

Deep Learning (and Deep Thinking) for QCD

Jesse Thaler



QCD@LHC 2019, University at Buffalo — July 15, 2019

Deep Learning

Inpainting



Corrupted



Deep image prior

increased computational power and large data sets

[Ulyanov, Vedaldi, Lempitsky, [1711.10925](#)]

Deep Learning (or Deep Thinking?)

Inpainting



Corrupted



Deep image prior

Using randomly initialized neural network (!)

Progress made by **understanding the structure** of problems
(not just **increased computational power** and large data sets)

[Ulyanov, Vedaldi, Lempitsky, [1711.10925](https://arxiv.org/abs/1711.10925)]

Deep Learning for QCD?

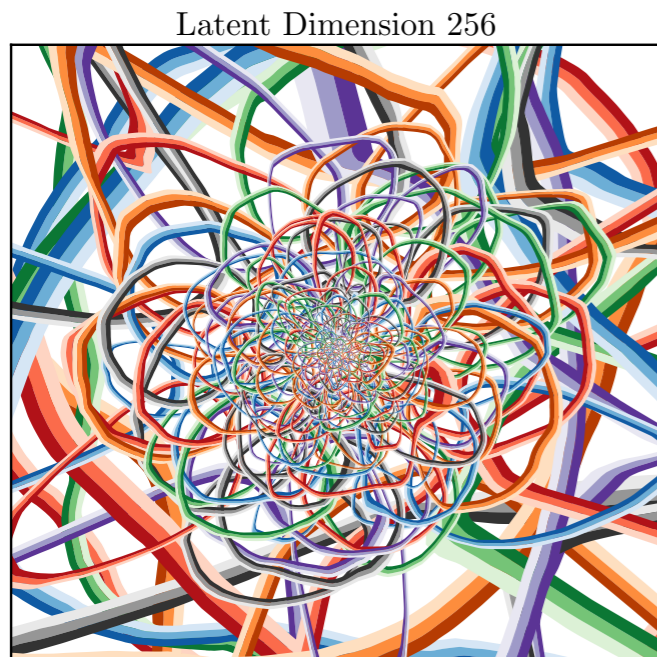
& other advanced data analysis strategies

New insights into structure of jets?
Robust handles on hadronic final states?

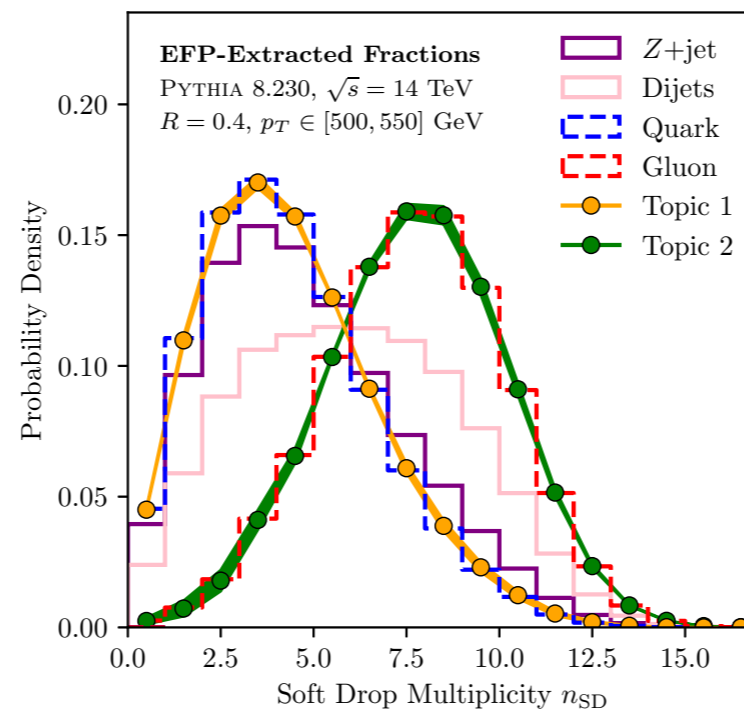
Three case studies from my research group

See also broader [ML4Jets](#) community

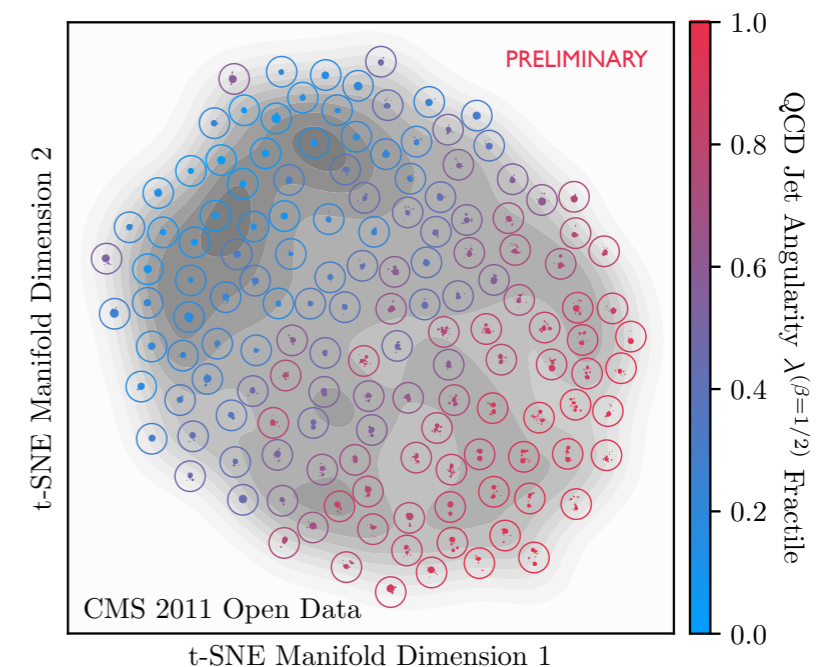
Energy Flow Networks



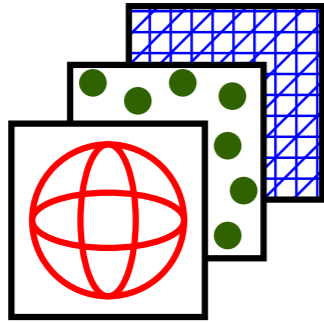
Jet Topics



(Energy Mover's Distance)



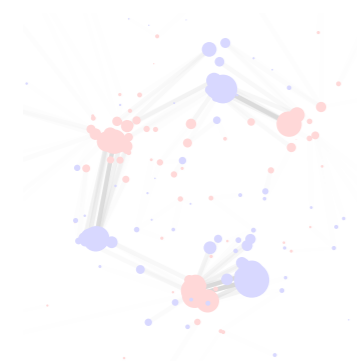
[Komiske, Metodiev, JDT, [1810.05165](#); Metodiev, JDT, [1802.00008](#); Komiske, Metodiev, JDT, [1809.01140](#);
Komiske, Metodiev, JDT, [1902.02346](#); Komiske, Mastandrea, Metodiev, Naik, JDT, in preparation]



Into the Network



Data Ex Machina



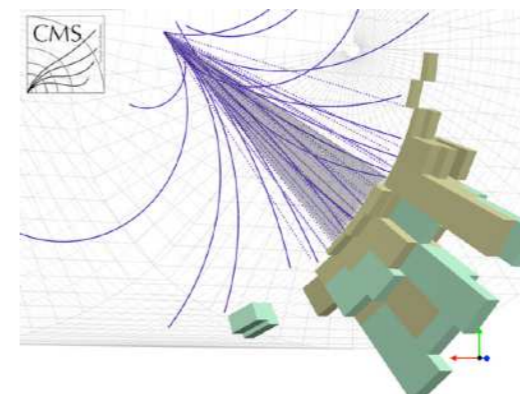
(The Space of Jets)

Cartoon of Machine Learning



E.g.: **Problem** = Minimize loss function
Solution = Multi-layer neural network
Strategy = Stochastic gradient descent

For most of this talk: \mathcal{J} = “jet”

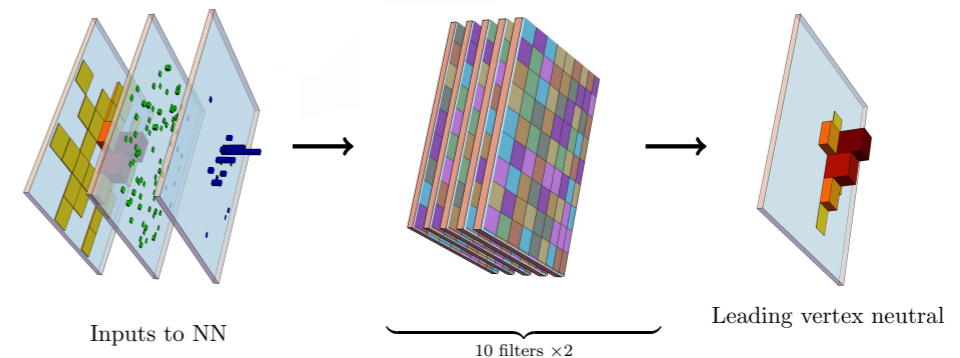


Examples of Supervised Learning

Regression

e.g. *PUMML for pileup mitigation*

[Komiske, Metodiev, Nachman, Schwartz, [1707.08600](#);
see also Arjona Martínez, Cerri, Pierini, Spiropulu, Vlimant, [1810.07988](#)]



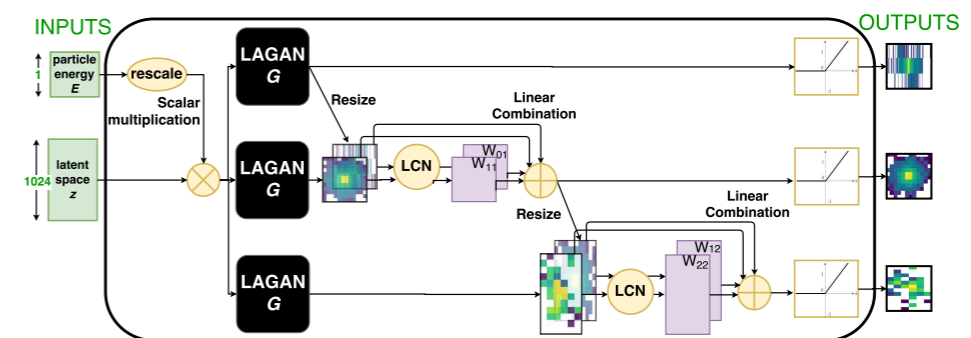
Labeled data: Objects J with property x

Solution: Map from J to x

Generation

e.g. *CaloGAN for fast detector simulation*

[Paganini, de Oliveira, Nachman, [1705.02355](#), [1712.10321](#);
see also de Oliveira, Michela Paganini, Nachman, [1701.05927](#)]

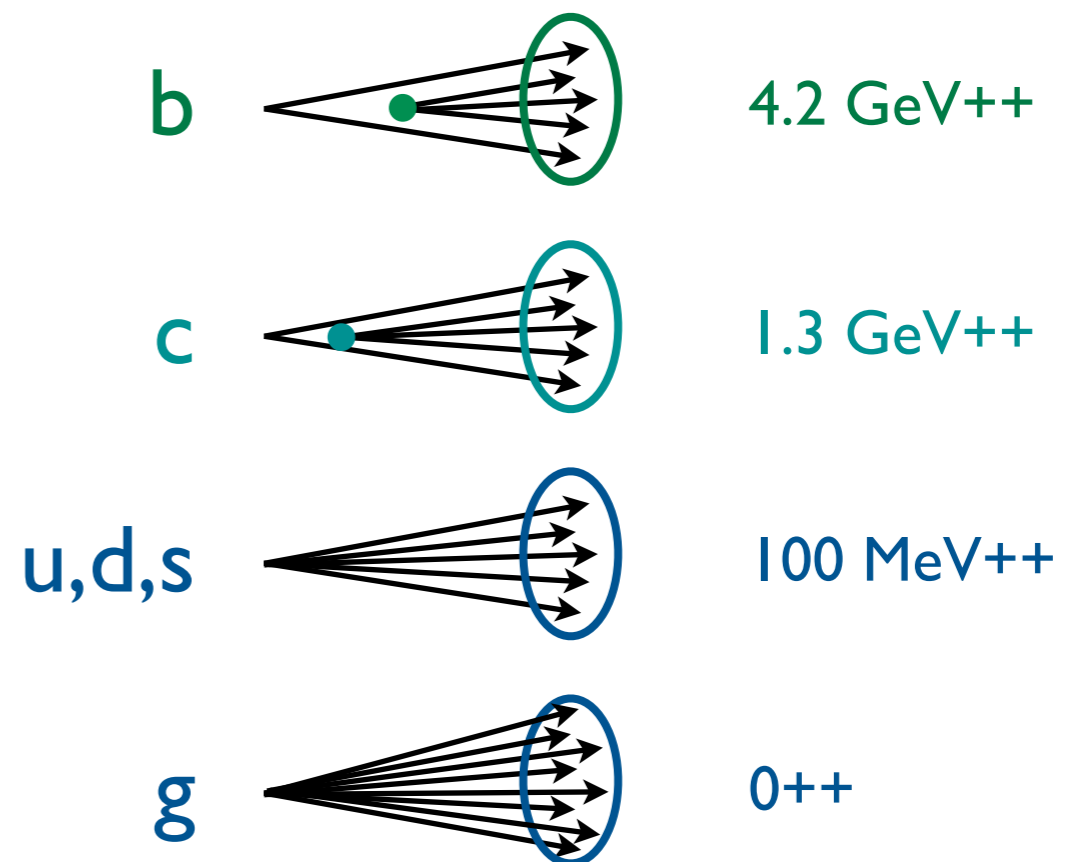
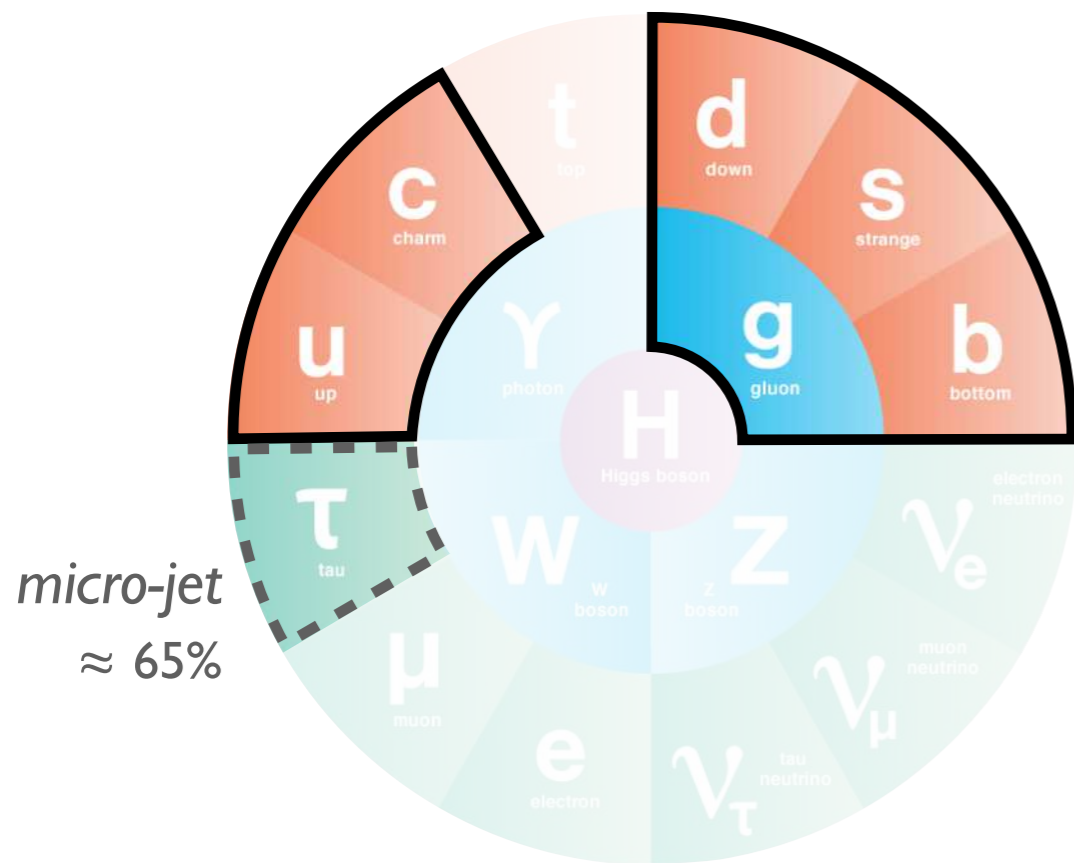


Labeled data: Objects J with property x

Solution: Map (conditioned on x)
from noise to J

Jet Classification

Key supervised learning task at LHC

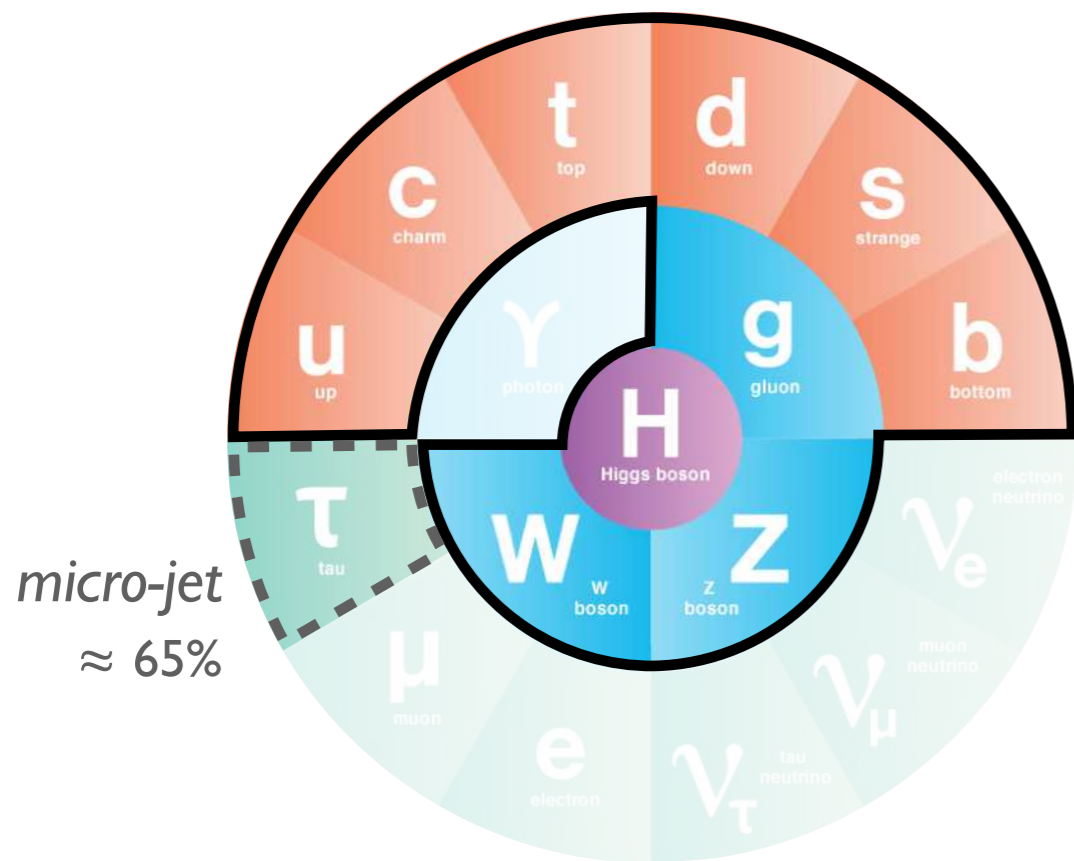


++ = Mass from QCD Radiation

[see review in Larkoski, Mout, Nachman, [1709.04464](#)]

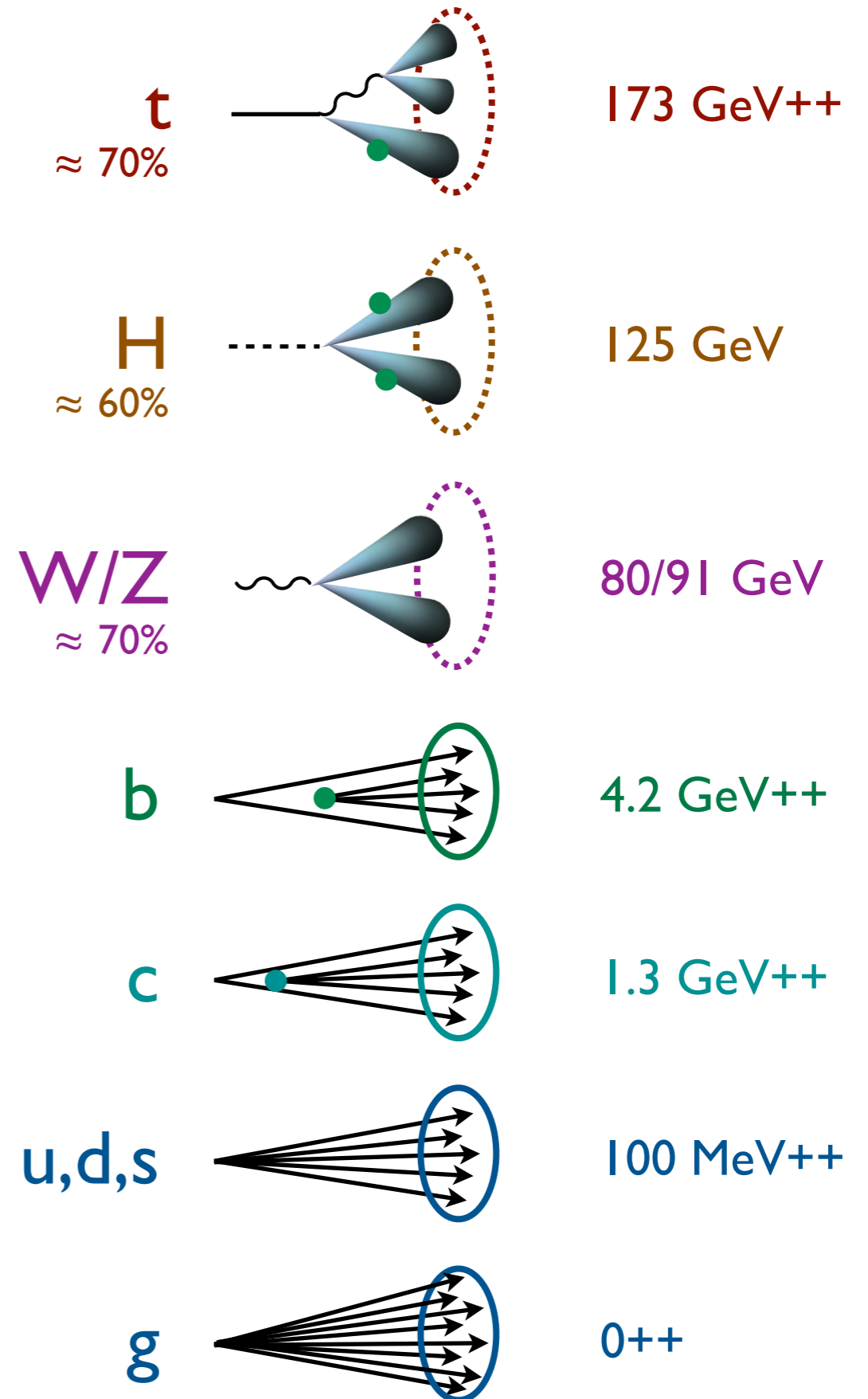
Jet Classification

Key supervised learning task at LHC



++ = Mass from QCD Radiation

[see review in Larkoski, Mout, Nachman, [1709.04464](#)]



BOSTON 2019

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

Local Organizing Committee:

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Philip Harris (MIT)
Yen-Jie Lee (MIT)
Matthew Schwartz (Harvard)
Jesse Thaler (MIT)

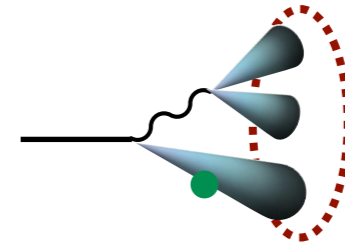
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Ayana Arce (Duke)
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July 22-26, 2019
Stata Center, MIT

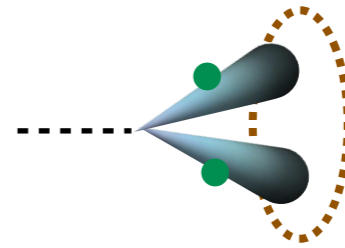
<https://indico.cern.ch/e/boost2019>

t
 $\approx 70\%$



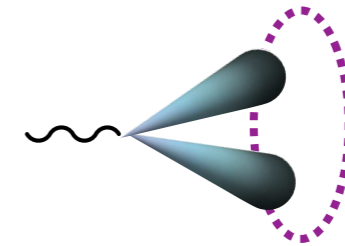
173 GeV++

H
 $\approx 60\%$



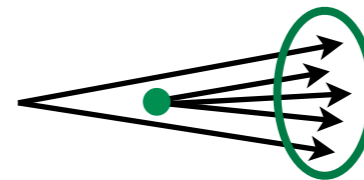
125 GeV

W/Z
 $\approx 70\%$



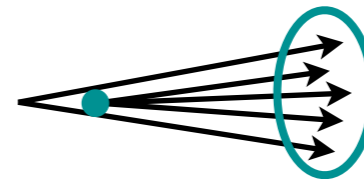
80/91 GeV

b



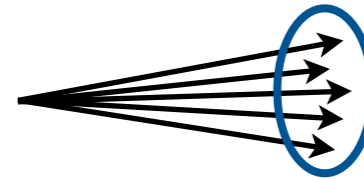
4.2 GeV++

c



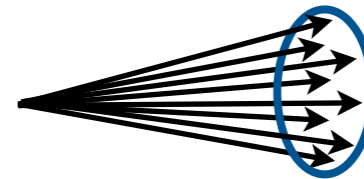
1.3 GeV++

u, d, s



100 MeV++

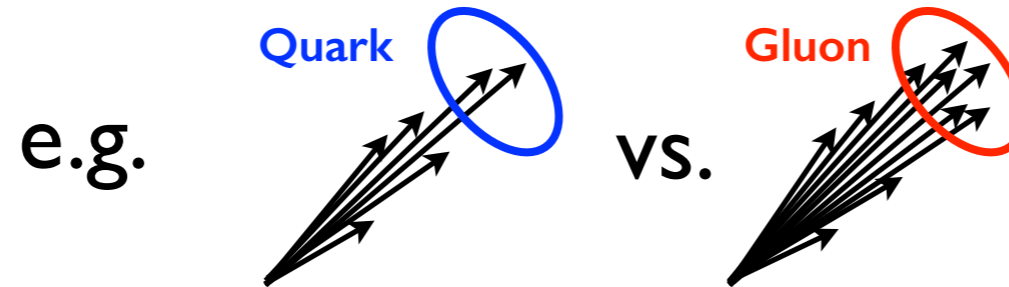
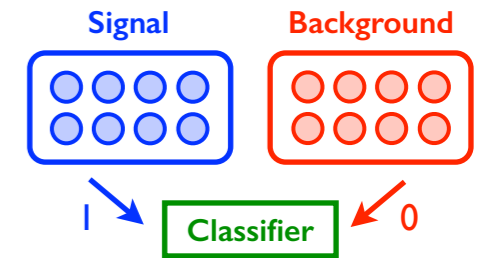
g



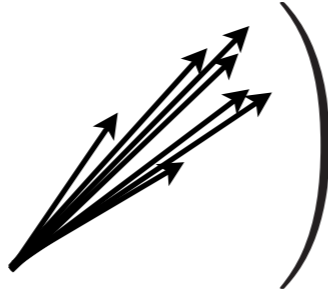
0++

Binary Classification

Much more in backup



assuming trustable
training data
(more later...)

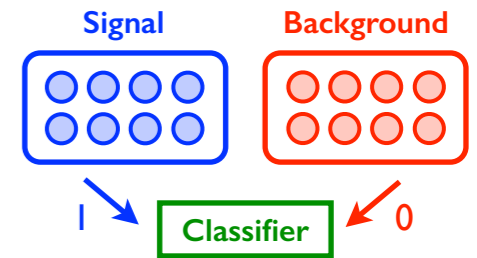
Find h  such that

$$h(\text{Quark}) = 1$$
$$h(\text{Gluon}) = 0$$

Best you can do: $h(\mathcal{J}) = \frac{p(\mathcal{J}|\text{Q})}{p(\mathcal{J}|\text{Q}) + p(\mathcal{J}|\text{G})}$
(Neyman-Pearson lemma)

Jet Classification Studies

Mix and match



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

Loss Function

Classifier

Inputs

Signal vs. Background

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

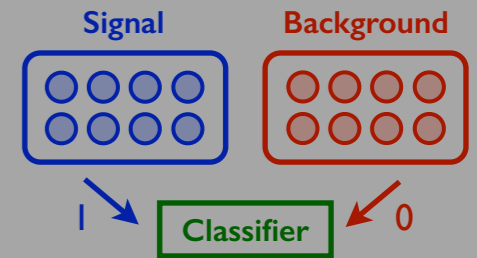
- High-Level Features
- Basis of High-Level Features
- Jet Image
- Multi-channel Jet Image
- Abstract Jet Image
- Sorted Four-Vectors
- Clustered Four-Vectors
- Lund Plane Emissions
- Kitchen Sink
- ...

- | | | |
|------------------------|-----|------------------|
| 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. | ... |

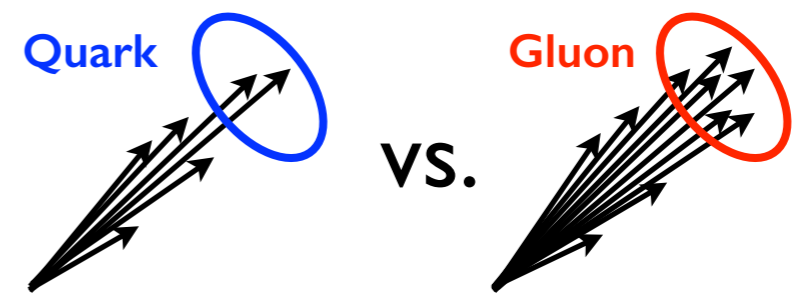
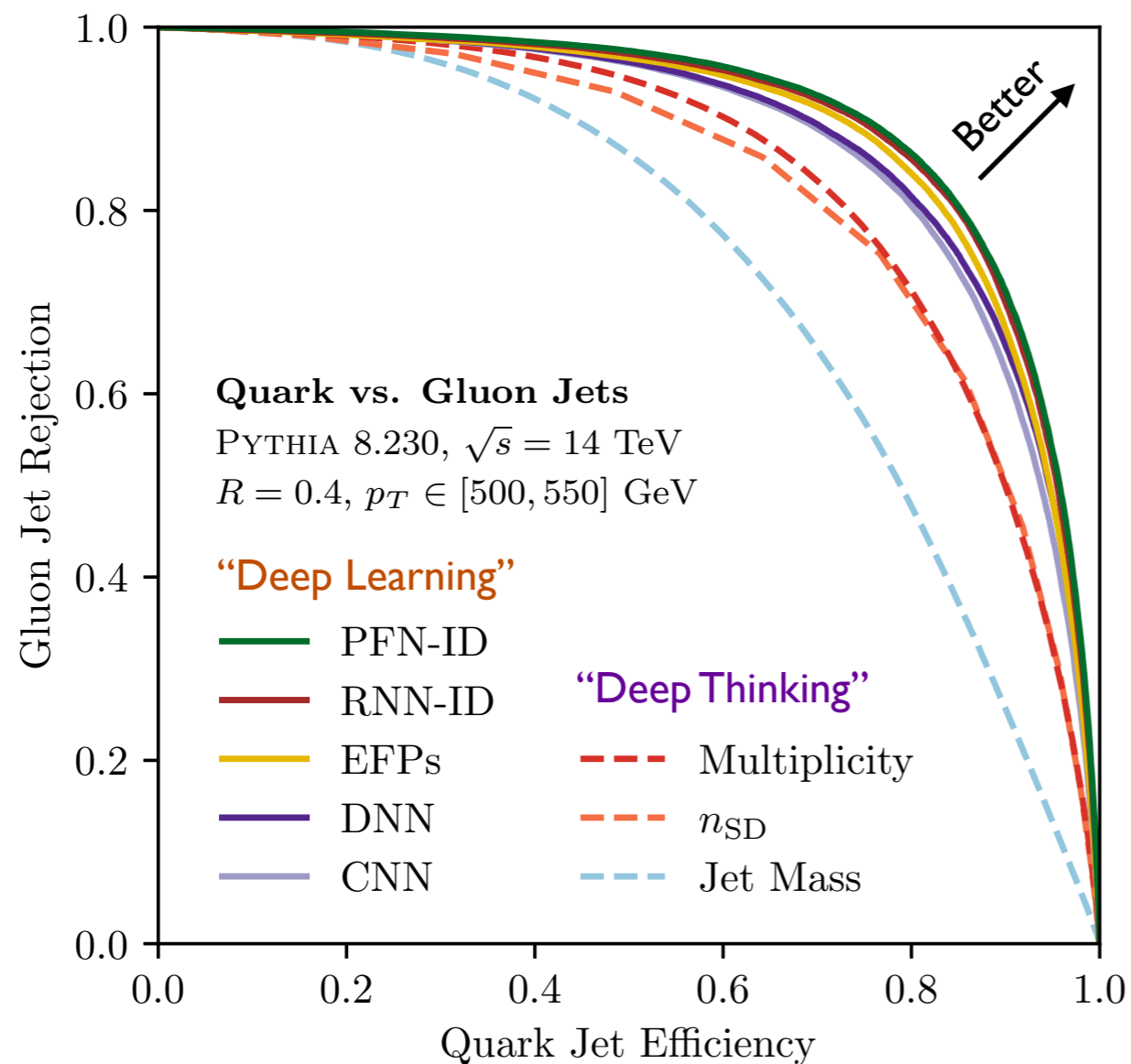
[Lönblad, Peterson, Rognvaldsson, [PRL 1990](#), ..., Cogan, Kagan, Strauss, Schwartzman, [1407.5675](#); Almeida, Backović, Cliche, Lee, Perelstein, [1501.05968](#); de Oliveira, Kagan, Mackey, Nachman, Schwartzman, [1511.05190](#); Baldi, Bauer, Eng, Sadowski, Whiteson, [1603.09349](#); Conway, Bhaskar, 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](#); Parkes, 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, Soye, [1807.04758](#); Moore, Nordström, Varma, Fairbairn, [1807.04769](#); plus many ATLAS/CMS performance studies; plus my friends who will scold me for forgetting their paper (and not updating this after July 23, 2018)]

Jet Classification Studies

Mix and match



The “Hello, World!” of Jet Classification



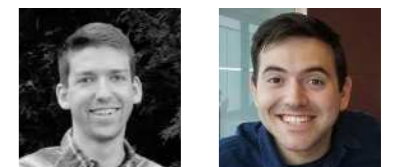
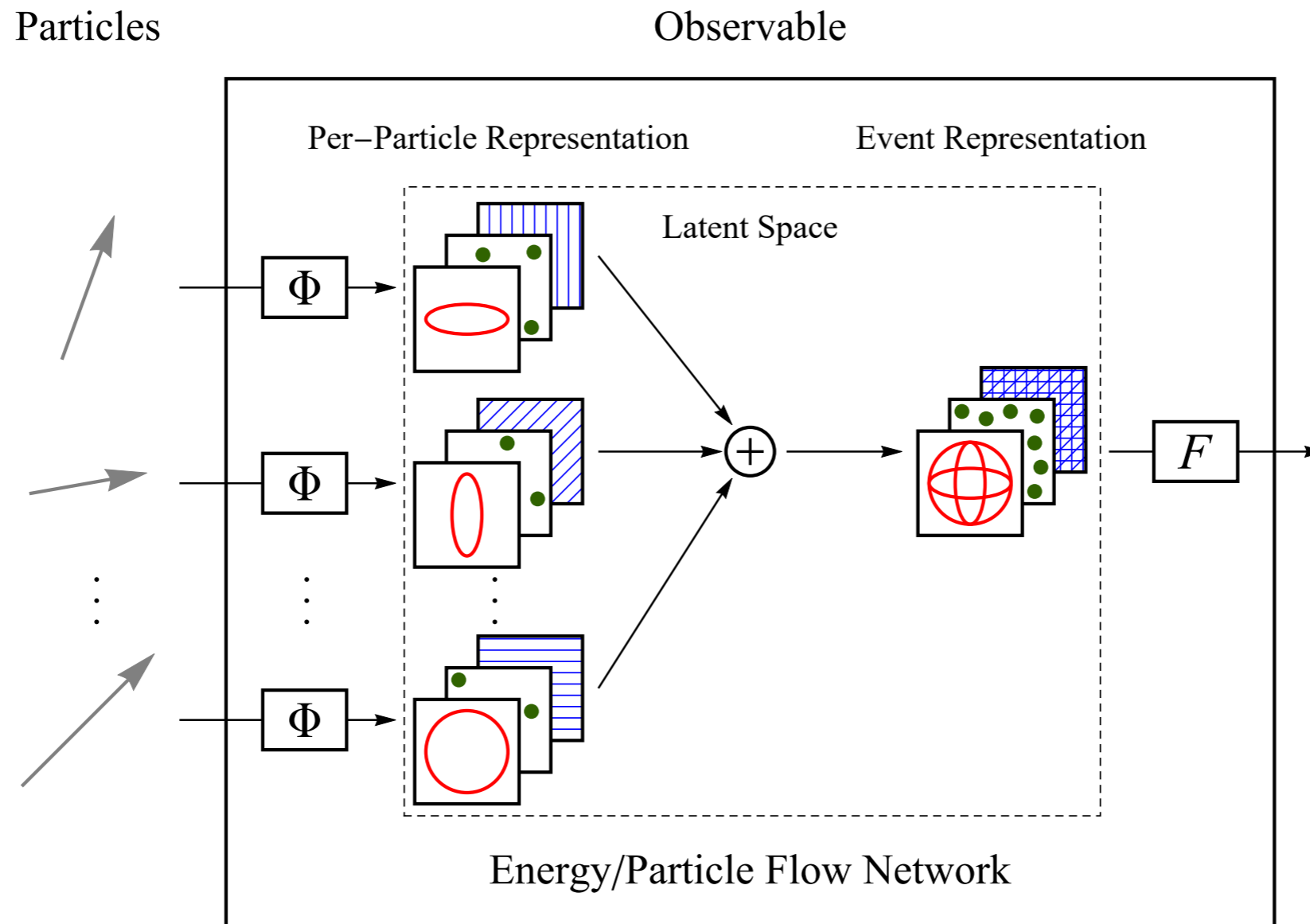
Substantial gains from deep learning... but why?

[Komiske, Metodiev, JDT, [1810.05165](#)]

Introducing Energy Flow Networks

An architecture designed for interpretability

(see backup for detailed architecture)



[Komiske, Metodiev, JDT, [1810.05165](#);
special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, [1703.06114](#)]

Introducing Energy Flow Networks

(see backup for detailed architecture)

An architecture designed for interpretability

$$S(\mathcal{J}) = F(V_1, V_2, \dots, V_\ell) \quad V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} p_{Ti} \Phi_a(y_i, \phi_i)$$

Latent space of dim ℓ

Linear weights

Parametrized with **Neural Networks**

Flexible enough to describe any* **IRC-safe** observable
(assuming large enough ℓ)

Generalization: Particle Flow Networks (aka “Deep Sets”)

[Komiske, Metodiev, JDT, [1810.05165](#);
special case of Zaheer, Kottur, Ravanbakhsh, Póczos, Salakhutdinov, Smola, [1703.06114](#)]

Introducing Energy Flow Networks

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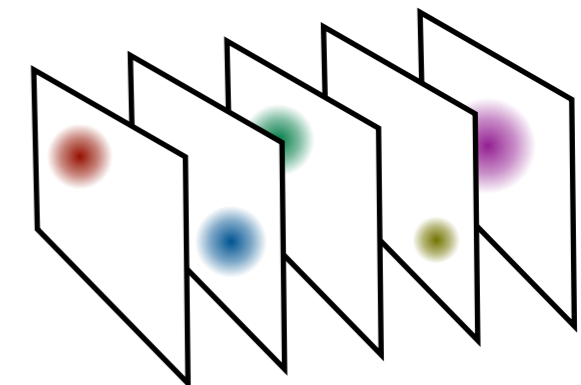
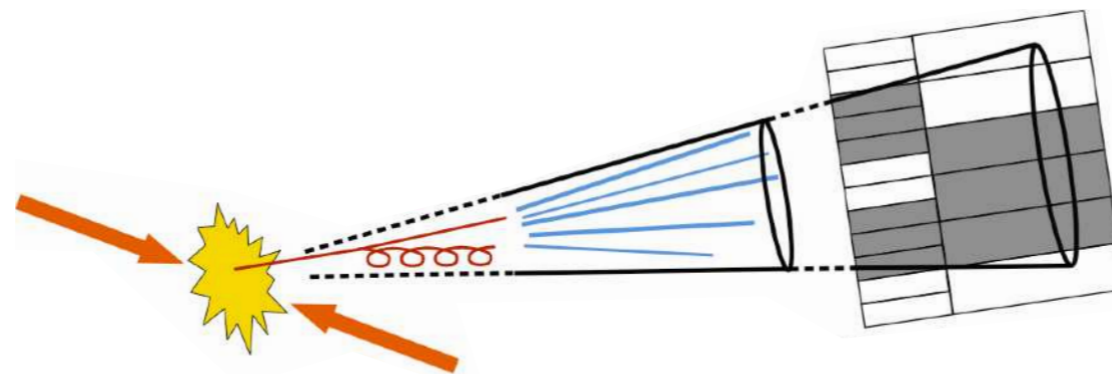
Visualization Strategy

$$S(\mathcal{J}) = F(V_1, V_2, \dots, V_\ell)$$

↑
Difficult to visualize
(unless ℓ is small)

$$V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} p_{Ti} \Phi_a(y_i, \phi_i)$$

↑
Easy to plot these!



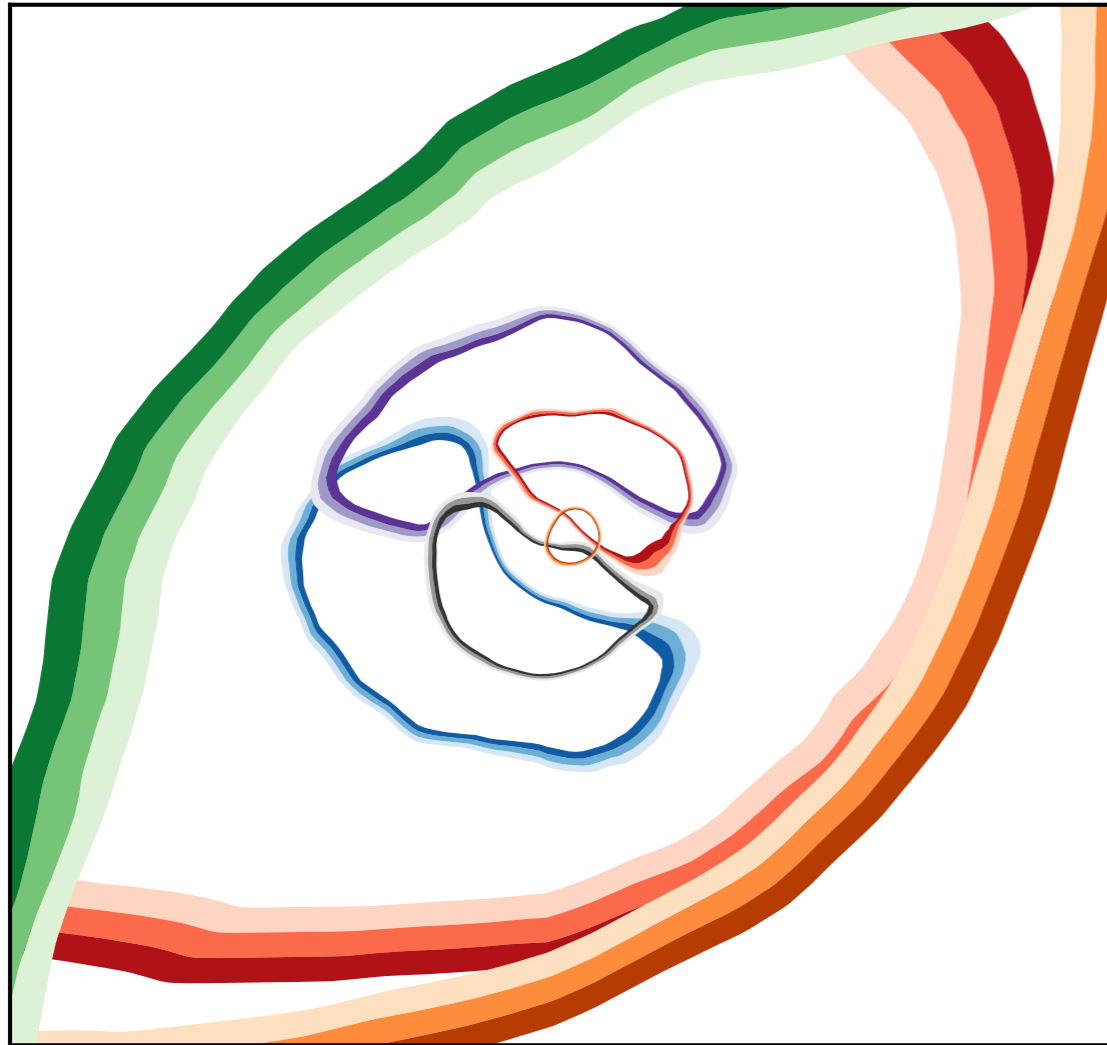
(similar to CNN
filter activation)

[Komiske, Metodiev, JDT, [1810.05165](#);
special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, [1703.06114](#)]

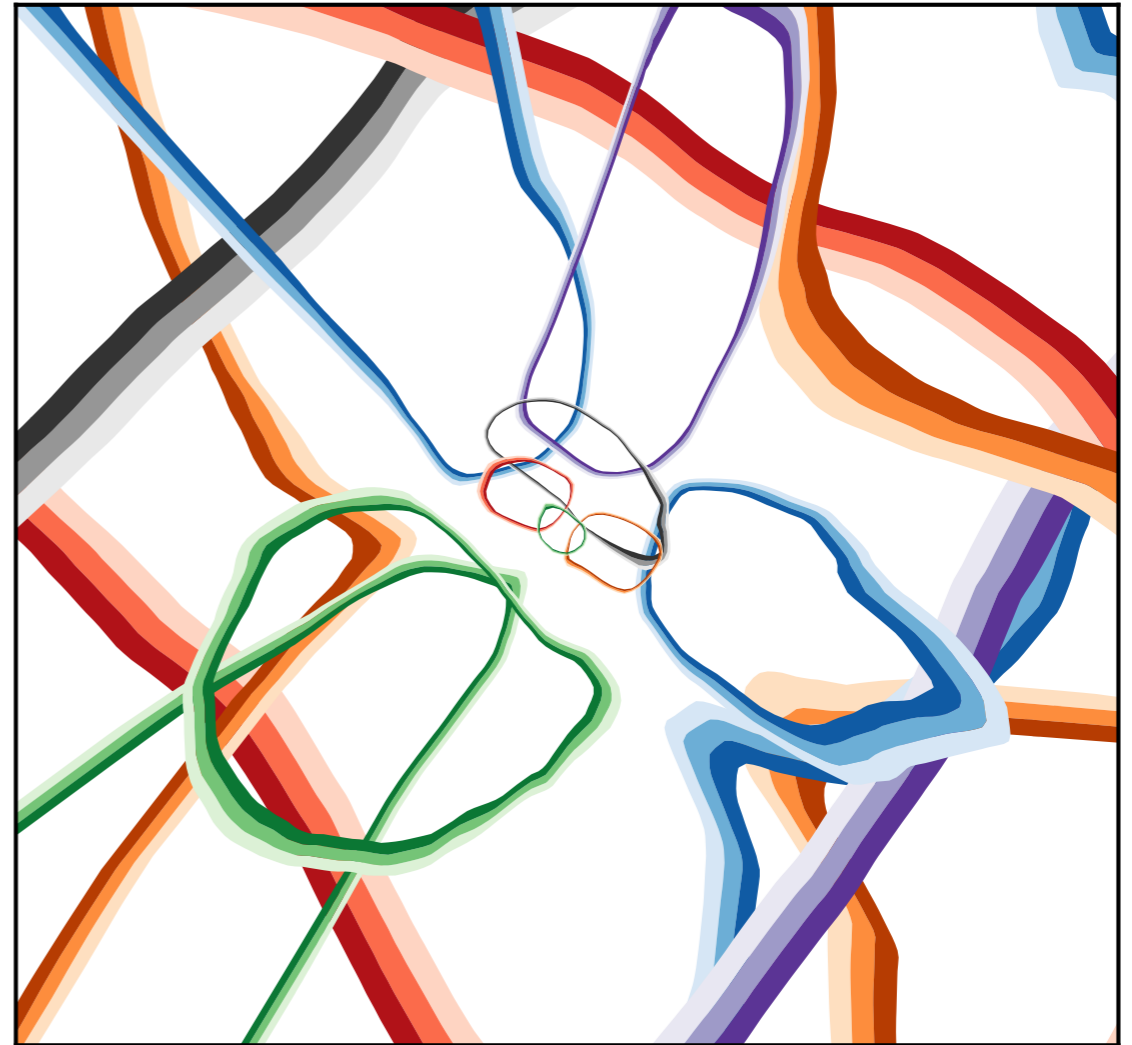
Psychedelic Network Visualization

(see backup for
how these are made)

Latent Dimension 8



Latent Dimension 16

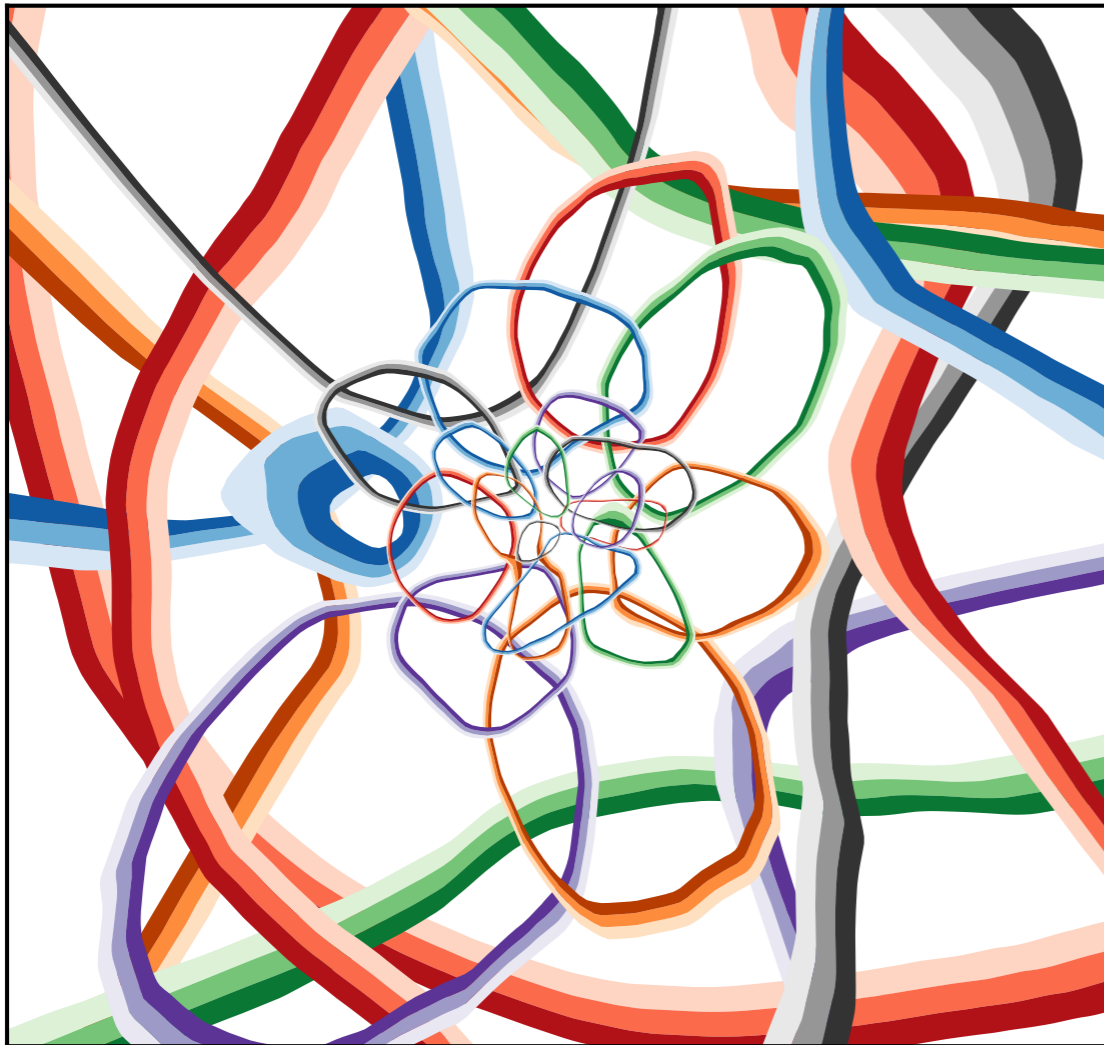


For the case of **quark** vs. **gluon** classification

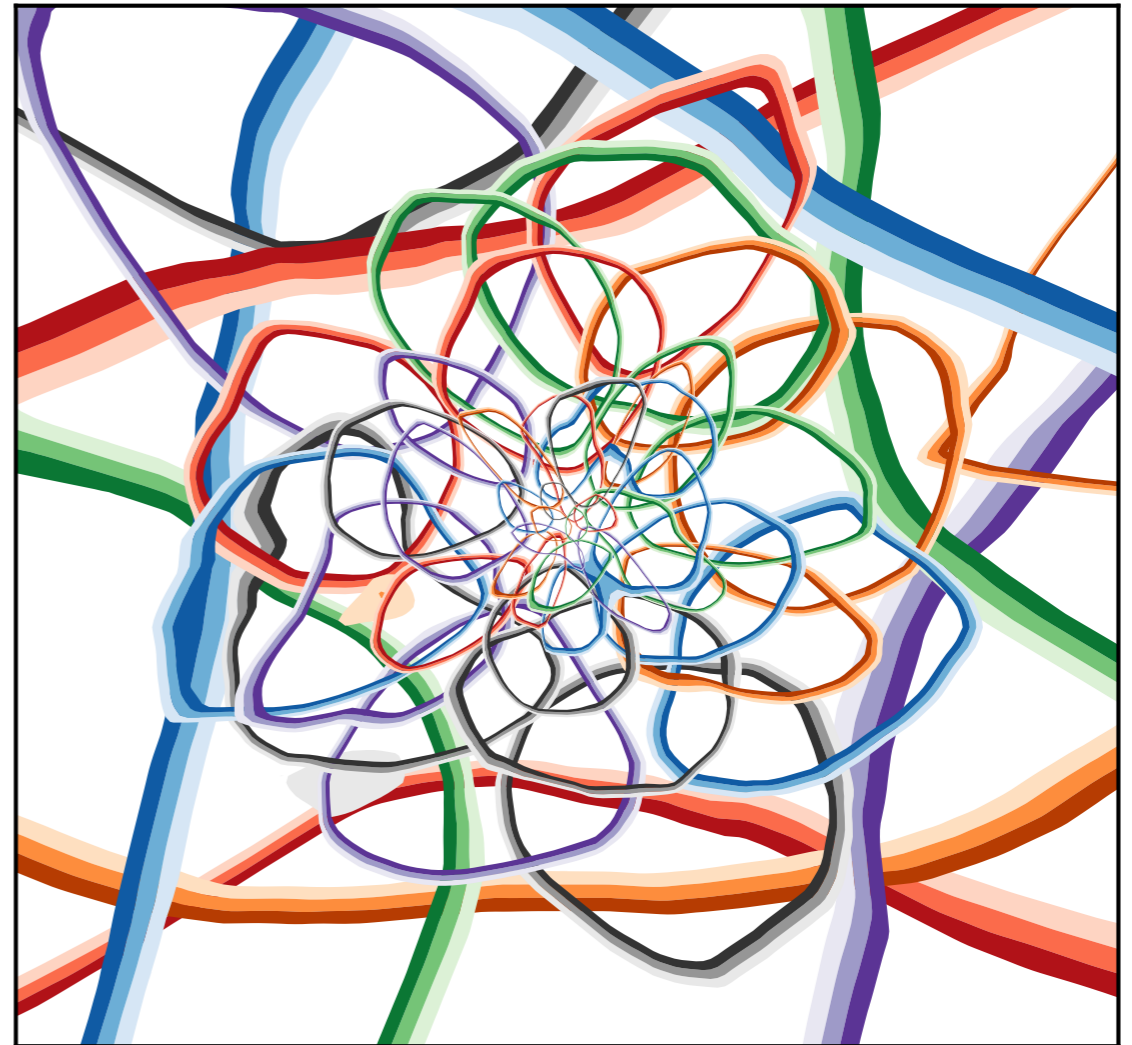
Psychedelic Network Visualization

(see backup for
how these are made)

Latent Dimension 32



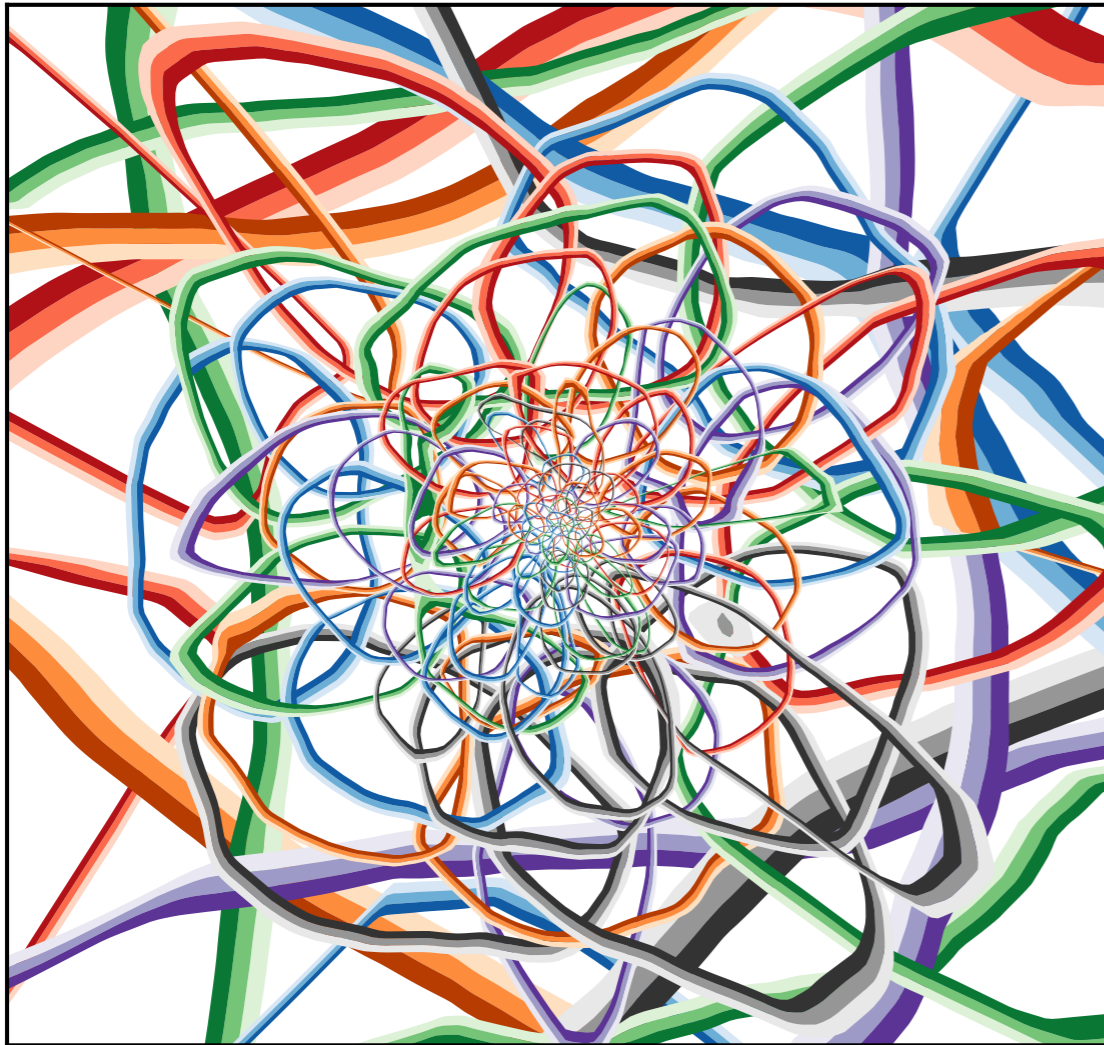
Latent Dimension 64



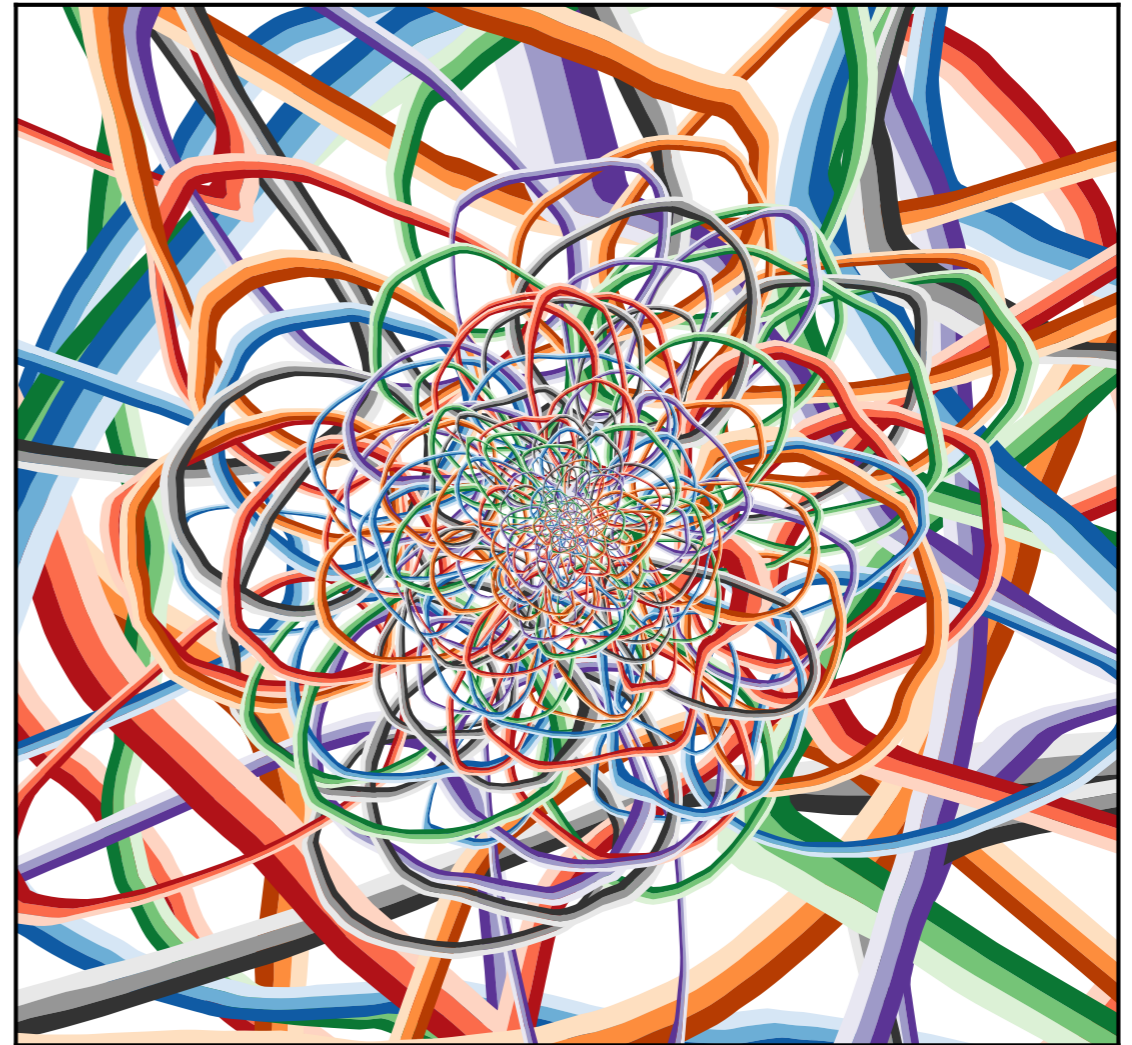
Psychedelic Network Visualization

(see backup for
how these are made)

Latent Dimension 128

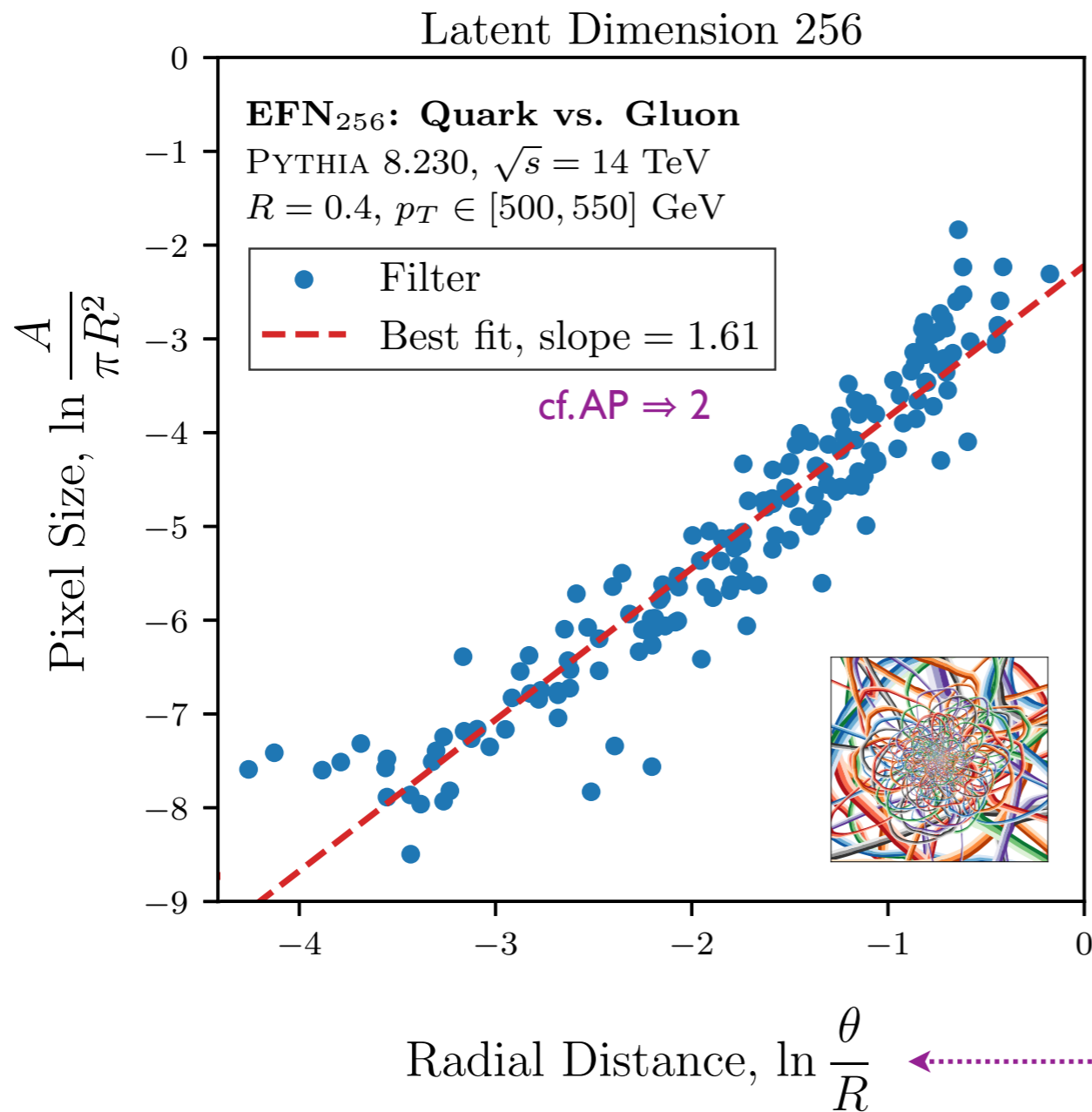
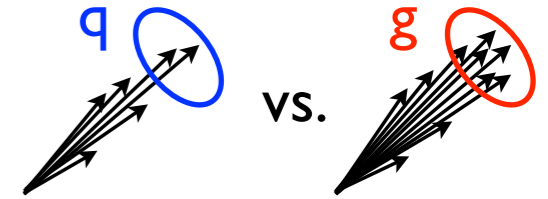


Latent Dimension 256



Singularity structure of QCD!

Putting the AI in Altarelli-Parisi



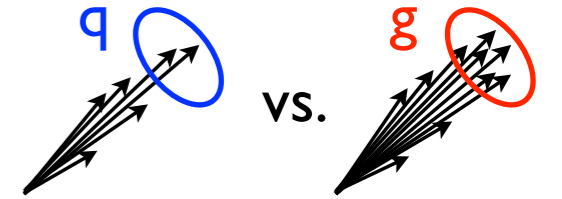
$C_q = 4/3$
 $C_g = 3$

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

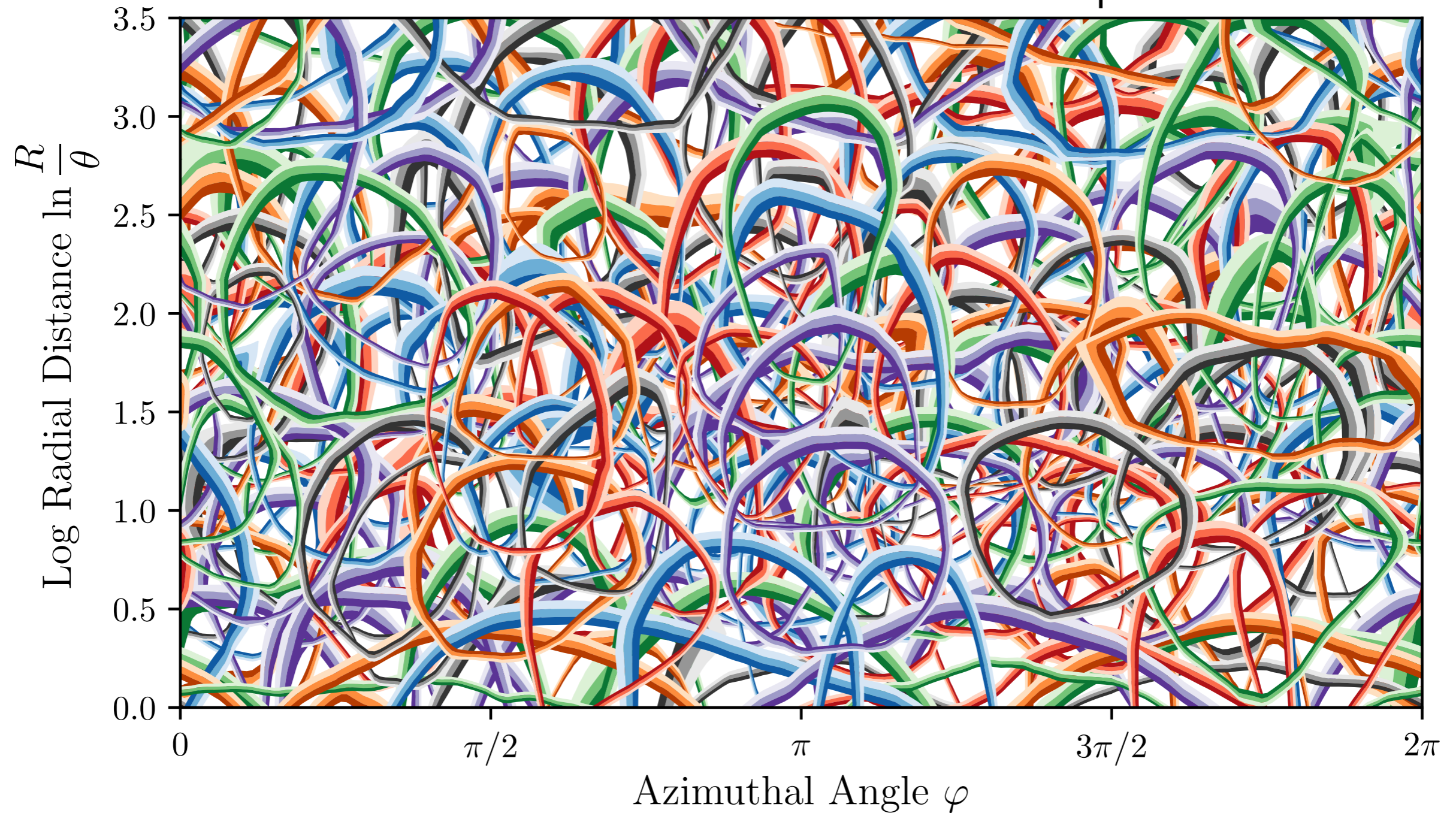
Collinear Soft

[Komiske, Metodiev, JDT, 1810.05165]

Suitable for Framing



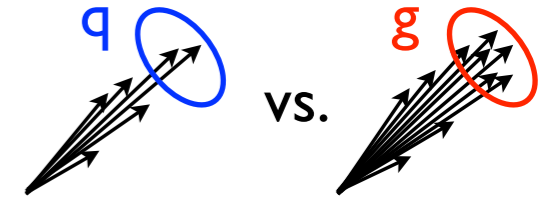
Coordinate transformation to the emission plane



[Komiske, Metodiev, JDT, [1810.05165](#); see also Dreyer, Salam, Soyez, [1807.04758](#)]

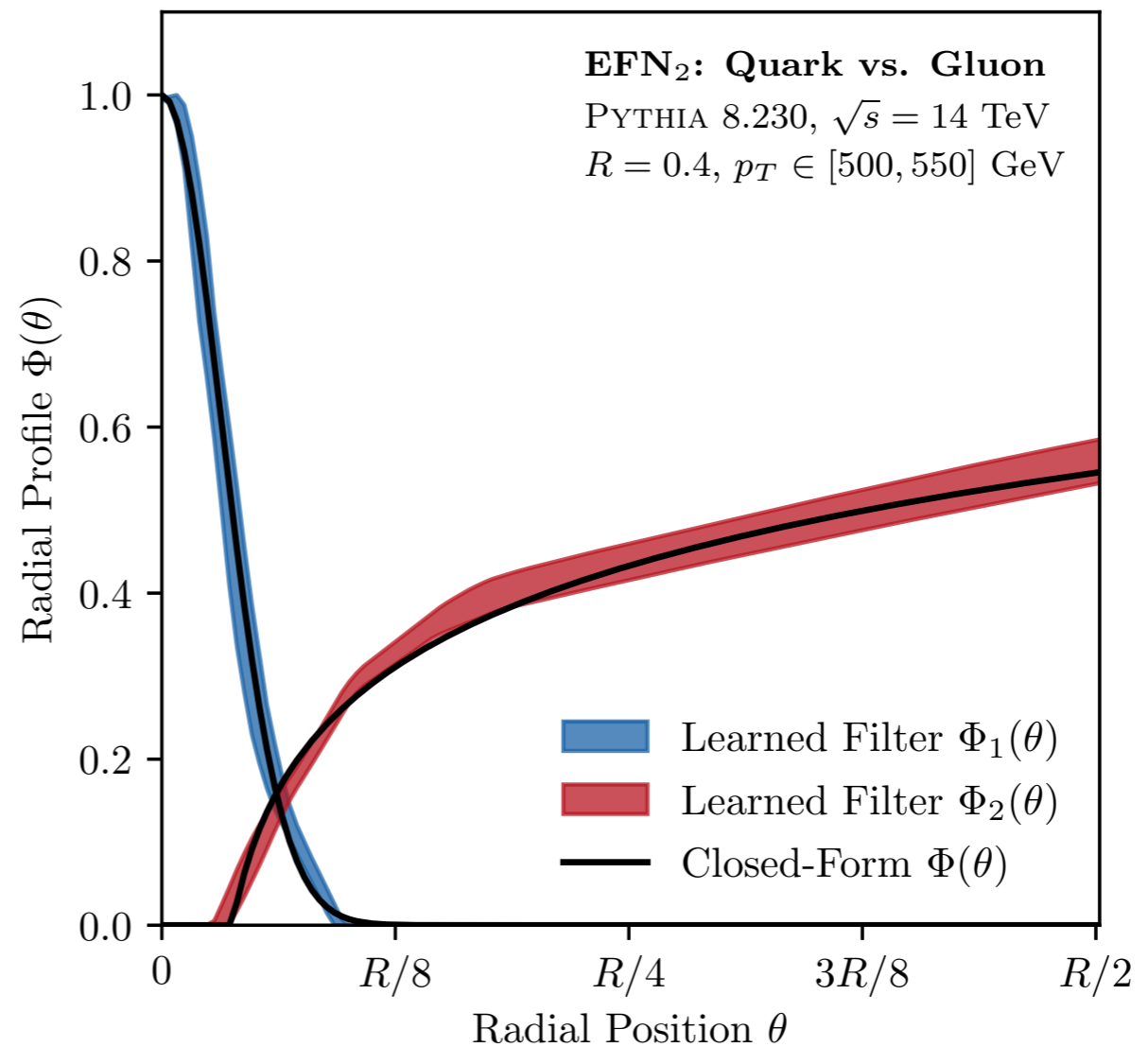
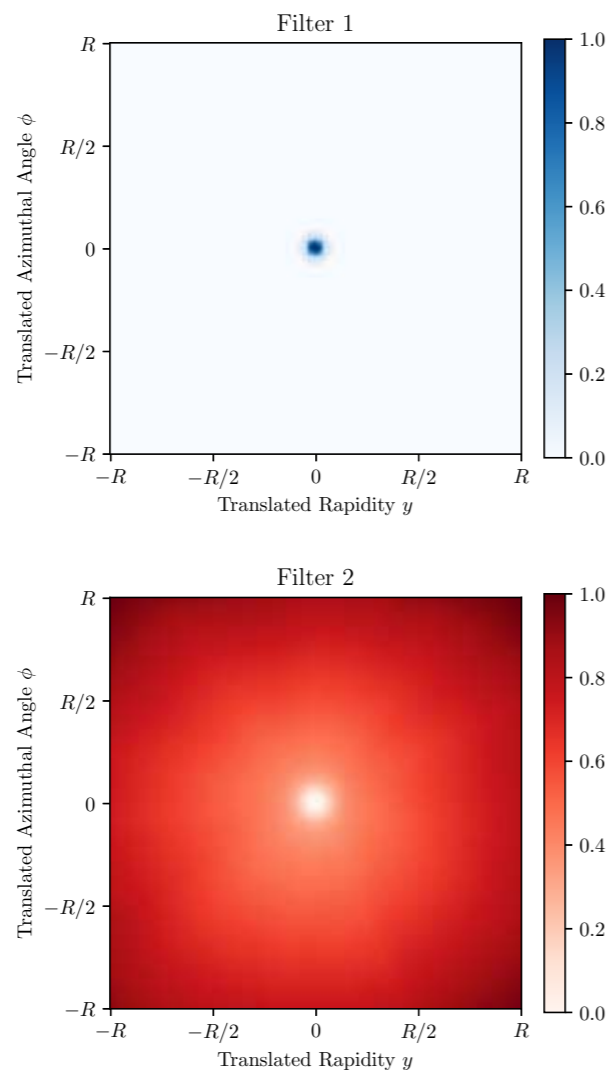
*“Ok, but did you really learn something
you didn’t already know?”*

Learning from the Machine



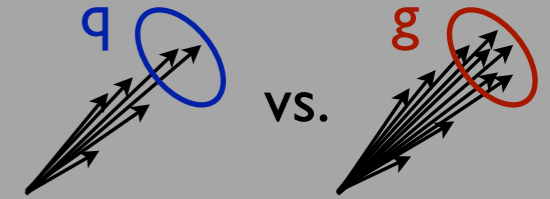
For $\ell = 2$ EFN, radial moments: $\sum_{i \in \text{jet}} z_i f(\theta_i)$

cf. Angularities:
 $f(\theta) = \theta^\beta$



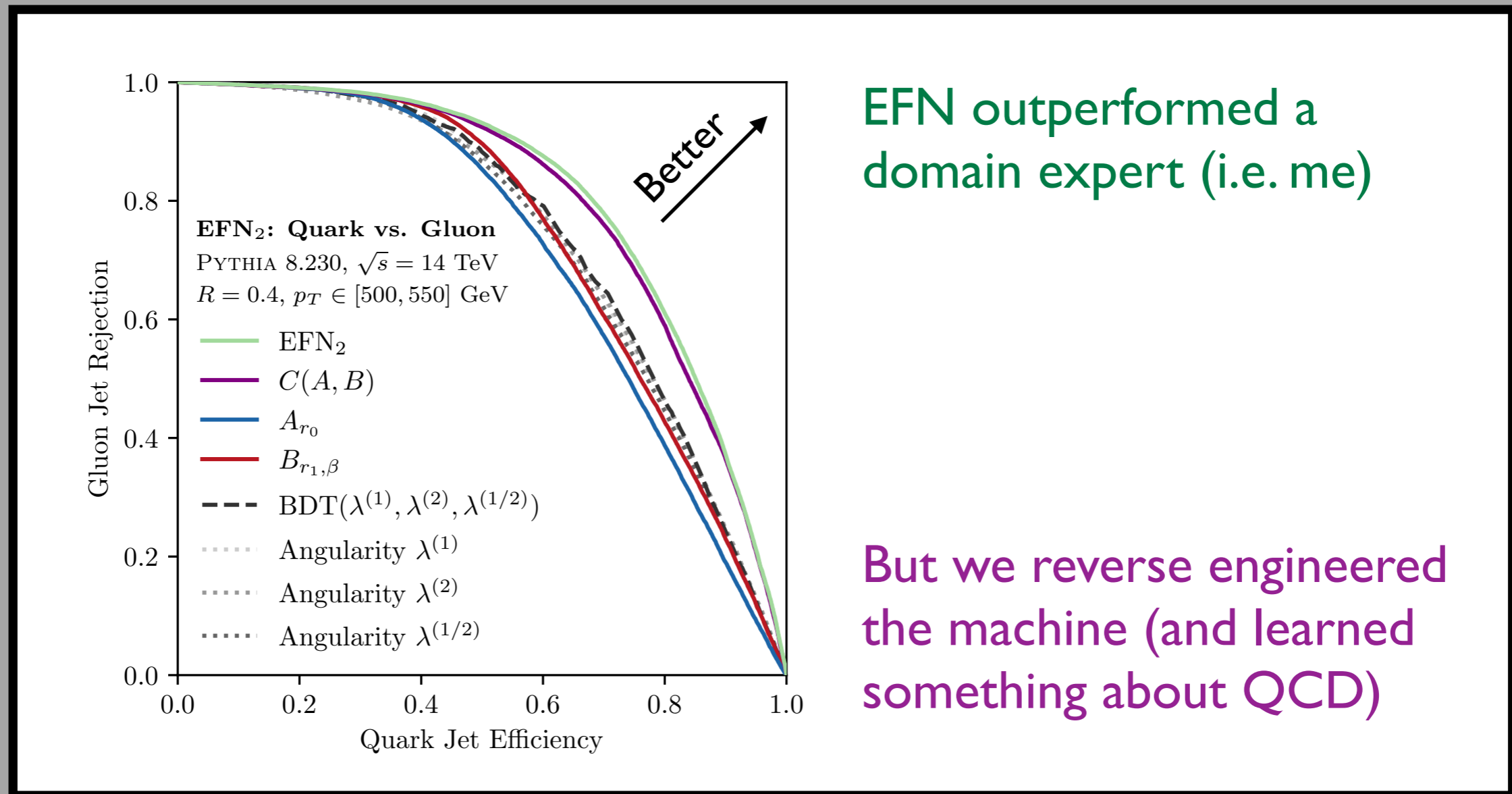
[Komiske, Metodiev, JDT, [1810.05165](#);
 cf. Larkoski, JDT, Waalewijn, [1408.3122](#); using Berger, Kucs, Sterman, [hep-ph/0303051](#); Ellis, Vermilion, Walsh, Hornig, Lee, [1001.0014](#)]

Learning from the Machine



For $\ell = 2$ EFN, radial moments: $\sum_{i \in \text{jet}} z_i f(\theta_i)$

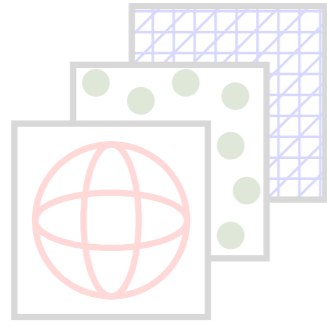
cf. Angularities:
 $f(\theta) = \theta^\beta$



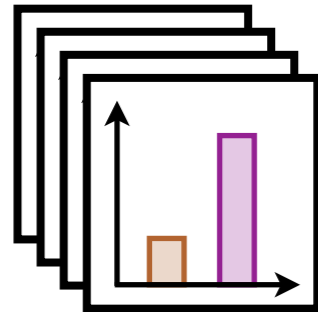
EFN outperformed a domain expert (i.e. me)

But we reverse engineered the machine (and learned something about QCD)

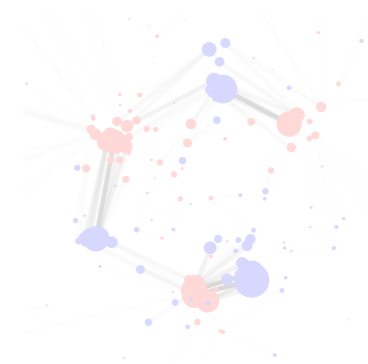
[Komiske, Metodiev, JDT, [1810.05165](#);
 cf. Larkoski, JDT, Waalewijn, [1408.3122](#); using Berger, Kucs, Sterman, [hep-ph/0303051](#); Ellis, Vermilion, Walsh, Hornig, Lee, [1001.0014](#)]



Into the Network



Data Ex Machina



(The Space of Jets)

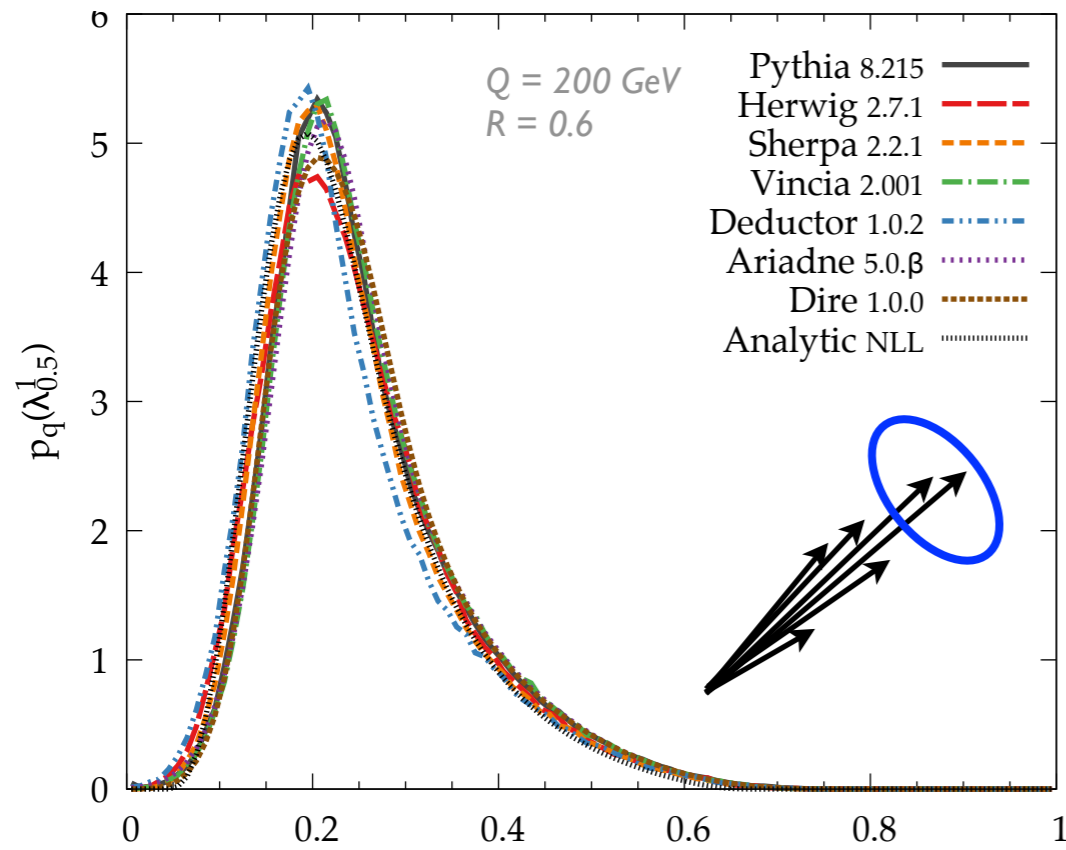
“Ok, but isn’t supervised learning only as reliable as your training samples?”

Uncertainties in Monte Carlo Samples?

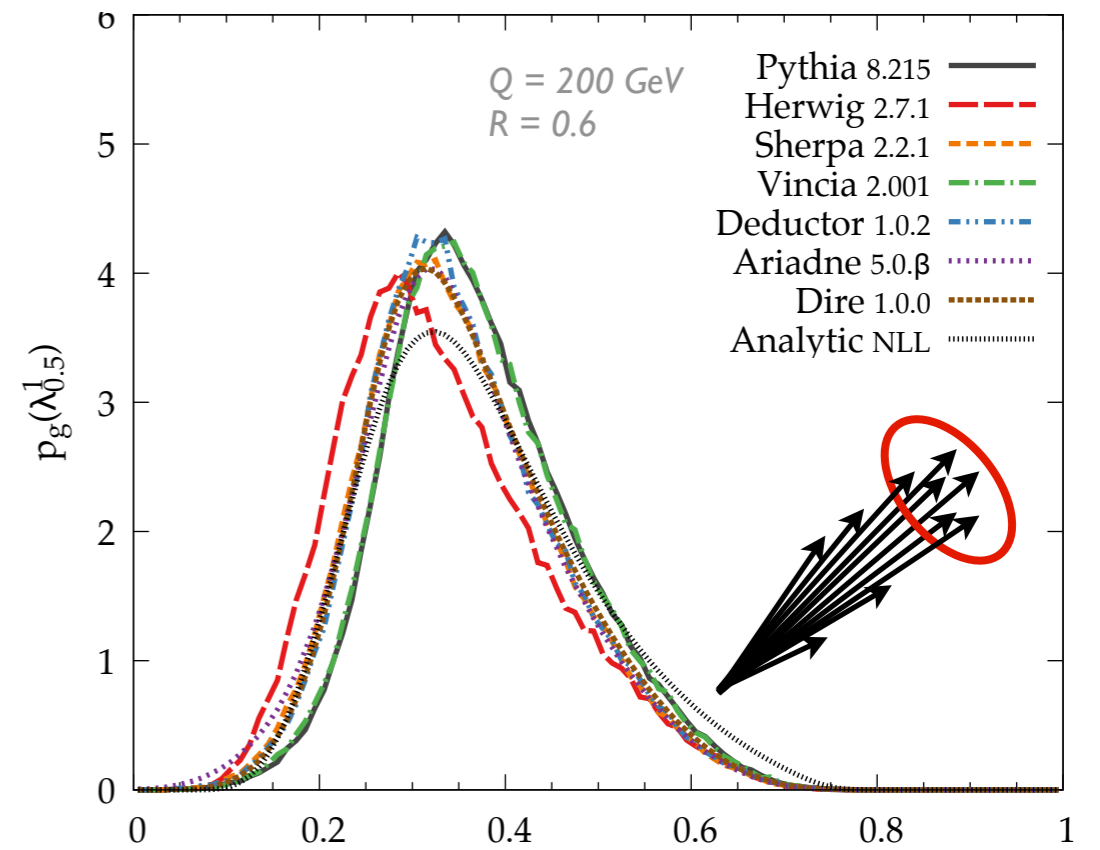
$e^+e^- \rightarrow$ quarks ($C_F = 4/3$)

VS.

$e^+e^- \rightarrow$ gluons ($C_A = 3$)



$$\text{LHA} = \sum_i z_i \sqrt{\theta_i}$$



$$\text{LHA} = \sum_i z_i \sqrt{\theta_i}$$

Large shower variations (esp. gluon jets, hard to tune from LEP)

[Gras, Hoeche, Kar, Larkoski, Lönnblad, Plätzer, Siódmok, Skands, Soyer, JDT, [1704.03878](#); see progress in Reichelt, Richardson, Siódmok, [1708.01491](#)]

What are “Quarks” and “Gluons” anyways?

Color triplet vs. Color octet?

But jet constituents are *color-singlet hadrons!*

What is a Quark Jet?

From lunch/dinner discussions

Les Houches 2015
(& 2017 & 2019 & ...)

<p>Ill-Defined</p> <p>↓</p> <p>Well-Defined</p>	<p>What people sometimes think we mean</p> <p>↑</p> <p>Quark as noun</p> <p>↓</p> <p>Quark as adjective</p> <p>↑</p> <p>What we mean</p>	<p>A quark parton</p> <p>A Born-level quark parton</p> <p>The initiating quark parton in a final state shower</p> <p>An eikonal line with baryon number $1/3$ and carrying triplet color charge</p> <p>A quark operator appearing in a hard matrix element in the context of a factorization theorem</p> <p>A parton-level jet object that has been quark-tagged using a soft-safe flavored jet algorithm (automatically collinear safe if you sum constituent flavors)</p> <p>A phase space region (as defined by an unambiguous hadronic fiducial cross section measurement) that yields an enriched sample of quarks (as interpreted by some suitable, though fundamentally ambiguous, criterion)</p>
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Jesse Thaler — Report of the Les Houches Quark/Gluon Subgroup 3

[Gras, Hoeche, Kar, Larkoski, Lönnblad, Plätzer, Siódmok, Skands, Soyez, JDT, [1704.03878](#); slide from Soyez, JDT, Freytsis, Gras, Kar, Lönnblad, Plätzer, Siódmok, Skands, Soper, [1605.04692](#)]

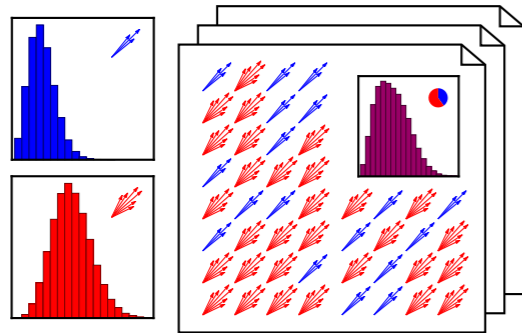
Data ex Machina

“A seemingly unsolvable problem is suddenly and abruptly resolved by an unexpected and seemingly unlikely occurrence, typically so much as to seem contrived”

[slogan from Eric Metodiev; quote from Deus ex machina on Wikipedia]

Enter Unsupervised Learning

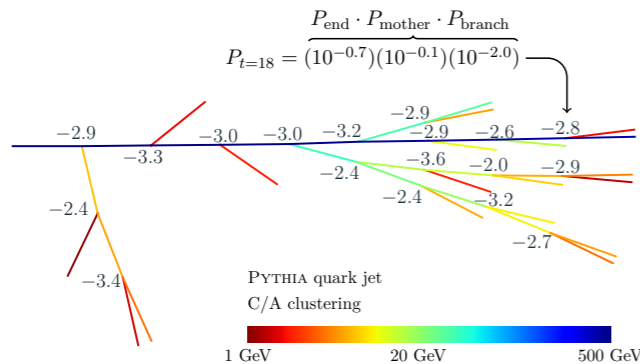
Learning from *unlabeled* (or barely labeled) data



Jet Topics

Blind Source Separation

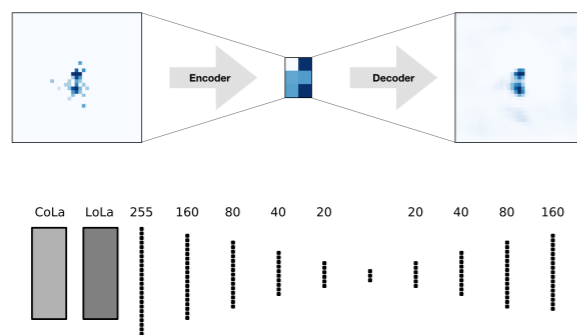
[Metodiev, JDT, [1802.00008](#); Komiske, Metodiev, JDT, [1809.01140](#);
see also Metodiev, Nachman, JDT, [1708.02949](#); Dillon, Faroughy, Kamenik, [1904.04200](#)]



JUNIPR

Probability Modeling

[Andreassen, Feige, Frye, Schwartz, [1804.09720](#), [1906.10137](#);
see also Monk, [1807.03685](#)]



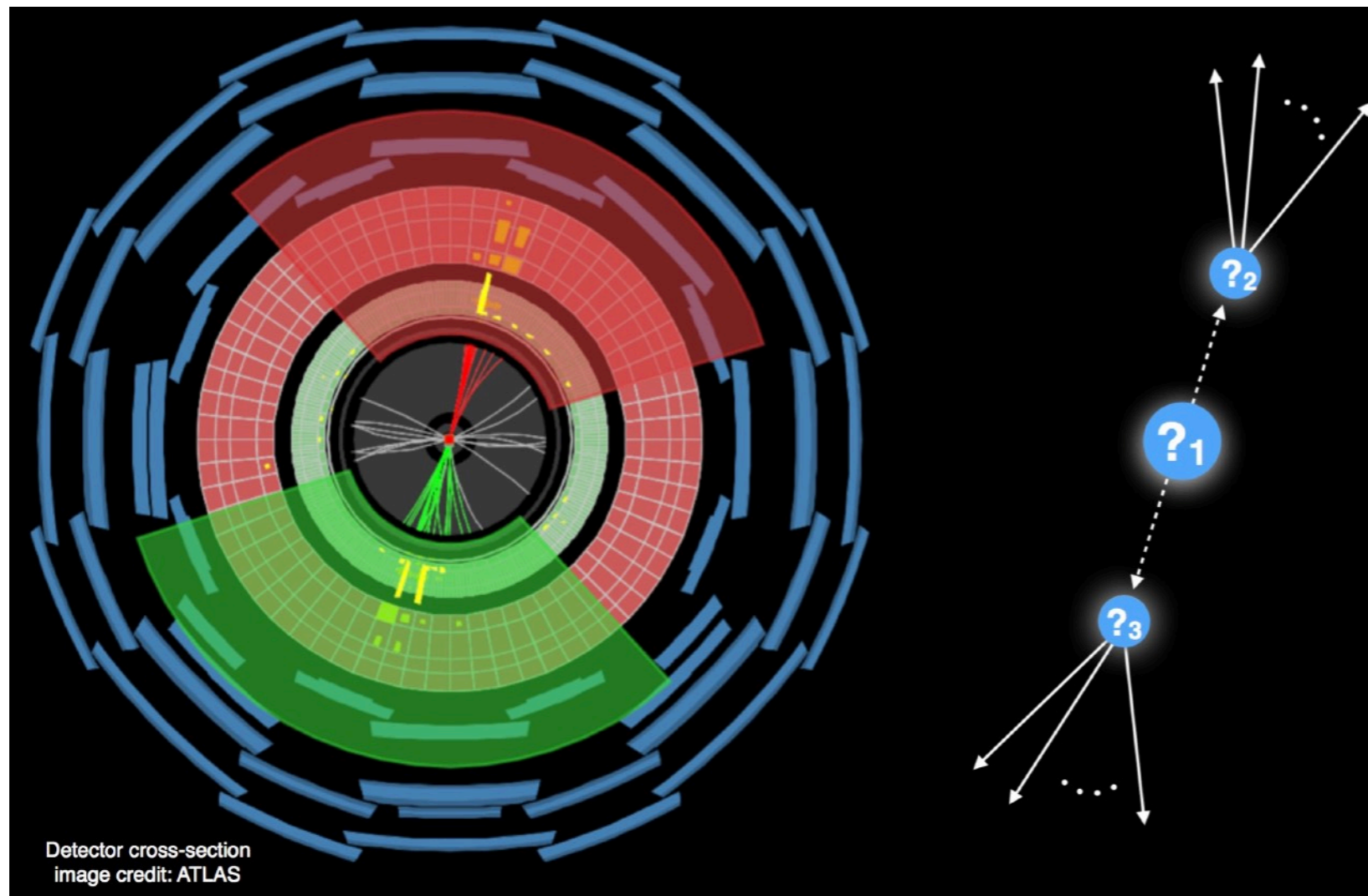
Autoencoders

Anomaly Detection

[Hajer, Li, Liu, Wang, [1807.10261](#); Heibel, Kasieczka, Plehn, Thompson, [1808.08979](#);
Farina, Nakai, Shih, [1808.08992](#); Cerri, Nguyen, Pierini, Spiropulu, Vlimant, [1811.10276](#);
see also Collins, Howe, Nachman, [1805.02664](#), [1902.02634](#); De Simone, Jacques, [1807.06038](#)]

LHC Olympics 2020

@ ML4Jets, NYU, January 15-17

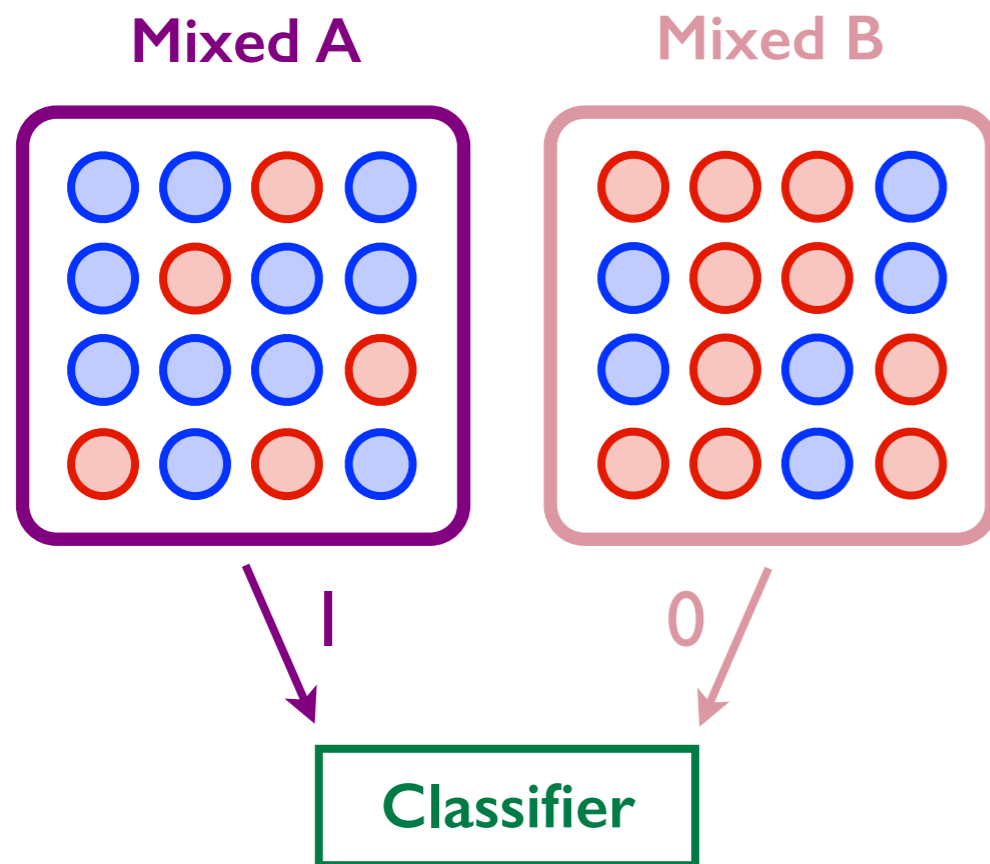


*An opportunity to stress test new **anomaly detection** strategies*

Biases from Training on Simulation?

Train directly on mixed data!

$$p_{\text{mixed}}(\vec{x}) = f_q p_{\text{quark}}(\vec{x}) + (1 - f_q) p_{\text{gluon}}(\vec{x})$$



$$h_{\text{mixed}}(\vec{x}) = \frac{p_A(\vec{x})}{p_A(\vec{x}) + p_B(\vec{x})}$$

$$\neq$$

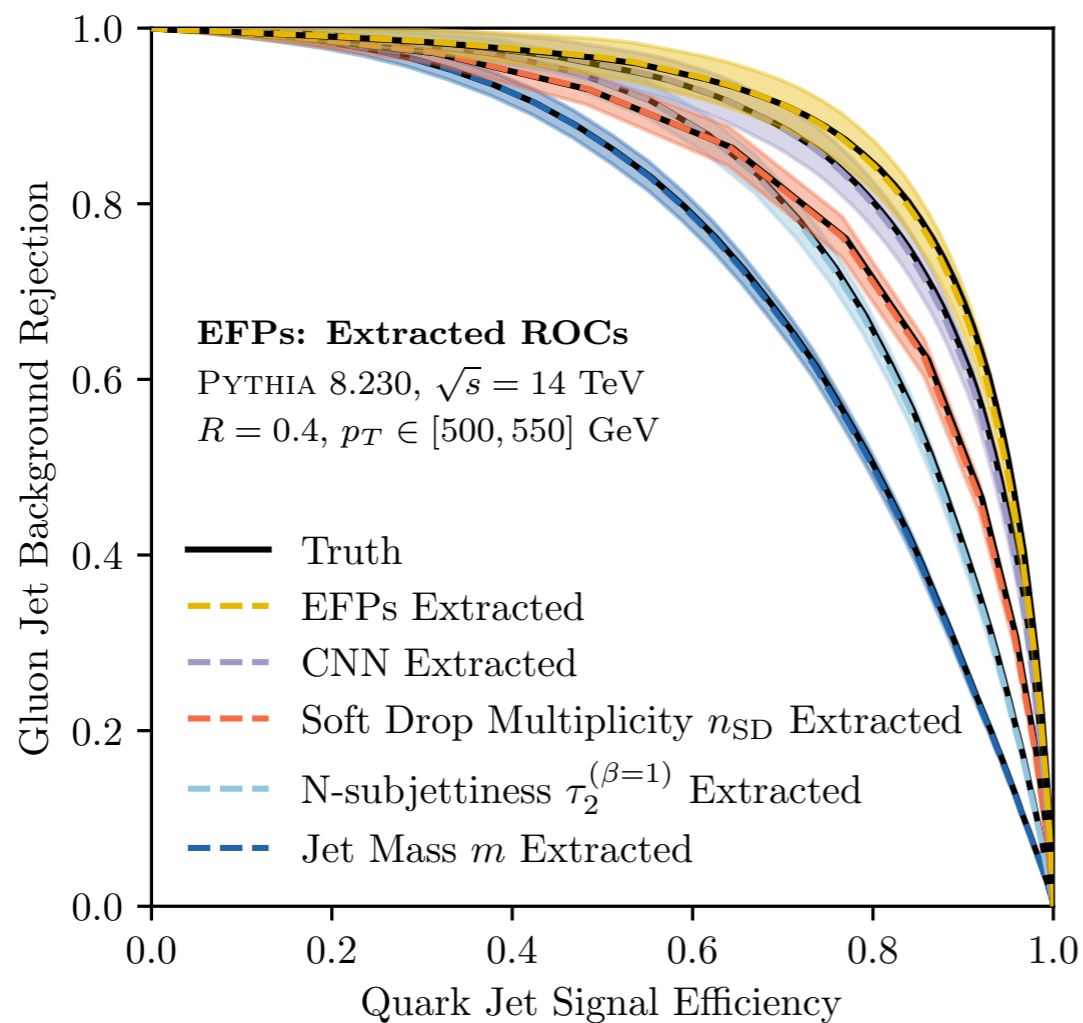
$$h_{\text{pure}}(\vec{x}) = \frac{p_q(\vec{x})}{p_q(\vec{x}) + p_g(\vec{x})}$$

but... $\frac{\partial h_{\text{mixed}}(\vec{x})}{\partial h_{\text{pure}}(\vec{x})} > 0$

[Metodiev, Nachman, JDT, [1708.02949](#);
see also Blanchard, Flaska, Handy, Pozzi, Scott, [1303.1208](#); Cranmer, Pavez, Louppe, [1506.02169](#); Dery, Nachman, Rubbo, Schwartzman, [1702.00414](#);
Cohen, Freytsis, Ostdiek, [1706.09451](#); Komiske, Metodiev, Nachman, Schwartz, [1801.10158](#); Collins, Howe, Nachman, [1805.02664](#), [1902.02634](#)]

Biases from Training on Simulation?

*Train directly on **mixed data**!*



CWoLa:
Classification Without Labels

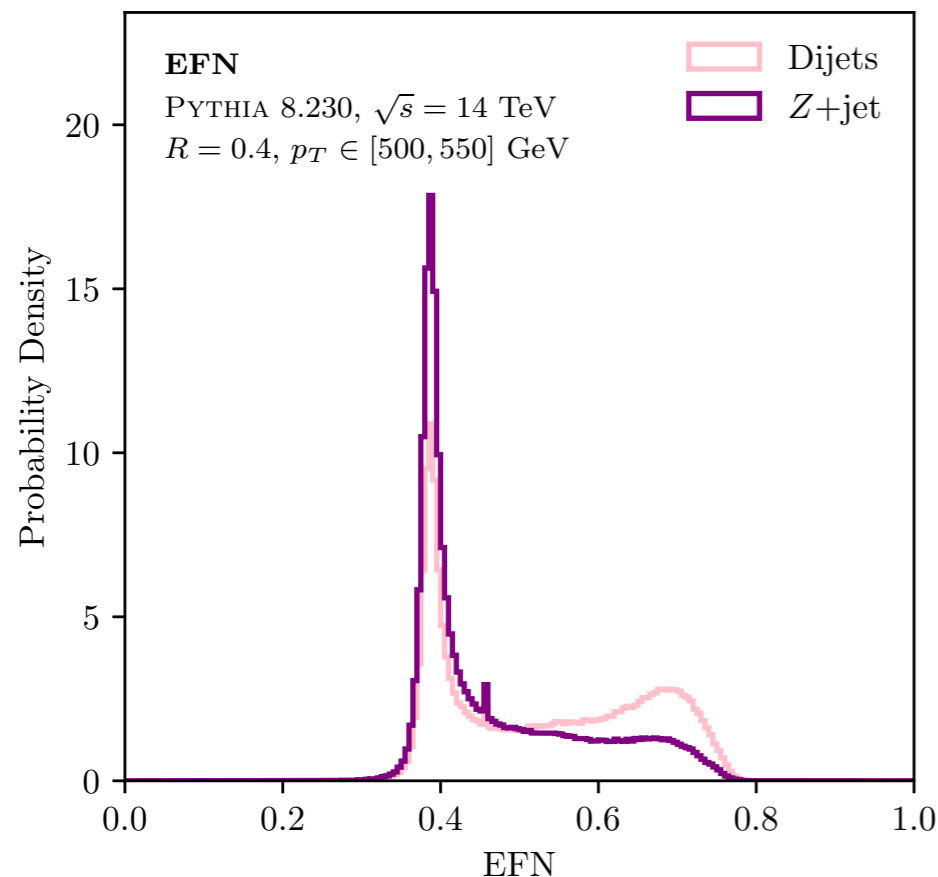
Robust tagging performance
(plus data-driven tricks to calibrate working points and estimate systematic uncertainties)

[Komiske, Metodiev, JDT, [1809.01140](#)]

[Metodiev, Nachman, JDT, [1708.02949](#);
see also Blanchard, Flaska, Handy, Pozzi, Scott, [1303.1208](#); Cranmer, Pavez, Louppe, [1506.02169](#); Dery, Nachman, Rubbo, Schwartzman, [1702.00414](#);
Cohen, Freytsis, Ostdiek, [1706.09451](#); Komiske, Metodiev, Nachman, Schwartz, [1801.10158](#); Collins, Howe, Nachman, [1805.02664](#), [1902.02634](#)]

Ambiguous Definition of Jet Categories?

Use classifiers to *define* categories!



Extract optimal jet categories from data, solely* from assumption they exist (!)

Mutual Irreducibility

“Anchor bins”:
Pure representatives exist for each category (even if very rare)

Sample Independence

Mixed samples have different category fractions but same category properties

$$h_{\text{pure}} \in [0, 1]$$

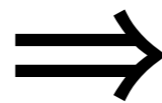
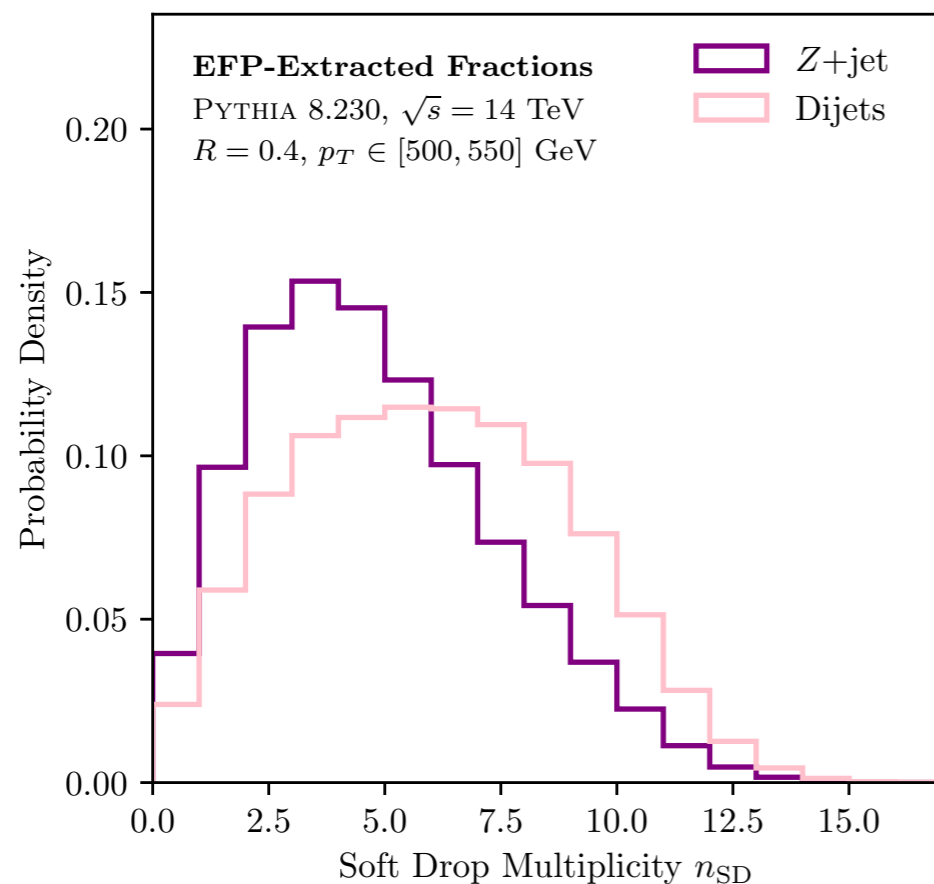
$$h_{\text{mixed}} \in \left[\frac{f_g^A}{f_g^A + f_g^B}, \frac{f_q^A}{f_q^A + f_q^B} \right]$$

[Metodiev, JDT, [1802.00008](#); Komiske, Metodiev, JDT, [1809.01140](#); using Katz-Samuels, Blanchard, Scott, [1710.01167](#)]

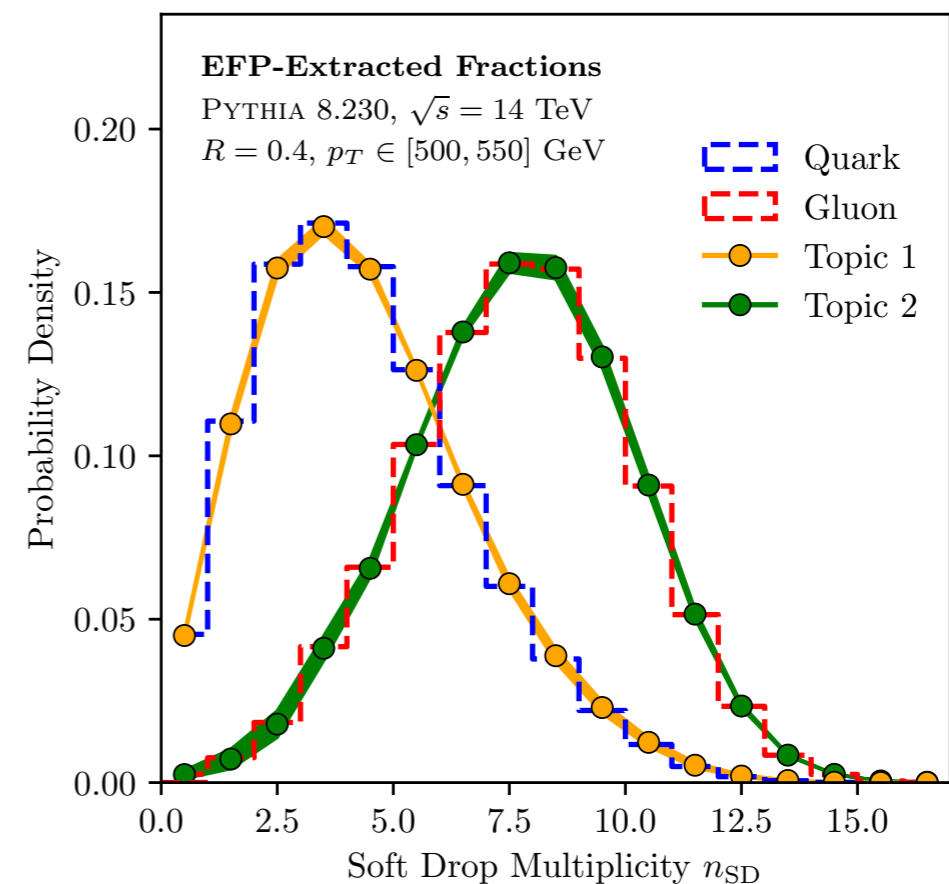
Ambiguous Definition of Jet Categories?

Use classifiers to *define* categories!

Z+jet vs. dijet



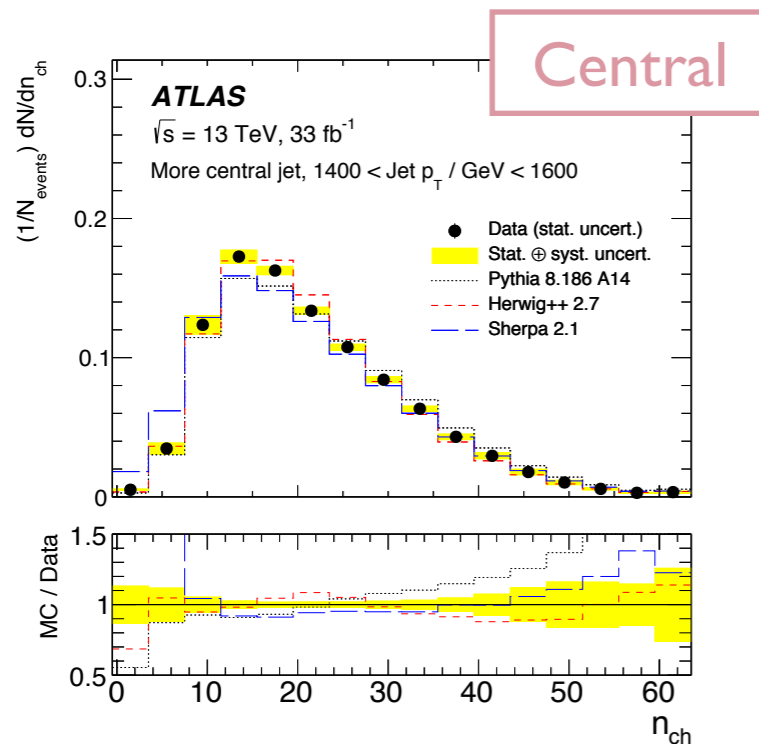
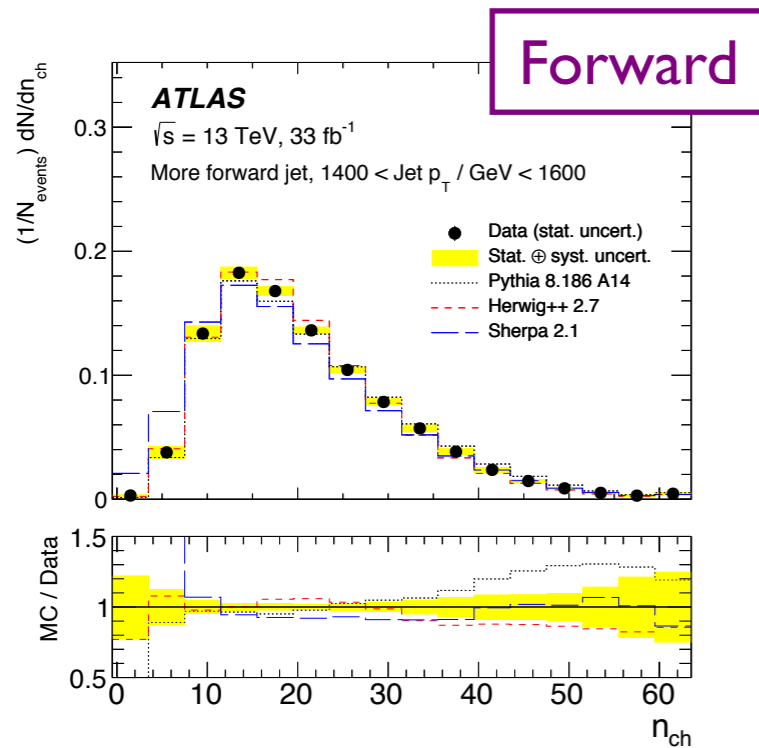
Topic 1 vs. Topic 2



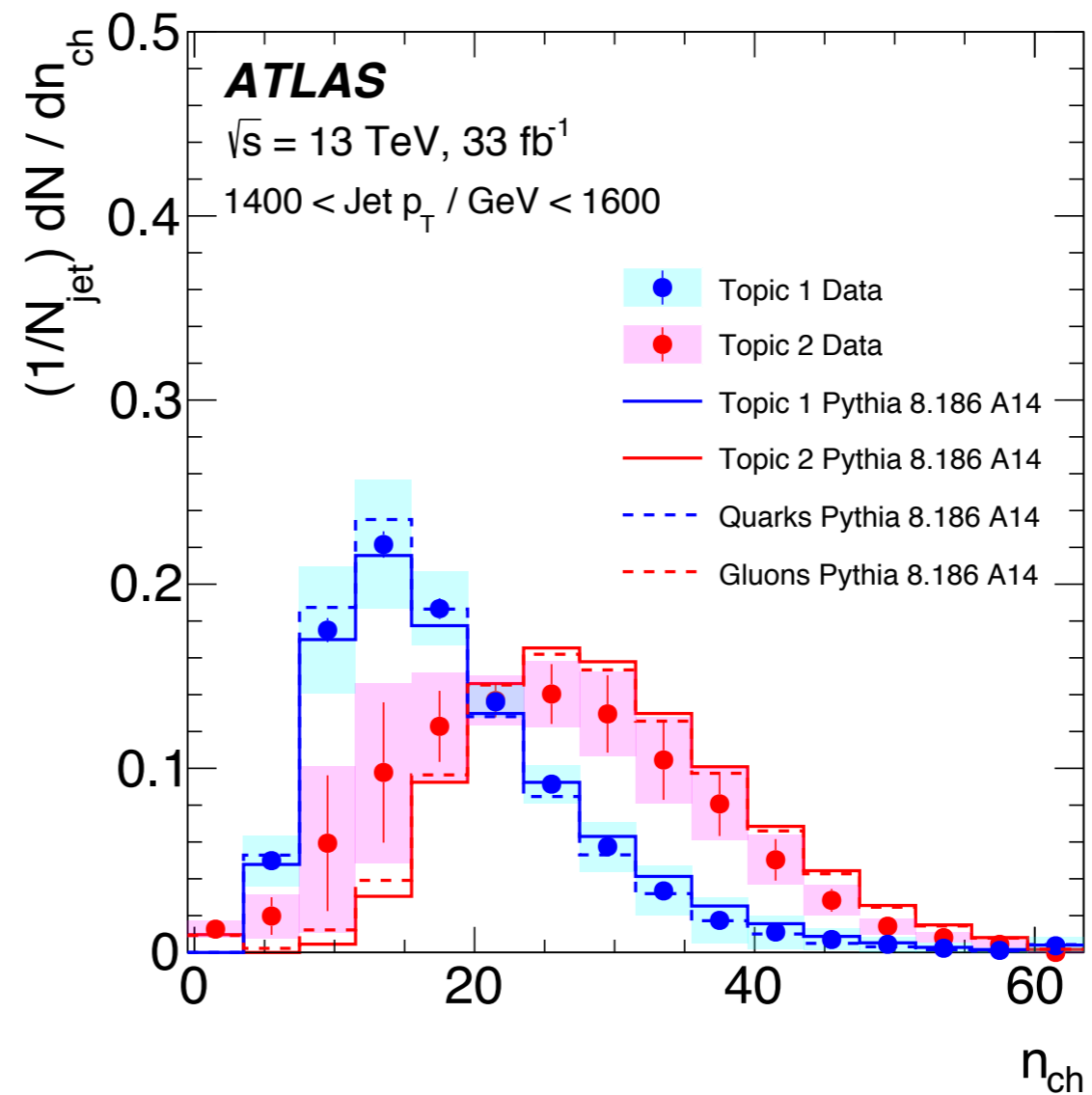
⇒ Operational Definition of “Quark” vs. “Gluon”

“Ok, but do you really think these techniques will ever be applied to real LHC data?”

First Jet Topics Result from ATLAS



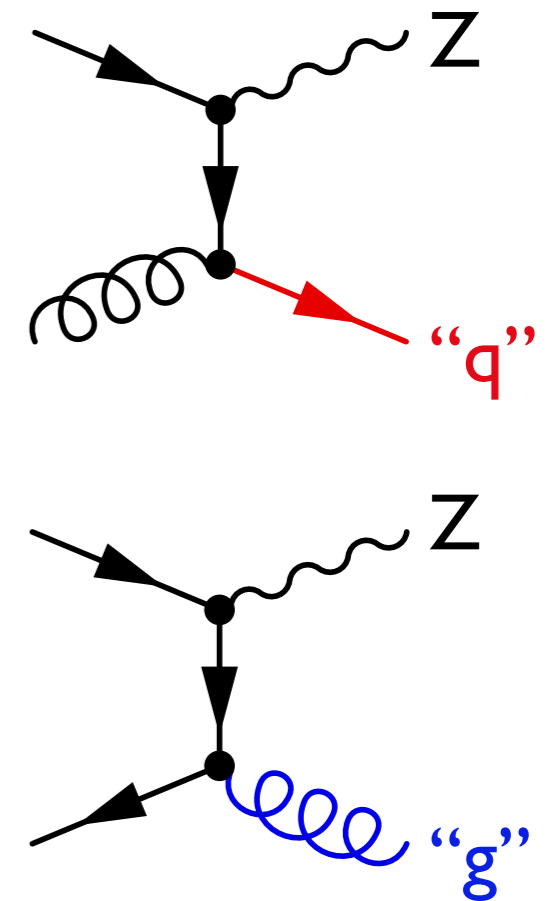
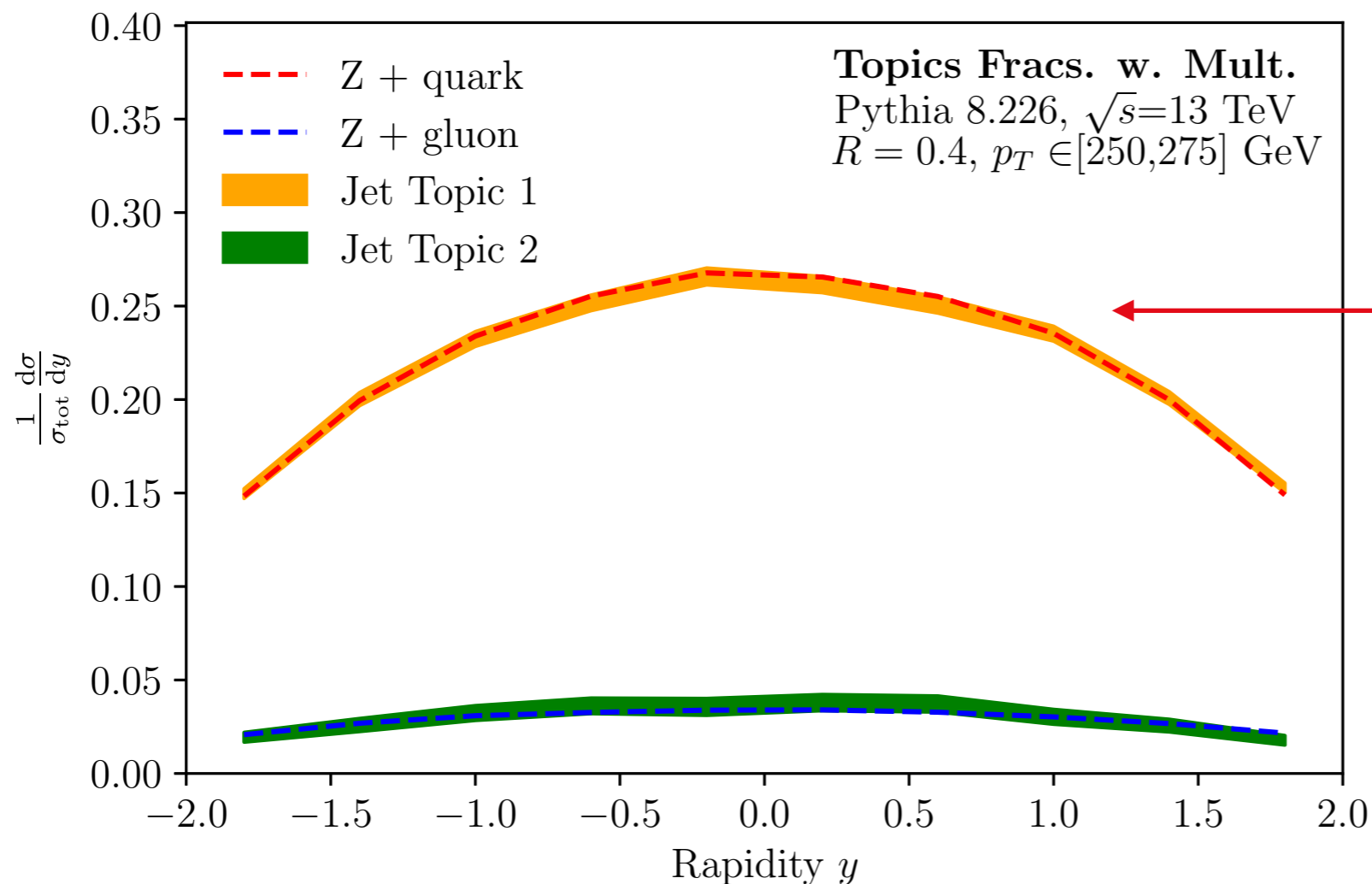
Track multiplicity for “Topic 1” and “Topic 2”



[ATLAS, 1906.09254]

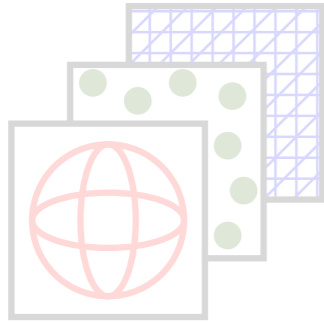
“Parton”-Labeled Cross Sections?

Potential boon for PDF extraction at colliders



Key Challenges: Sample dependence from color coherence
Limited statistics in anchor bin region
Defining jet topics at fixed order

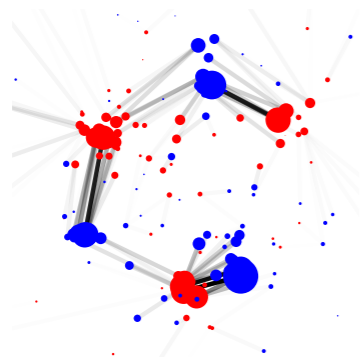
[Metodiev, JDT, 1802.00008]



Into the Network



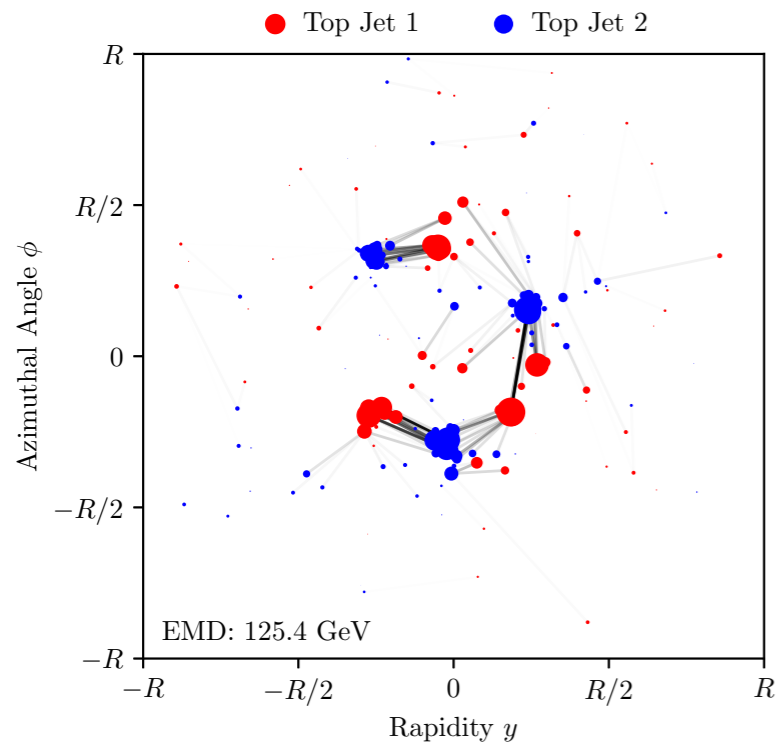
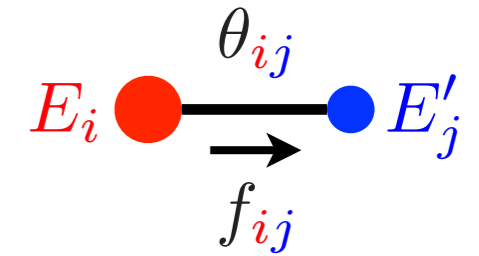
Data Ex Machina



(The Space of Jets)

The Energy Mover's Distance

Closely related to 1-Wasserstein metric



Optimal transport between energy flows...

$$\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \underbrace{\sum_i \sum_j f_{ij} \frac{\theta_{ij}}{R}}_{\text{Cost to move energy}} + \underbrace{\left| \sum_i E_i - \sum_j E'_j \right|}_{\text{Cost to create energy}}$$

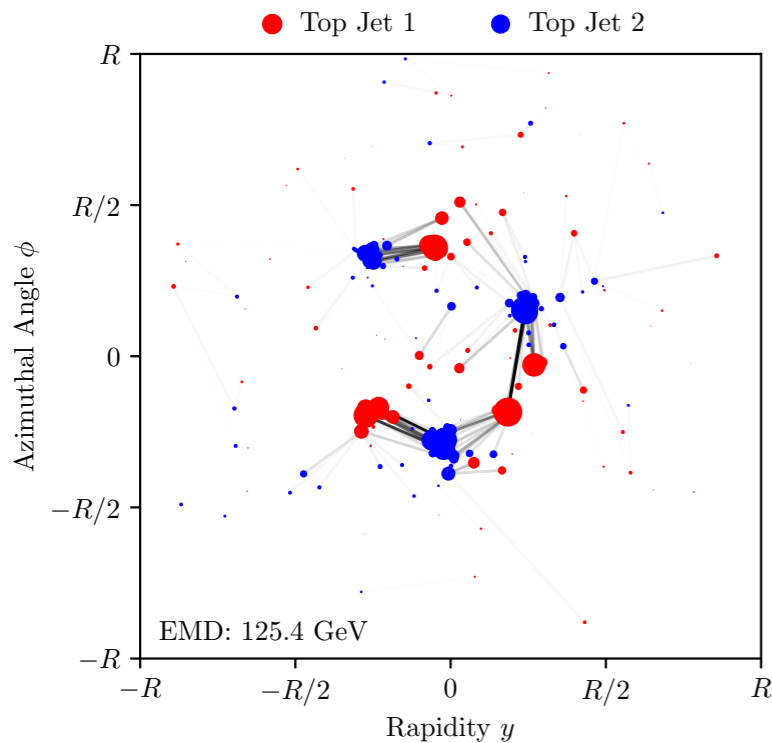
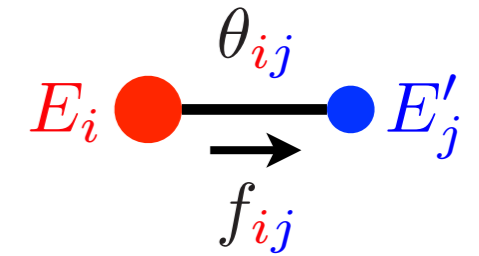
in GeV

[Komiske, Metodiev, JDT, 1902.02346;

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

The Energy Mover's Distance

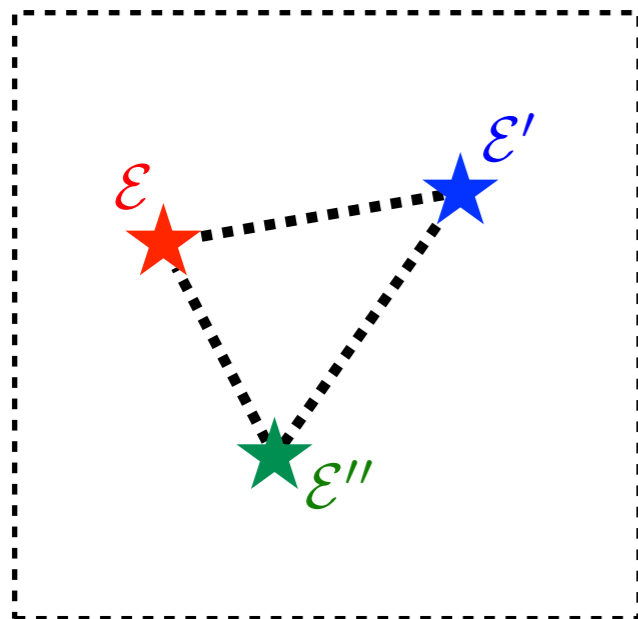
Closely related to 1-Wasserstein metric



Optimal transport between energy flows...

$$\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \underbrace{\sum_i \sum_j f_{ij} \frac{\theta_{ij}}{R}}_{\text{Cost to move energy}} + \underbrace{\left| \sum_i E_i - \sum_j E'_j \right|}_{\text{Cost to create energy}}$$

↑
in GeV



...defines a metric on the space of events

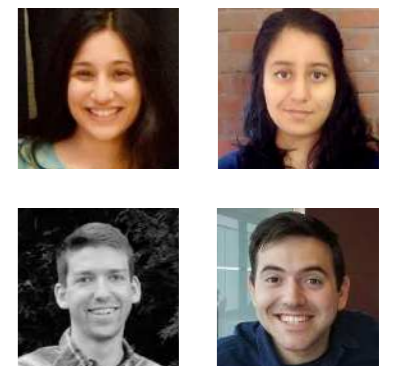
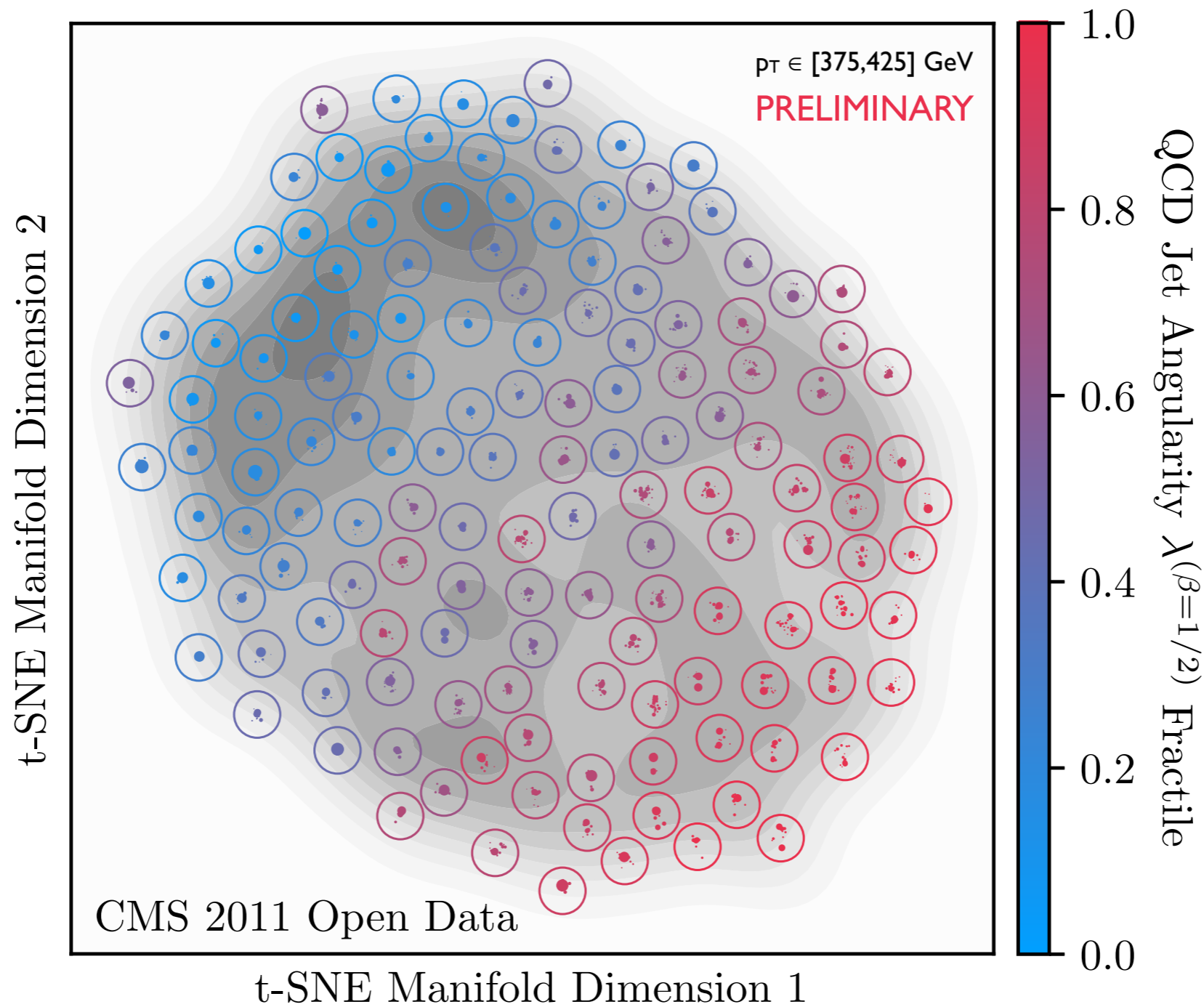
$$0 \leq \text{EMD}(\mathcal{E}, \mathcal{E}') \leq \text{EMD}(\mathcal{E}, \mathcal{E}'') + \text{EMD}(\mathcal{E}', \mathcal{E}'')$$

(assuming $R \geq \theta_{\max}/2$, i.e. $R \geq$ jet radius for conical jets)

[Komiske, Metodiev, JDT, 1902.02346;

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

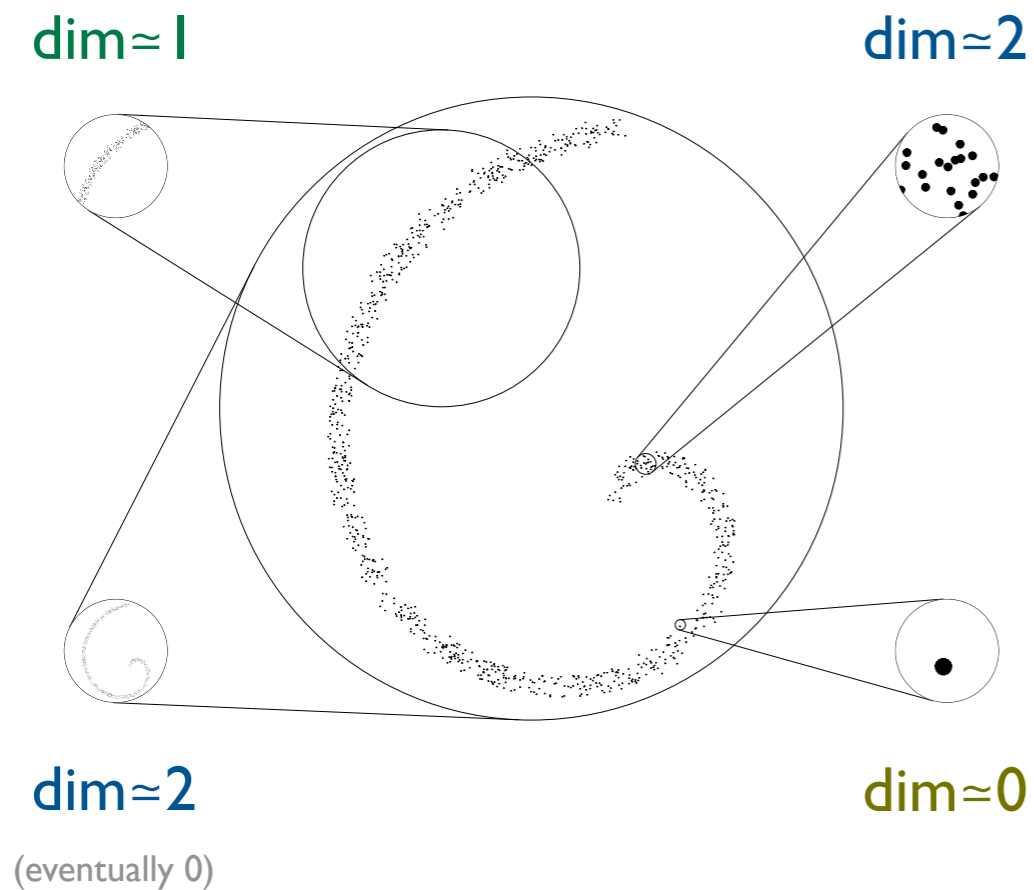
The Space of Quark/Gluon Jets



[Komiske, Mastandrea, Metodiev, Naik, JDT, in preparation]

Quantifying Dimensionality

Correlation Dimension: $\dim(Q) = Q \frac{\partial}{\partial Q} \ln \sum_i \sum_j \Theta(\text{EMD}(\mathcal{E}_i, \mathcal{E}_j) < Q)$



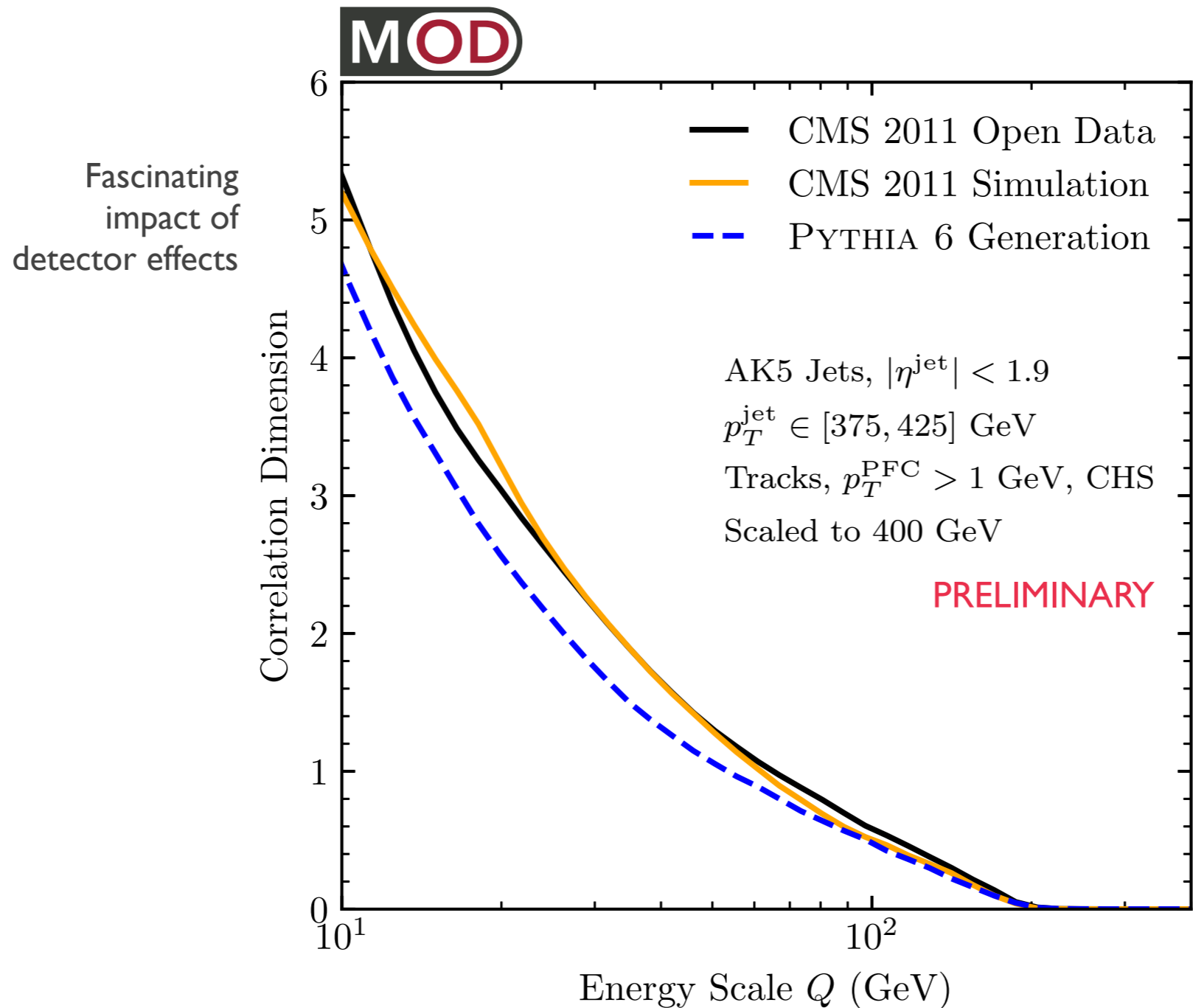
$$N_{\text{neighbors}}(r) \sim r^{\text{dim}}$$

\Downarrow

$$\dim(r) \sim r \frac{\partial}{\partial r} \ln N_{\text{neighbors}}(r)$$

[Grassberger, Procaccia, [PRL 1983](#); Kégl, [NIPS 2002](#)]

The Dimension of Quark/Gluon Jets



[Komiske, Mastandrea, Metodiev, Naik, JDT, in preparation]

Preliminary Calculation

Leading Log:

(single log, since dim has derivative)

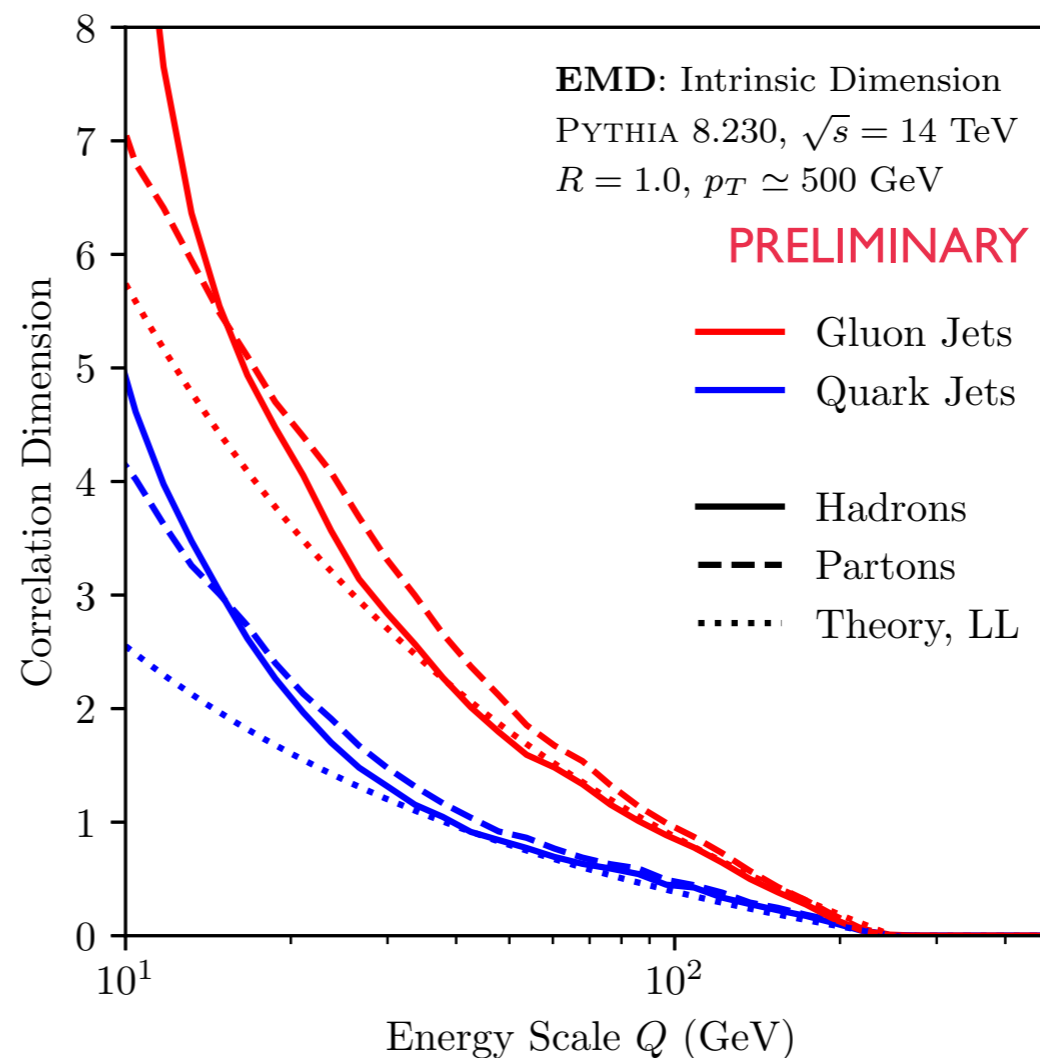
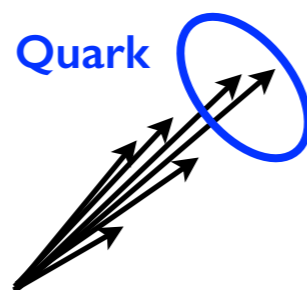
$$\dim_i(Q) \simeq -\frac{8\alpha_s}{\pi} C_i \ln \frac{Q}{p_T}$$

↑
Color Factor

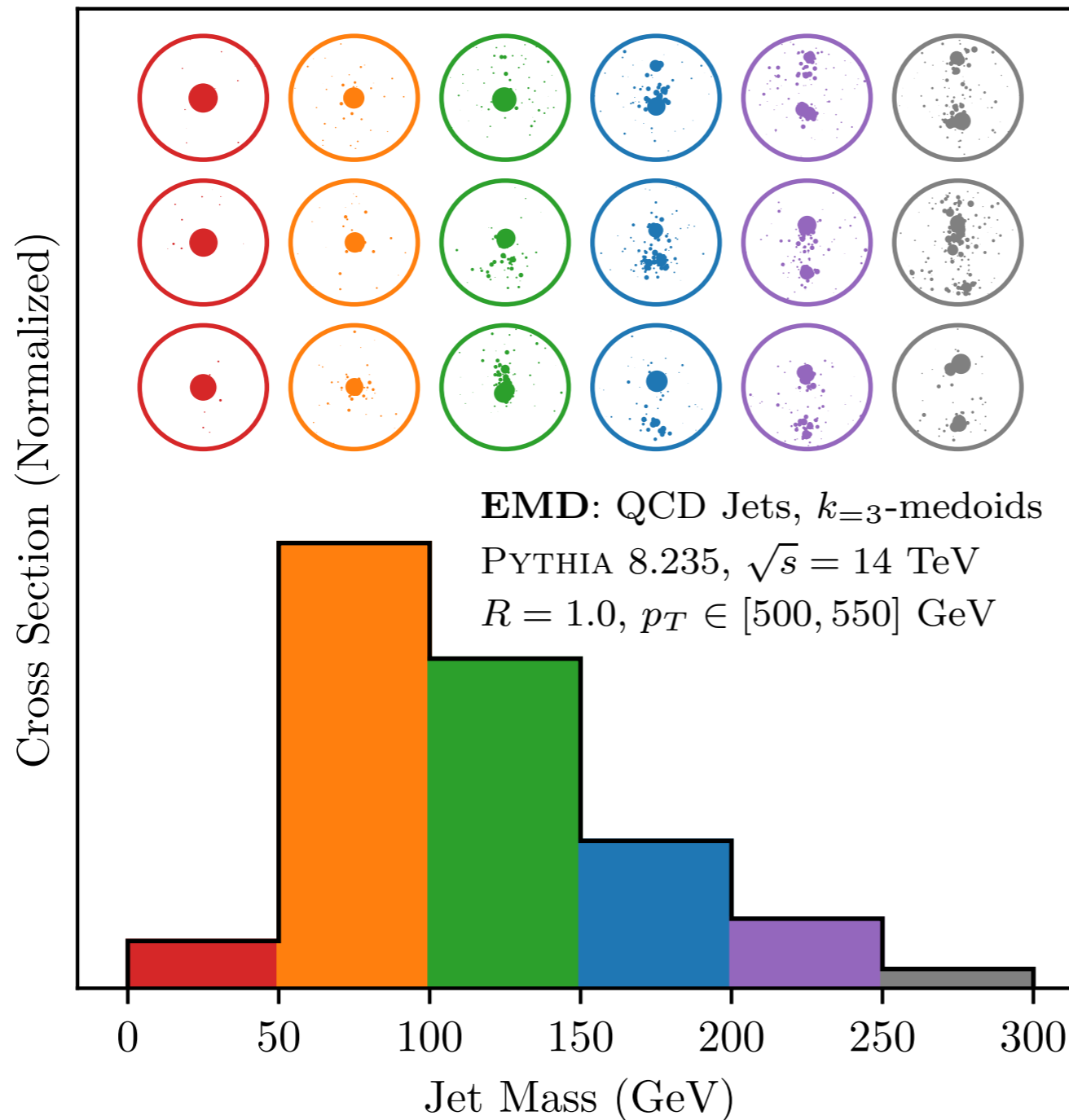
$$C_A = 3$$



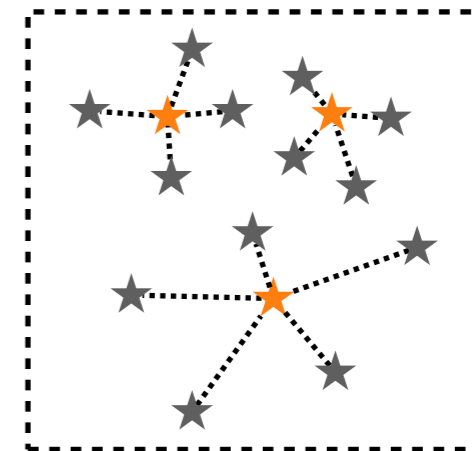
$$C_F = 4/3$$



Histograms meet Event Displays



3-medoid: Three most representative jets in each bin

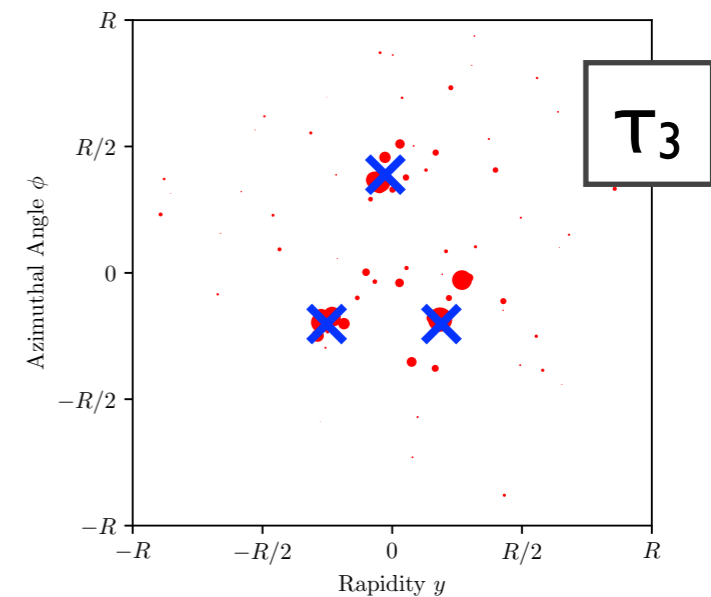
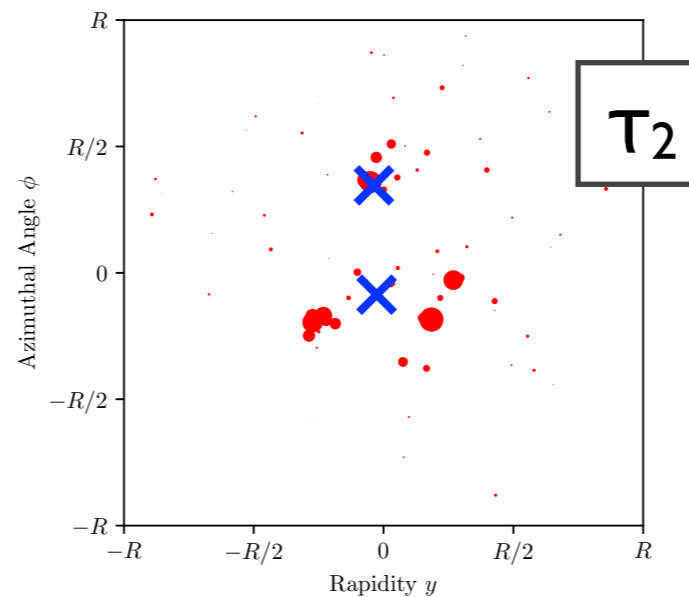
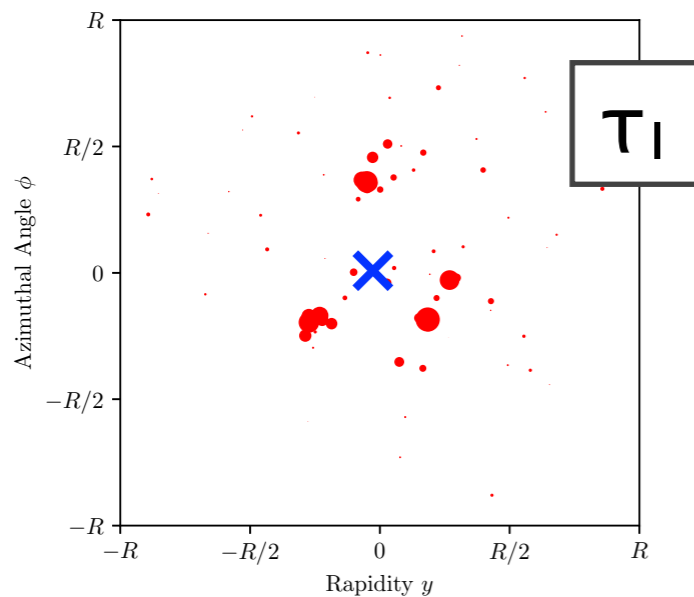


[Komiske, Metodiev, JDT, [1902.02346](#)]

Insight into N-subjettiness

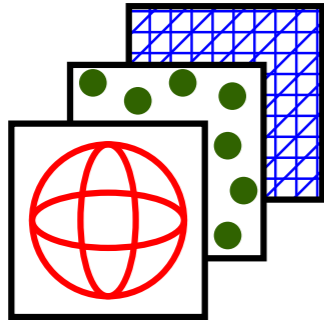
$$\tau_N^{(\beta)}(\mathcal{E}) = \min_{N \text{ axes}} \sum_i E_i \min \left\{ \theta_{1,i}^\beta, \theta_{2,i}^\beta, \dots, \theta_{N,i}^\beta \right\}$$

↑
IRC safe
↑
kind of arbitrary



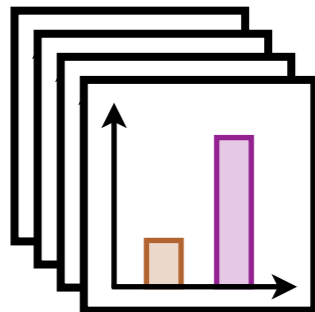
[JDT, Van Tilburg, [1011.2268](#), [1108.2701](#);
based on Brandt, Dahmen, [ZPC 1979](#); Stewart, Tackmann, Waalewijn, [1004.2489](#)]

Summary



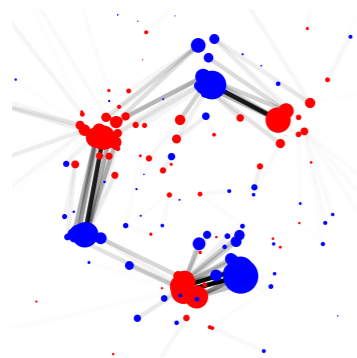
Into the Network

Designing architectures around symmetries and interpretability



Data Ex Machina

Unsupervised learning to interpret hadronic final states



(The Space of Jets)

Computational geometry as a new collider data analysis strategy



Patrick Komiske



Eric Metodiev

(Theoretical)
High Energy
Physics

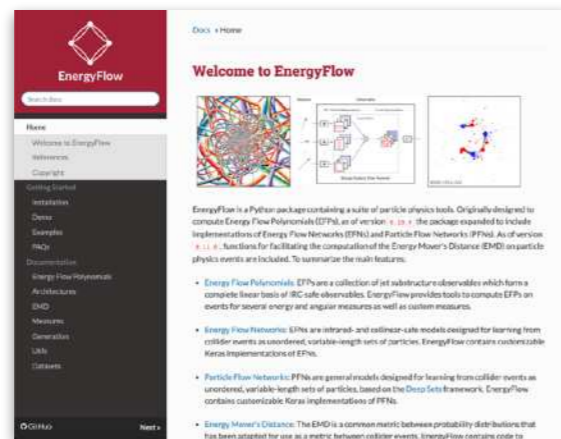


Mathematics,
Statistics,
Computer Science



Energy Flow Package

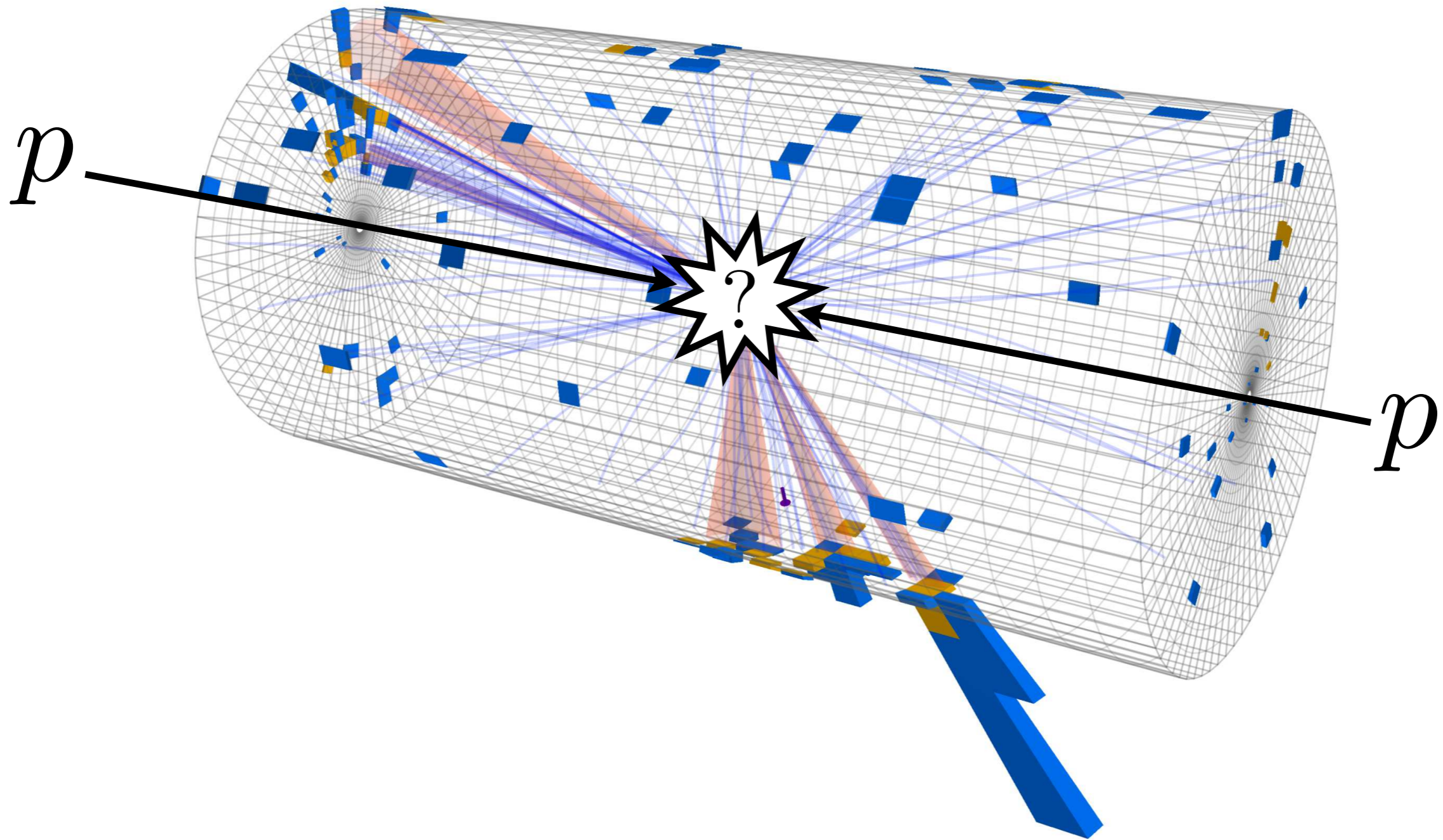
<https://energyflow.network/>



Backup Slides

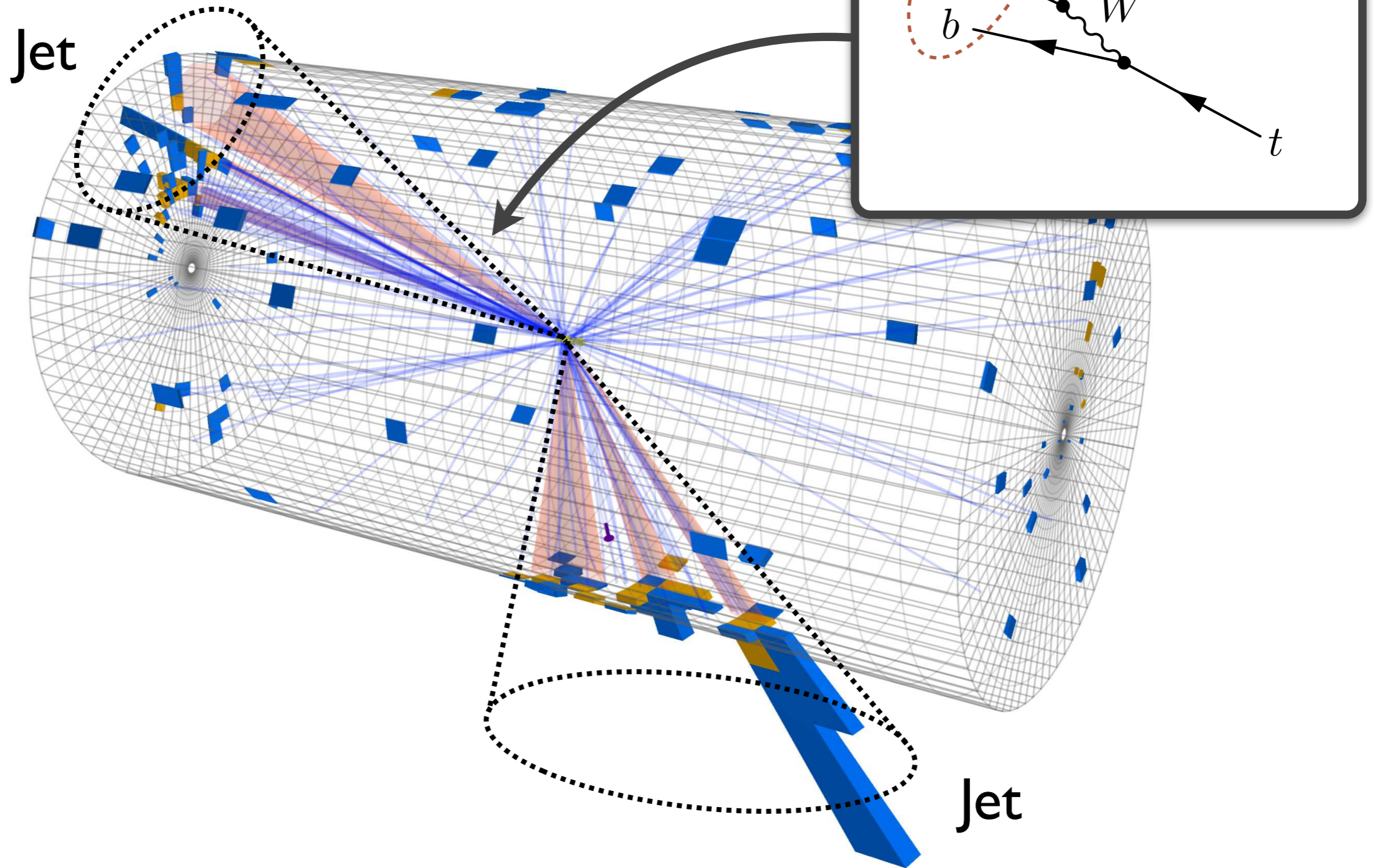


CMS Experiment at LHC, CERN
Data recorded: Sun Jul 12 07:25:11 2015 CEST
Run/Event: 251562 / 111132974
Lumi section: 122
Orbit/Crossing: 31722792 / 2253





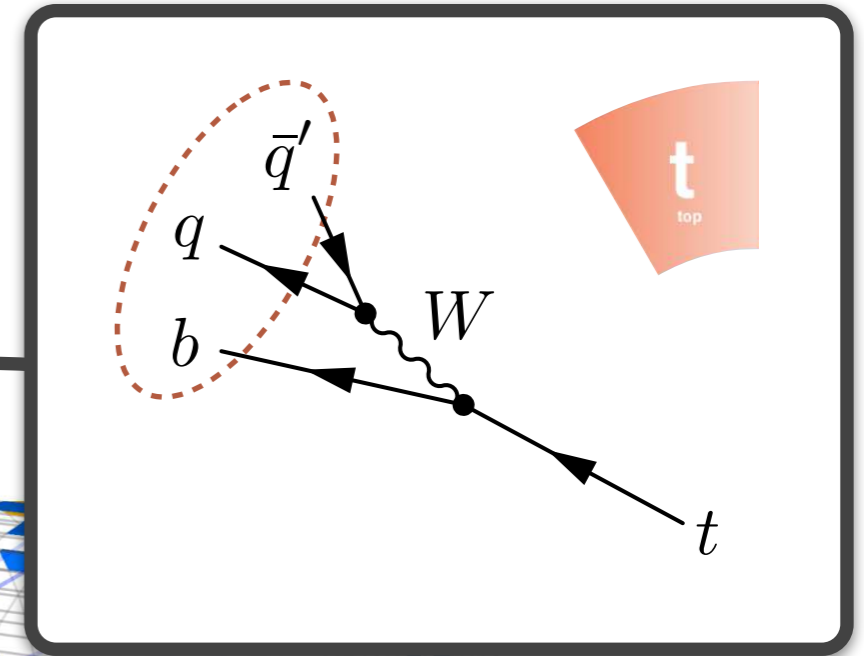
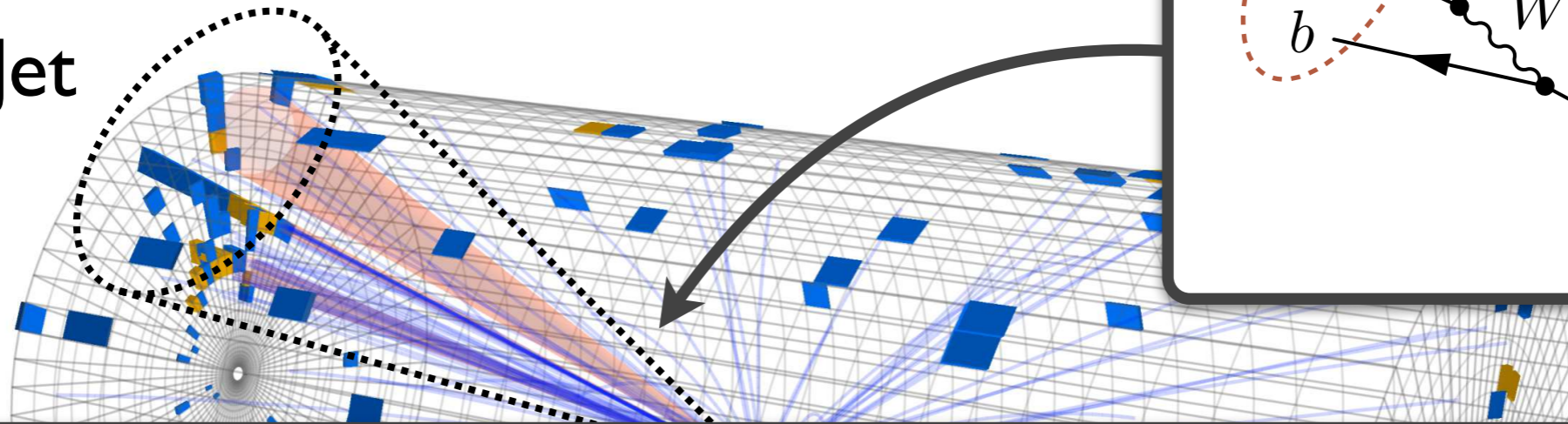
CMS Experiment at LHC, CERN
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CMS Experiment at LHC, CERN
 Data recorded: Sun Jul 12 07:25:11 2015 CEST
 Run/Event: 251562 / 111132974
 Lumi section: 122
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Jet



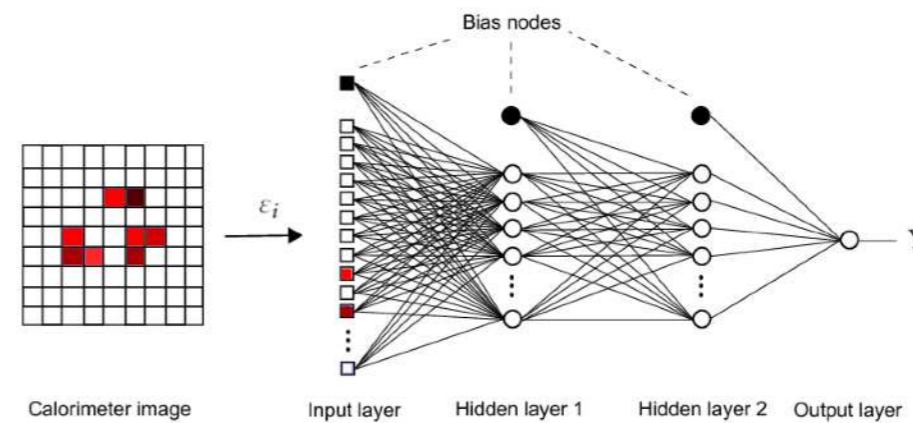
“Deep Thinking”?

[e.g. JDT, Van Tilburg, [1011.2268](#), [1108.2701](#);
 rephrased in language of Komiske, Metodiev, JDT, [1902.02346](#)]

$$\tau_N(\mathcal{J}) = \min_{|\mathcal{J}'|=N} \text{EMD}(\mathcal{J}, \mathcal{J}')$$

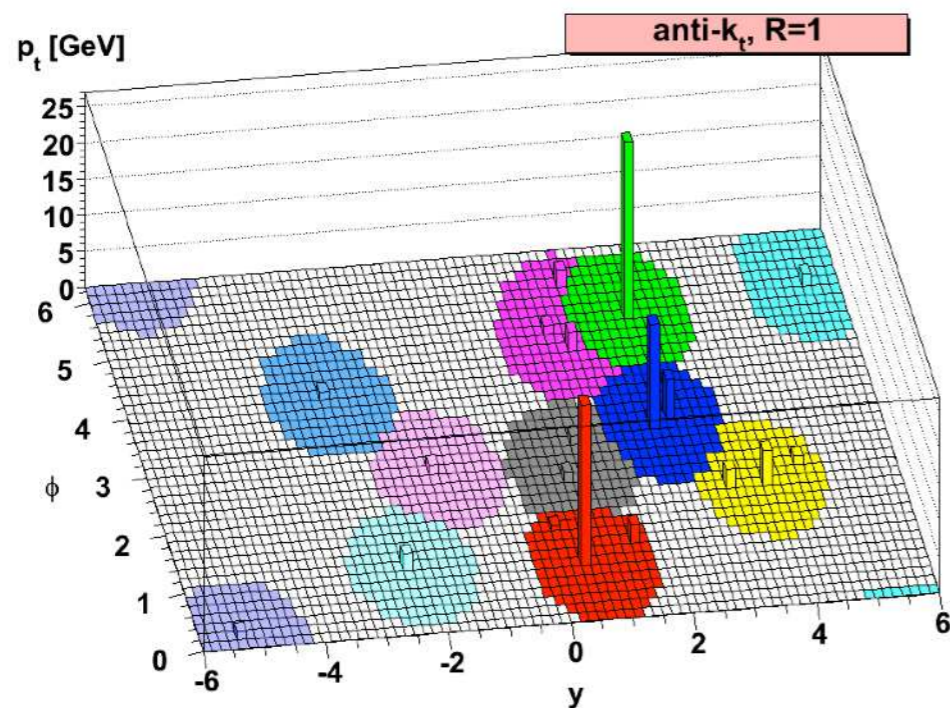
“Deep Learning”?

[e.g. Almeida, Backović, Cliche, Lee, Perelstein, [1501.05968](#);
 review in Kasieczka, Plehn, et al., [1902.09914](#)]

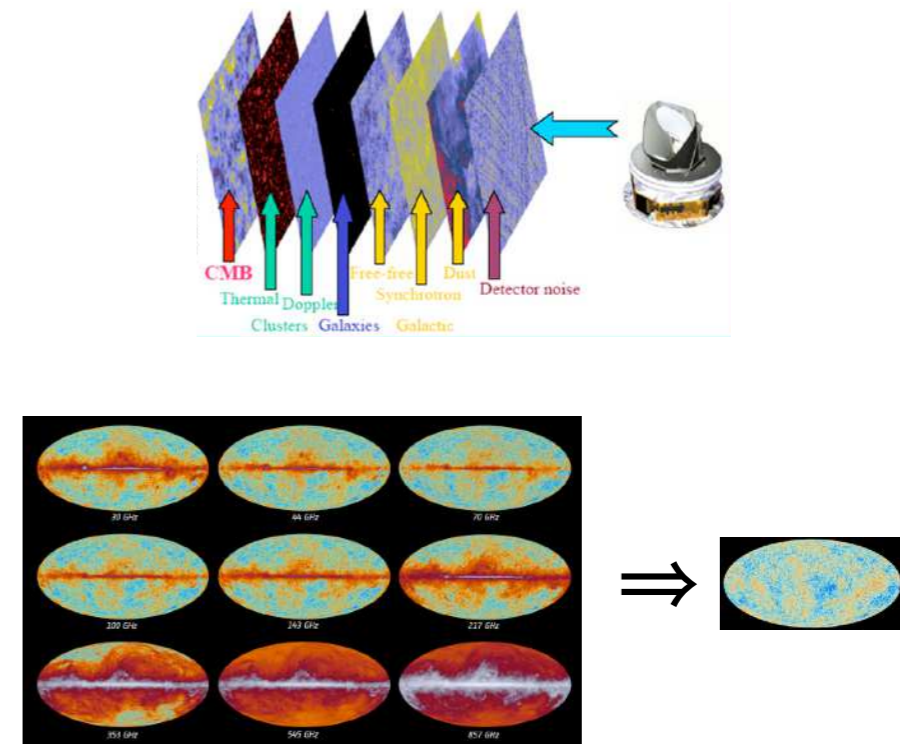


Examples of Unsupervised Learning

Clustering



Topic Modeling

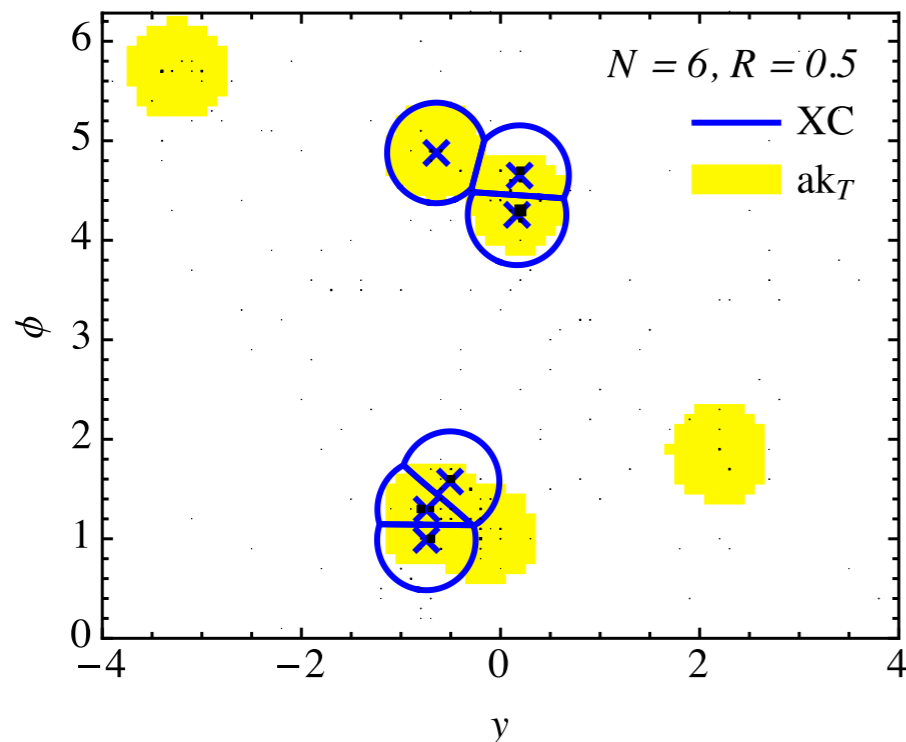


(Approximate) *solutions* to *properly specified problems*

[figures from Cacciari, Salam, Soyez, 0802.1189; Planck Outreach]

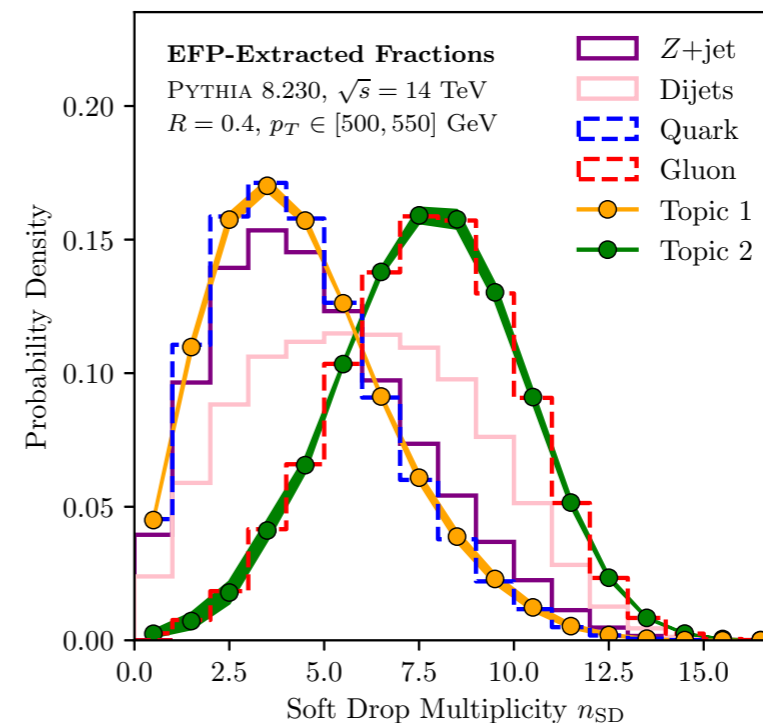
Examples of Unsupervised Learning

XCone Jet Finding



“Find N axes that minimize N -jettiness”

Jet Topics



“Find two mutually irreducible distributions”

[Stewart, Tackmann, JDT, Vermilion, Wilkason, [1508.01516](#); based on Stewart, Tackmann, Waalewijn, [1004.2489](#)]
[Metodiev, JDT, [1802.00008](#); Komiske, Metodiev, JDT, [1809.01140](#); see also Dillon, Faroughy, Kamenik, [1904.04200](#)]

(Approximate) *solutions* to *properly specified problems*

[figures from Cacciari, Salam, Soyez, [0802.1189](#); Planck Outreach]

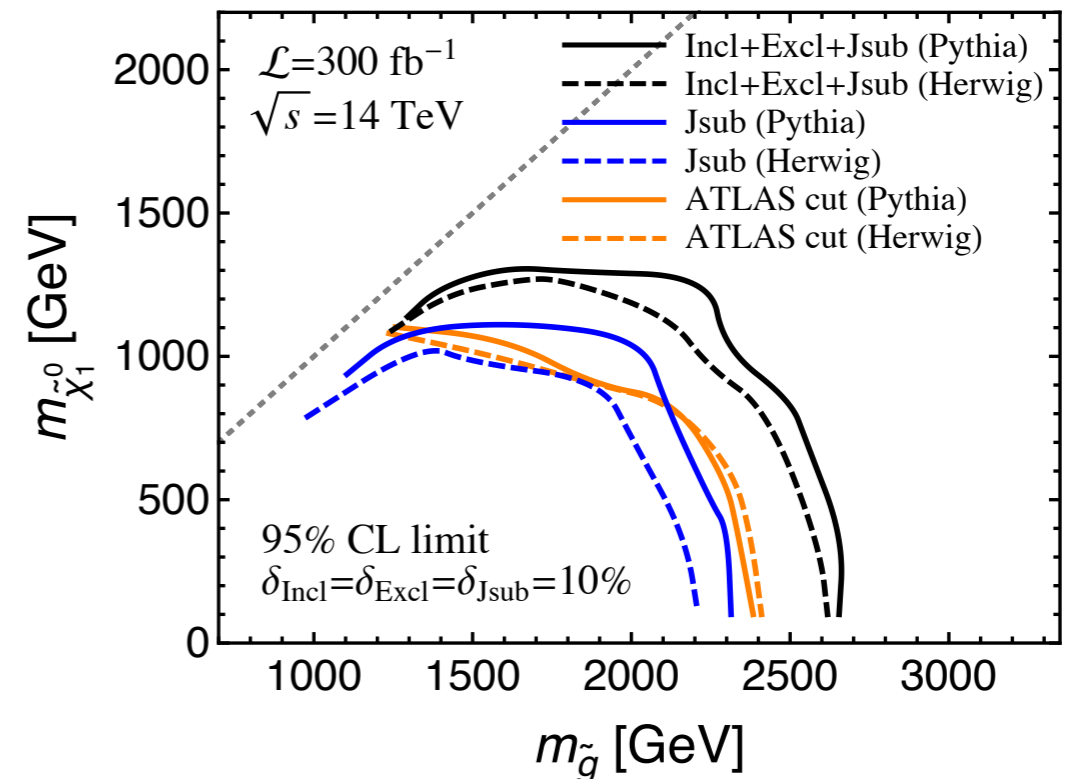
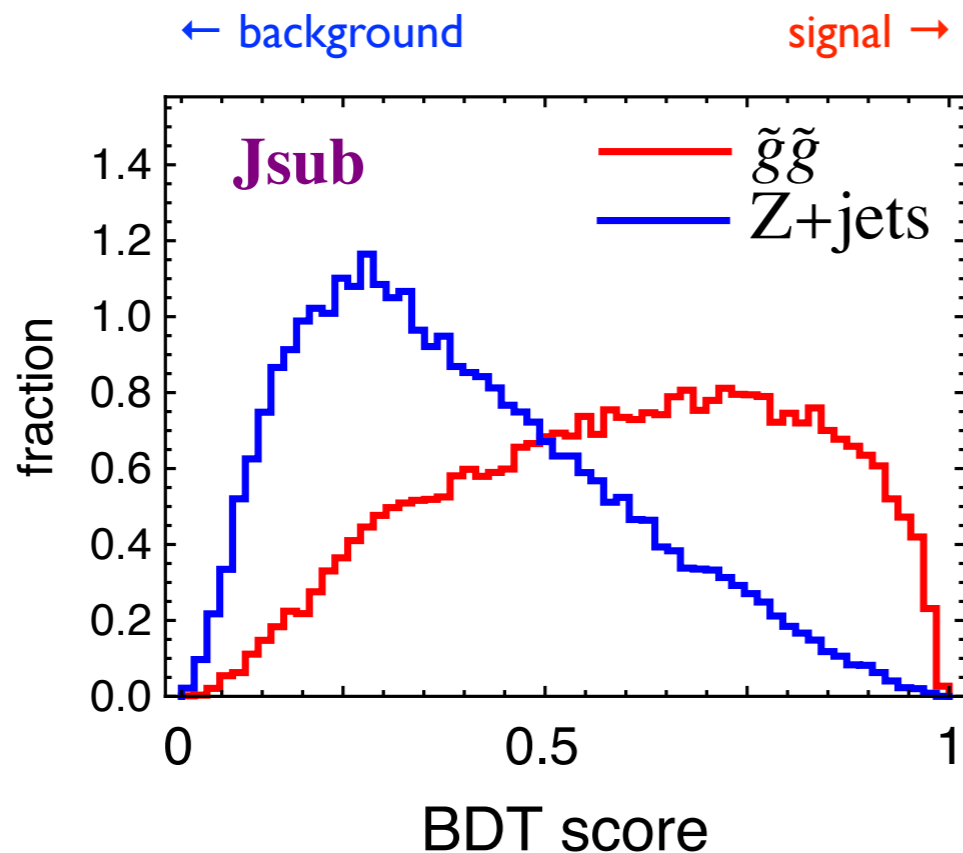
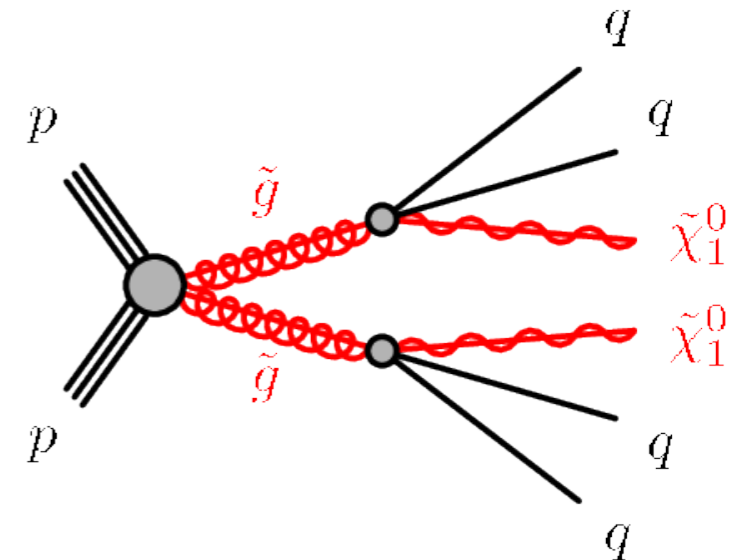
E.g. SUSY Search for Gluino Pairs

Classifier: Boosted decision tree (for each of 4 jets)

Inputs: Jet mass, width, track multiplicity

Signal: Quark enriched ($C_F = 4/3$)

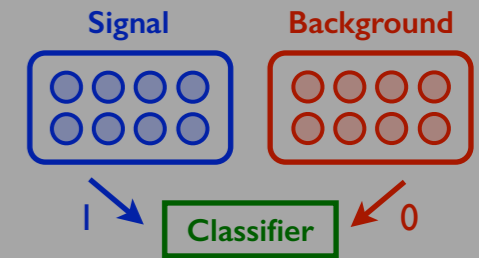
Background: Gluon enriched ($C_A = 3$)



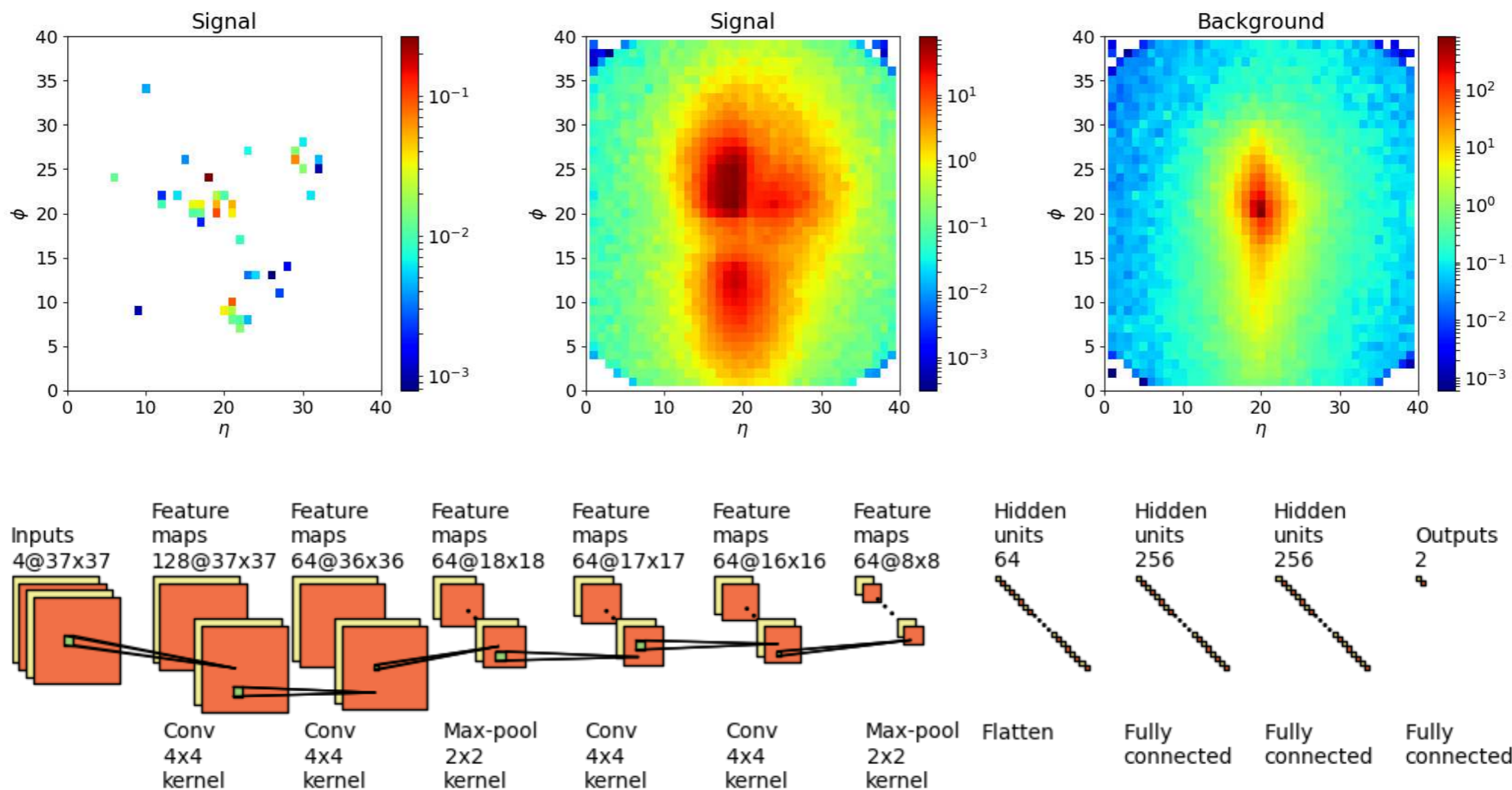
[Bhattacharjee, Mukhopadhyay, Nojiri, Sakakie, Webber, [1609.08781](#)]

Jet Classification Studies

Mix and match

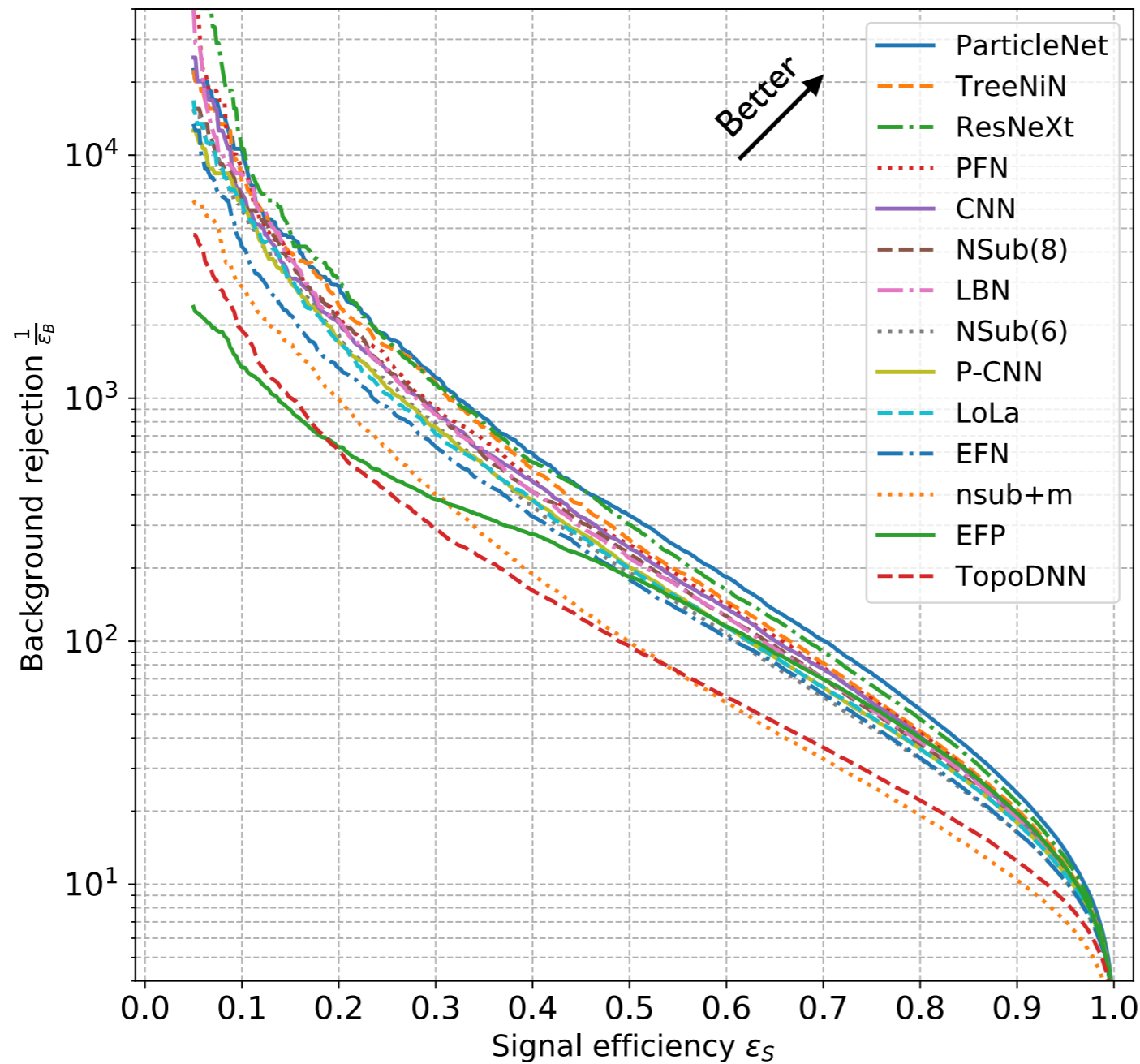
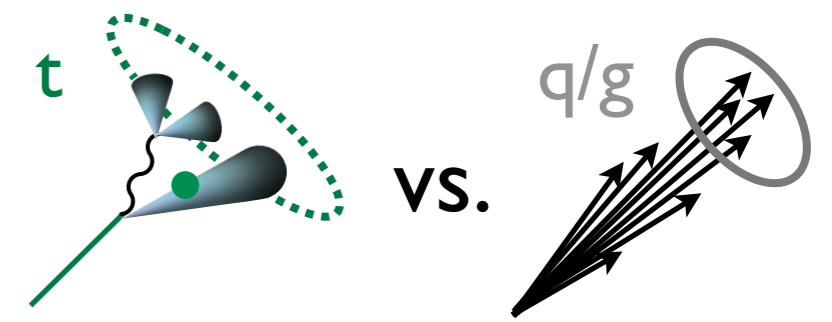


Deep Learning: Jet Image Strategy with CNNs



[Macaluso, Shih [1803.00107](#); building off Kasieczka, Plehn, Russell, Schell, [1701.08784](#); based on Cogan, Kagan, Strauss, Schwartzman, [1407.5675](#); de Oliveira, Kagan, Mackey, Nachman, Schwartzman, [1511.05190](#)]

Throwing Down the Gauntlet

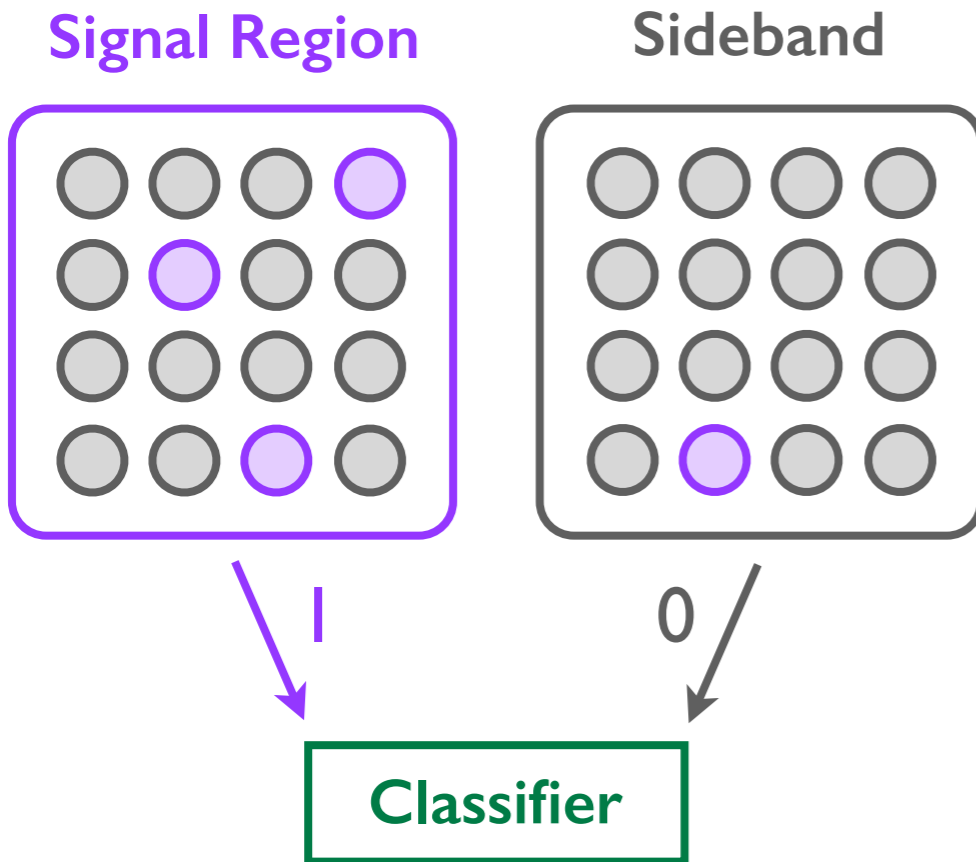
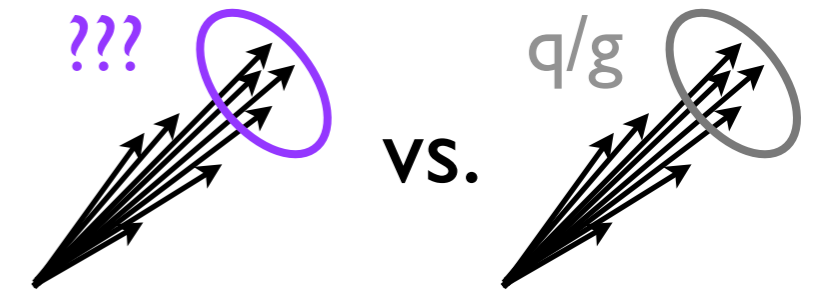


← “Deep Pockets”
 ← Previous slide
 ← Deep Sets
 ← “Deep Thinking”

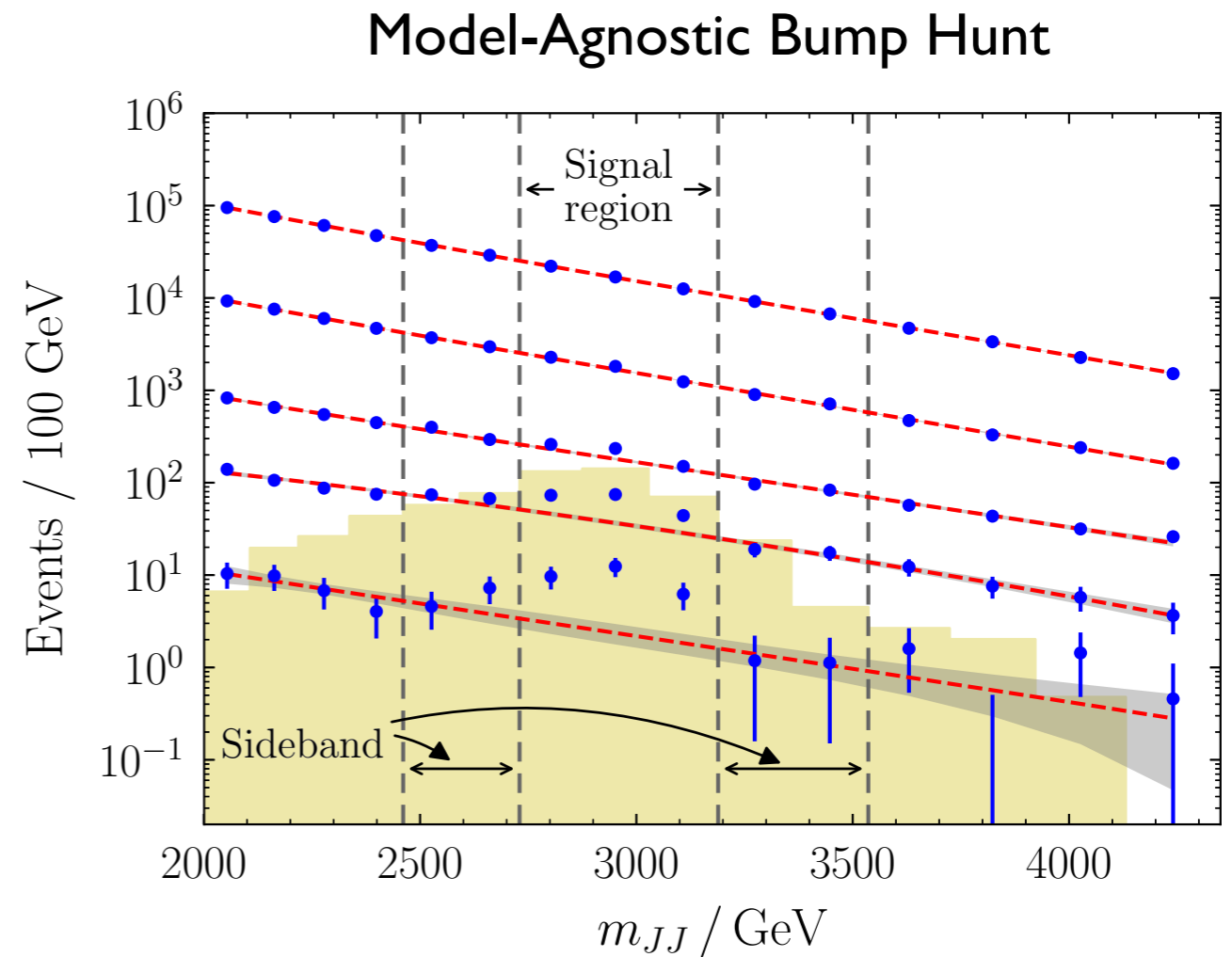
[Kasieczka, Plehn, et al., [1902.09914](#);
 comparison of [JDT, Van Tilburg, 1011.2268, 1108.2701](#); [Xie, Girshick, Dollár, Tu, He, 1611.05431](#); CMS-DP-2017-049; Pearkes, Fedorko, Lister, Gay, [1704.02124](#);
 Butter, Kasieczka, Plehn, Russell, [1707.08966](#); Komiske, Metodiev, JDT, [1712.07124](#); [Macaluso, Shih 1803.00107](#); Moore, Nordström, Varma, Fairbairn [1807.04769](#);
 Komiske, Metodiev, JDT, [1810.05165](#); Erdmann, Geiser, Rath, Rieger, [1812.09722](#); Qu, Gouskos, [1902.08570](#); Macaluso, Cranmer, to appear]

CWoLa Hunting

Using “Classification Without Labels”

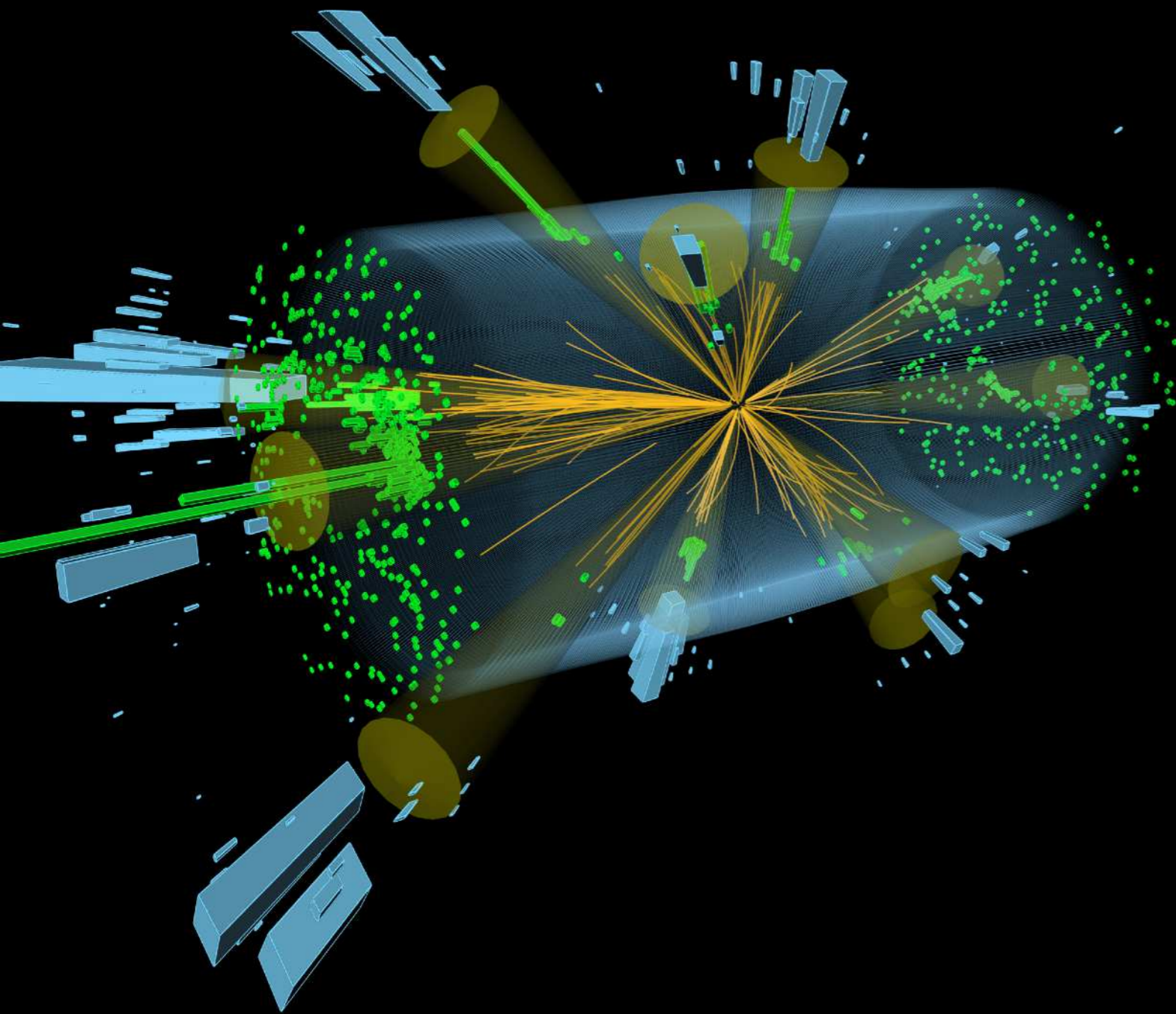


With enough data, monotonic
w.r.t. optimal classifier (!)



[Collins, Howe, Nachman, [1805.02664](#), [1902.02634](#); using Metodiev, Nachman, [JDT, 1708.02949](#); see also Blanchard, Flaska, Handy, Pozzi, Scott, [1303.1208](#); Cranmer, Pavez, Louppe, [1506.02169](#)]

What is a Collision Event?



T E H M

	●		γ	photon
●	●		e^{\pm}	electron
●	●	●	μ^{\pm}	muon
●	●	●	π^{\pm}	pion
●	●	●	K^{\pm}	kaon
	●	●	K_L^0	K-long
●	●	●	p/\bar{p}	proton
	●	●	n/\bar{n}	neutron

elementary

composite

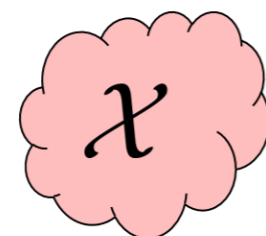
Point Cloud



[Popular Science, 2013]

Meanwhile in ML-Land: Deep Sets

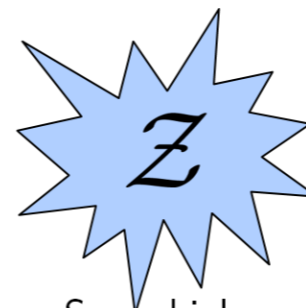
Theorem 2 A function $f(X)$ operating on a set X having elements from a countable universe, is a valid set function, i.e., **invariant** to the permutation of instances in X , iff it can be decomposed in the form $\rho\left(\sum_{x \in X} \phi(x)\right)$, for suitable transformations ϕ and ρ .



Original space

Variable-Length
Unordered Set
of Particles

$$\xleftrightarrow[\text{Homeomorphism}]{z = E(X) = \sum_{x \in X} \phi(x)}$$



Some higher dim space

Additive
Latent Space

$$\xrightarrow[\text{Continuous map}]{\rho(z) = f(E^{-1}(z))}$$

\mathbb{R}

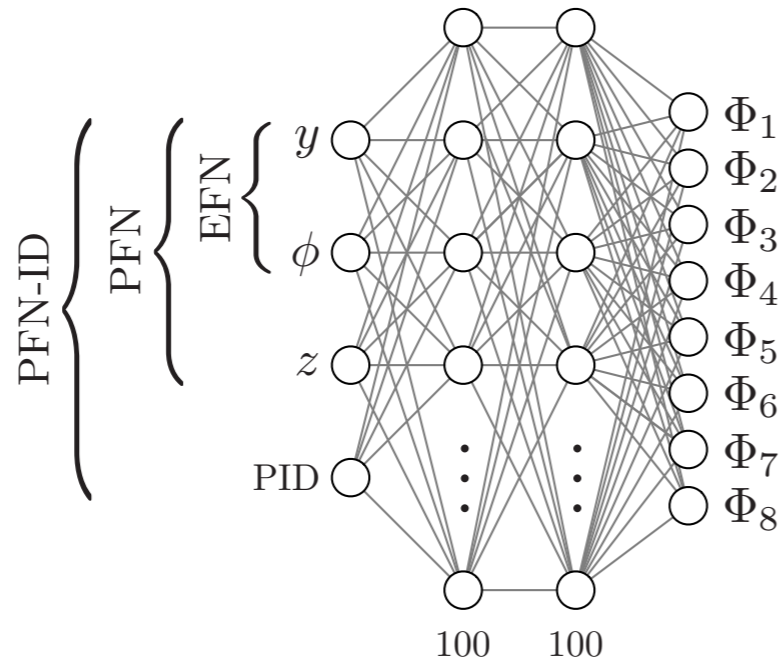
Target space

Generic
Observable

[Zaheer, Kottur, Ravanbakhsh, Póczos, Salakhutdinov, Smola, [1703.06114](#); see also Vinyals, Bengio, Kudlur, [1511.06391](#); Qi, Su, Mo, Guibas, [1612.00593](#)]

Technical Implementation

Per-Particle Network: Φ

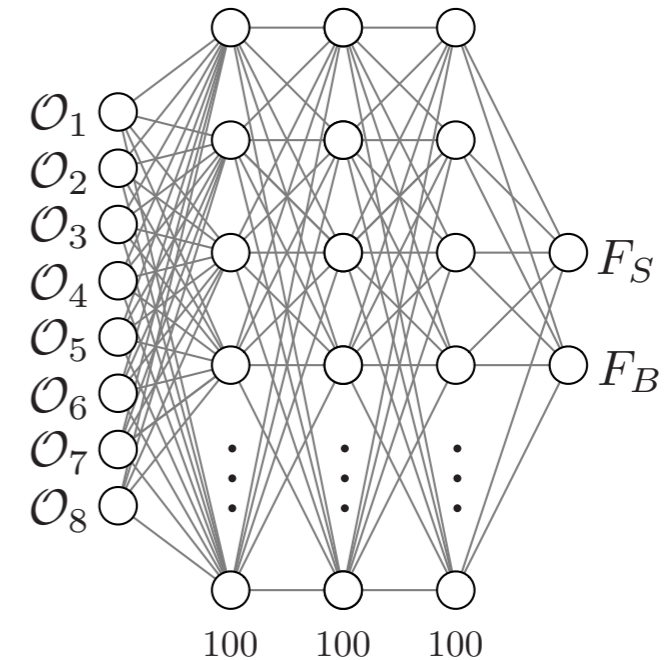


Per-Jet (Latent Space):

$$\text{EFN: } \mathcal{O}_a = \sum_{i \in \text{jet}} z_i \Phi_a(y_i, \phi_i) \quad z_i = \frac{p_{Ti}}{\sum_j p_{Tj}}$$

$$\text{PFN: } \mathcal{O}_a = \sum_{i \in \text{jet}} \Phi_a(y_i, \phi_i, z_i, \text{PID}_i)$$

Latent Combiner: F

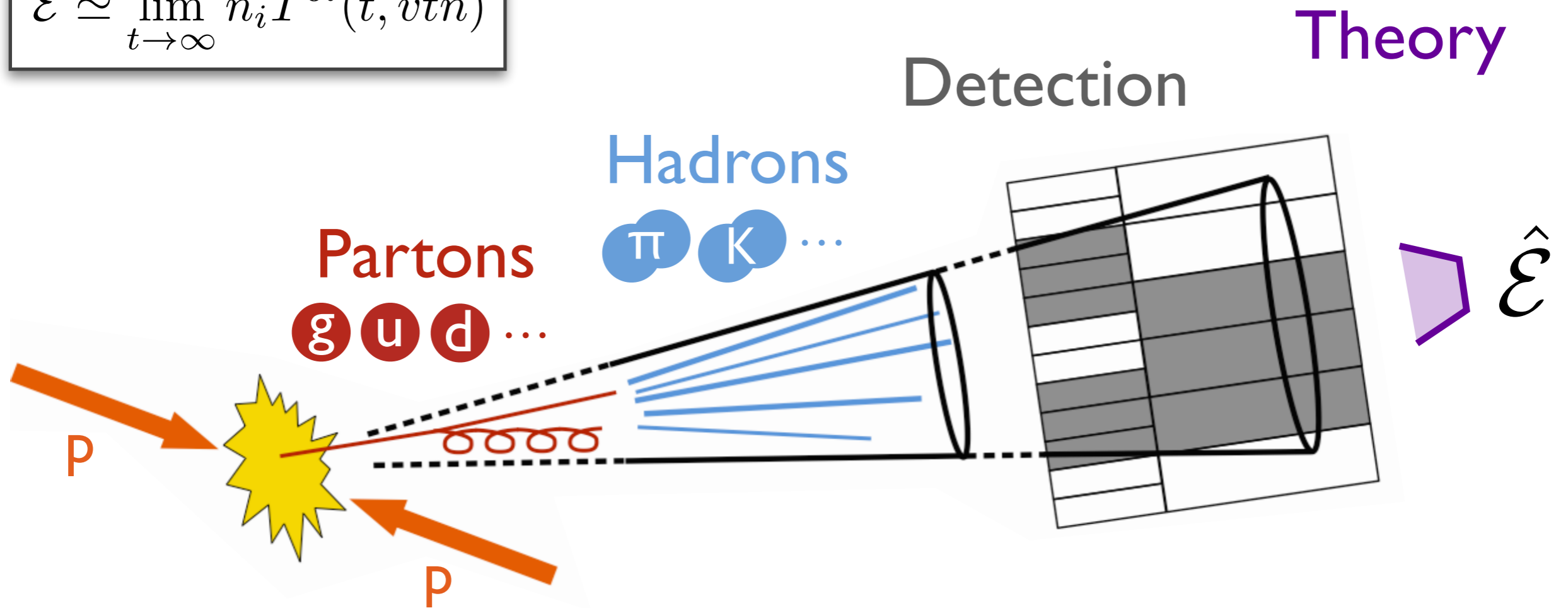


Final Discriminant:

$$\text{softmax}(F_S, F_B)$$

Focus on Energy Flow

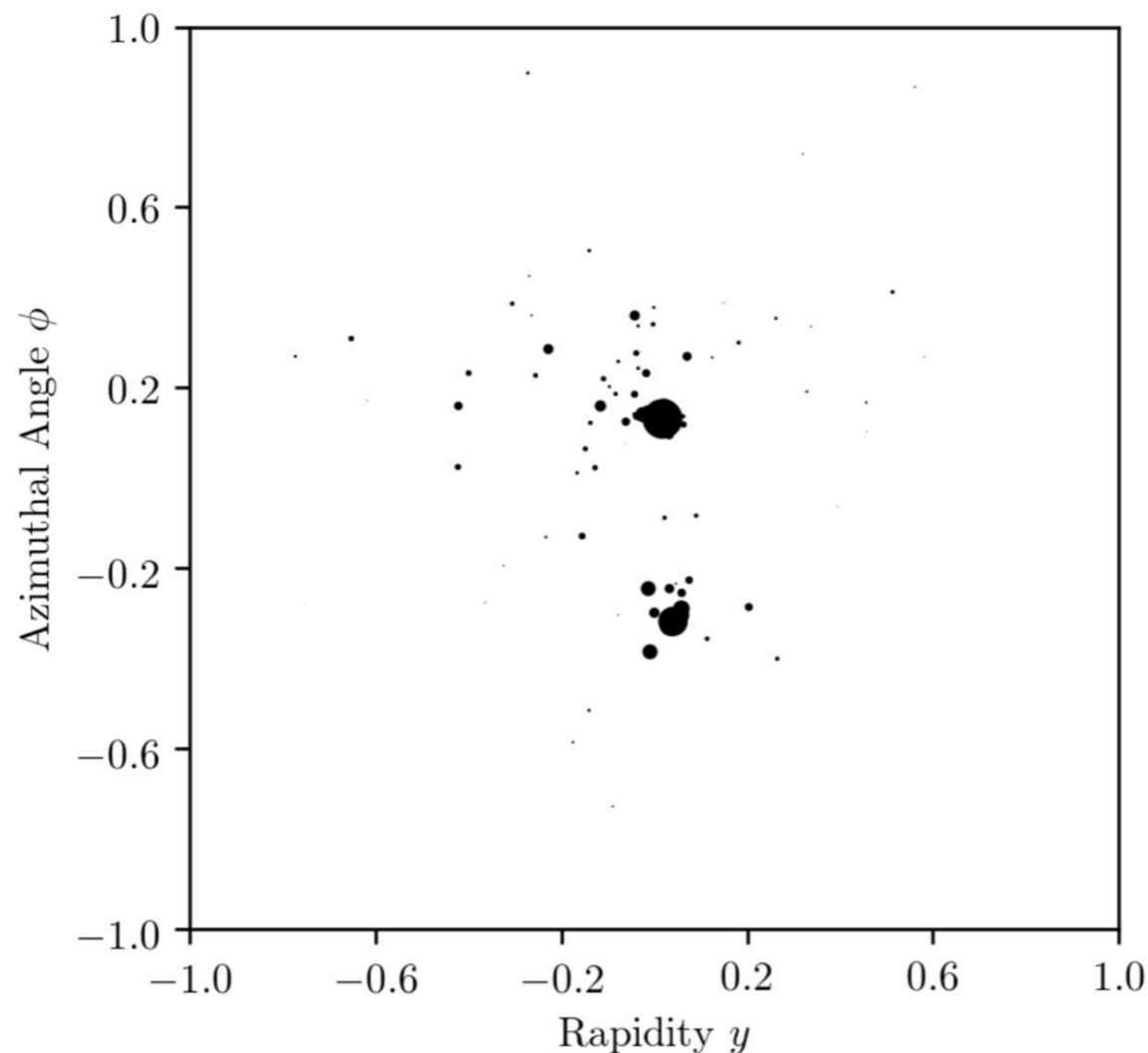
$$\hat{\mathcal{E}} \simeq \lim_{t \rightarrow \infty} \hat{n}_i T^{0i}(t, vt\hat{n})$$



*Stress-energy flow: Measure of event/jet structure robust to non-perturbative and detector effects (i.e. **IRC safe**)*

[Sveshnikov, Tkachov, [hep-ph/9512370](#); Hofman, Maldacena, [0803.1467](#); Mateu, Stewart, [JDT, 1209.3781](#); Komiske, Metodiev, [JDT, 1712.07124](#), [1810.05165](#)]

Focus on Energy Flow



Represent jet as:

$$\rho(\hat{p}) = \sum_{i \in \text{jet}} E_i \delta(\hat{p} - \hat{p}_i)$$

Energy (pT) Direction (y,φ)

Safe to infrared & collinear splittings
No flavor/charge information
No pixelation needed

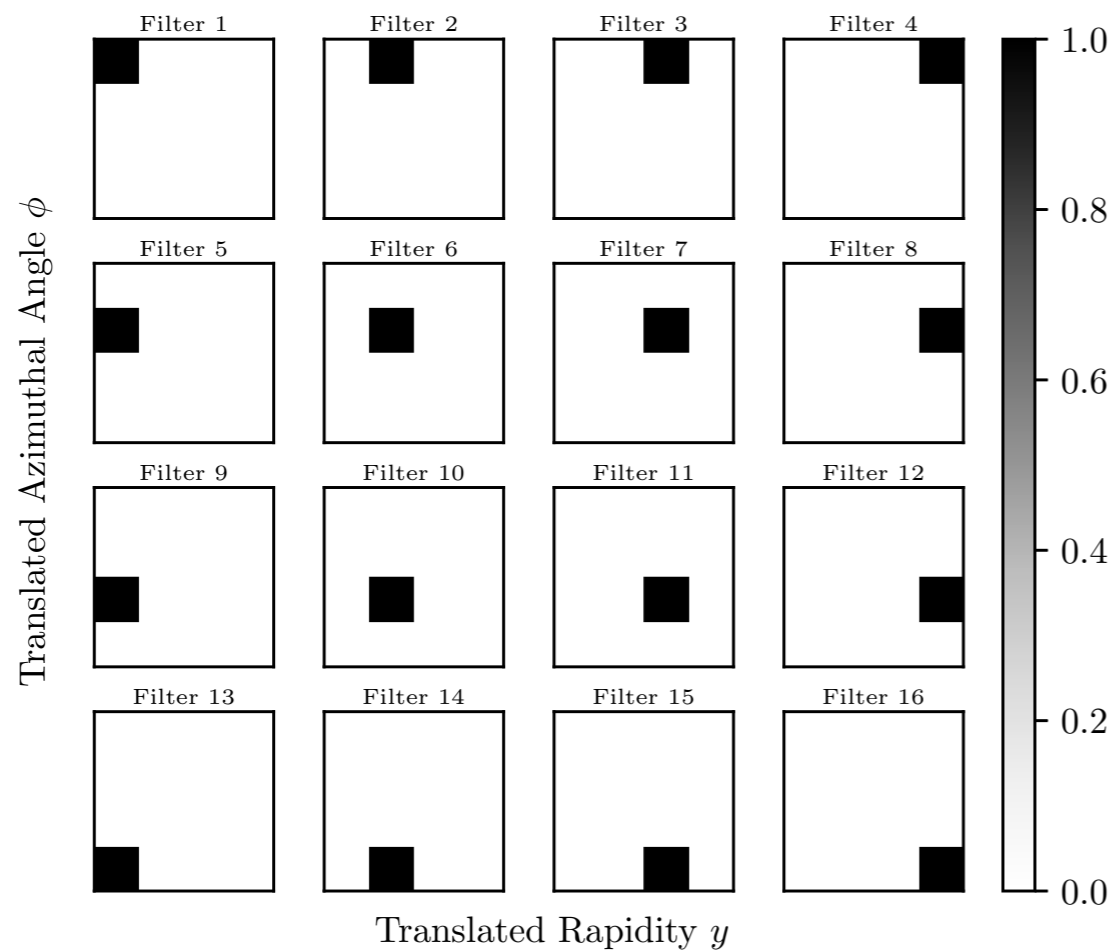
*Stress-energy flow: Measure of event/jet structure
robust to non-perturbative and detector effects (i.e. IRC safe)*

Latent Space Visualization

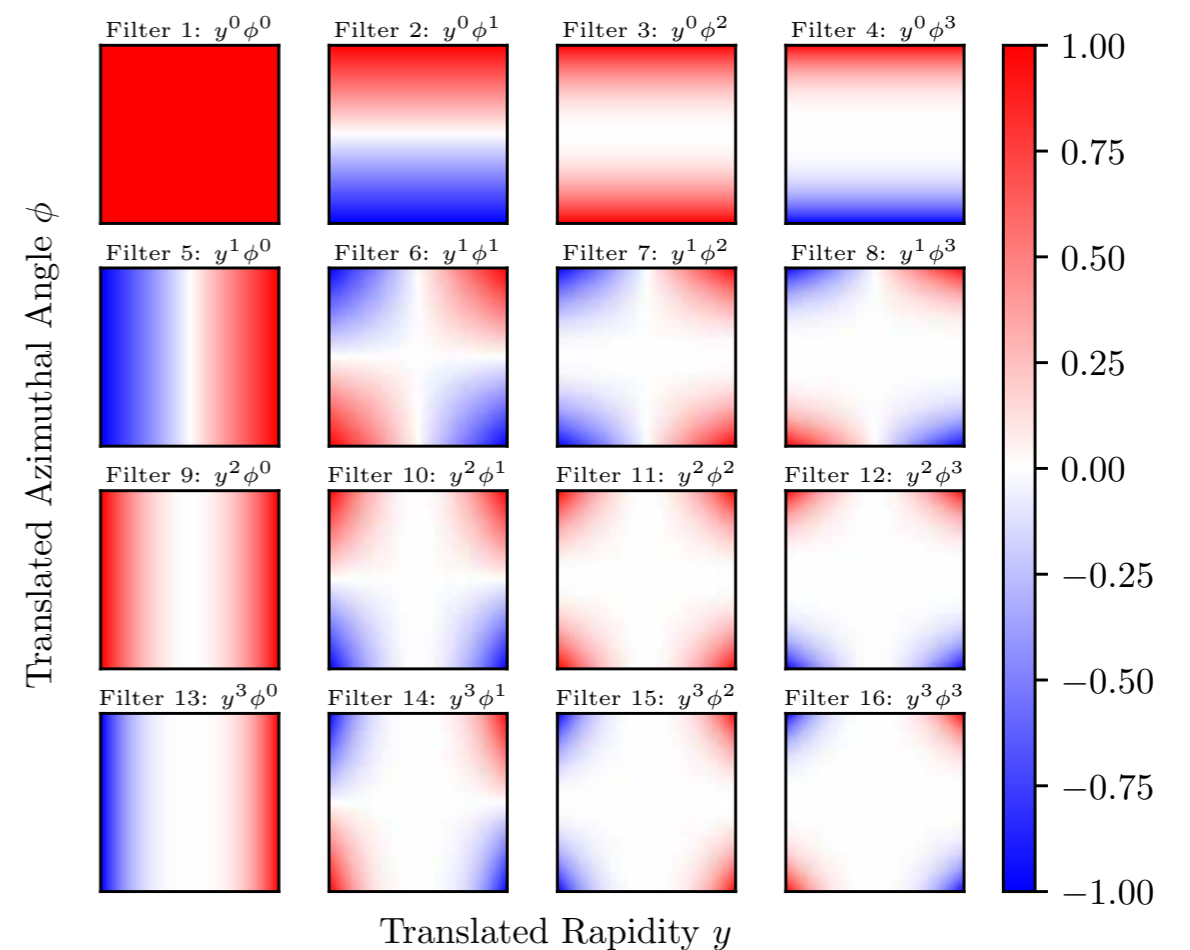
$$\mathcal{O}(\{p_i^\mu\}) = F(\mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_\ell)$$

$$\text{IRC-safe: } \mathcal{O}_a = \sum_{i \in \text{jet}} E_i \Phi_a(\hat{p}_i)$$

Calorimeter Pixels



Radiation Moments

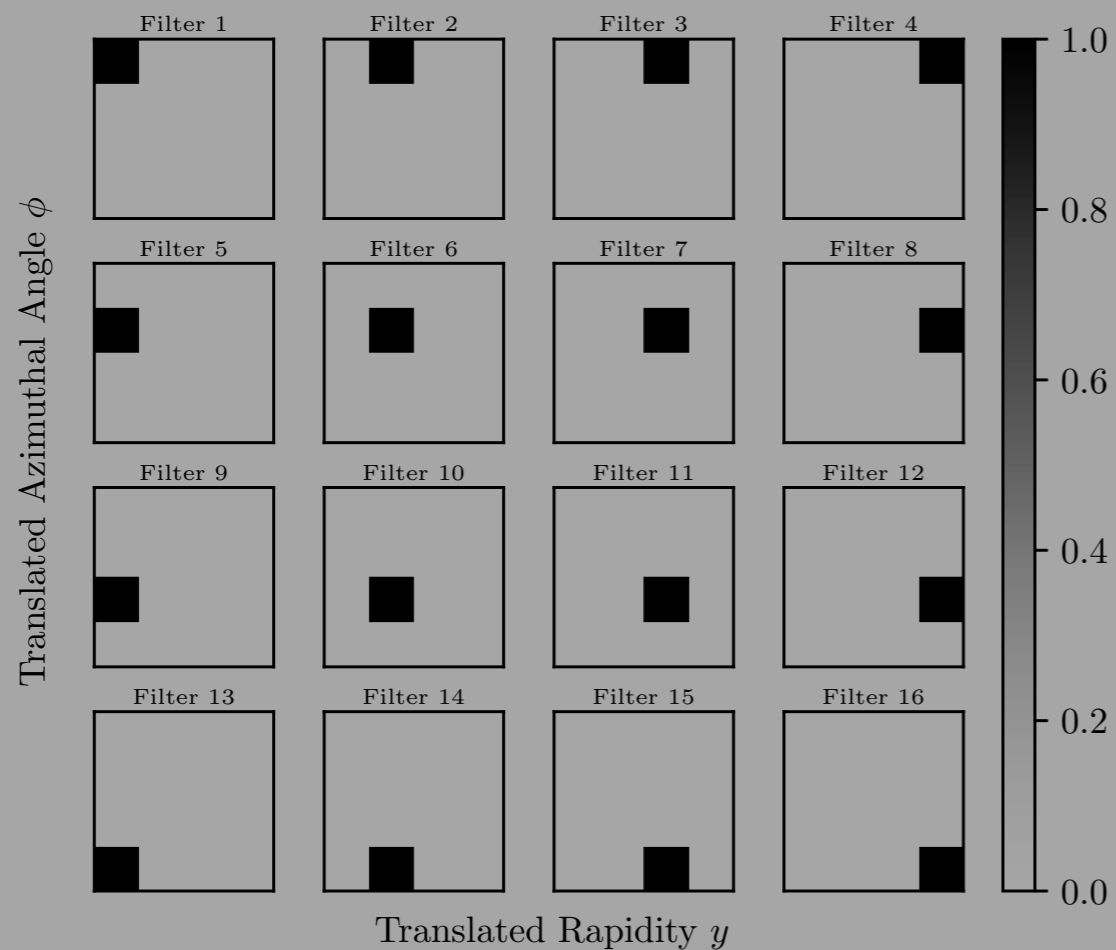


Latent Space Visualization

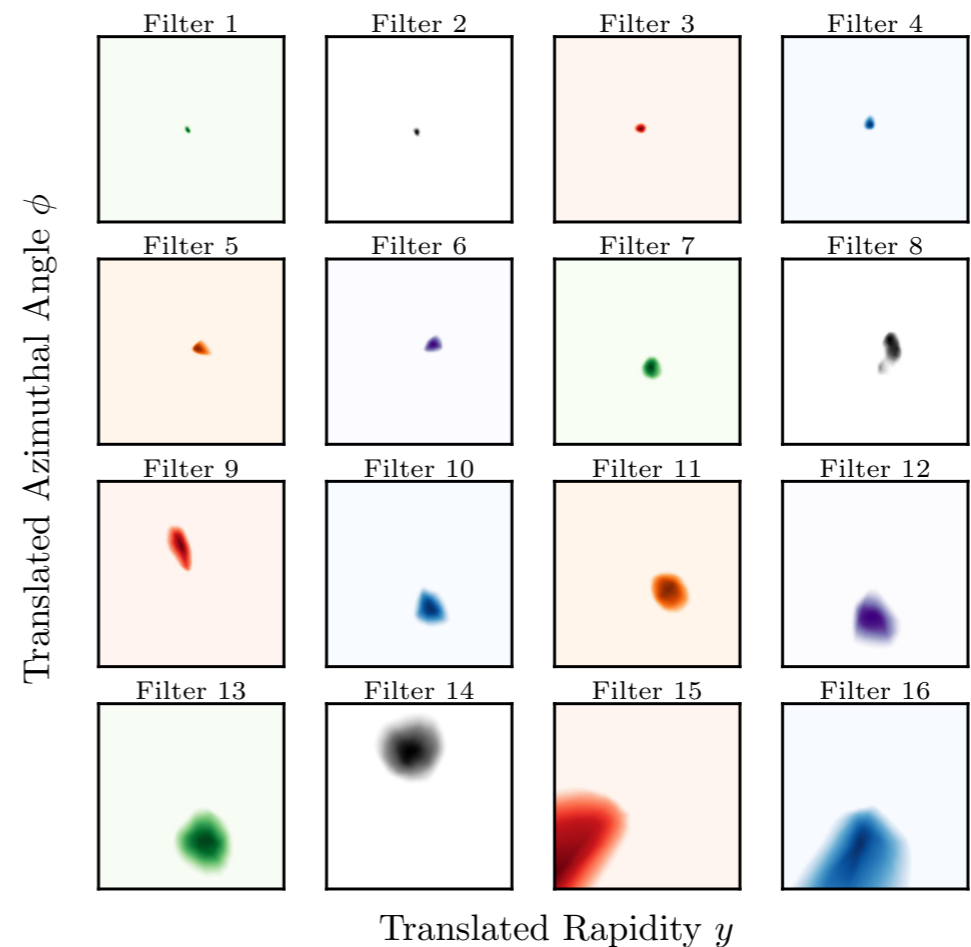
$$\mathcal{O}(\{p_i^\mu\}) = F(\mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_\ell)$$

$$\text{IRC-safe: } \mathcal{O}_a = \sum_{i \in \text{jet}} E_i \Phi_a(\hat{p}_i)$$

Calorimeter Pixels

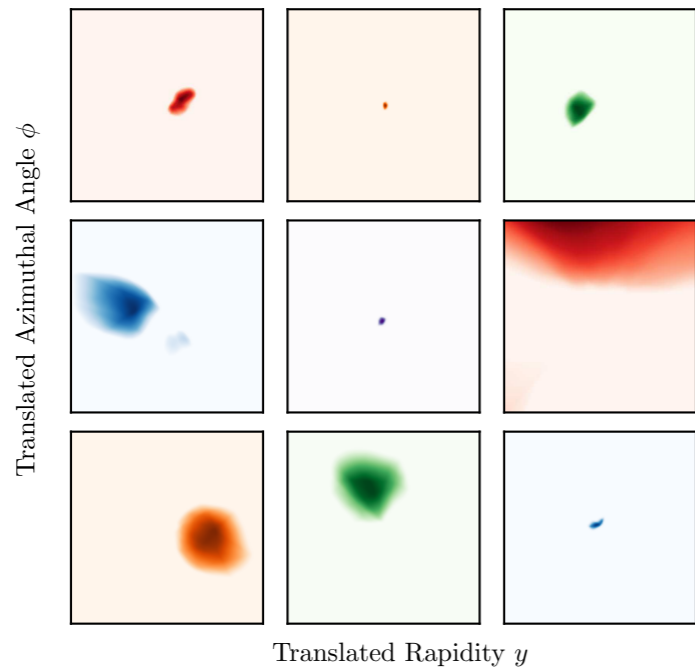


EFNs: Dynamic Pixelation

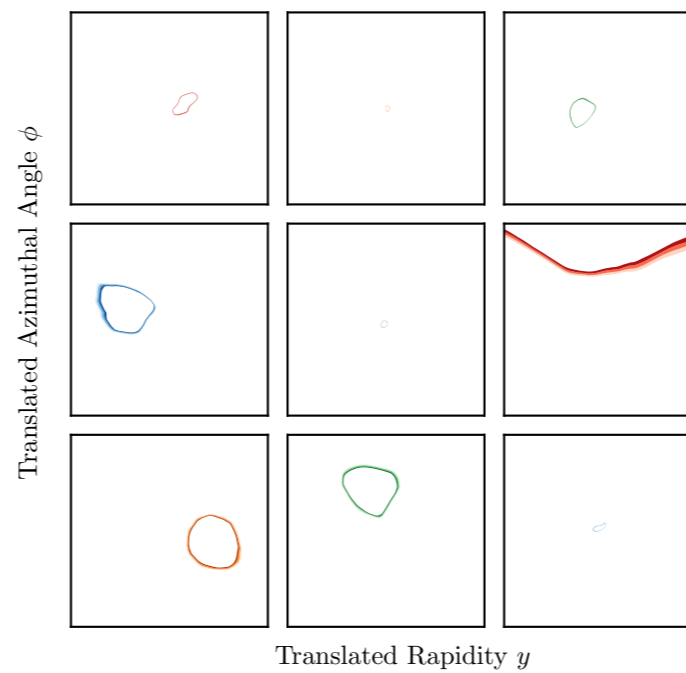


Psychedelic Network Visualization

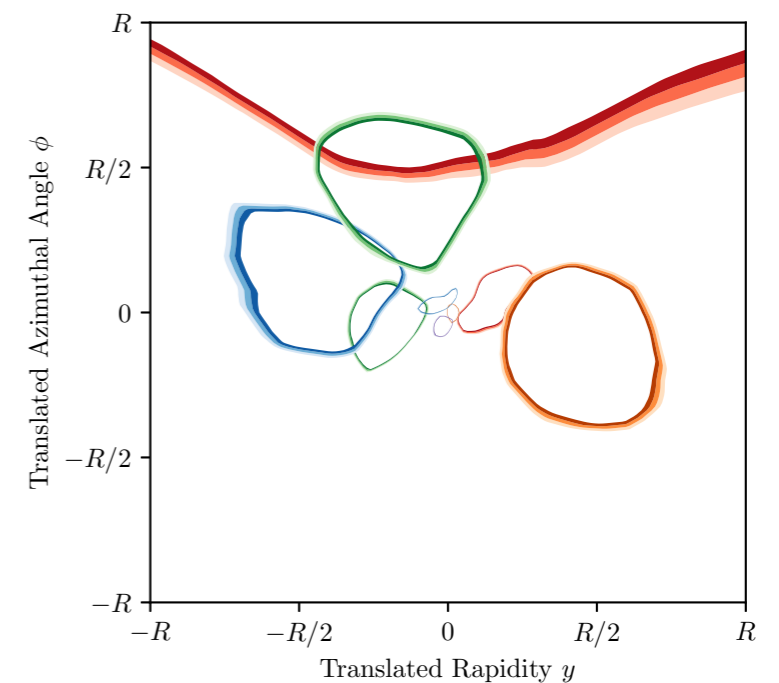
Latent Filters



50% Contours



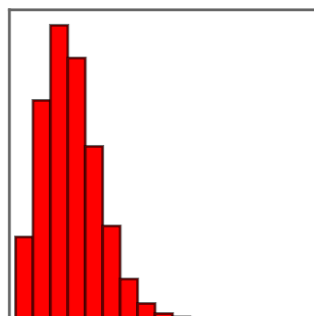
Overlay



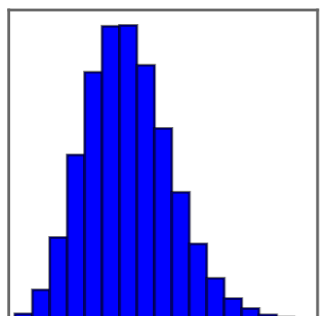
Generation (Easy)



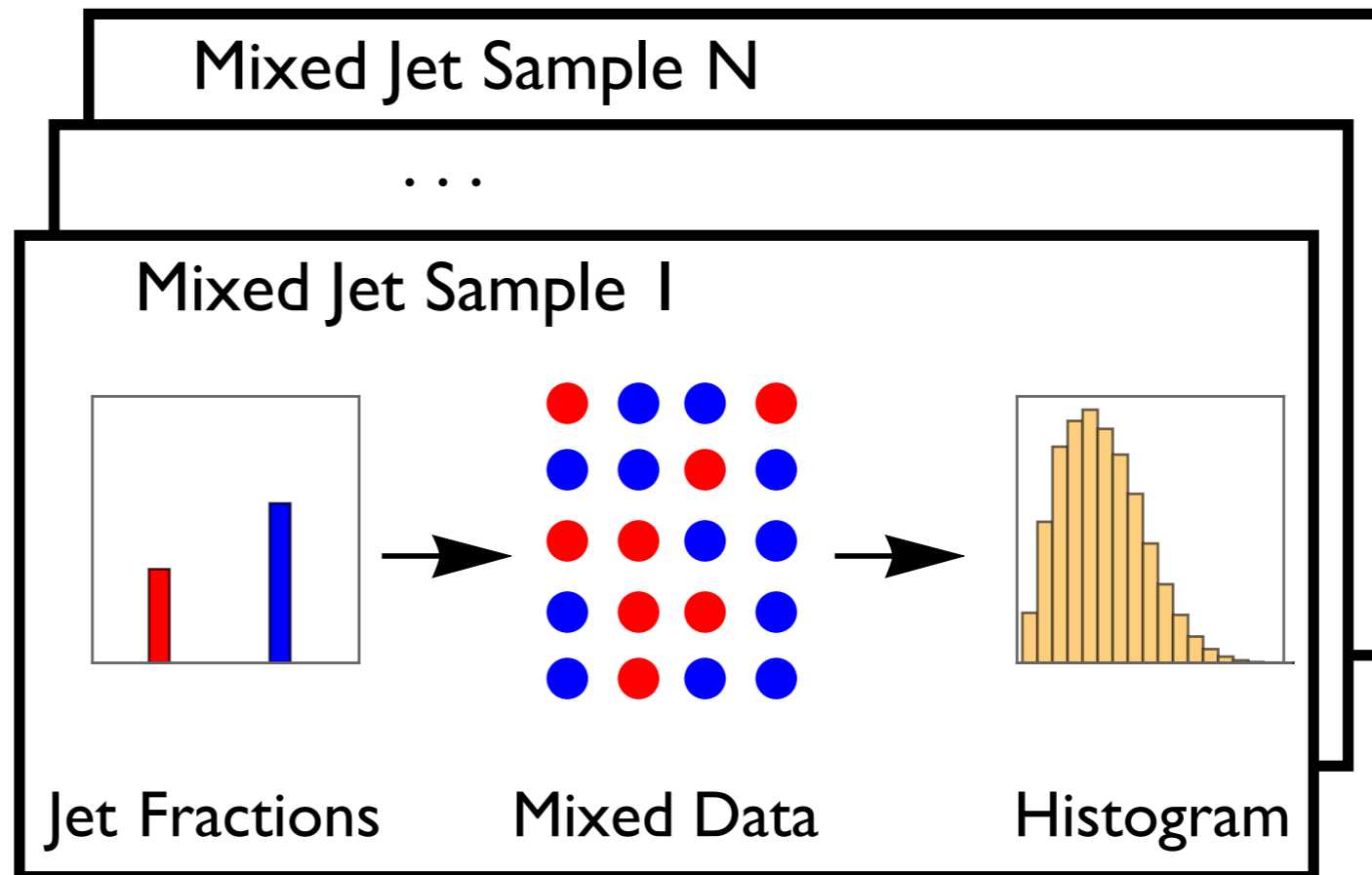
Jet Topics



Quark Jet



Gluon Jet



Demixing (Impossible?)

Topic Modeling

Topics

gene	0.04
dna	0.02
genetic	0.01
...	

life	0.02
evolve	0.01
organism	0.01
...	

brain	0.04
neuron	0.02
nerve	0.01
...	

data	0.02
number	0.02
computer	0.01
...	

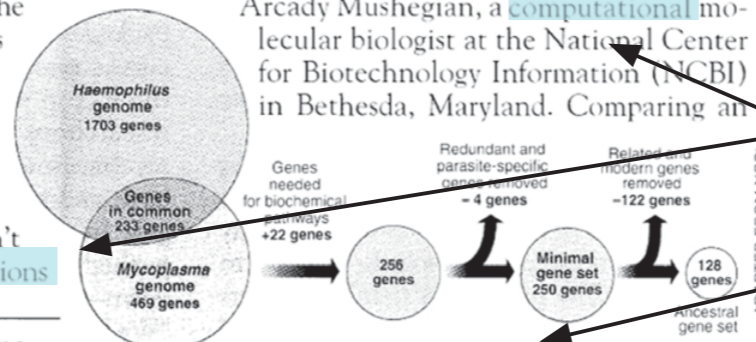
Documents

Seeking Life's Bare (Genetic) Necessities

COLD SPRING HARBOR, NEW YORK— How many **genes** does an **organism** need to **survive**? Last week at the genome meeting here,* two genome researchers with radically different approaches presented complementary views of the basic genes needed for **life**. One research team, using **computer** analyses to compare known **genomes**, concluded that today's **organisms** can be sustained with just 250 genes, and that the earliest life forms required a mere 128 **genes**. The other researcher mapped genes in a simple parasite and estimated that for this organism, 800 genes are plenty to do the job—but that anything short of 100 wouldn't be enough.

Although the numbers don't match precisely, those **predictions**

"are not all that far apart," especially in comparison to the 75,000 **genes** in the human genome, notes Siv Andersson of Uppsala University in Sweden, who arrived at the 800 number. But coming up with a consensus answer may be more than just a **genetic numbers** game, particularly as more and more **genomes** are completely mapped and sequenced. "It may be a way of organizing any newly **sequenced genome**," explains Arcady Mushegian, a **computational** molecular biologist at the National Center for Biotechnology Information (NCBI) in Bethesda, Maryland. Comparing an

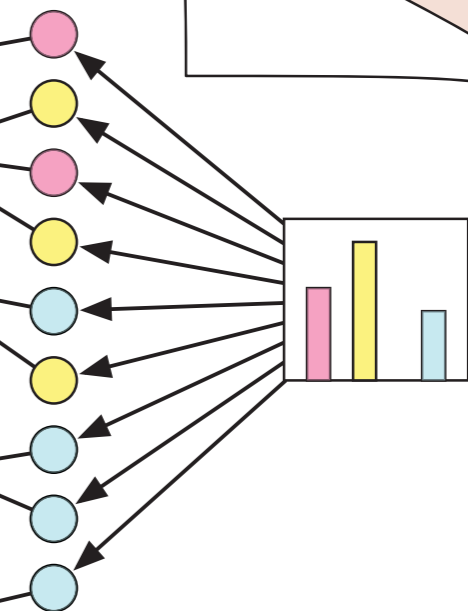


* Genome Mapping and Sequencing, Cold Spring Harbor, New York, May 8 to 12.

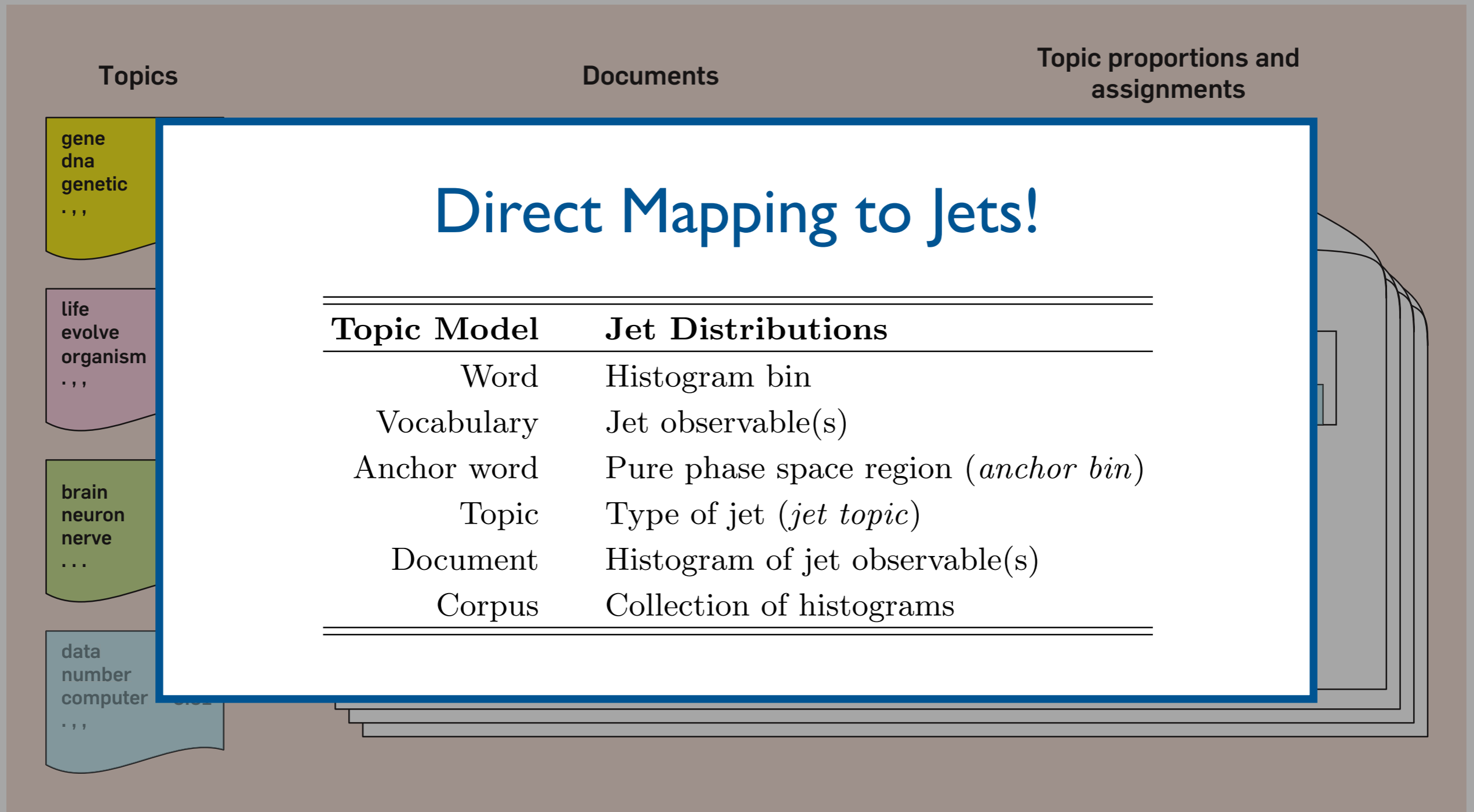
Stripping down. Computer analysis yields an estimate of the minimum modern and ancient genomes.

SCIENCE • VOL. 272 • 24 MAY 1996

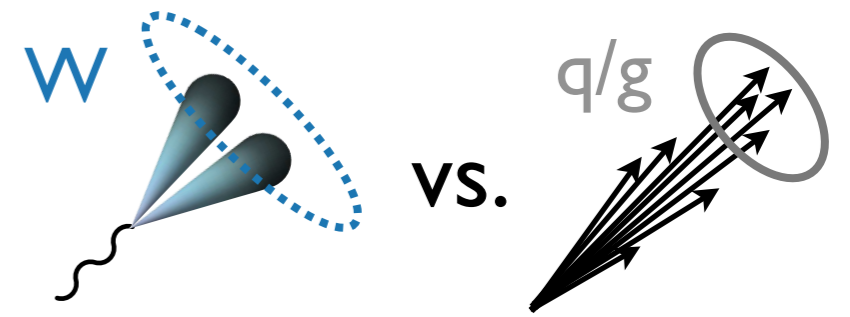
Topic proportions and assignments



Topic Modeling

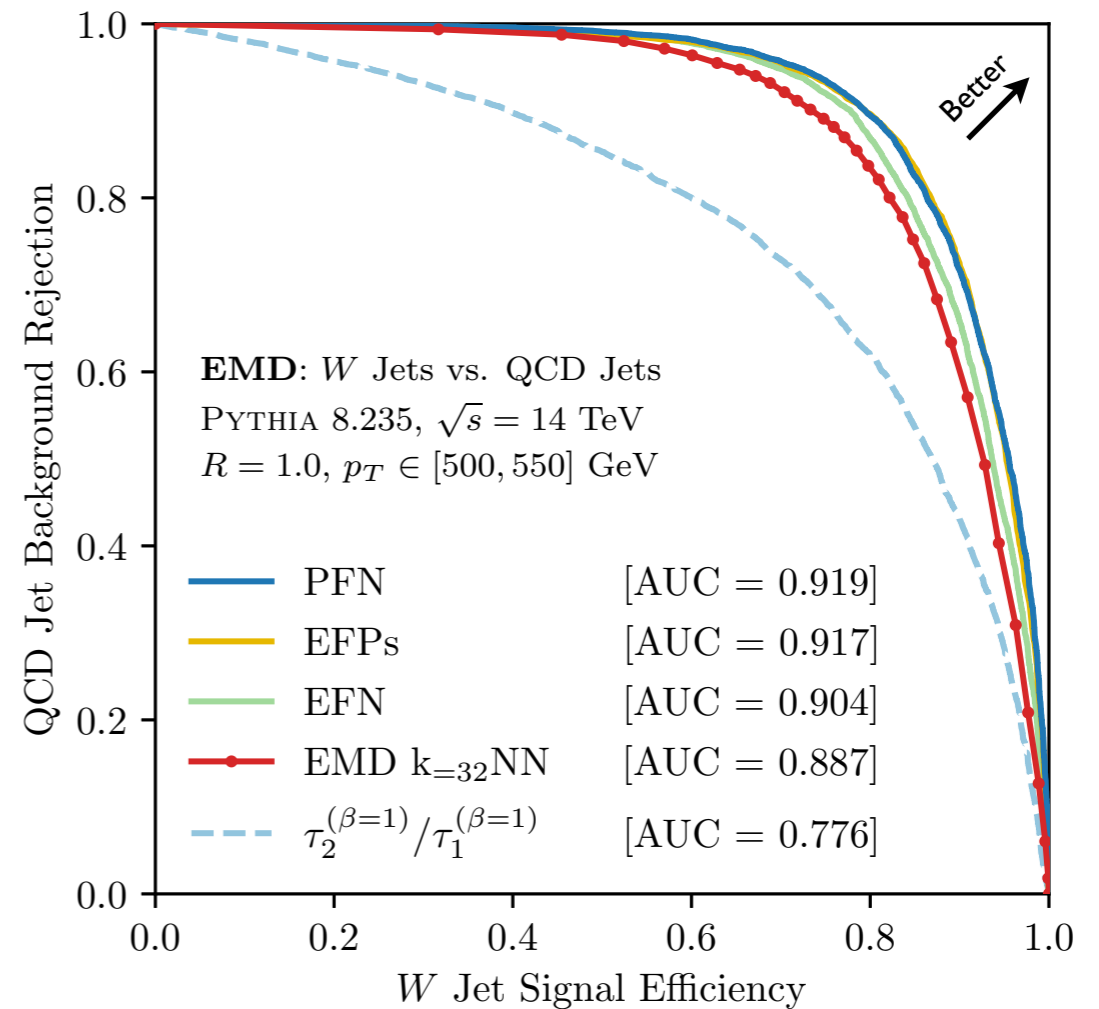
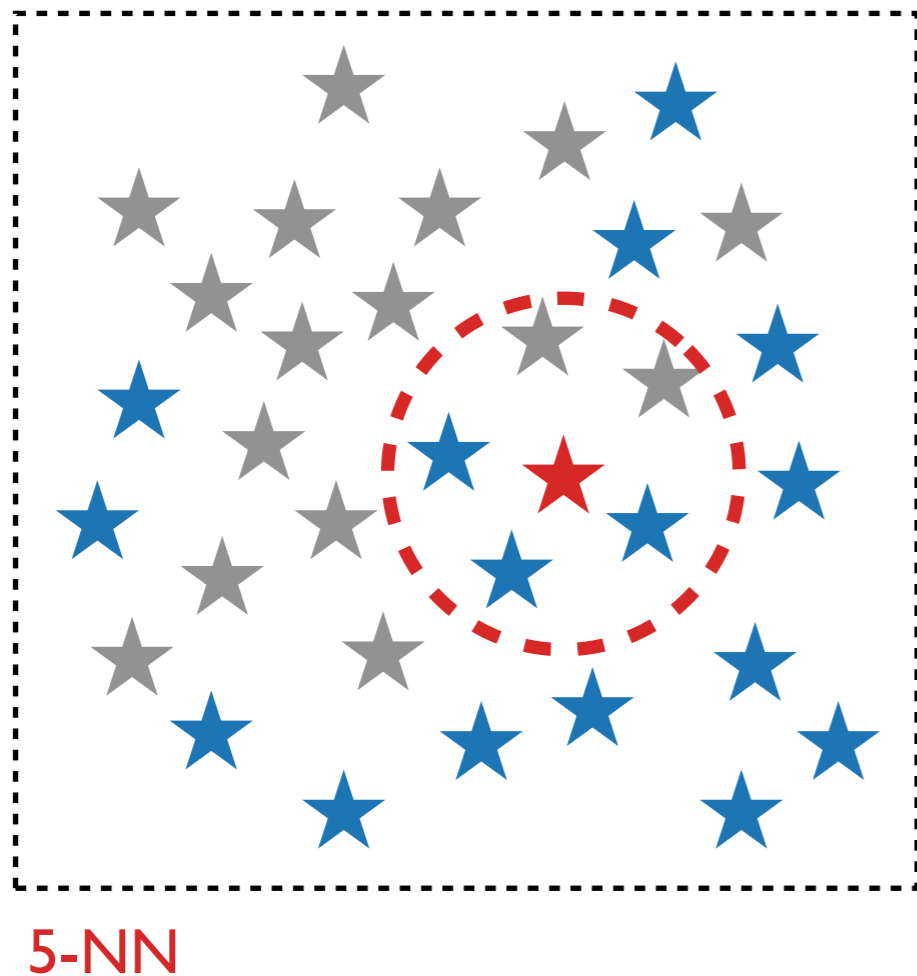


Revisiting Jet Classification



Estimate jet label by **k nearest neighbors** in training data

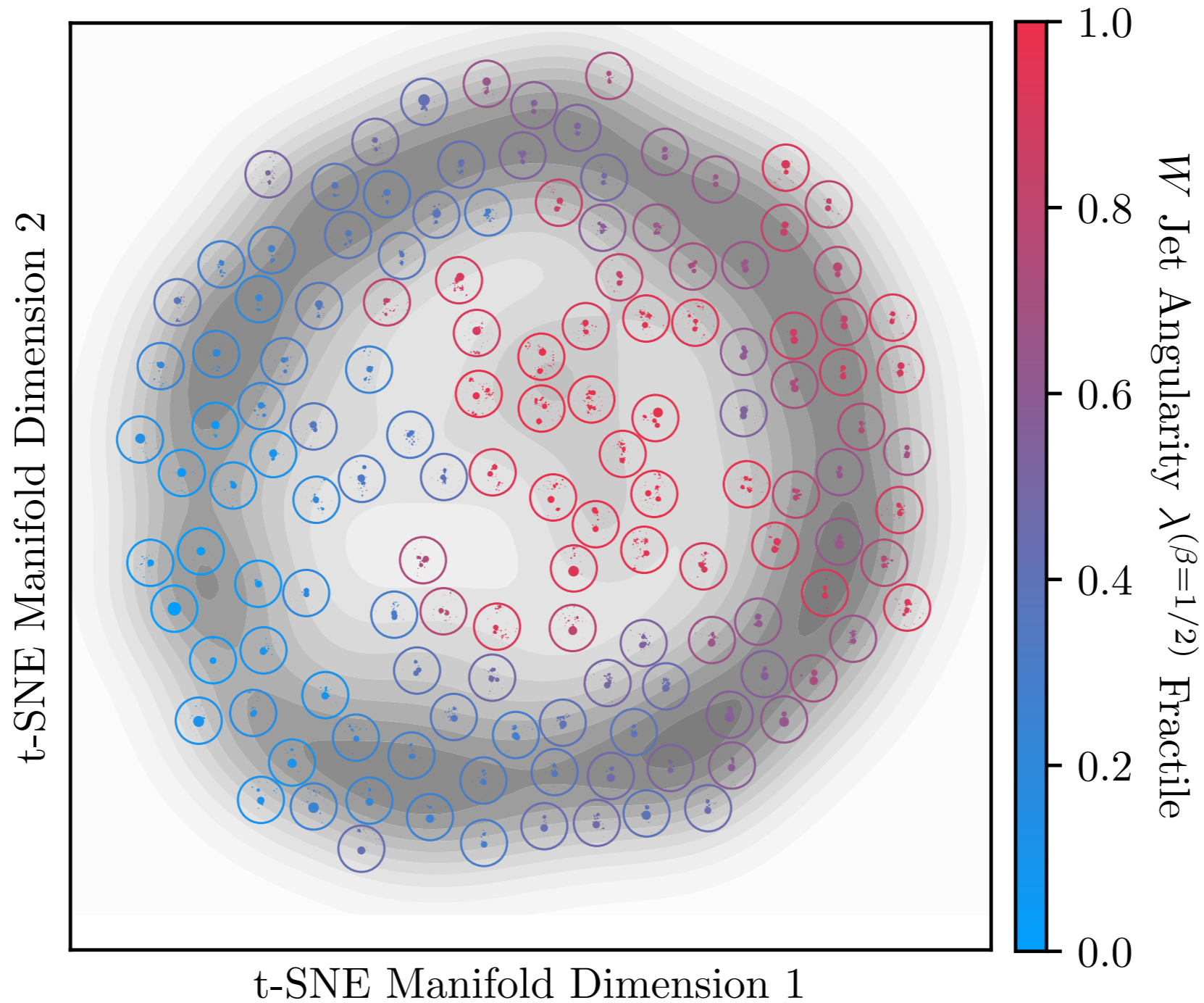
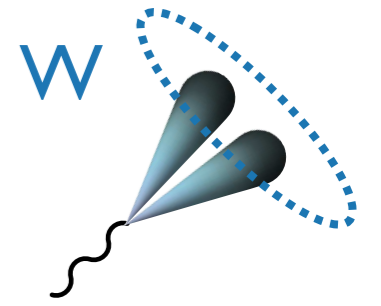
Approaches performance of **modern machine learning**



[Komiske, Metodiev, JDT, 1902.02346;

comparison to JDT, Van Tilburg, 1011.2268, 1108.2701; Komiske, Metodiev, JDT, 1712.07124, 1810.05165]

The Space of Boosted W Bosons



[Komiske, Metodiev, JDT, [1902.02346](#)]