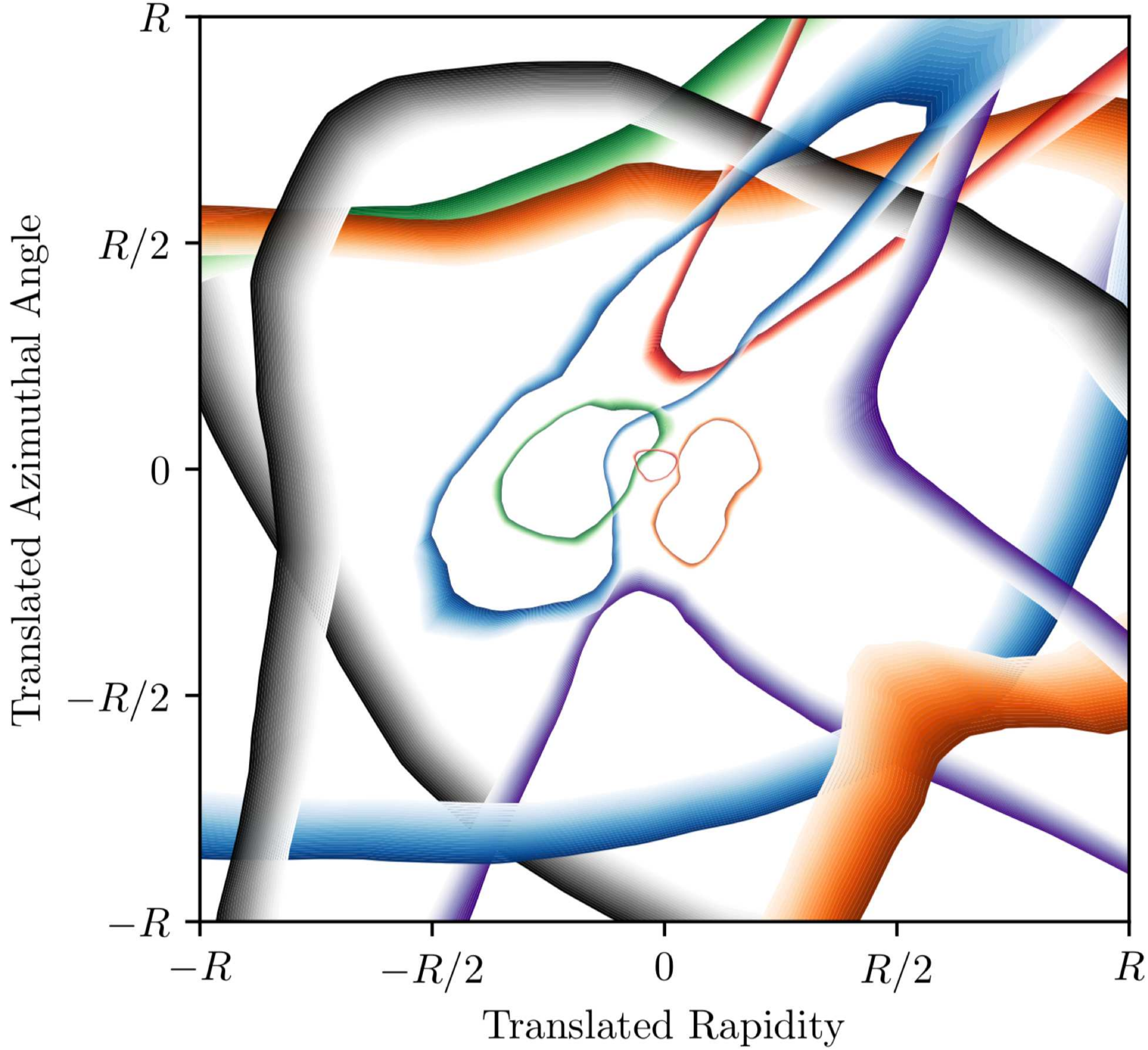


PRELIMINARY

Quark vs. Gluon
8 filters

Colored region is 10% around median

Visualizing the Filters – Quark vs. Gluon Jets

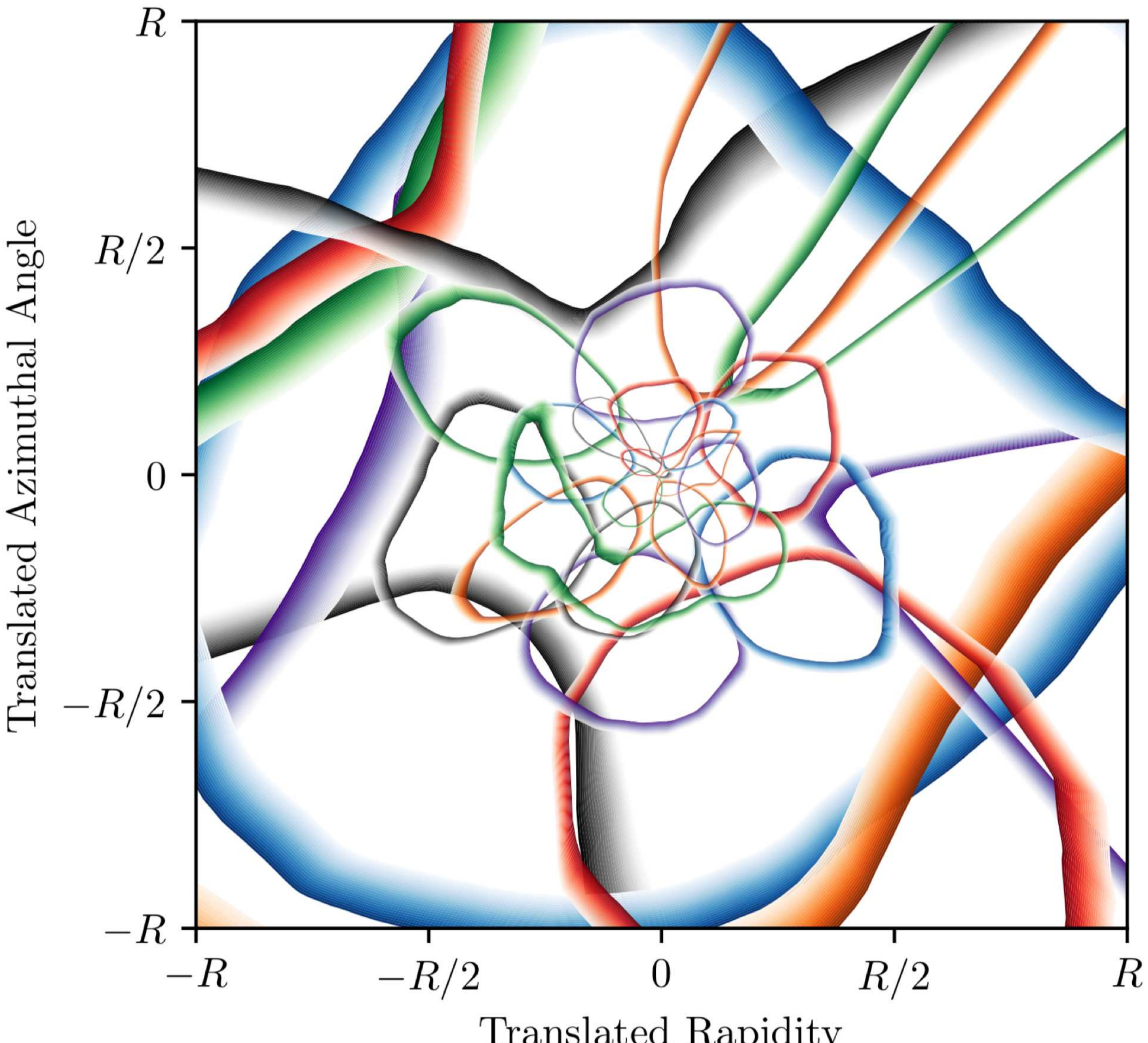


PRELIMINARY

Quark vs. Gluon
16 filters

Colored region is 10% around median

Visualizing the Filters – Quark vs. Gluon Jets

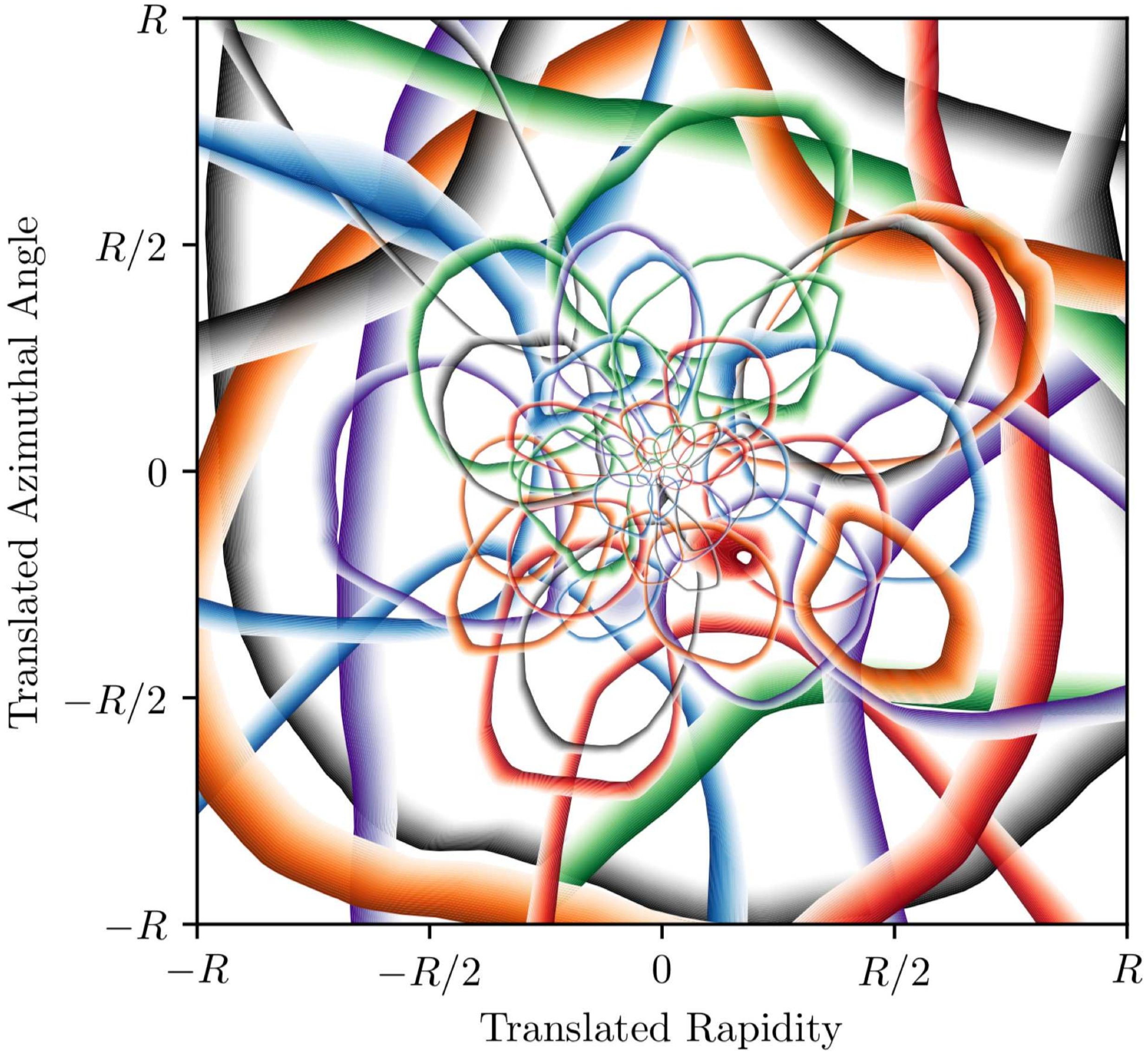


PRELIMINARY

Quark vs. Gluon
32 filters

Colored region is 10% around median

Visualizing the Filters – Quark vs. Gluon Jets

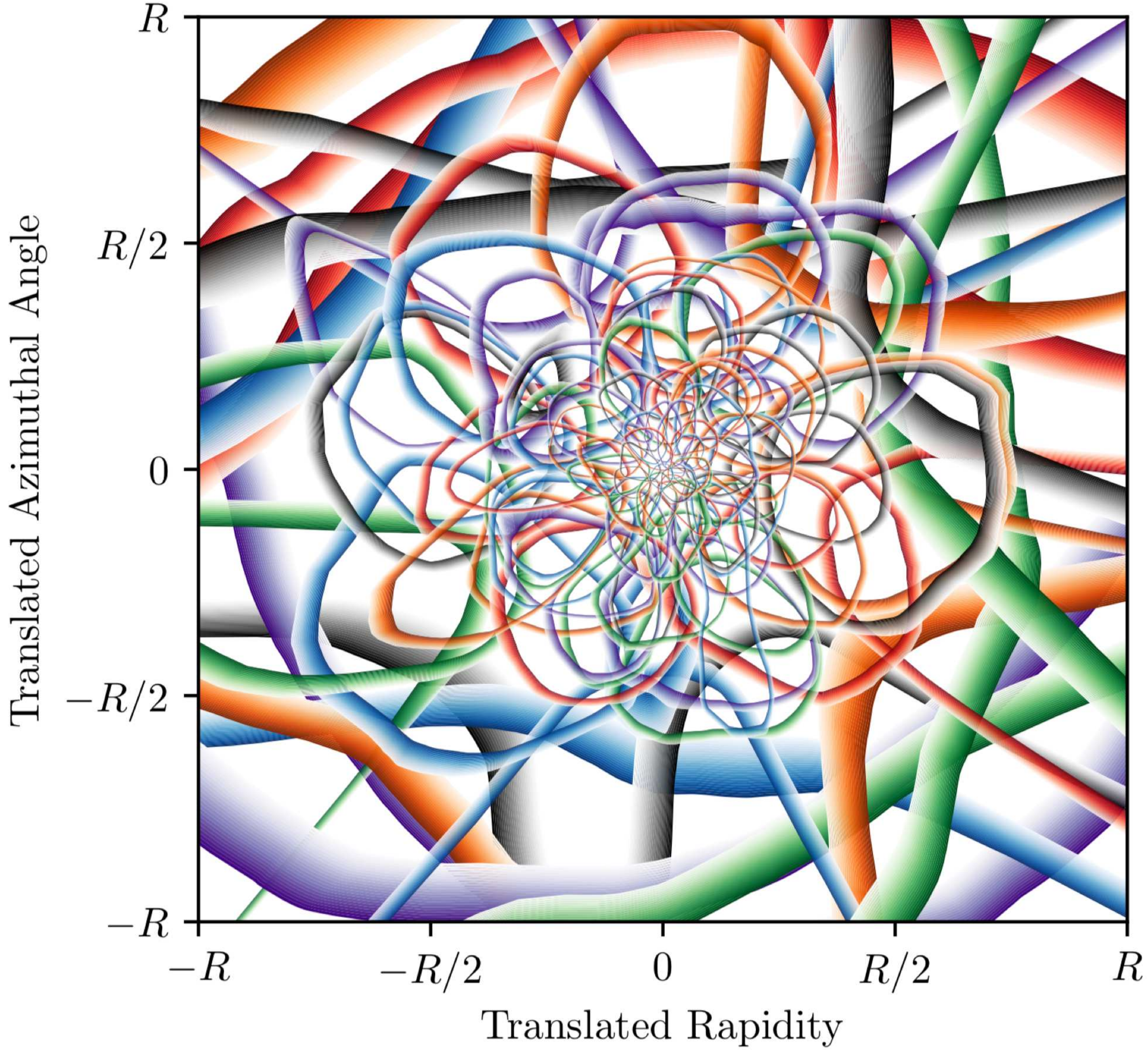


PRELIMINARY

Quark vs. Gluon
64 filters

Colored region is 10% around median

Visualizing the Filters – Quark vs. Gluon Jets

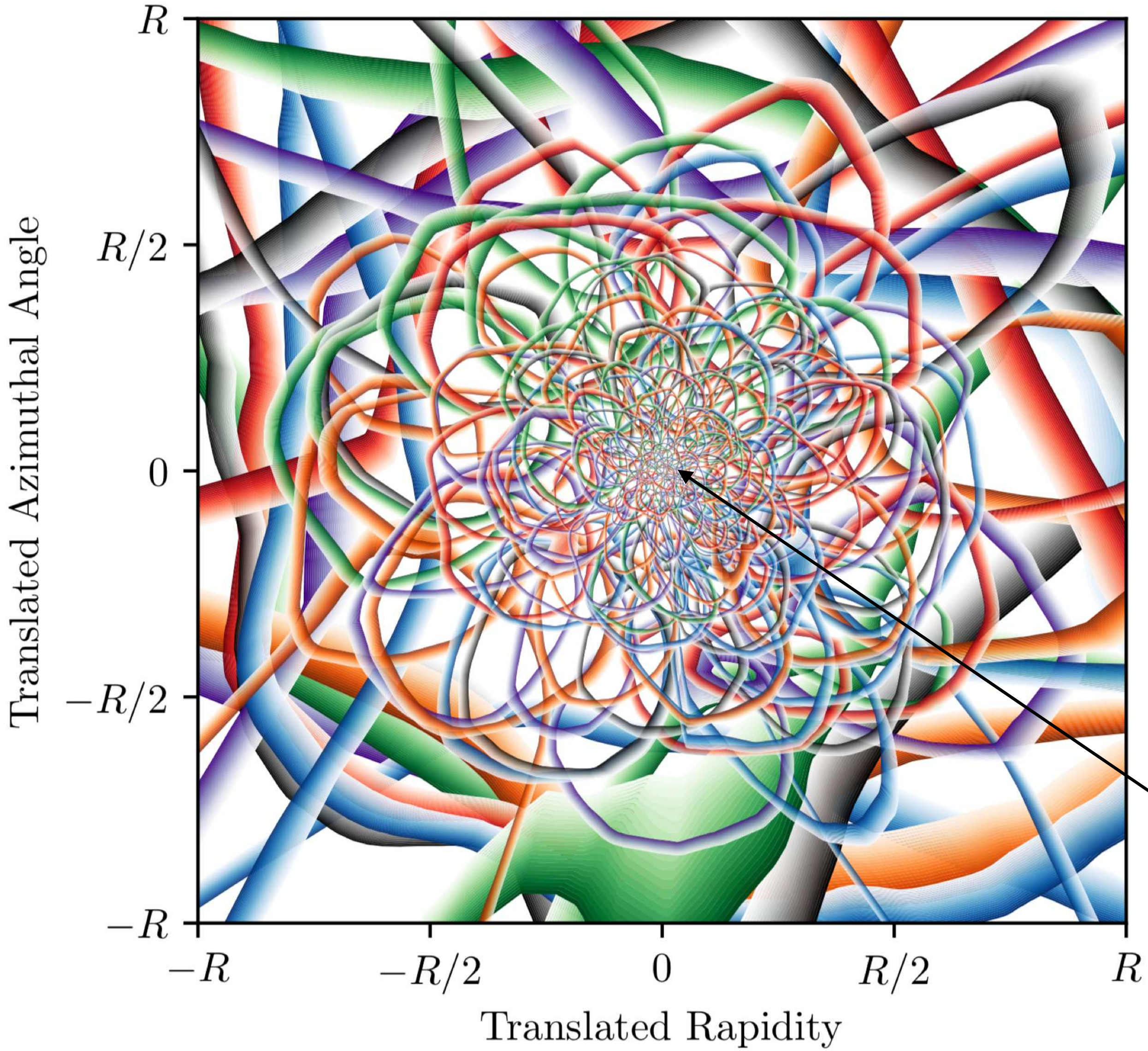


PRELIMINARY

Quark vs. Gluon
128 filters

Colored region is 10% around median

Visualizing the Filters – Quark vs. Gluon Jets



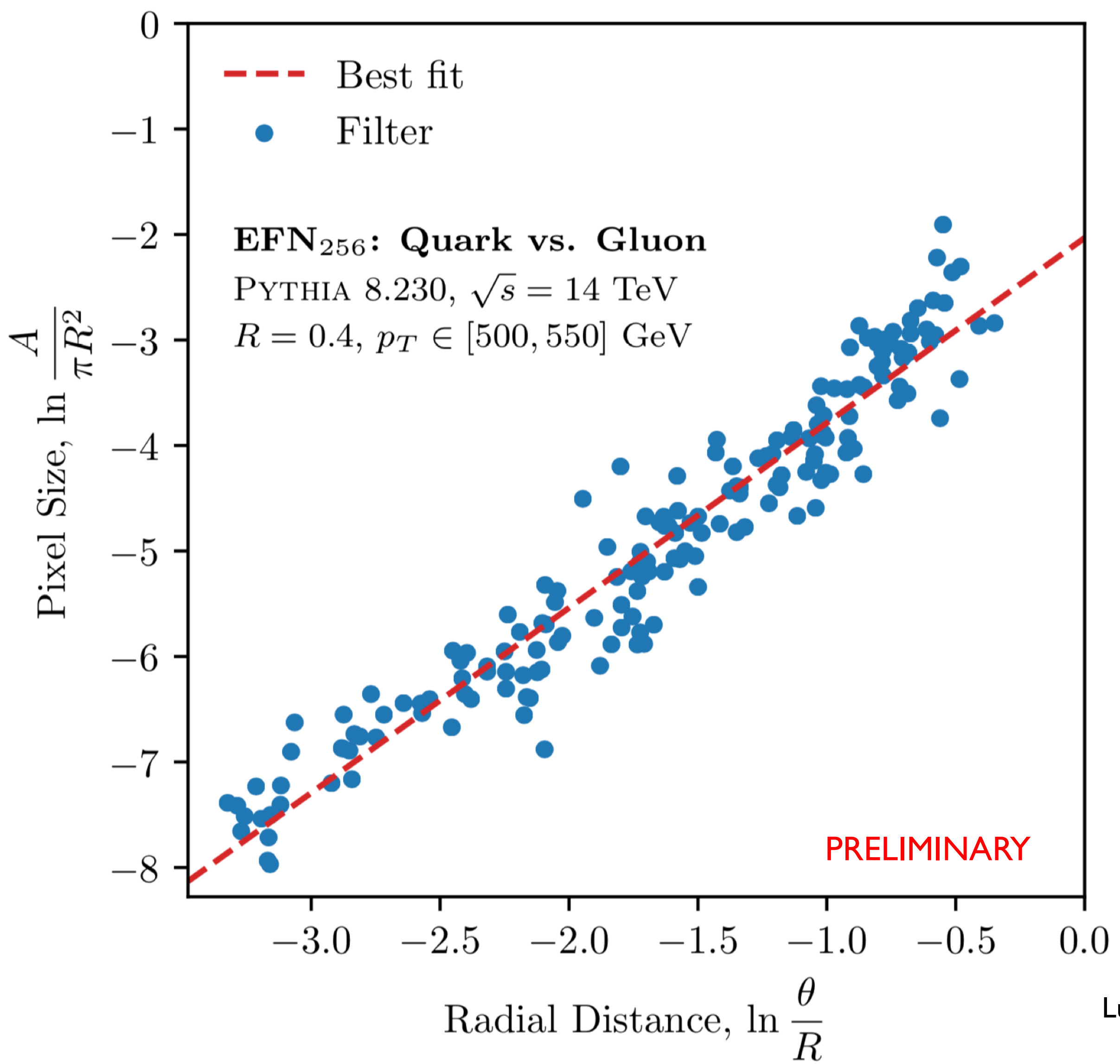
PRELIMINARY

Quark vs. Gluon
256 filters

Colored region is 10% around median

Singularity structure of QCD!

Measuring the Filters – Quark vs. Gluon Jets

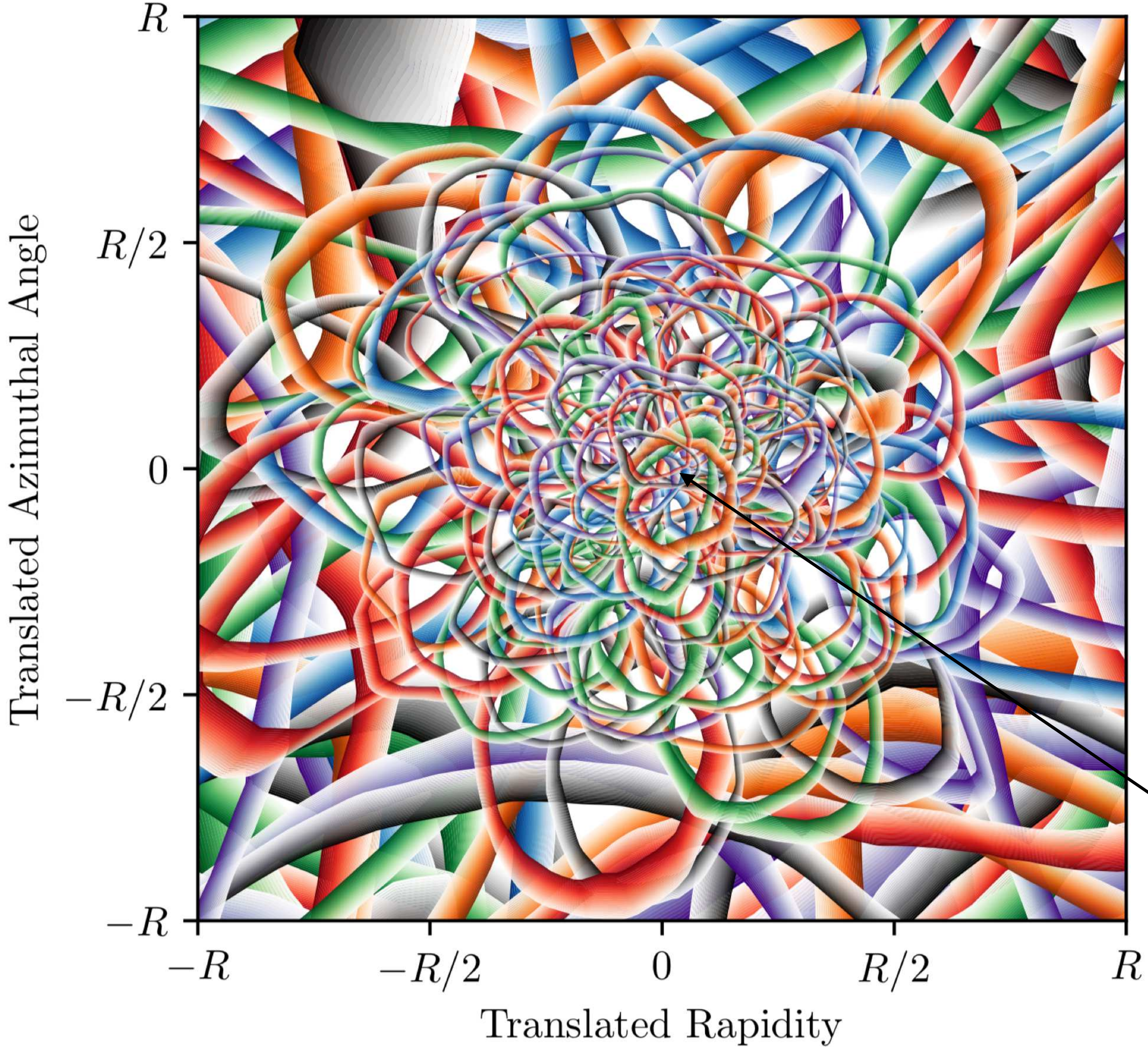


Power-law dependence between filter size and distance from center

Indicative that the model has learned a radial, logarithmic transform of a jet image (suggestive of Lund-plane jet images) (Stay tuned for F. Dreyer's talk!)

Lund jet images:
[F. Dreyer, G. Salam, G. Soyez, 1807.04758]

Visualizing the Filters – Top vs. QCD Jets

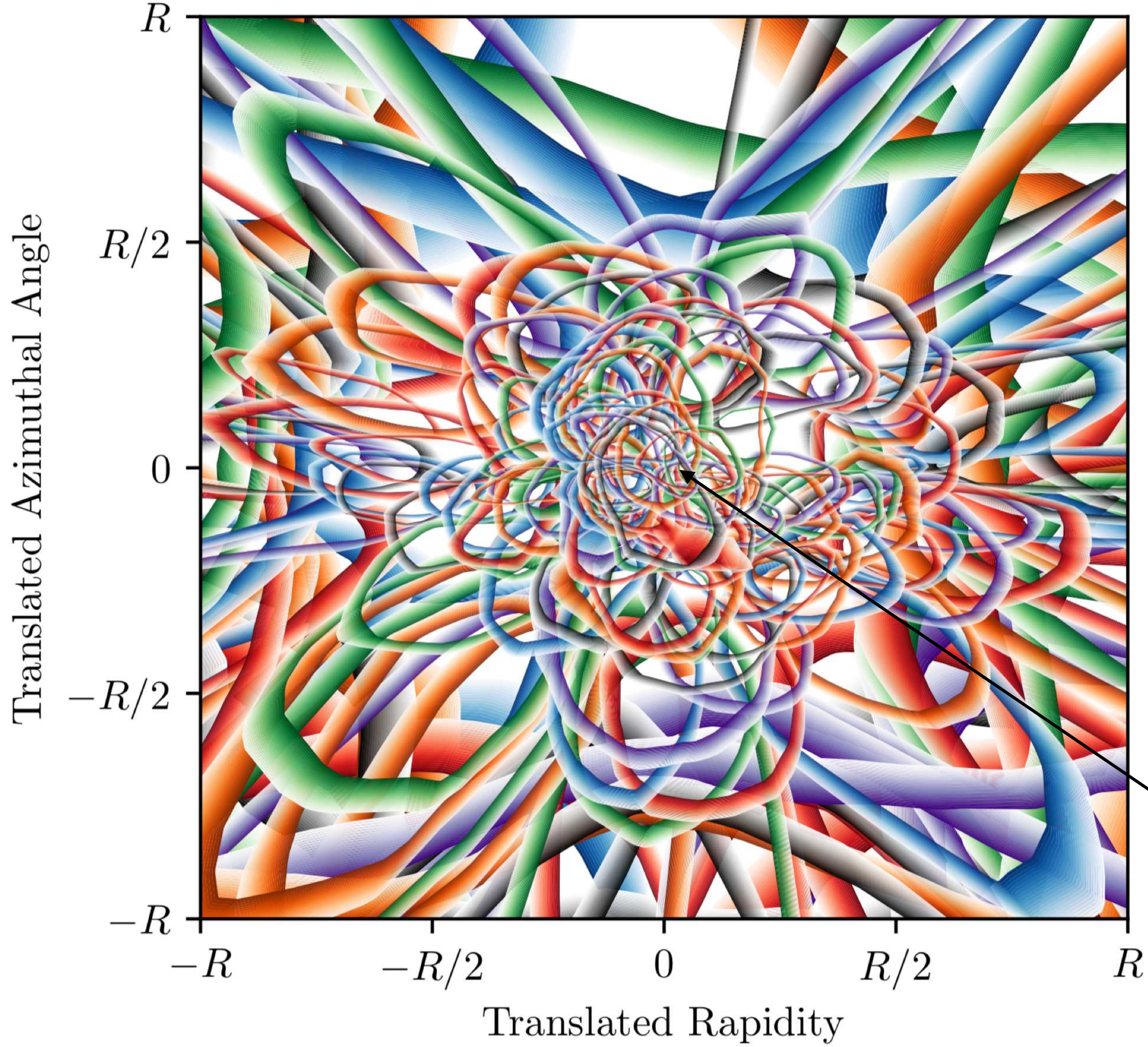


PRELIMINARY

Top vs. QCD
256 filters

No more central singularity structure!

Visualizing the Filters – Top vs. QCD Jets



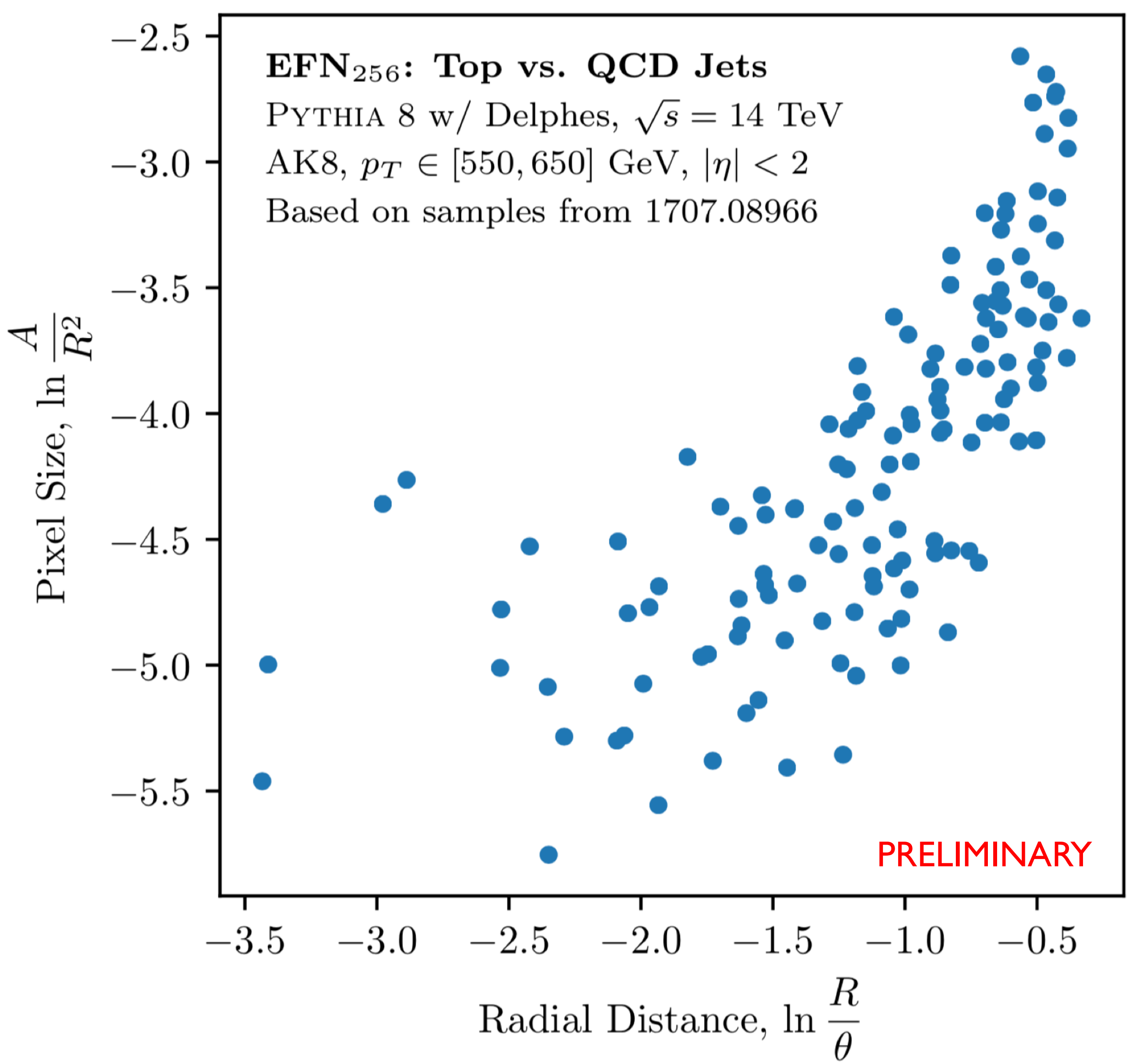
PRELIMINARY

Top vs. QCD
256 filters

Rotated and reflected - approximate rotational symmetry broken

No more central singularity structure!

Measuring the Filters – Top vs. QCD Jets



Not as much a power-law dependence

General trend that more central filters are smaller

Don't expect or see any central singularity structure

Program

Overture

Act I

- IRC Safe Jet Observables
- Energy Flow Polynomials
- Linear Classification Performance

Intermission

Act II

- Intrinsic Jet Symmetries
- Energy Flow Networks
- Opening the Box

Epilogue

Conclusions

Linear tagging with EFPs performs comparably to modern approaches

- Training is vastly simplified, convex global minimum, no hyperparameters, fully IRC safe
- EnergyFlow package allows for simple and fast evaluation

EFNs have the appropriate symmetries for variable length sets of particles

- Quark vs. gluon and top vs. QCD tagging performance is great
- Architecture just works out of the box

EFNs admit fascinating, interpretable visuals of what the model is doing

- Model has learned a Lund-plane-like particle embedding
- Singularity structure of QCD is organically discovered
- Effect of preprocessing is clearly seen in the top case

Everything has the same* performance

Recent work along these lines
[Moore, Nordstrom, Varma, Fairbairn, 1807.04769]

Models should be evaluated on more than just performance

- Connection to underlying physics, and eventually data, is most important
- EFPs and EFNs each have unique properties that make them attractive

See Eric Metodiev's talk for a use of both models with weak supervision

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See Eric Metodiev's talk for a use of both models with weak supervision

Ultimately, ML efficiently implements mathematical/statistical ideas that are grounded in physics

Azure

Backup Slides

What is IRC Safety?

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

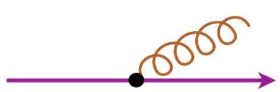
$$S(\{p_1^\mu, \dots, p_M^\mu\}) = \lim_{\epsilon \to 0} S(\{p_1^\mu, \dots, p_M^\mu, \epsilon p_{M+1}^\mu\}), \qquad \forall p_{M+1}^\mu$$

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 in QCD splitting function:



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

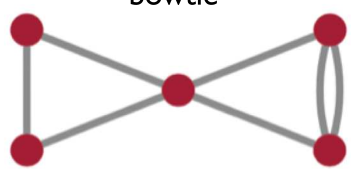
$$C_q = C_F = 4/3$$
$$C_g = C_A = 3$$

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

Multigraph/EFP Correspondence

Multigraph $\longleftrightarrow$ EFP

"bowtie"



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

j $\longleftrightarrow$ z_{i_j}

k l $\longleftrightarrow$ $\theta_{i_k i_l}$

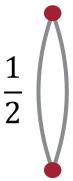
N	Number of vertices	$\longleftrightarrow$	N-particle correlator
d	Number of edges	$\longleftrightarrow$	Degree of angular monomial
χ	Treewidth + 1	$\longleftrightarrow$	Optimal VE Complexity

Connected $\longleftrightarrow$ Prime

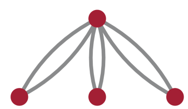
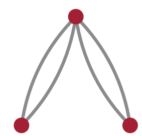
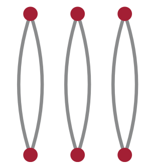
Disconnected $\longleftrightarrow$ Composite

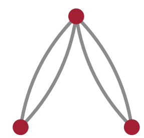
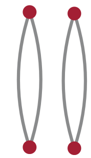
⋮

Familiar Jet Substructure Observables as EFPs

Scaled Jet Mass: $\frac{m_J^2}{p_{TJ}^2} = \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} z_{i_1} z_{i_2} (\cosh \Delta y_{i_1 i_2} - \cos \Delta\phi_{i_1 i_2}) = \frac{1}{2}$  $+ \cdots$

Jet Angularities: $\lambda^{(\alpha)} = \sum_{i}^{M} z_i \theta_i^{\alpha}$

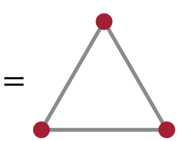
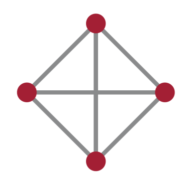
$\lambda^{(6)} =$  $- \frac{3}{2}$   $+ \frac{5}{8}$ 

$\lambda^{(4)} =$  $- \frac{3}{4}$ 

[C. Berger, T. Kucs, and G. Sterman, hep-ph/0303051]
[S. Ellis, *et al.*, 10010014]
[A. Larkoski, J. Thaler, and W. Waalewijn, 1408.3122]

Energy Correlation Functions(ECFs): $e_N^{(\beta)} = \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} \cdots \sum_{i_N=1}^{M} z_{i_1} z_{i_2} \cdots z_{i_N} \prod_{k<l \in \{1,\cdots,N\}} \theta_{i_k i_l}^{\beta}$

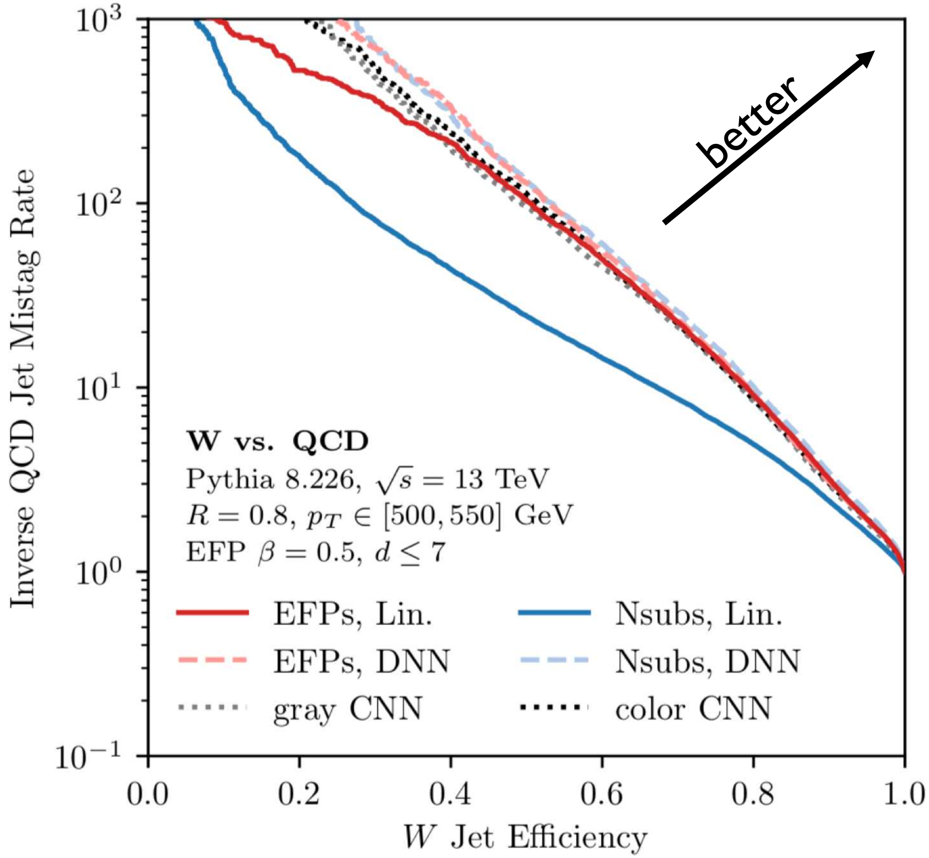
[A. Larkoski, G. Salam, and J. Thaler, 1305.0007]

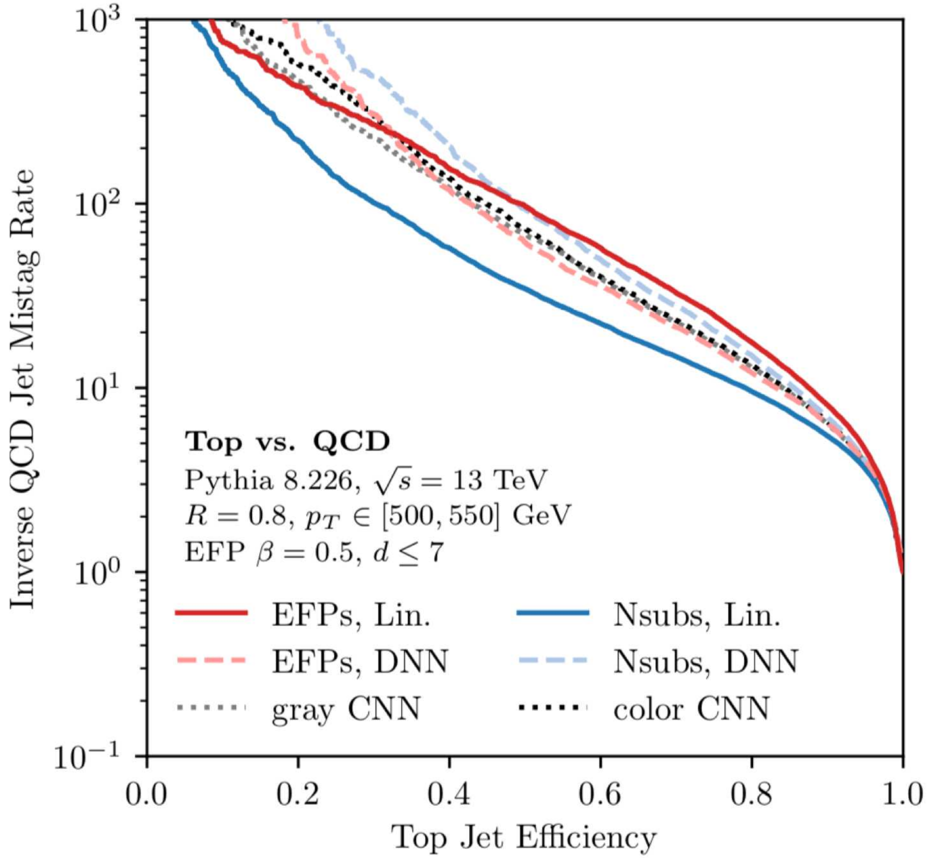
$e_2^{(\beta)} =$  $e_3^{(\beta)} =$  $e_4^{(\beta)} =$ 

and many more…

Jet Tagging Performance – 2-prong and 3-prong tagging

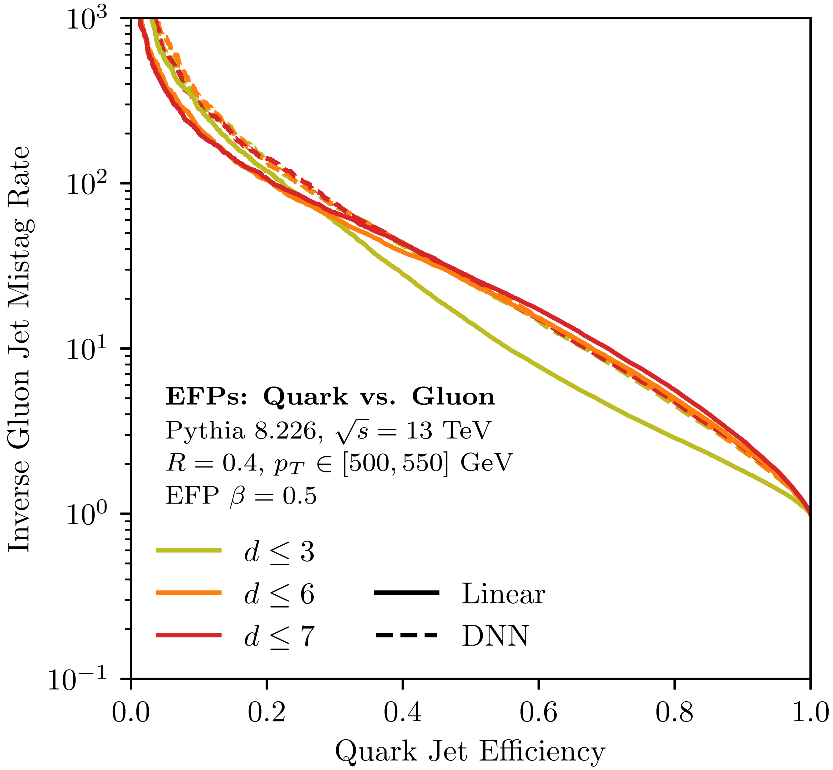
ROC curves for W vs. QCD and top vs. QCD jet tagging

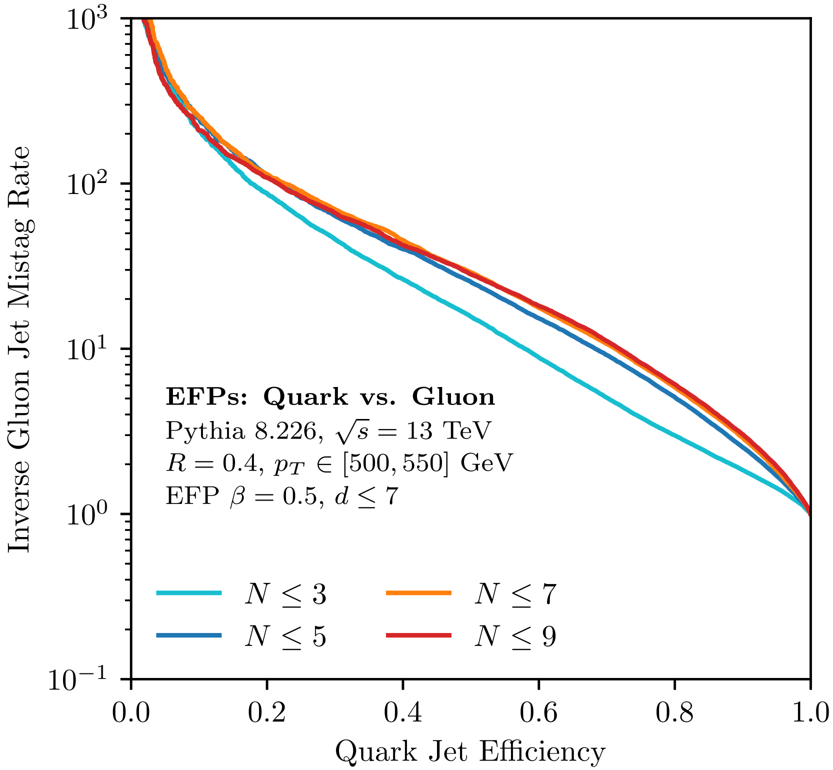




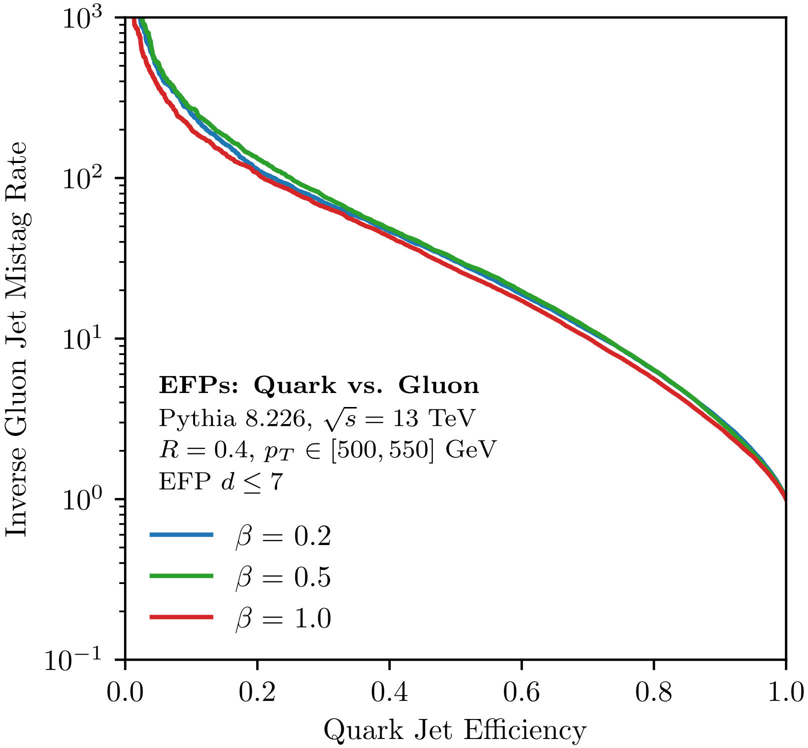
(Linear classification with EFPs) ~ (MML) for efficiency > 0.5!

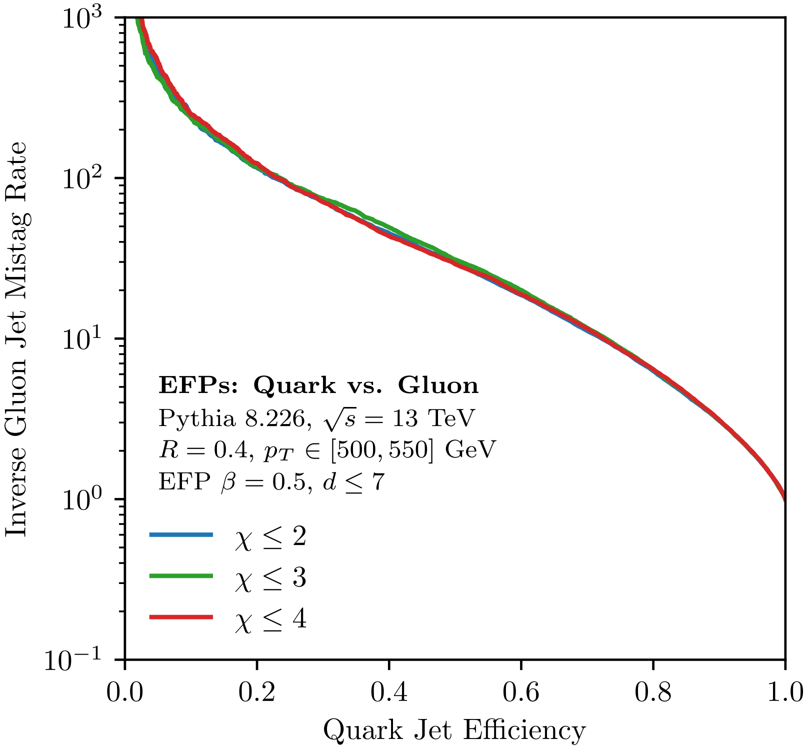
Additional EFP Tagging Plots – Quark vs. Gluon Jets



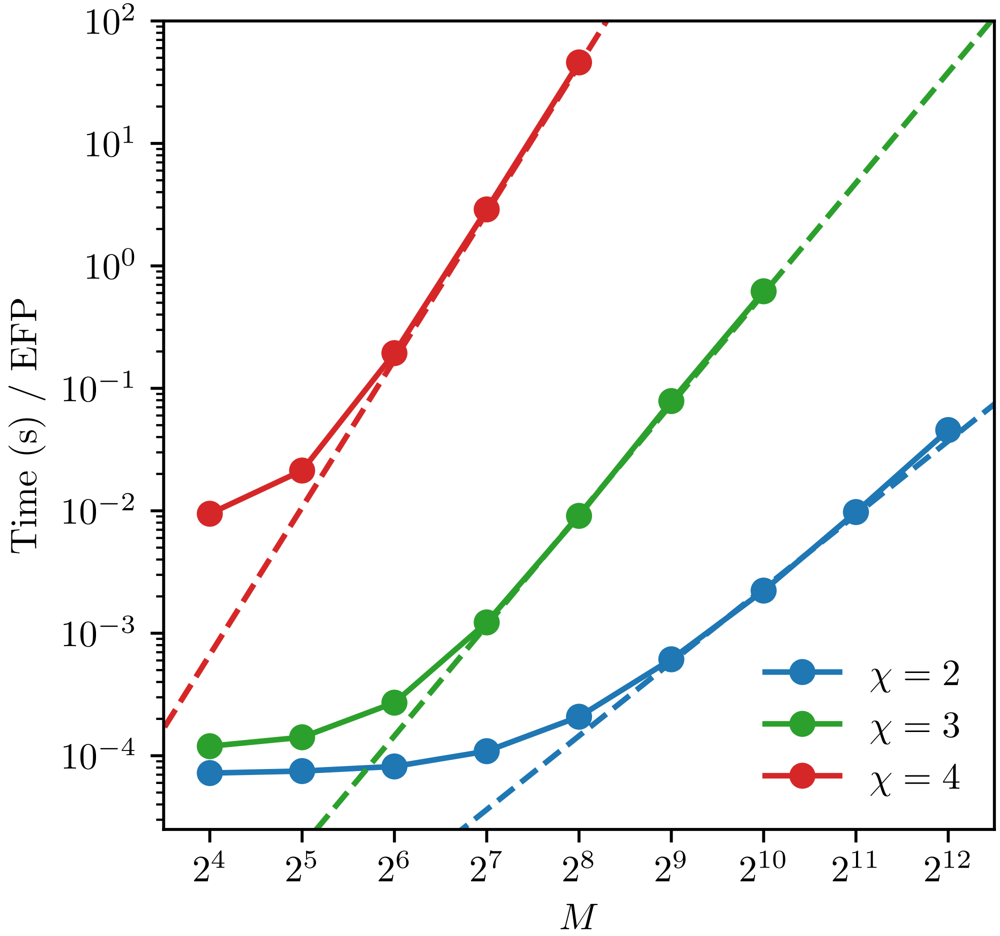


Additional EFP Tagging Plots – Quark vs. Gluon Jets





EFP Computation Timing with Variable Elimination



Linear Classification Performance – Top vs. QCD Jets