Collision Course

Particle Physics as a Machine-Learning Testbed

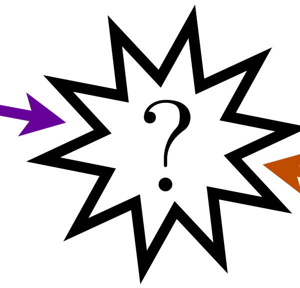
Jesse Thaler

Dark Universe Seminar, Brandeis University — February 14, 2019

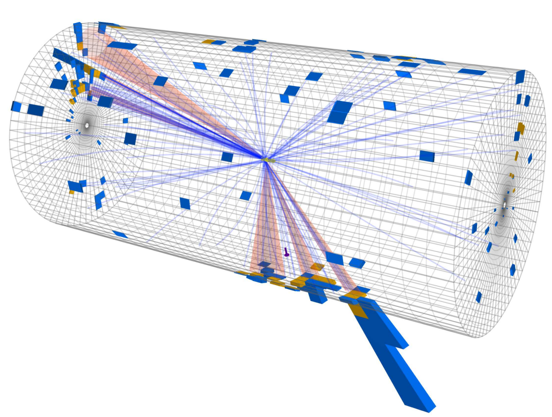
“Collision Course”

“Theoretical Physics for Machine Learning”
Aspen Center for Physics, January 2019

Theoretical
(High Energy)
Physics



Mathematics,
Statistics,
Computer Science

Could  *be the next*  *?*

Relevance for the Dark Universe

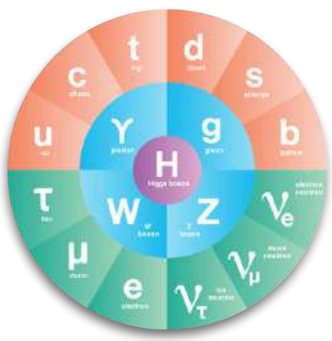
Can ML enhance the search for dark matter (and other BSM physics) at colliders?

Yes, almost every LHC analysis uses ML in some way
Today: Focus on jet classification tasks

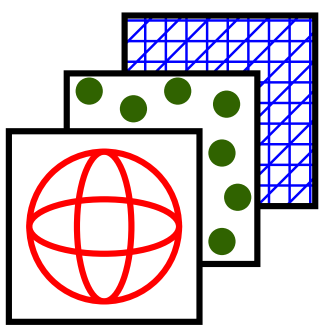
Can the collider approach to ML inform astrophysical/cosmological investigations?

Yes, with two broad lessons:
Match ML architecture to symmetry of dataset
Pursue ML alternatives when data has meta-structures

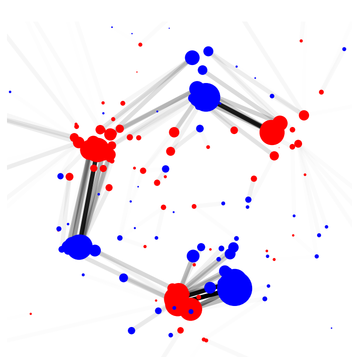
Outline



Particle Physics Primer

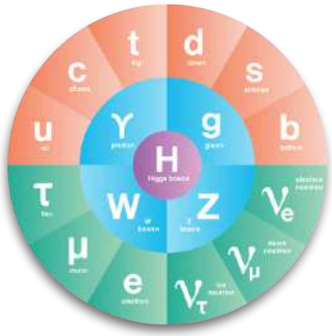


Point Clouds & Energy Flow Networks



(The Metric Space of Collider Events)

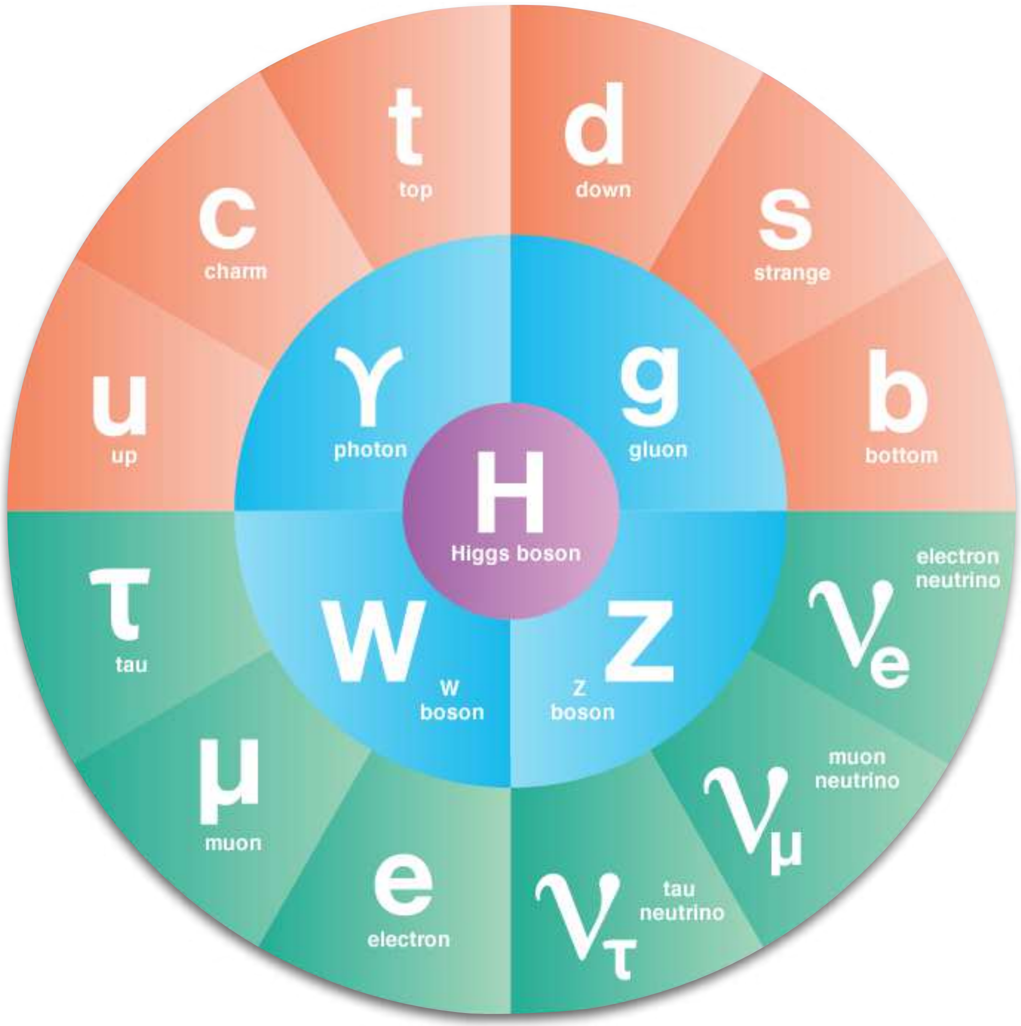
[Physics Valentines, Symmetry, Feb 2015]



Particle Physics Primer

Point Clouds & Energy Flow Networks

(The Metric Space of Collider Events)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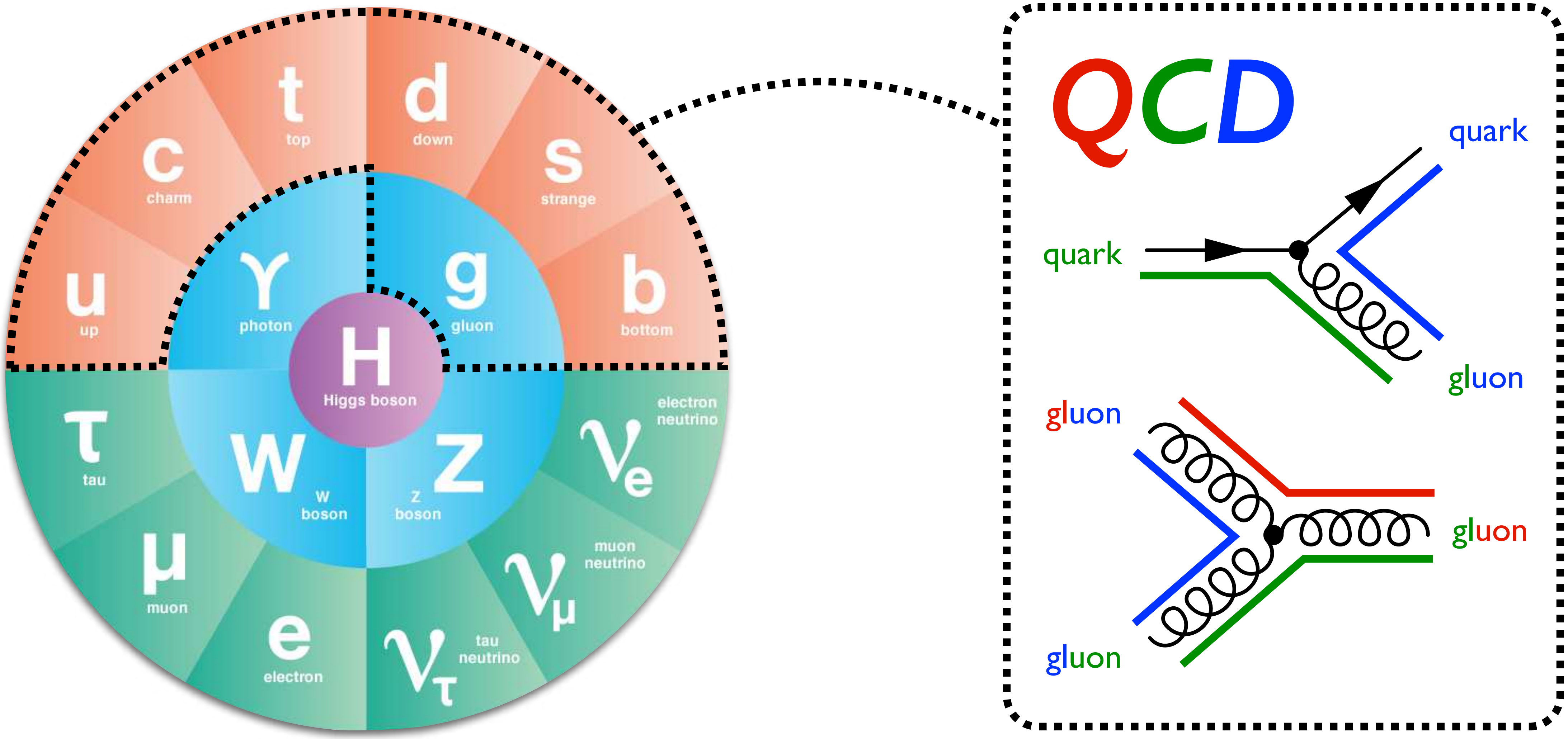
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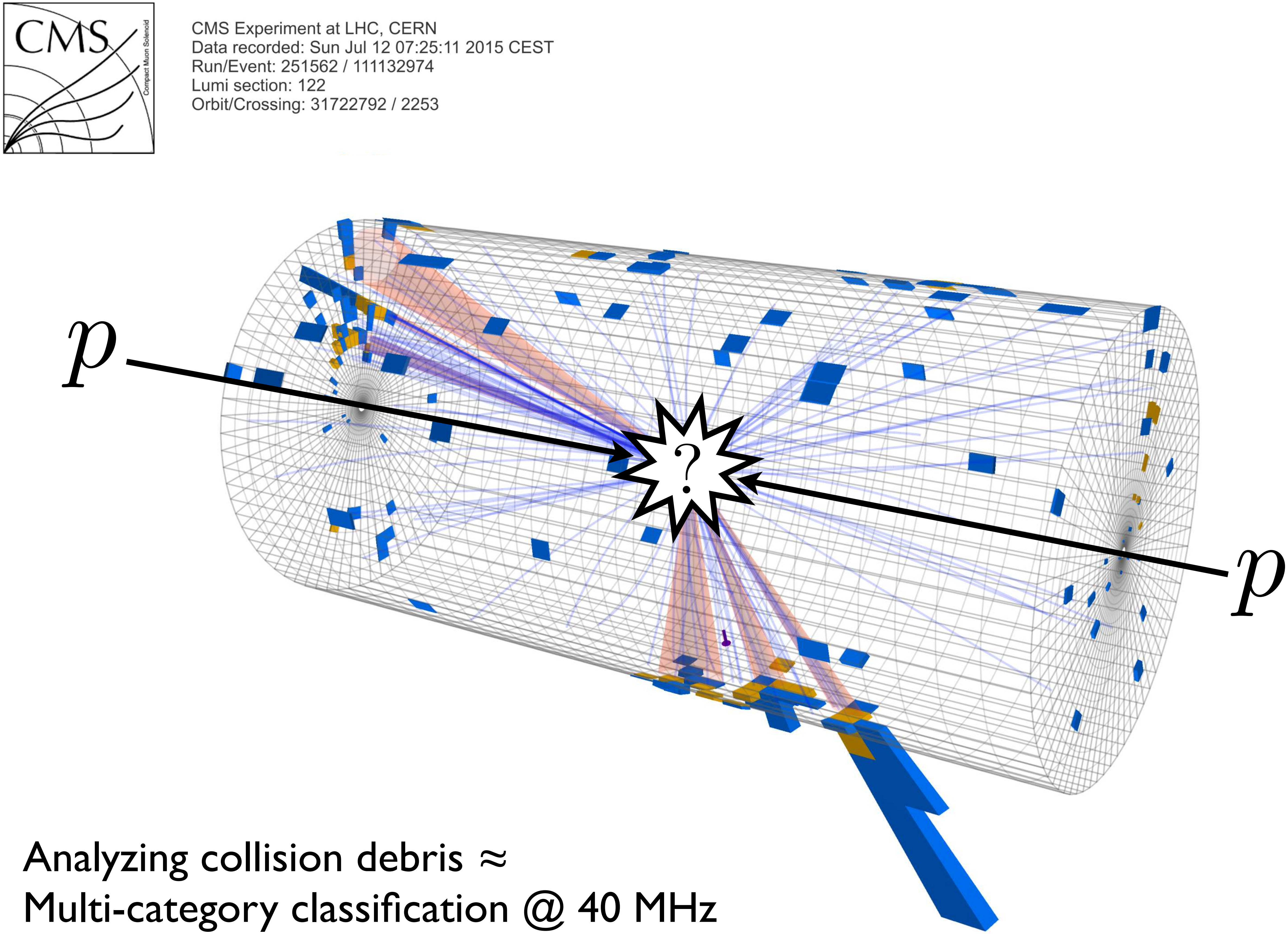
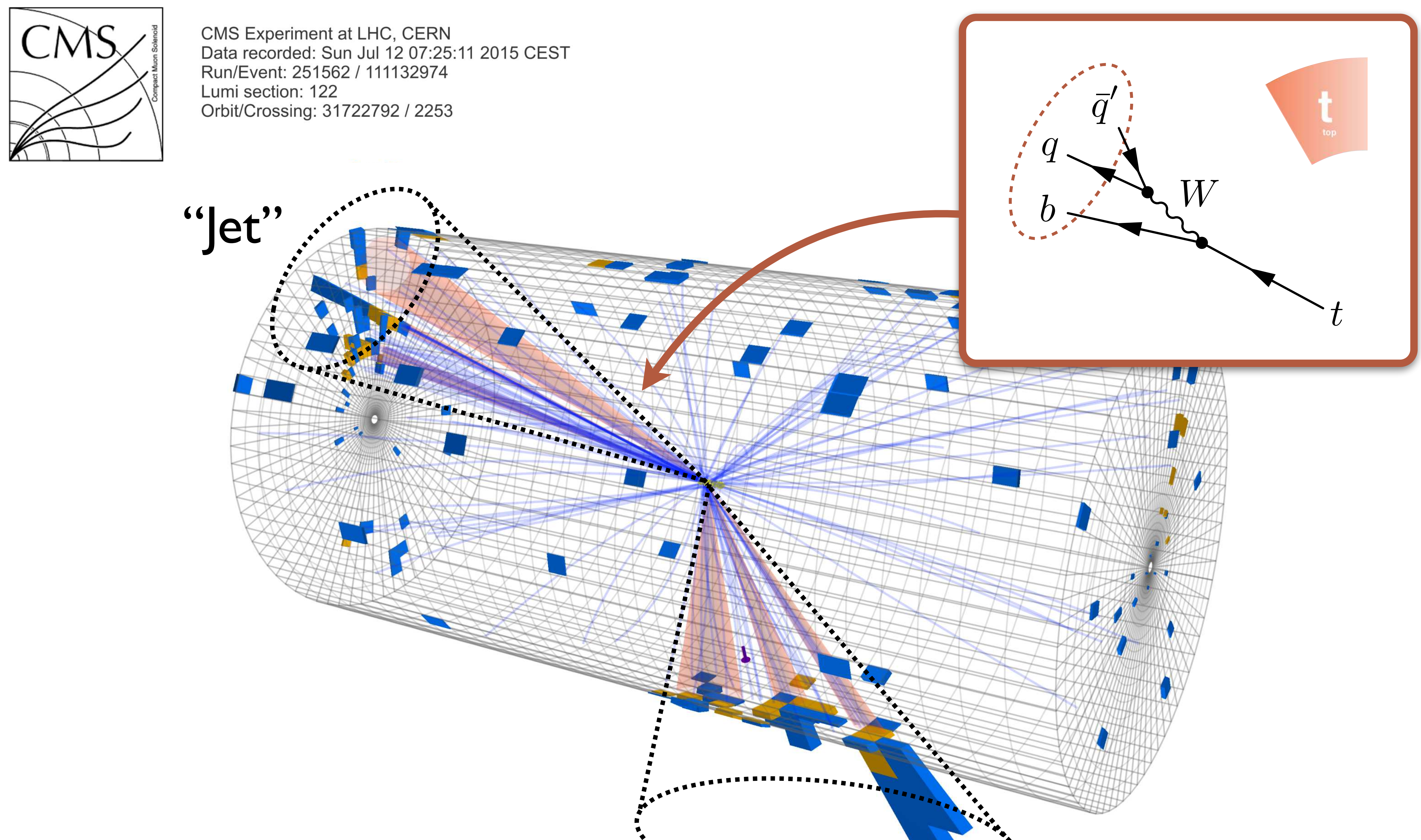


Analyzing collision debris ≈
Multi-category classification @ 40 MHz



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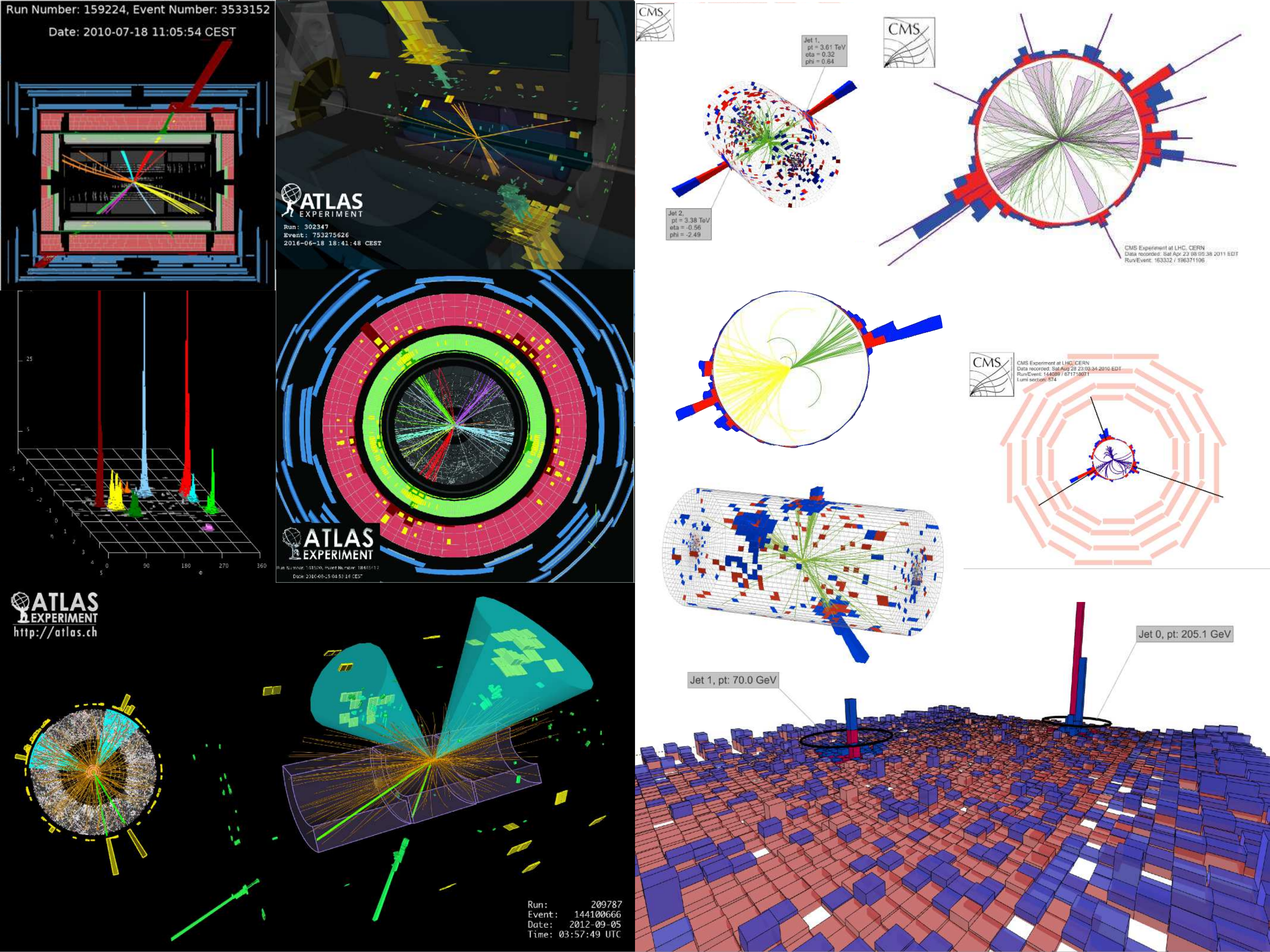
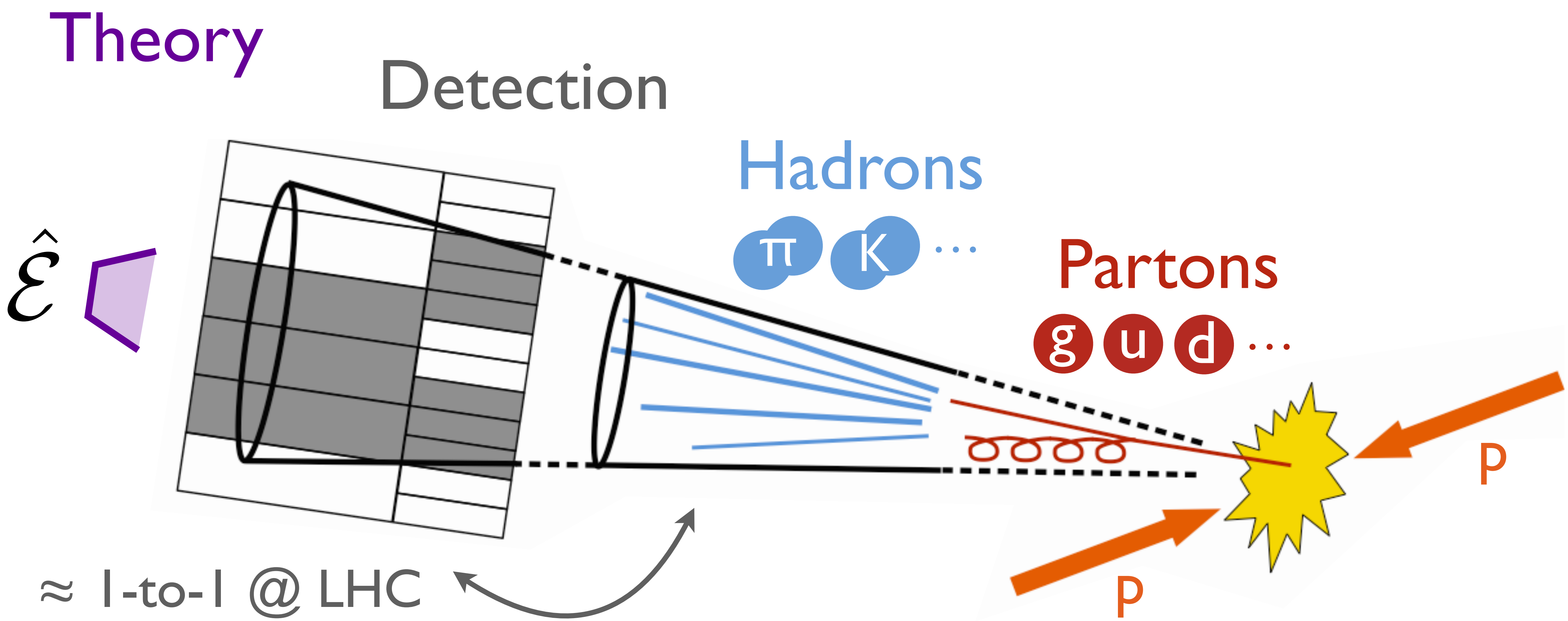
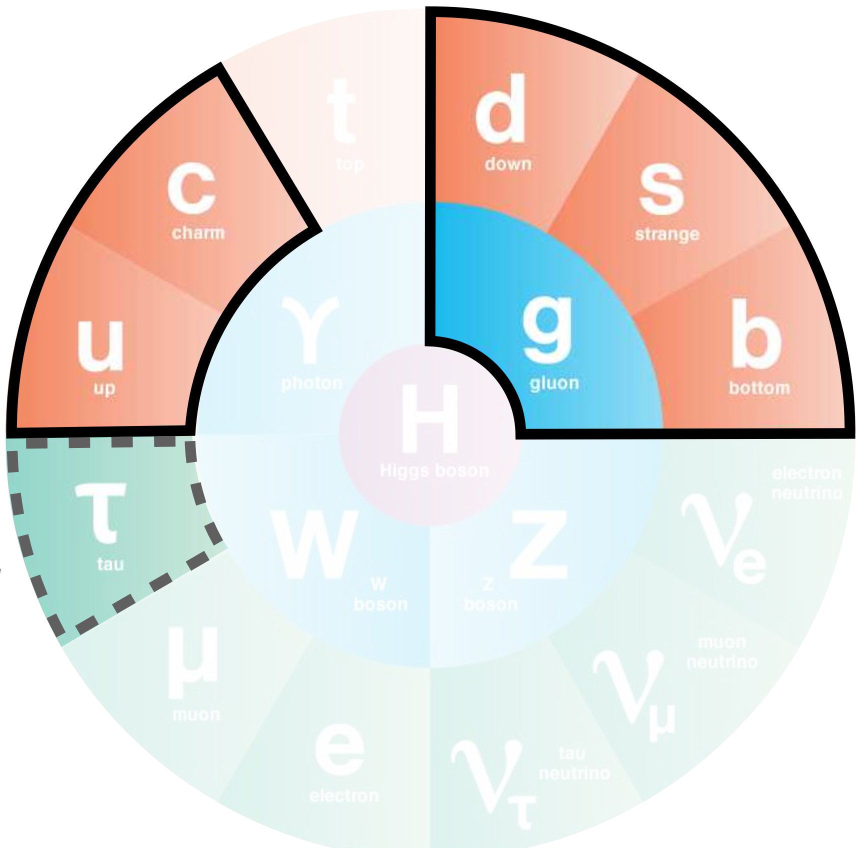


Run Number: 159224, Event Number: 3533152
Date: 2010-07-18 11:05:54 CEST
ATLAS
EXPERIMENT
Run: 302347
Event: 753275626
2016-06-18 18:41:48 CEST
CMS
Jet 1,
pt = 3.61 TeV
eta = 0.32
phi = 0.64
Jet 2,
pt = 3.38 TeV
eta = -0.56
phi = -2.49
CMS
ATLAS
EXPERIMENT
CMS
ATLAS
EXPERIMENT
http://atlas.ch
Run: 209787
Event: 144100666
Date: 2012-09-05
Time: 03:57:49 UTC
Jet 0, pt: 205.1 GeV
Jet 1, pt: 70.0 GeV



Stress-Energy Flow Operator: $\hat{\mathcal{E}} \simeq \lim_{t \to \infty} \hat{n}_i T^{0i}(t, vt\hat{n})$

[Sveshnikov, Tkachov, hep-ph/9512370; Hofman, Maldacena, 0803.1467; Mateu, Stewart, JDT, 1209.3781]



micro-jet
≈ 65%

Jets from QCD and the Standard Model

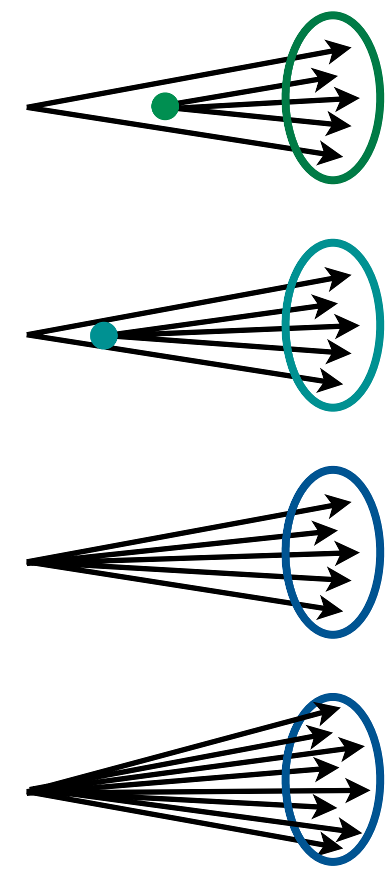
++ = Mass from QCD Radiation

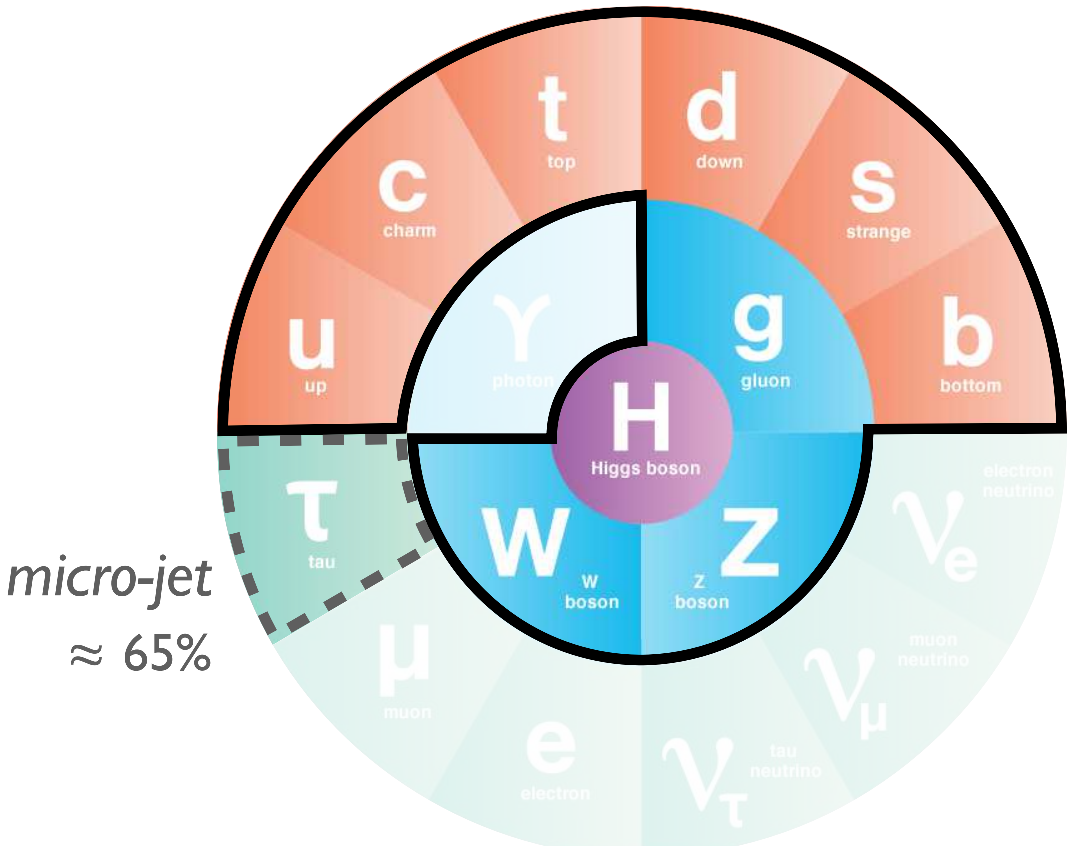
b — 4.2 GeV++

c — 1.3 GeV++

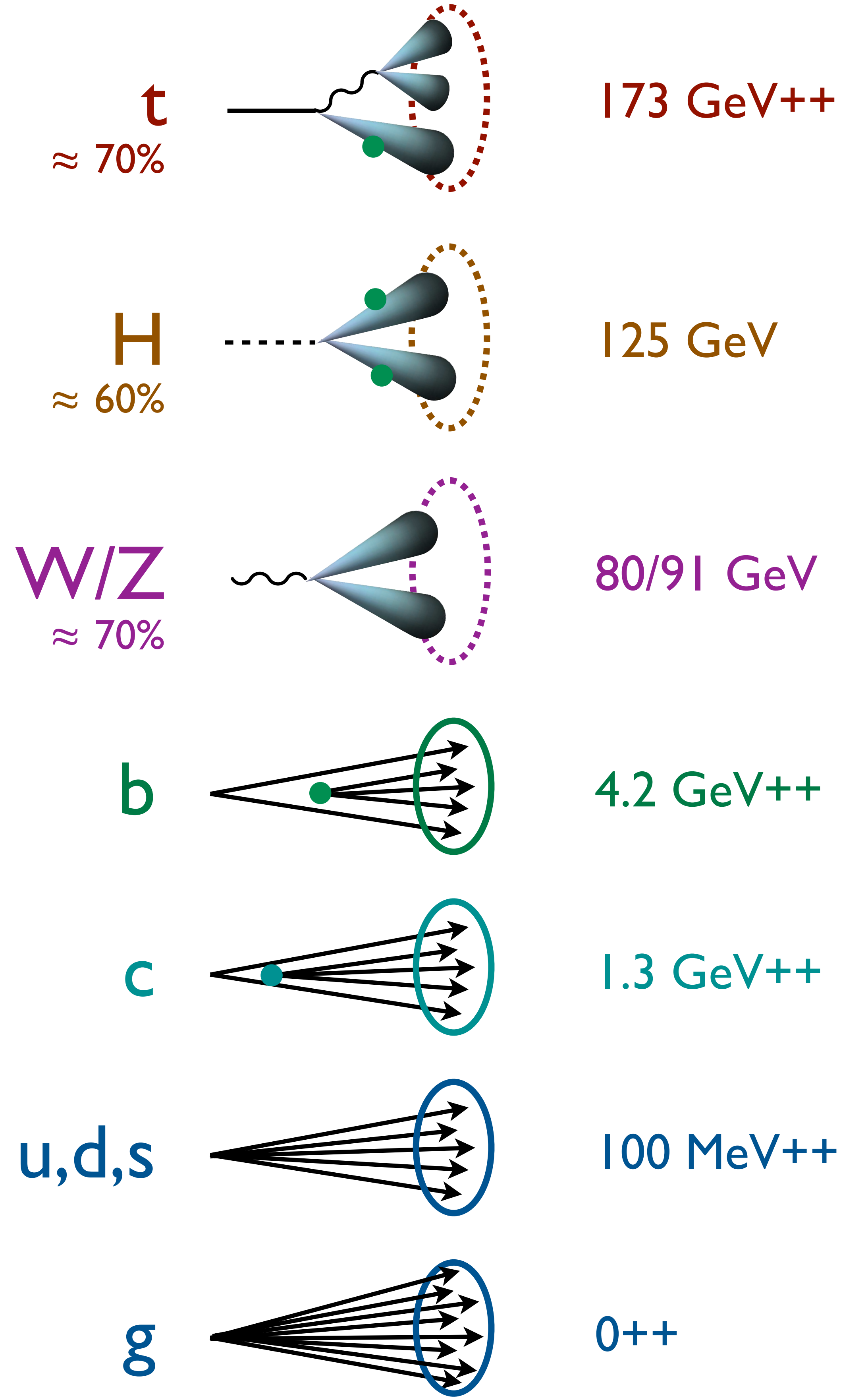
u,d,s — 100 MeV++

g — 0++





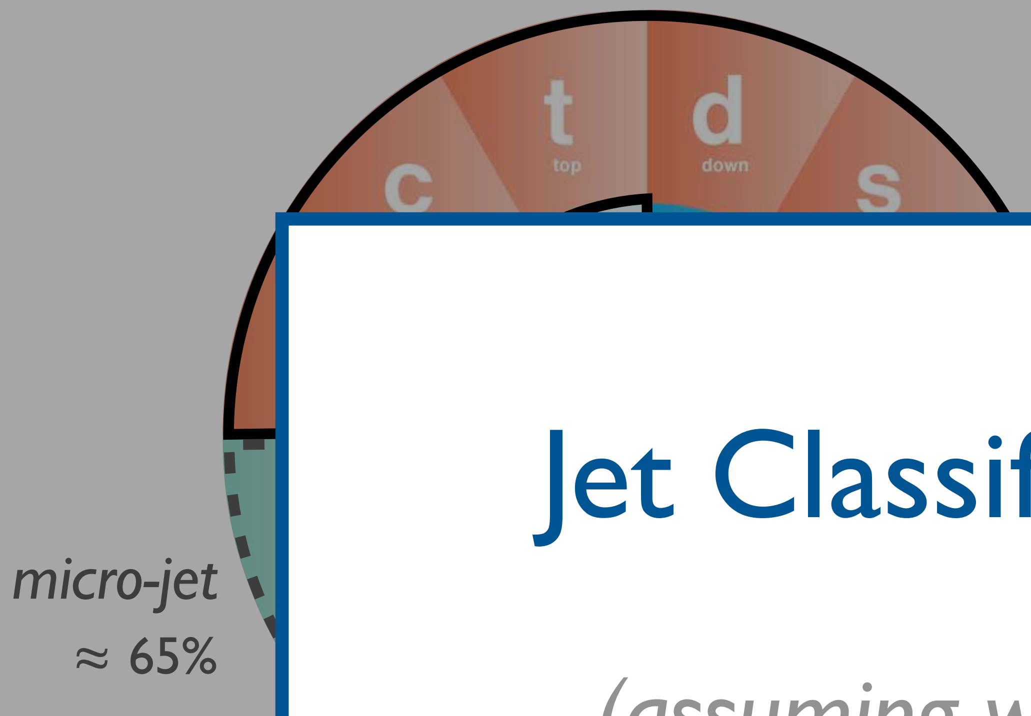
Jets from QCD and the Standard Model



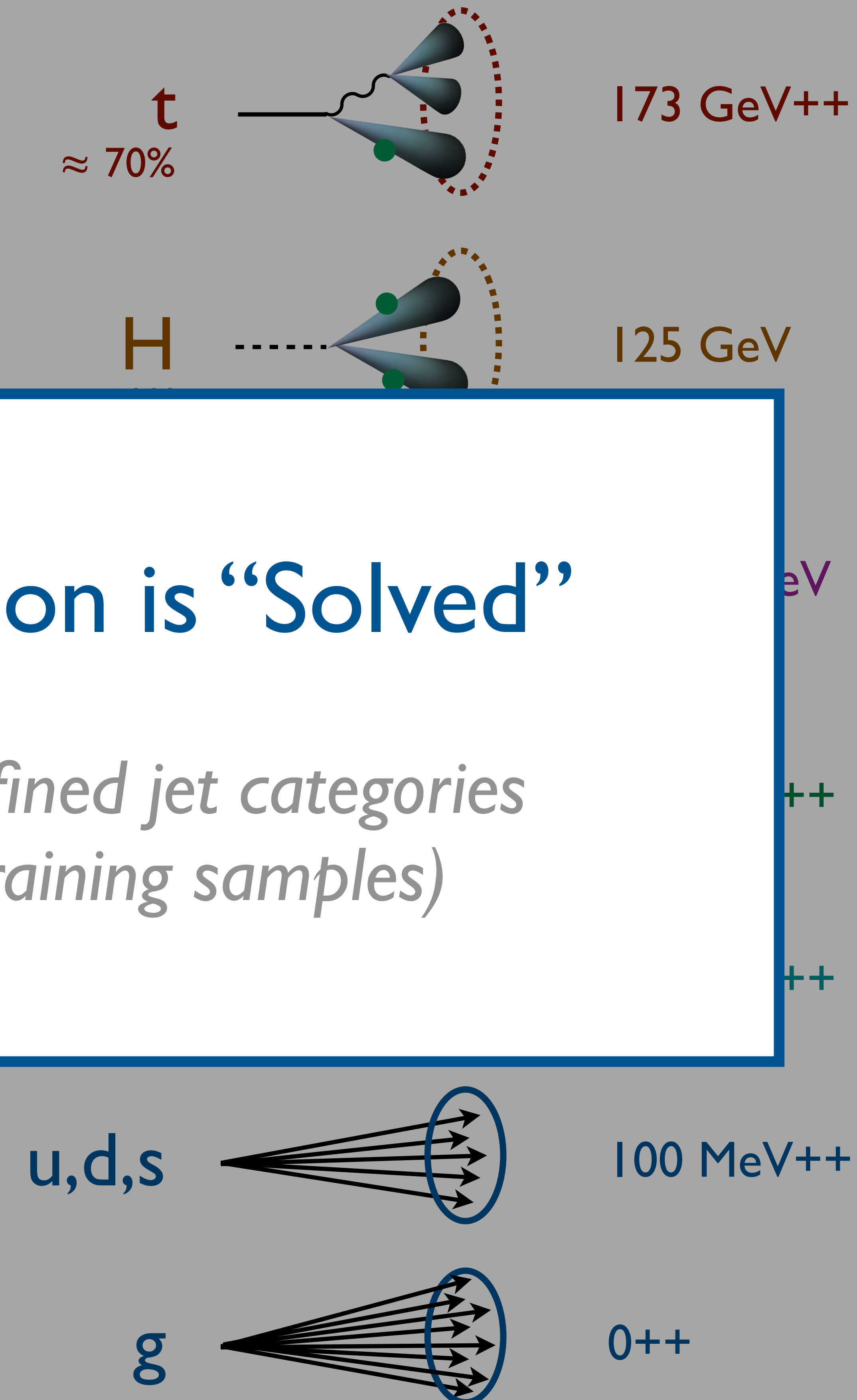
++ = Mass from QCD Radiation

Jet Classification is “Solved”

(assuming well-defined jet categories and trustable training samples)



the Standard Model



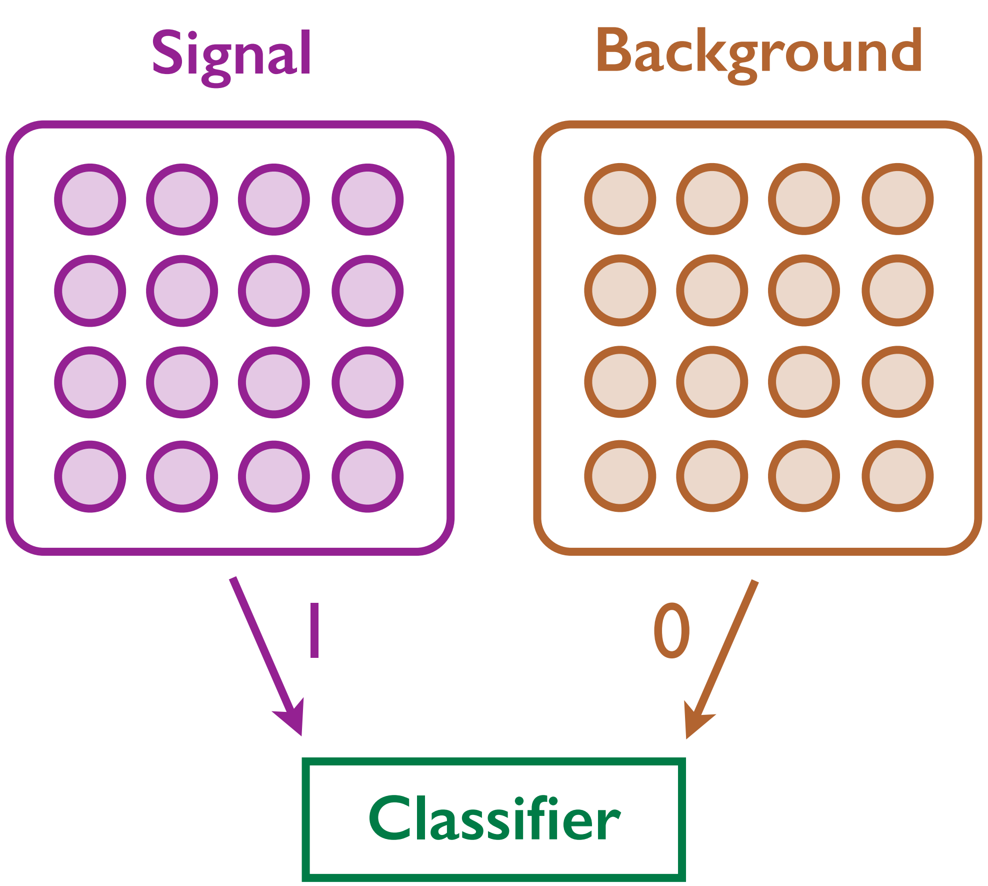
++ = Mass from QCD Radiation

A Cartoon of Machine Learning

For fully-supervised jet classification

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

Classifier Inputs



Minimize Loss Function

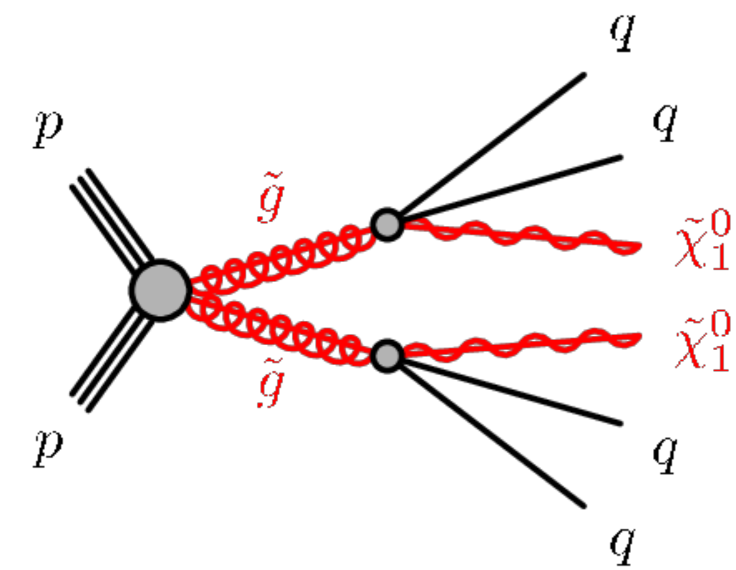
(assuming infinite training sets, and flexible enough functional form)

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

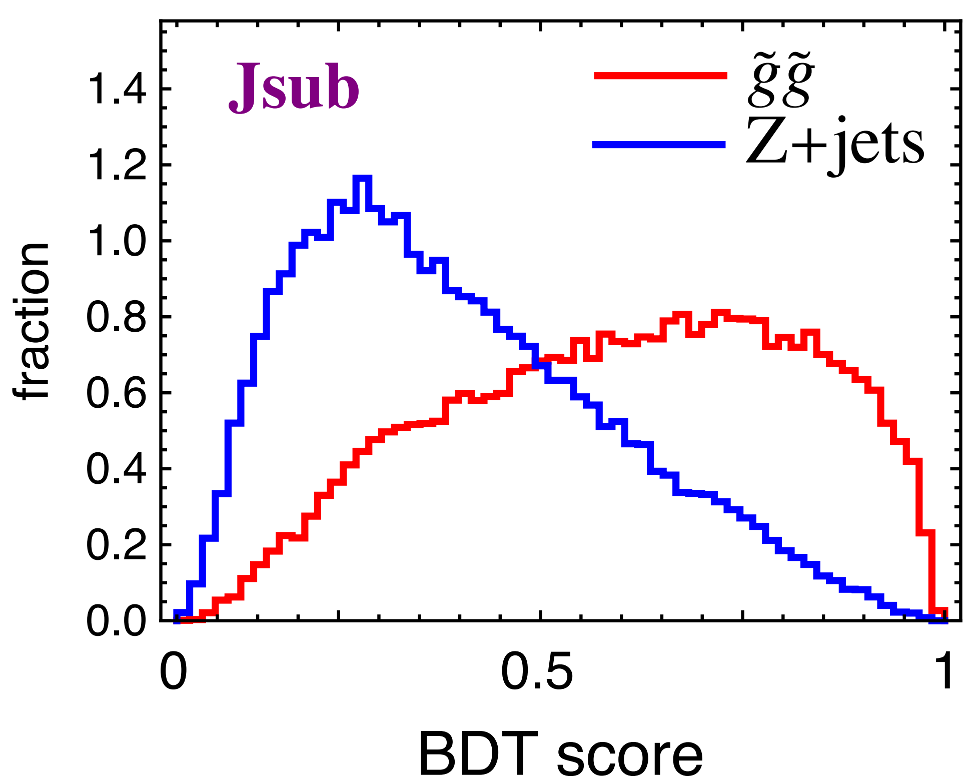
Optimal Classifier (Neyman–Pearson)

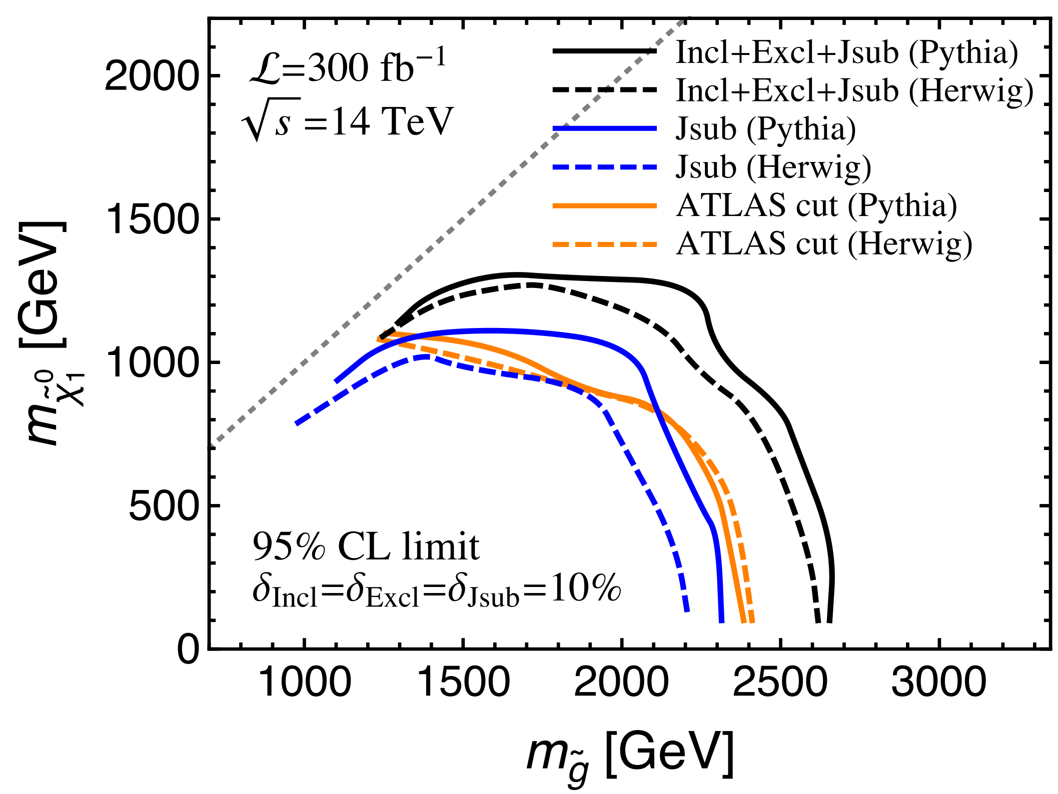
E.g. Search for Gluino Cascade to Dark Matter

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)



← background
signal →





[Bhattacherjee, Mukhopadhyay, Nojiri, Sakakie, Webber, 1609.08781]

Jet Classification Studies

Mix and match

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

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
…

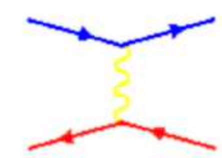
Signal vs. Background

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]

Particle Physics as ML Testbed

- *Huge datasets with reliable simulations*

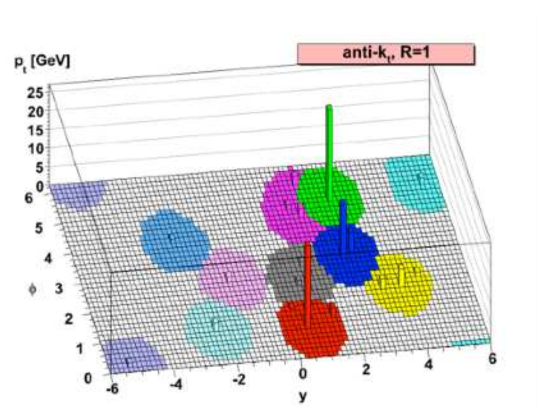
e.g.  with  +  + GEANT4 A SIMULATION TOOLKIT

MadGraph

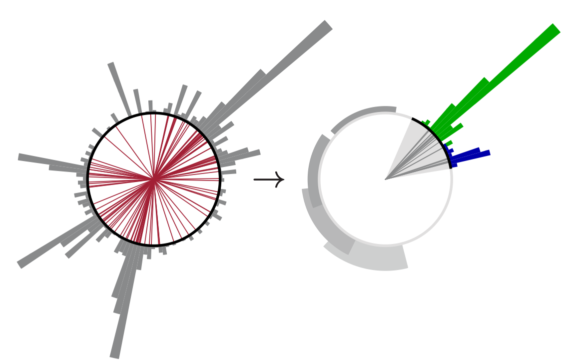
Pythia

- *Broad use of (un)supervised algorithms*

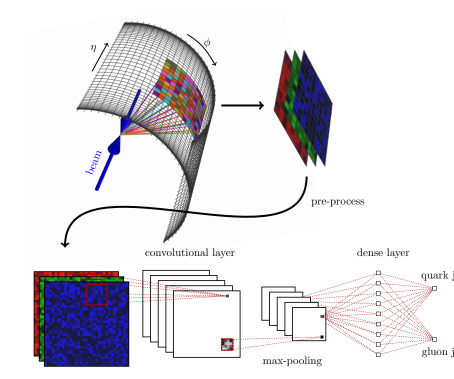
e.g.



Clustering



Noise Mitigation

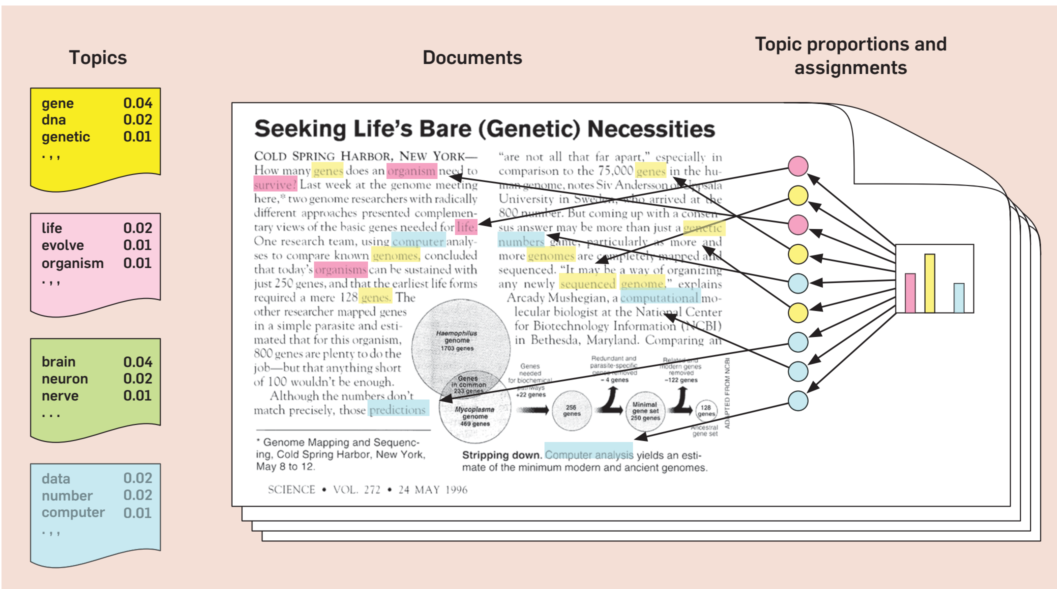


Machine Learning

- *Extensive domain knowledge and strong theory priors*

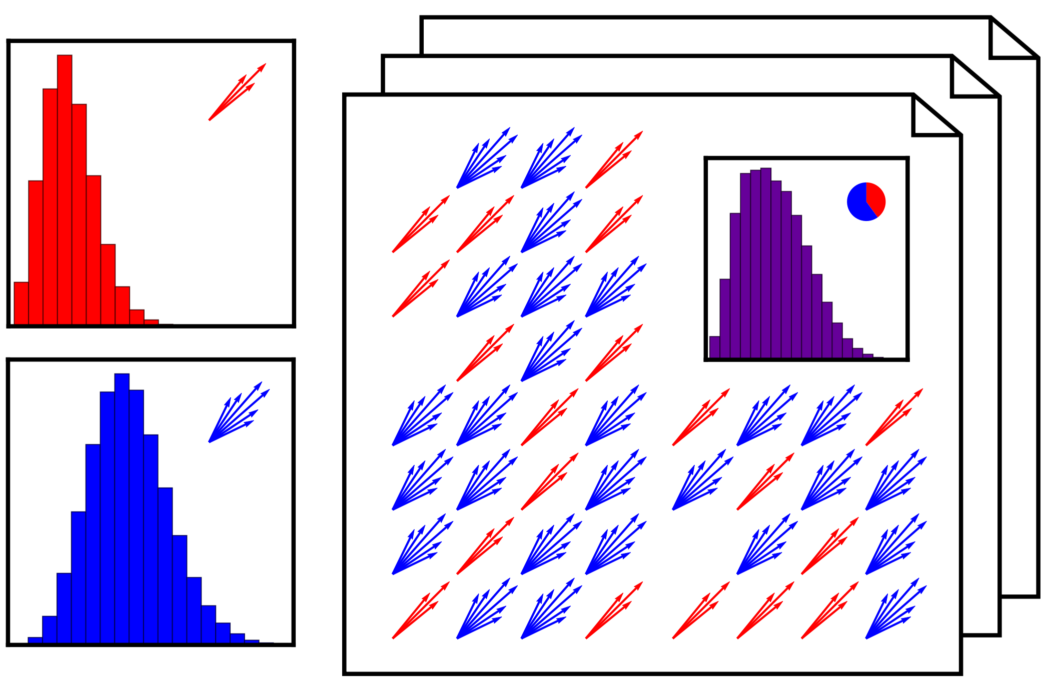
[figures from Cacciari, Salam, Soyez, 0802.1189; Larkoski, Marzani, JDT, Tripathee, Xue, 1704.05066; Komiske, Metodiev, Schwartz, 1612.01551]

E.g. Topic Modeling for Jets



Blind Source Separation:

Documents as bags of words
(which they really aren't)



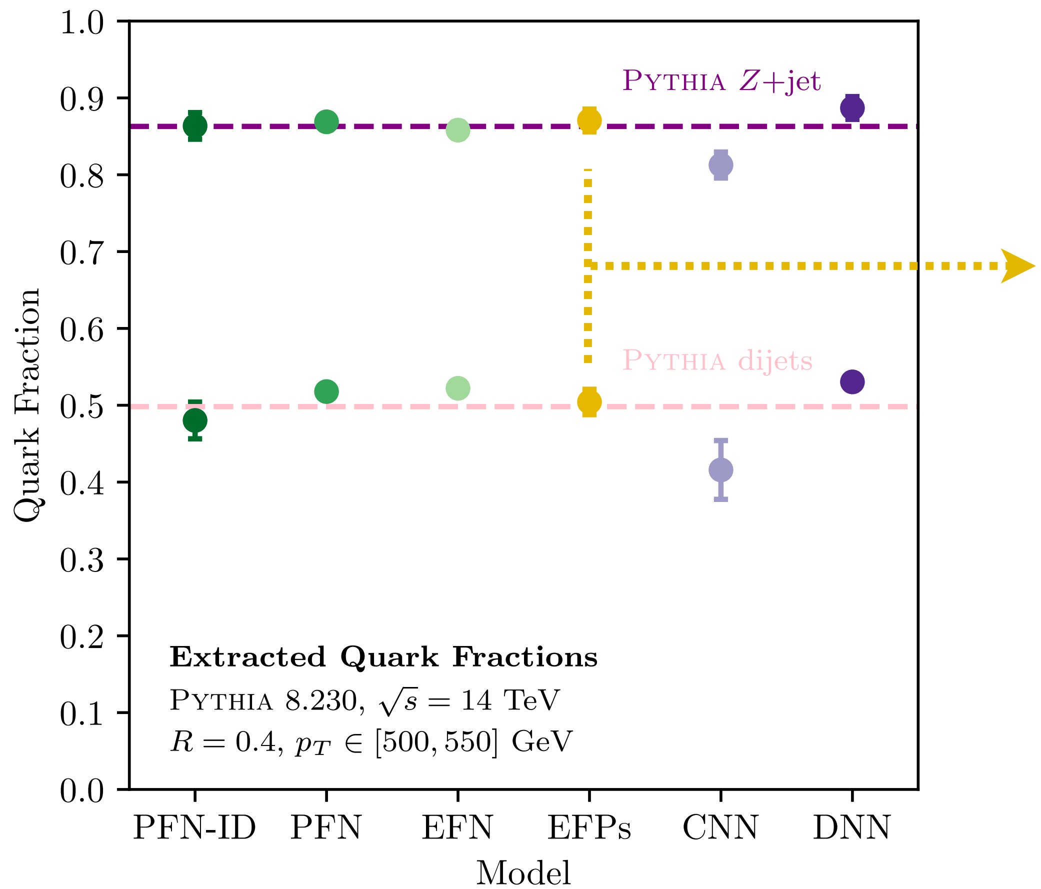
Quark/Gluon Separation:

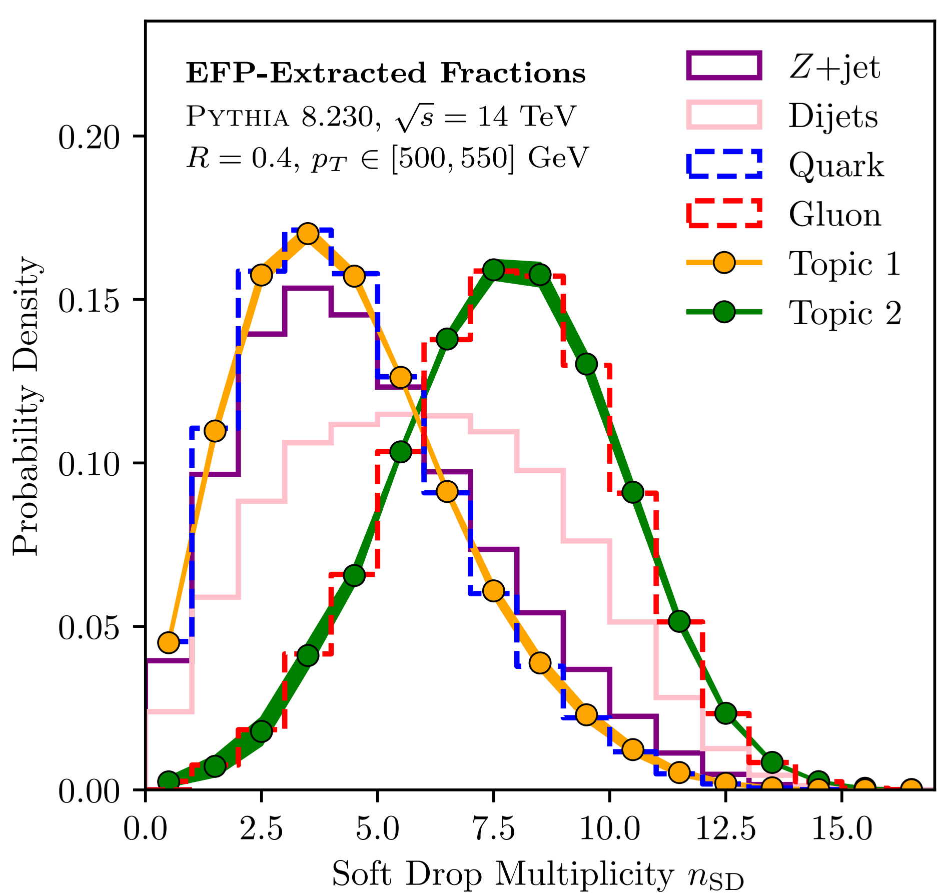
Jet histograms as mixtures of "mutually irreducible" categories
(which they really are)*

[Blei, CACM 2012; Metodiev, JDT, 1802.00008]

E.g. Topic Modeling for Jets

ML validation in complicated (but controlled) environment

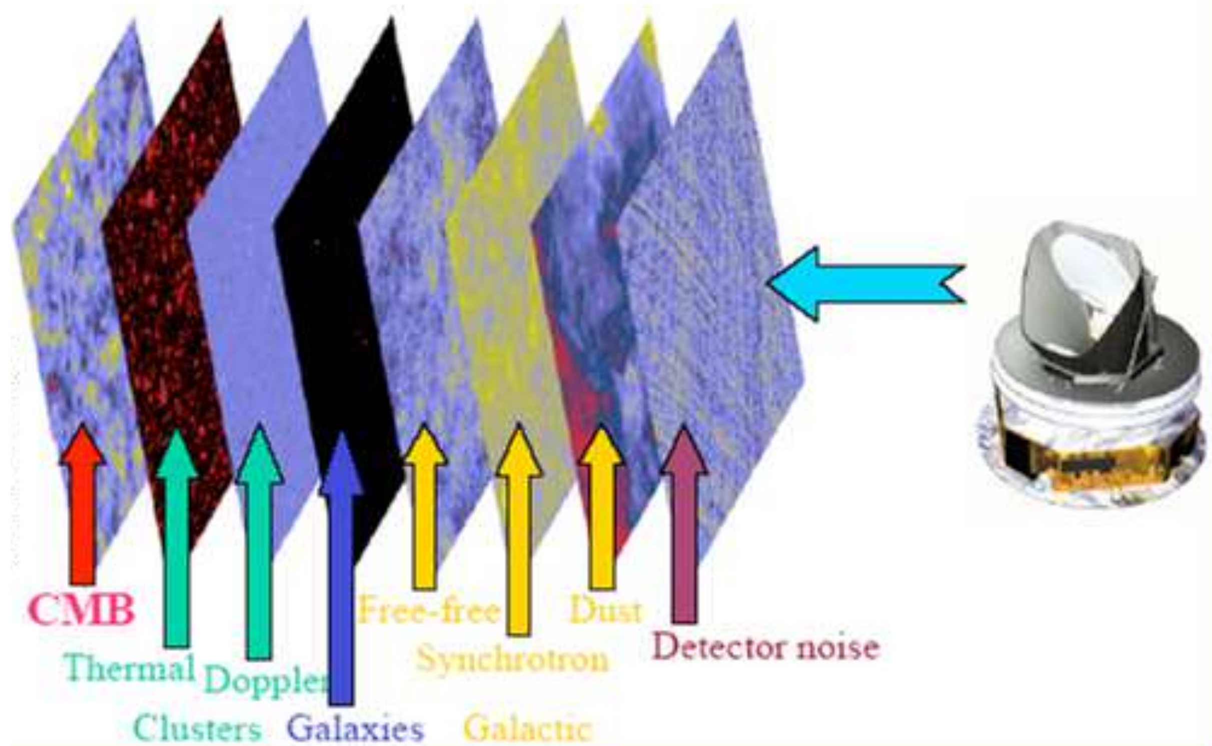


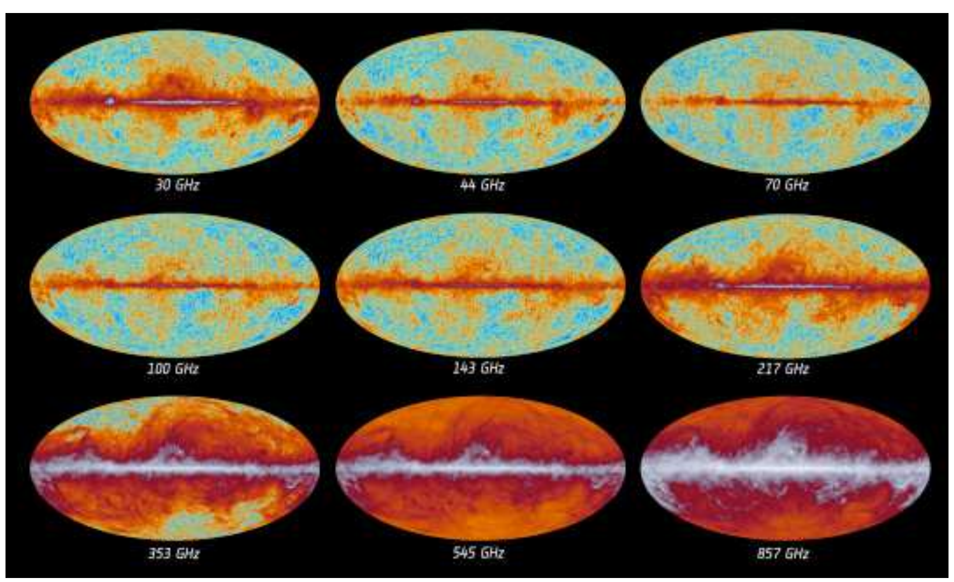


[Komiske, Metodiev, JDT, 1809.01140;
plotting Frye, Larkoski, JDT, Zhou, 1704.06266; Komiske, Metodiev, JDT, 1712.07124;
using Katz-Samuels, Blanchard, Scott, 1710.01167; Metodiev, Nachman, JDT, 1708.02949; Metodiev, JDT, 1802.00008]

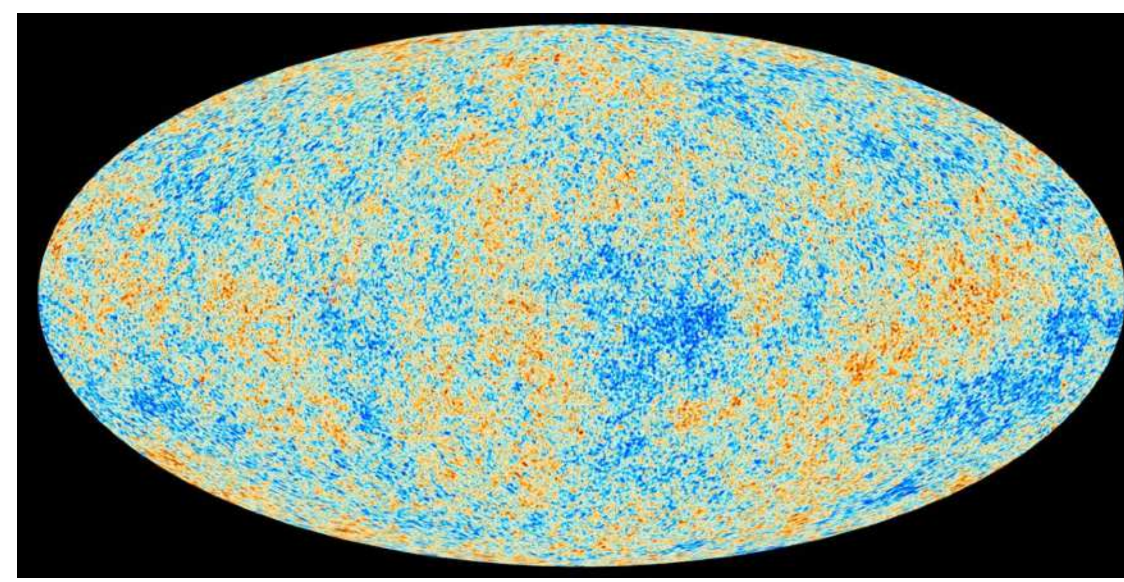
[Blei, CACM 2012; Metodiev, JDT, 1802.00008]

Related to CMB Foreground Separation



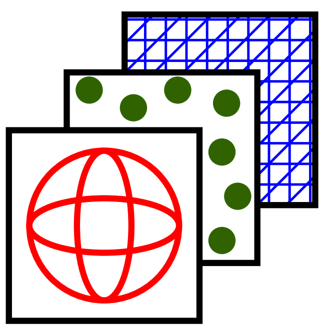


$\Rightarrow$



[Planck Outreach]

Particle Physics Primer



Point Clouds & Energy Flow Networks

(The Metric Space of Collider Events)

Relevance for the Dark Universe

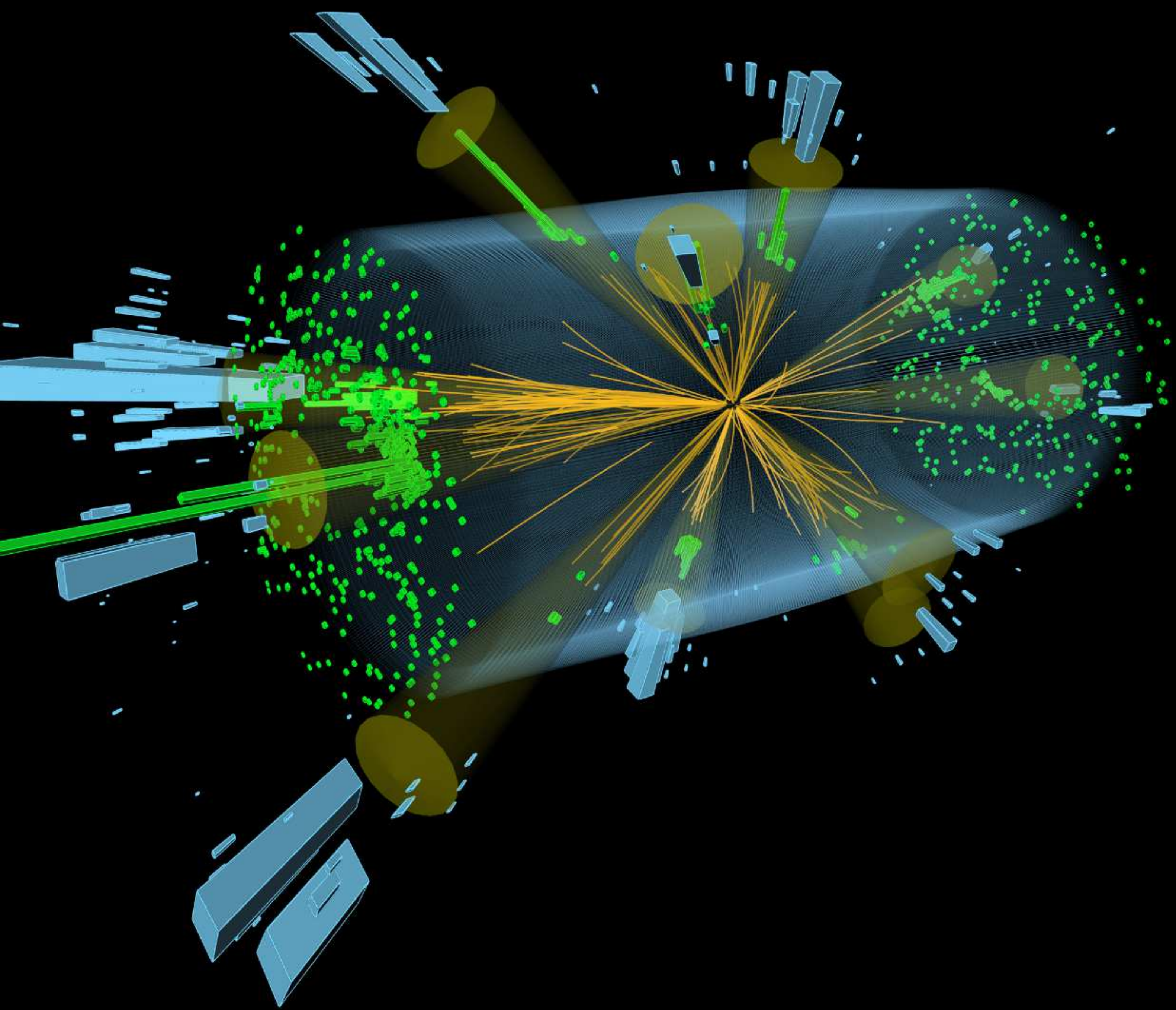
Can ML enhance the search for dark matter (and other BSM physics) at colliders?

Yes, almost every LHC analysis uses ML in some way
Today: Focus on jet classification tasks

Can the collider approach to ML inform astrophysical/cosmological investigations?

Yes, with two broad lessons:
Match ML architecture to symmetry of dataset
Pursue ML alternatives when data has meta-structures

What is a Collision Event?



T	E	H	M			
	●			γ	photon	elementary
●	●			$e^{\pm}$	electron	elementary
●	•	•	●	$\mu^{\pm}$	muon	elementary
●	•	●		$\pi^{\pm}$	pion	composite
●	•	●		$K^{\pm}$	kaon	composite
	•	●		K_L^0	K-long	composite
●	•	●		$p/\overline{p}$	proton	composite
	•	●		$n/\overline{n}$	neutron	composite

Point Cloud

[Popular Science, 2013]

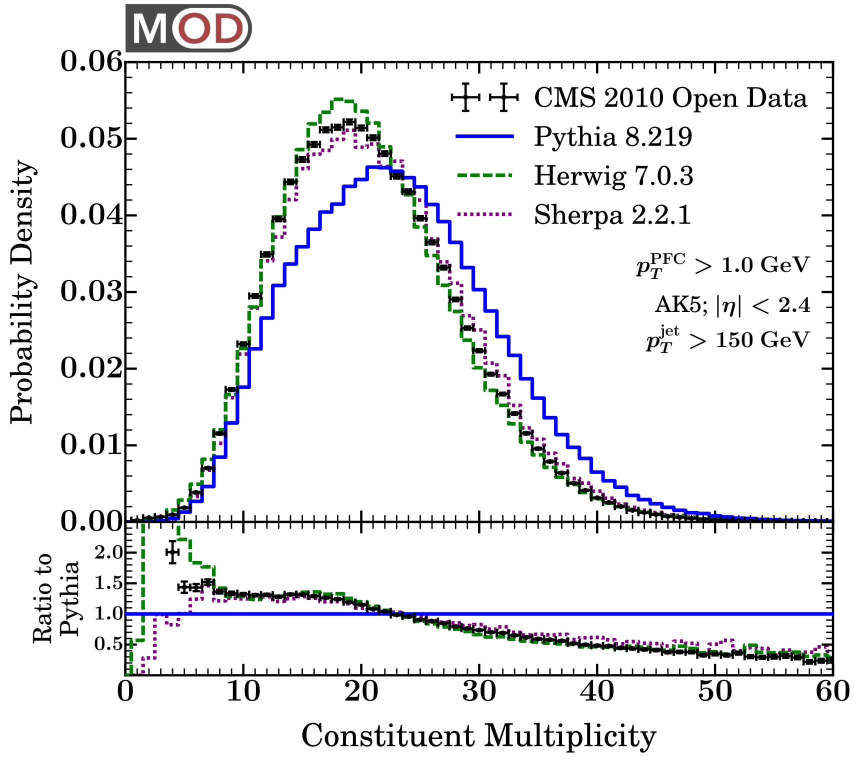
Key Fact #1: Events/Jets are Point Clouds

Jet constituents:

Particle-like objects

Variable-length

Unordered set QM



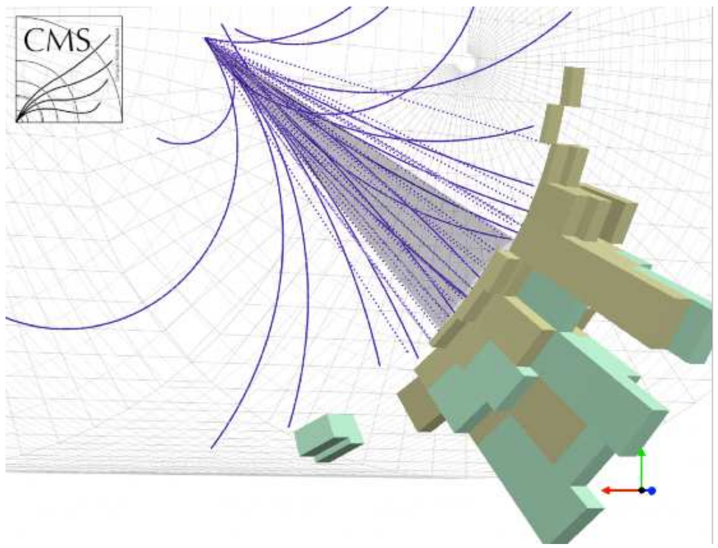
Per particle:

$\{E, p_x, p_y, p_z\}$ or $\{p_T, y, \Phi, m\}$

Flavor/charge labels

Vertex information

Quality criteria, etc.

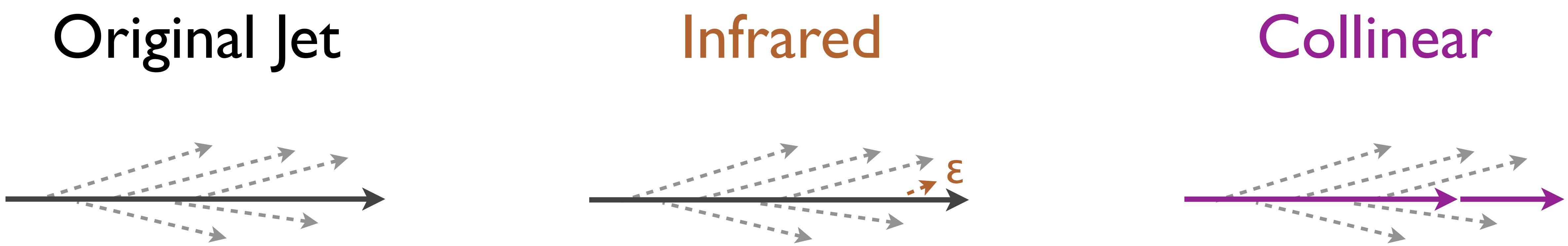


[plot from Tripathee, Xue, Larkoski, Marzani, JDT, 1704.05842]

Key Fact #2: IRC Safety is Important

Wide range of interesting observables are "safe"

Interesting ≈ Calculable in fixed-order perturbation theory



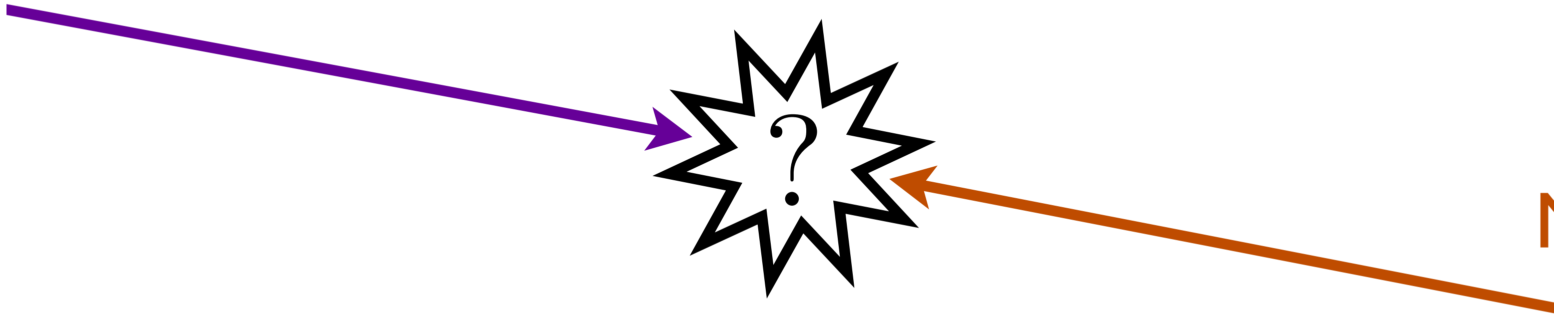
IRC Safe Observable: Insensitive to IR or C emissions

Enforces smooth interpolation between variable-length inputs (i.e. $N \rightarrow N-1$)

(optionally)

Bottom line: Jets are energy-weighted point clouds

Theoretical
(High Energy)
Physics



Mathematics,
Statistics,
Computer Science

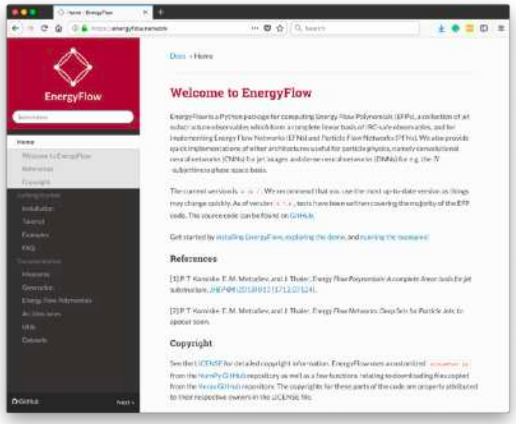
Patrick Komiske

Eric Metodiev

Theoretical (High Energy) Physics

?

Mathematics, Statistics, Computer Science



Energy Flow Networks

https://energyflow.network/

Theory Prior: Dissect Jets with Addition

Additive Observable: $\mathcal{O} = \sum_{i \in \text{jet}} \Phi(E_i, \vec{p}_i, \ldots)$

(relevant for factorization in SCET)

Permutation invariant by construction
Easily adapts to variable-length inputs
Can approximate Φ with neural networks
Can incorporate additional particle properties
Linear runtime in number of particles

Additive Safe Observable: $\mathcal{O} = \sum_{i \in \text{jet}} E_i \, \Phi(\hat{p}_i) \qquad \hat{p}_i = \frac{\vec{p}_i}{E_i}$

IRC safety guaranteed by energy weighting

Conjectured Generalization

Arbitrary permutation-symmetric observable?

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

Latent Additive Observables

$$\mathcal{O}_a = \sum_{i \in \text{jet}} \Phi_a(E_i, \vec{p}_i, \ldots)$$

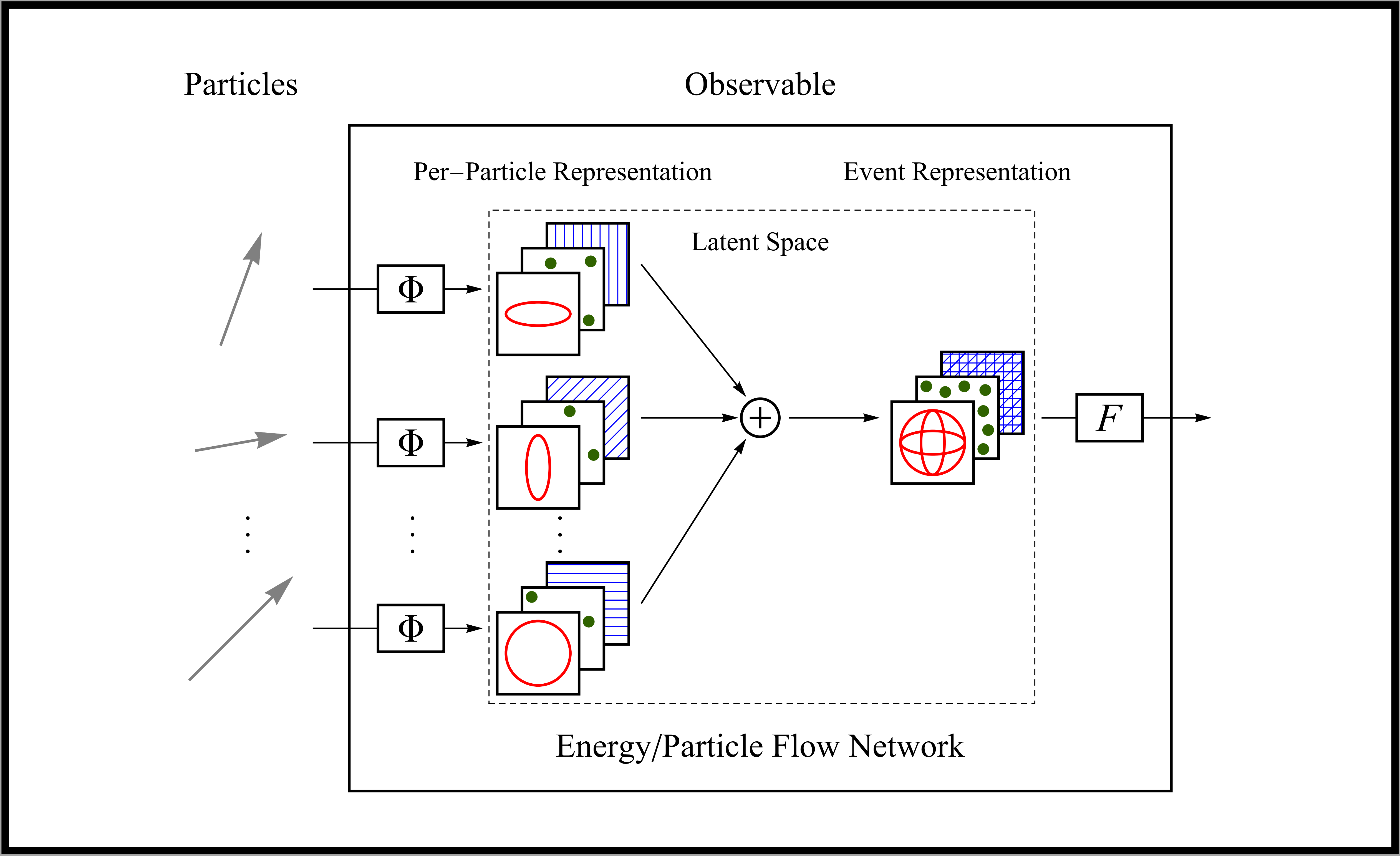
Energy / Particle Flow Networks

IRC-safe Φ

General Φ

[Komiske, Metodiev, JDT, 1810.05165]

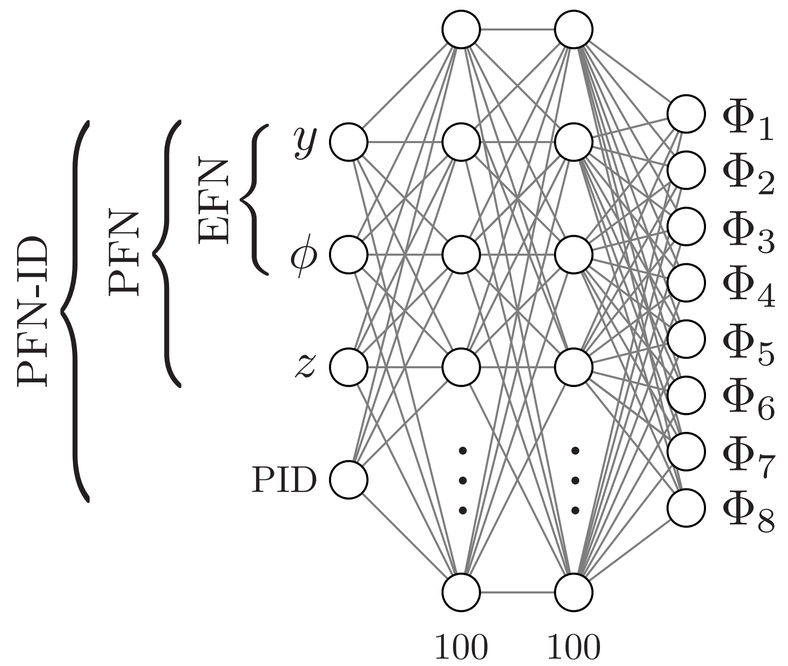
Conjectured Generalization



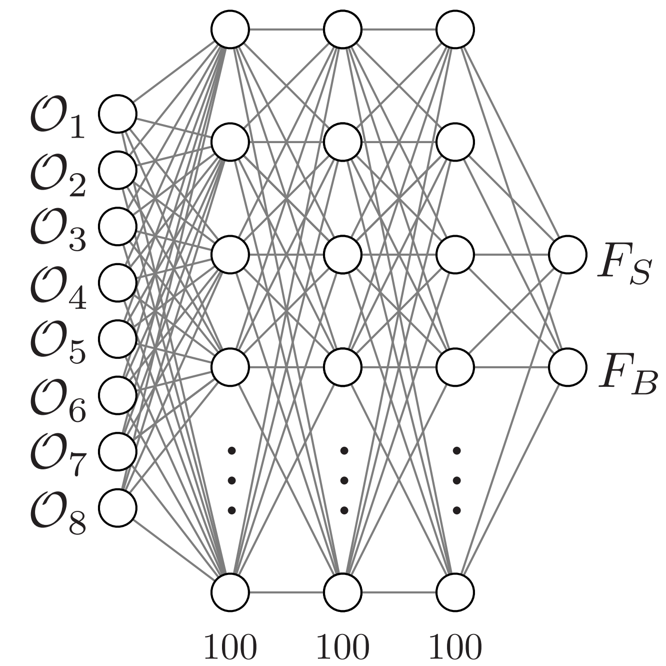
[Komiske, Metodiev, JDT, 1810.05165]

Conjectured Generalization

Per-Particle: Φ



Latent Combiner: F



Per-Jet (Latent Space):

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

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

Final Discriminant:

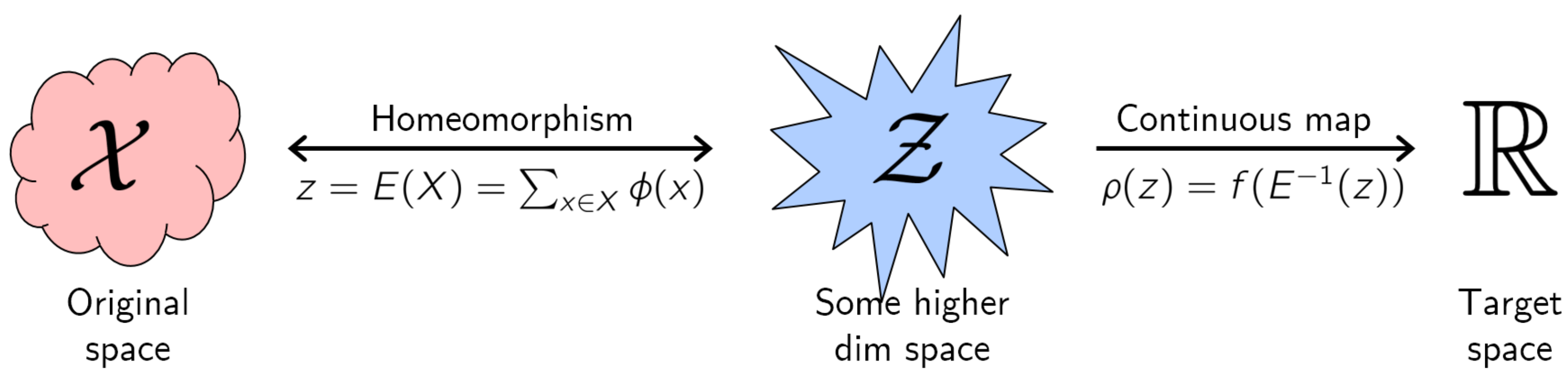
$$\text{softmax}(F_S, F_B)$$

[Komiske, Metodiev, JDT, 1810.05165]

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.*

(!)



Variable-Length Unordered Set of Particles

Additive Latent Space

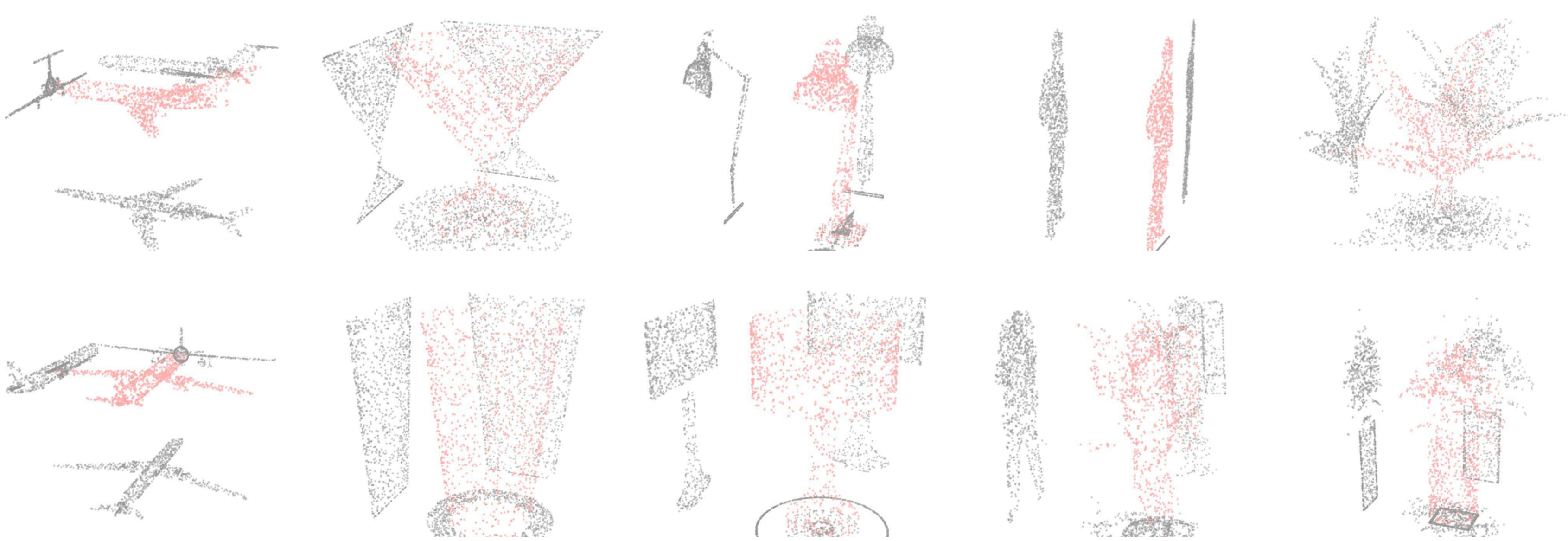
Generic Observable

[Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, 1703.06114]

Deep Sets for…

Celebrity Face Anomaly Detection

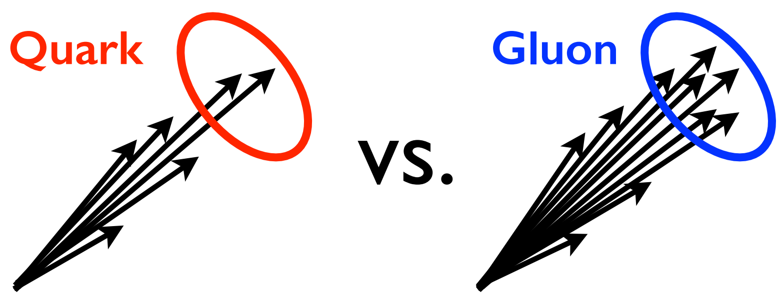
Point Cloud Classification



[Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, 1703.06114]

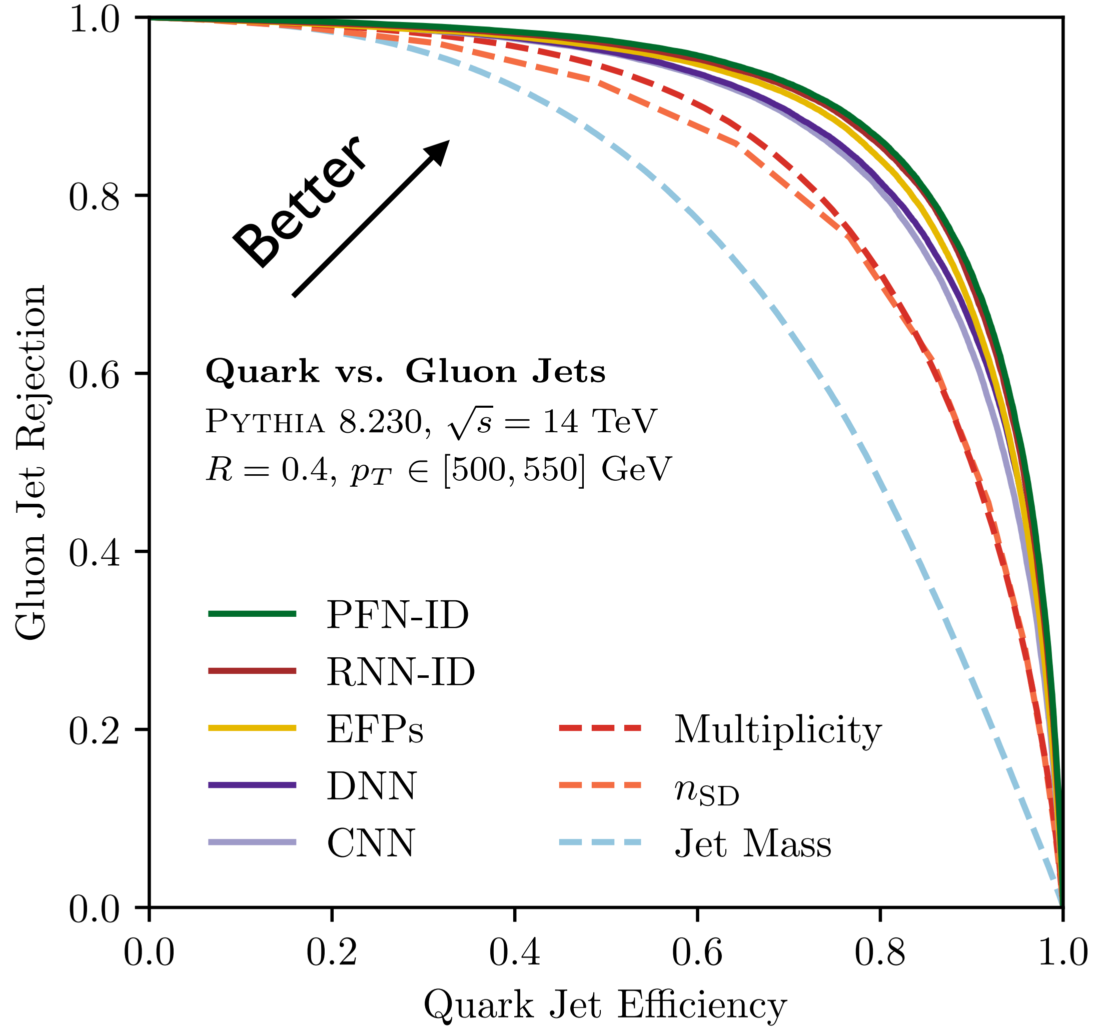
Deep Sets for Particle Jets

Q vs. G: The “Hello, World!” of jet classification



Theory prior:
Network must be exploiting
IRC singularity structure of QCD

Competitive with previous methods



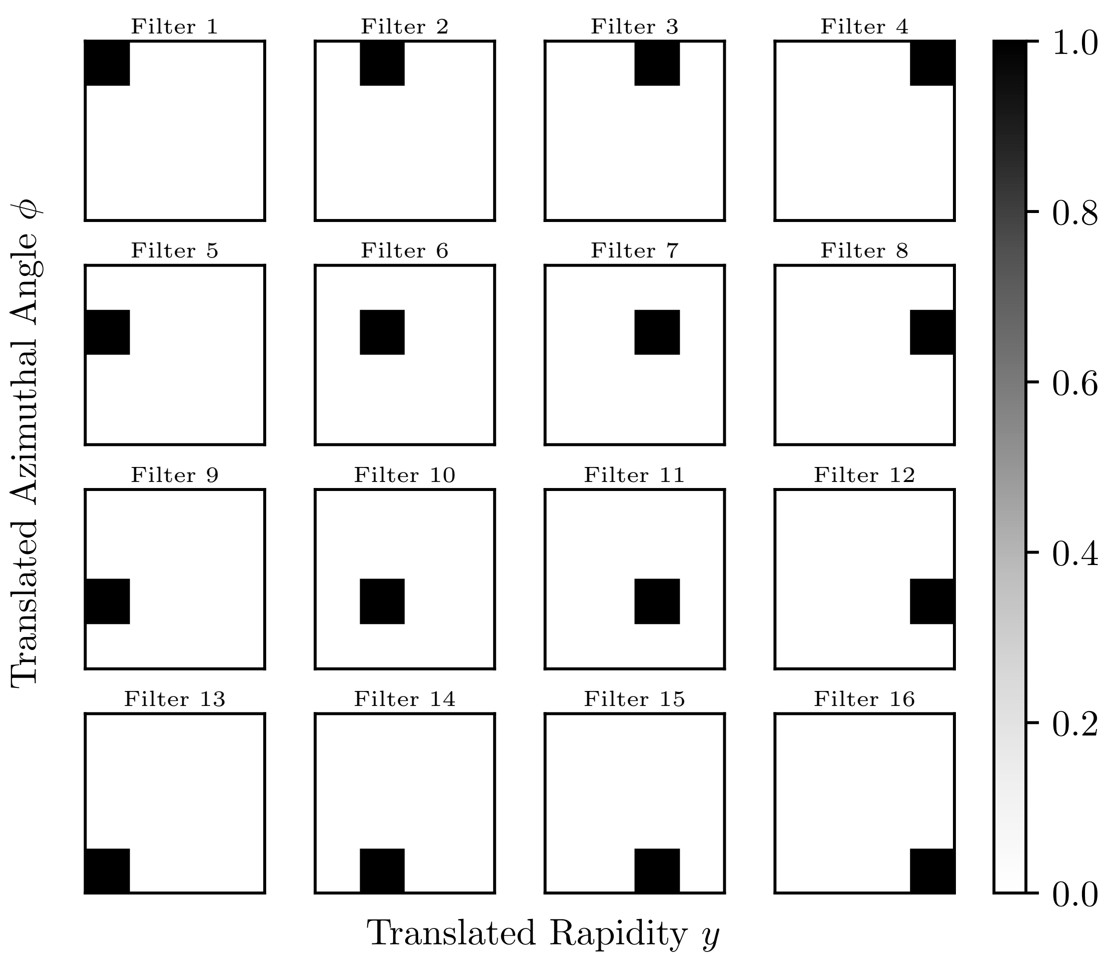
[Komiske, Metodiev, JDT, 1810.05165]

Latent Space Visualization

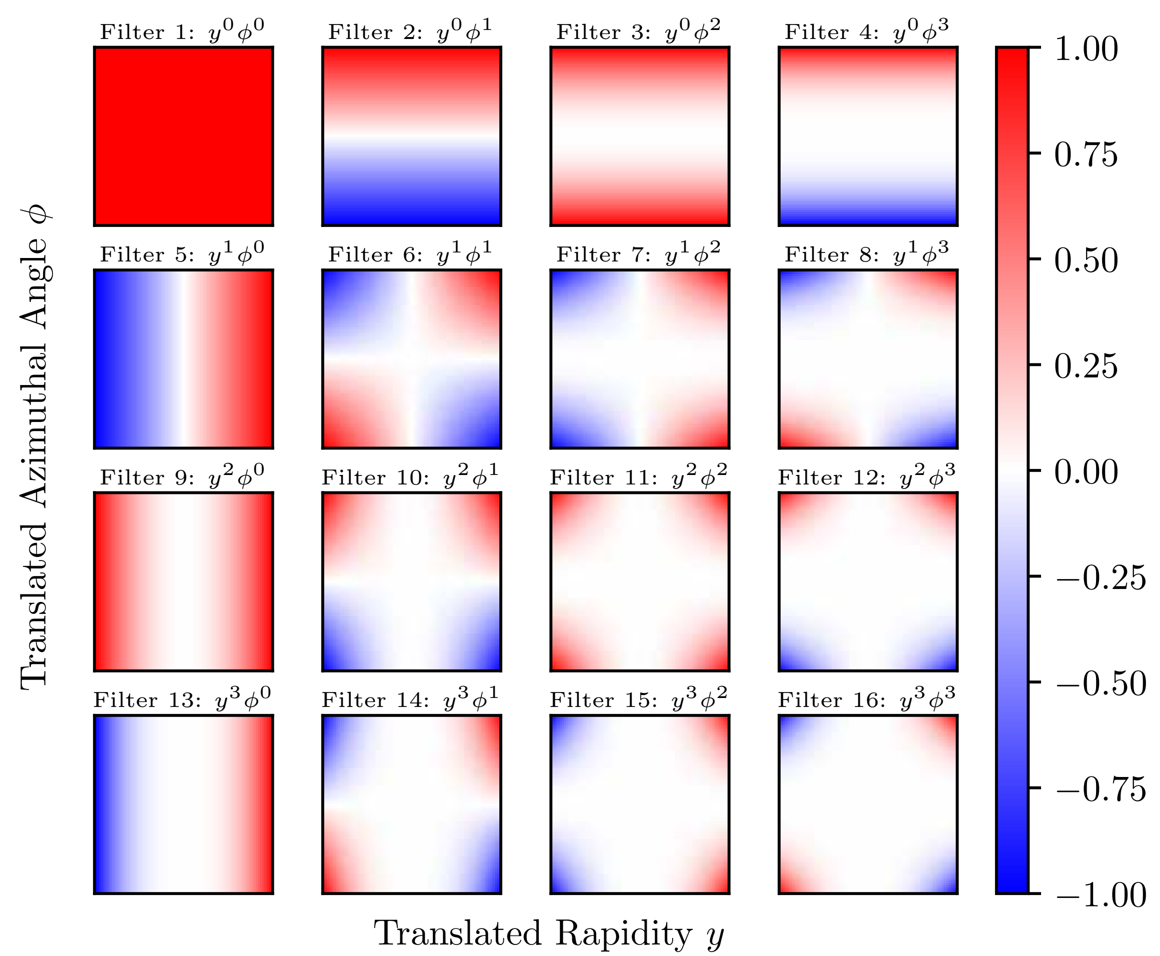
$$\mathcal{O}(\{p_i^\mu\}) = F(\mathcal{O}_1, \mathcal{O}_2, \ldots, \mathcal{O}_\ell)$$

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

Calorimeter Pixels



Radiation Moments



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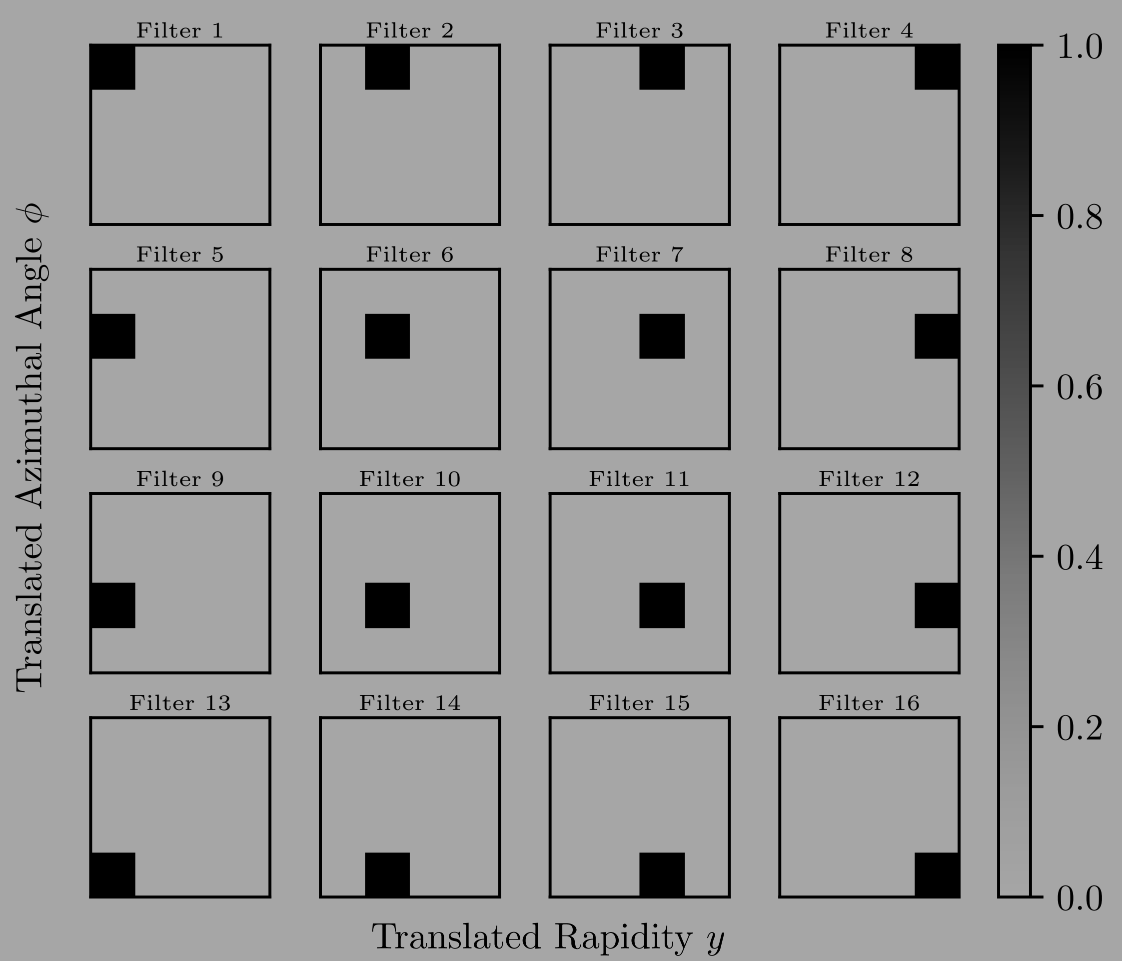
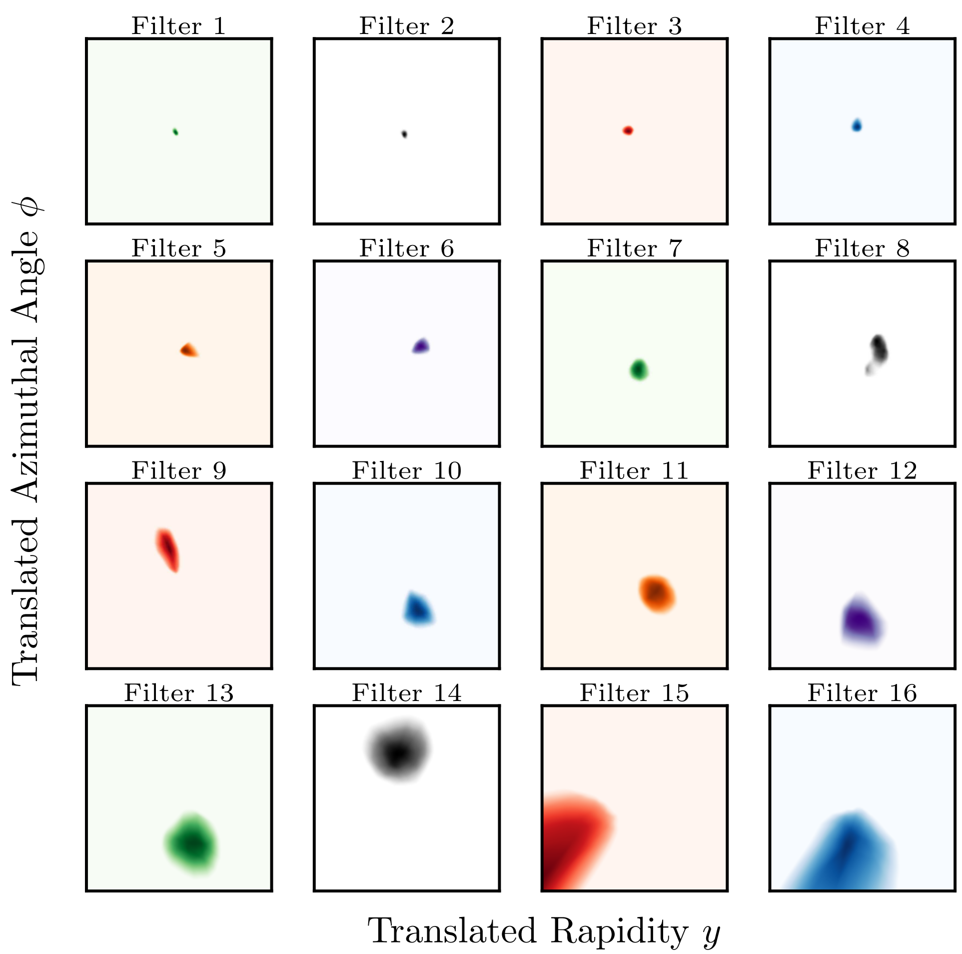
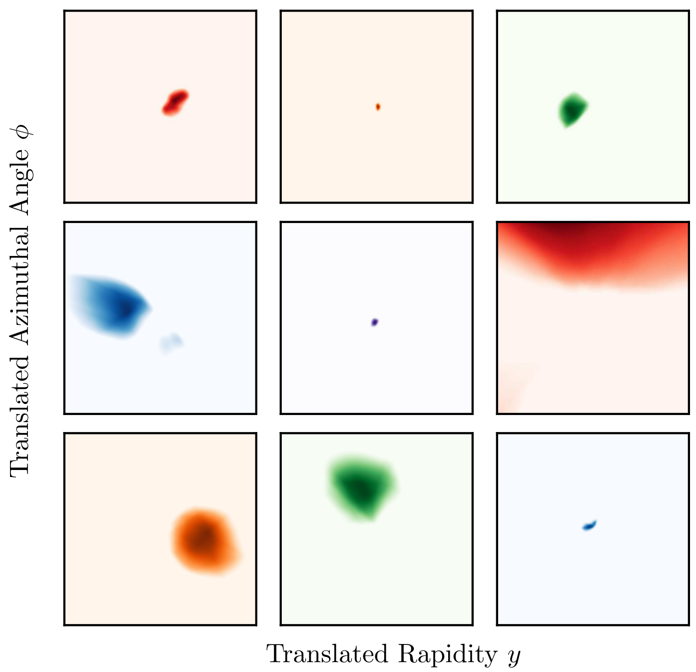


EFNs: Dynamic Pixelation

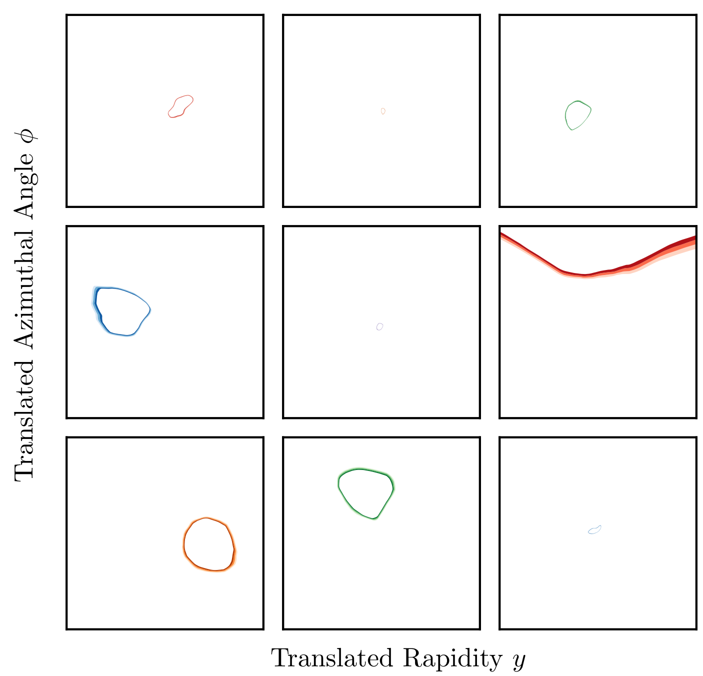


Psychedelic Network Visualization

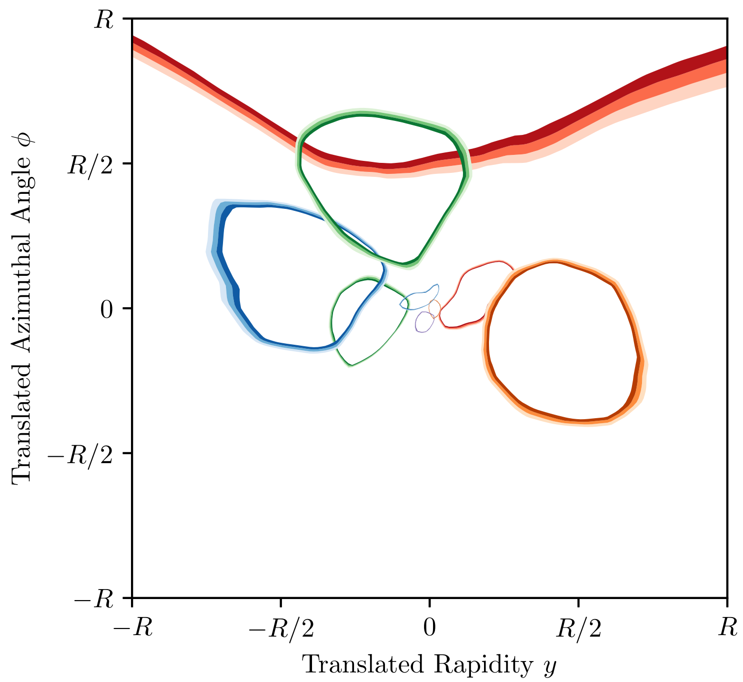
Latent Filters



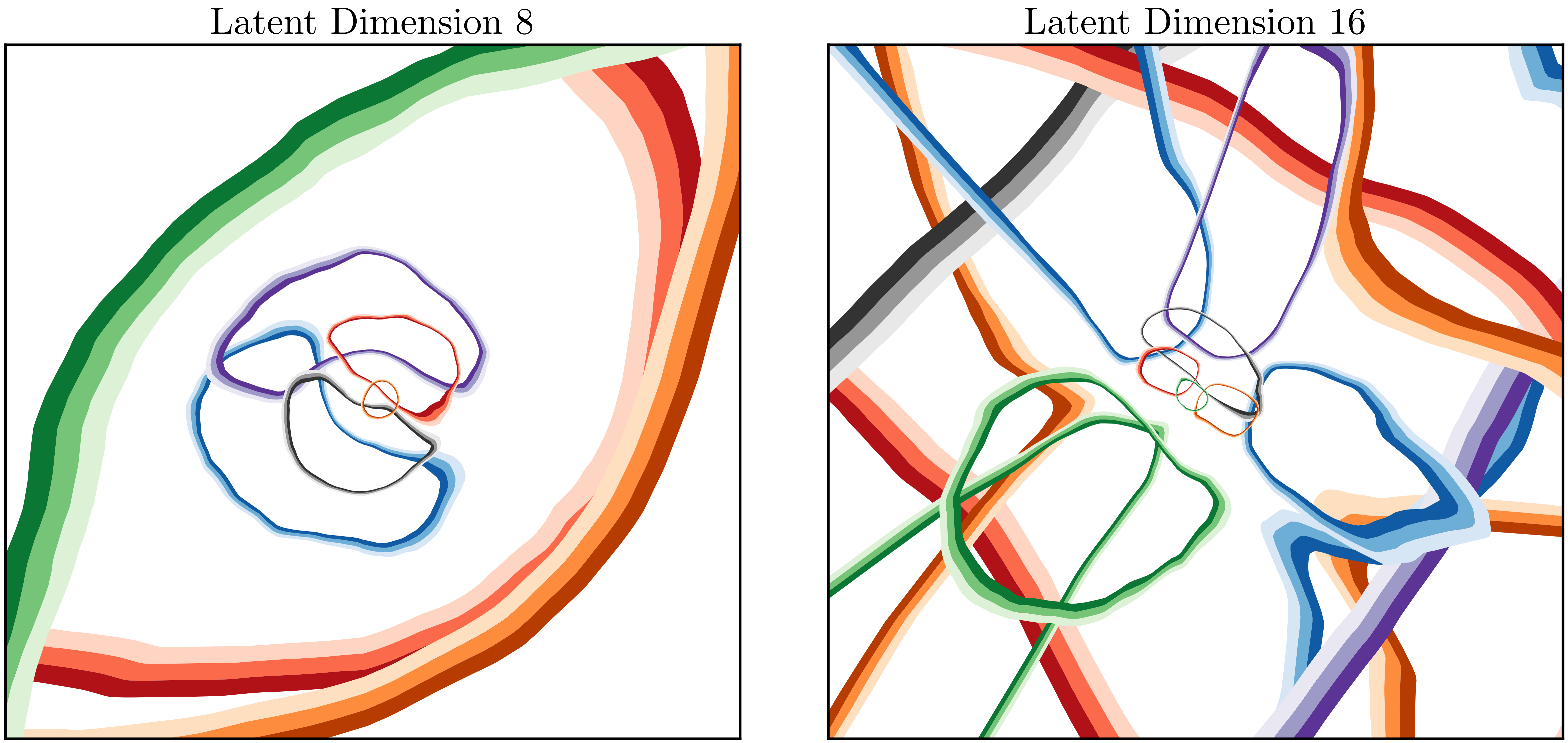
50% Contours



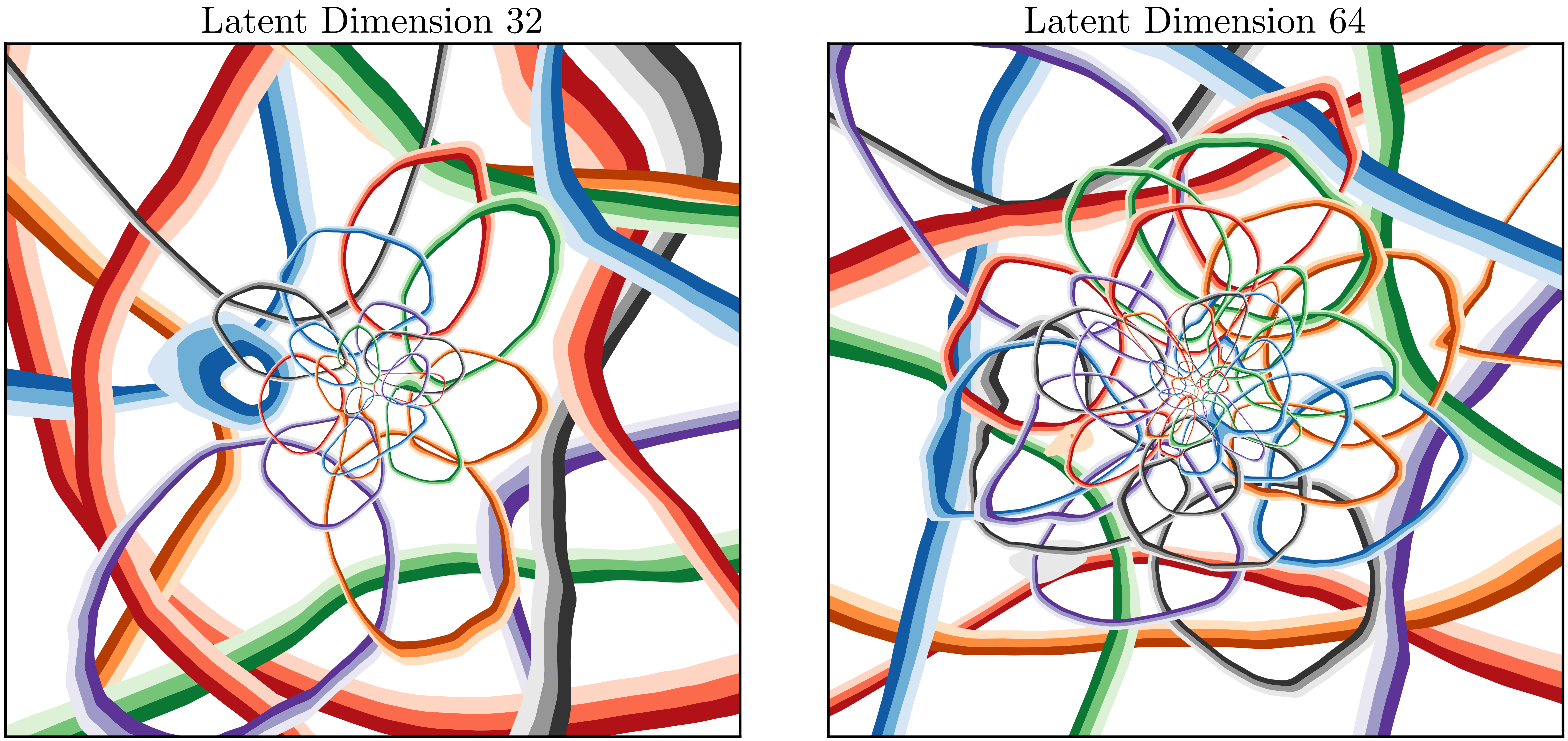
Overlay



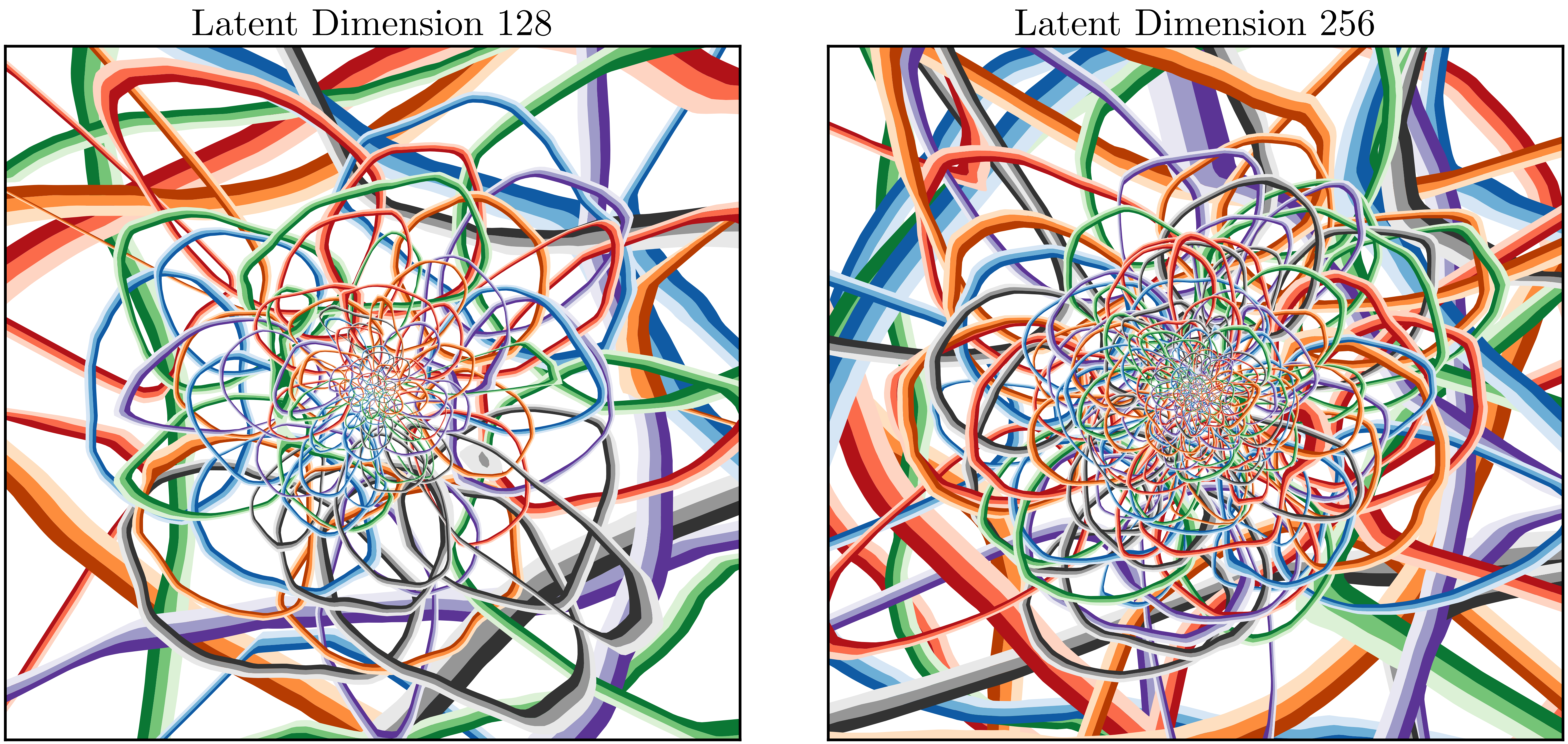
Psychedelic Network Visualization



Psychedelic Network Visualization

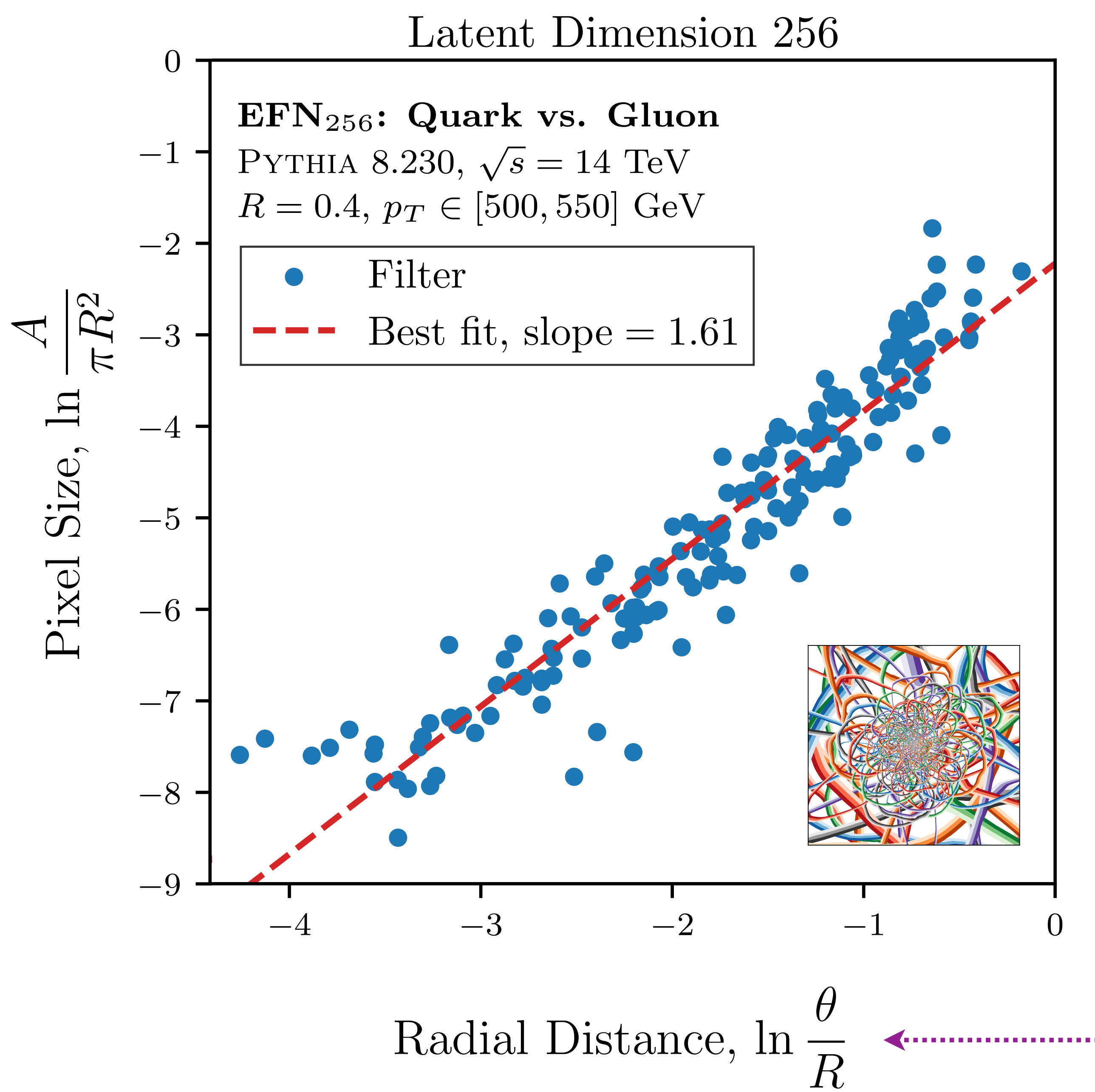


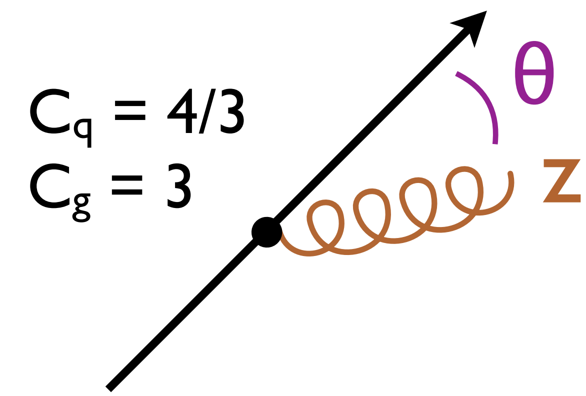
Psychedelic Network Visualization



Collinear singularity of QCD!

Learning the Singularity Structure of QCD

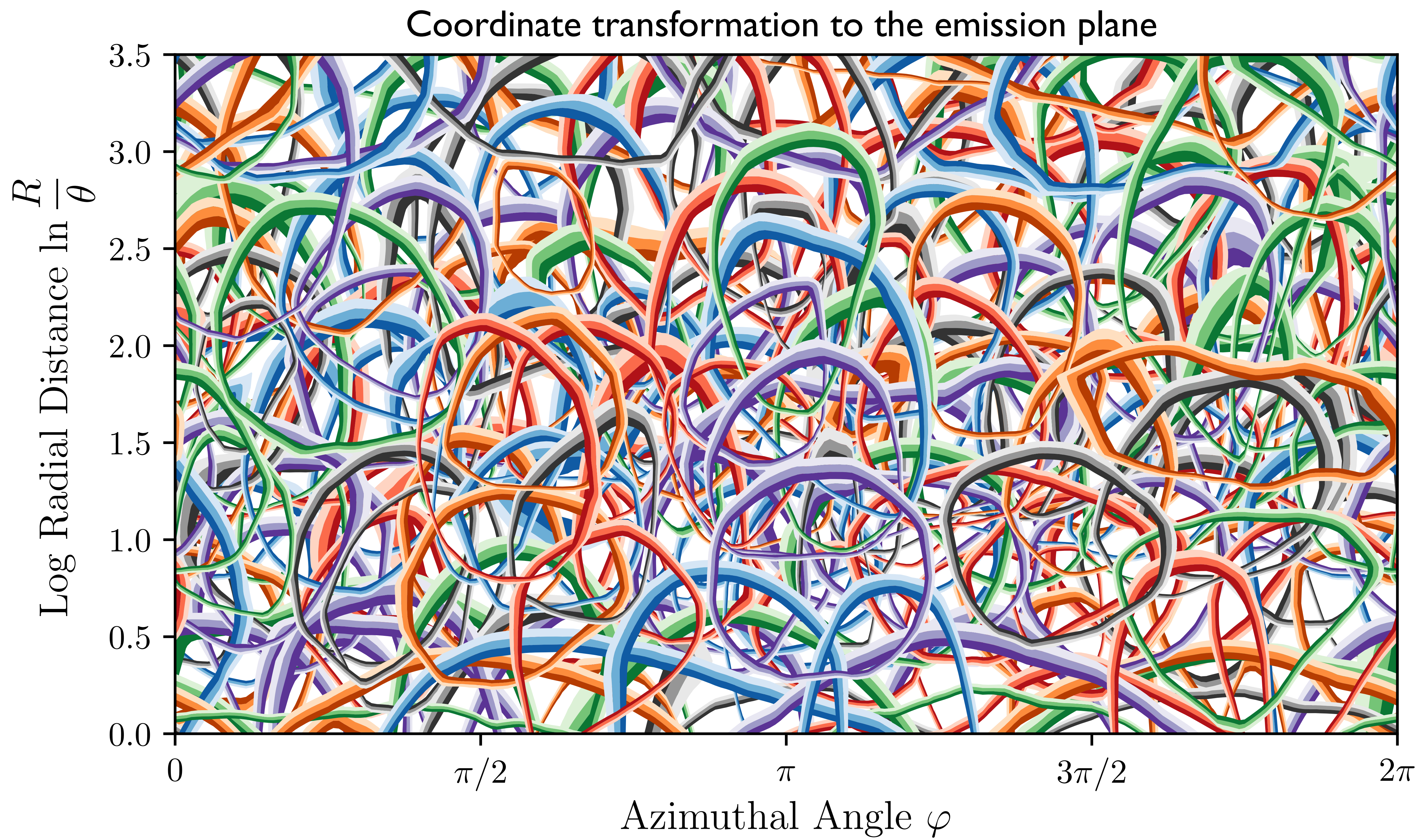




$$\mathrm{d}P_{i \to ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{\mathrm{d}\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{\mathrm{d}z}{z}}_{\text{Soft}}$$

[Komiske, Metodiev, JDT, 1810.05165]

Ready for the MoMA

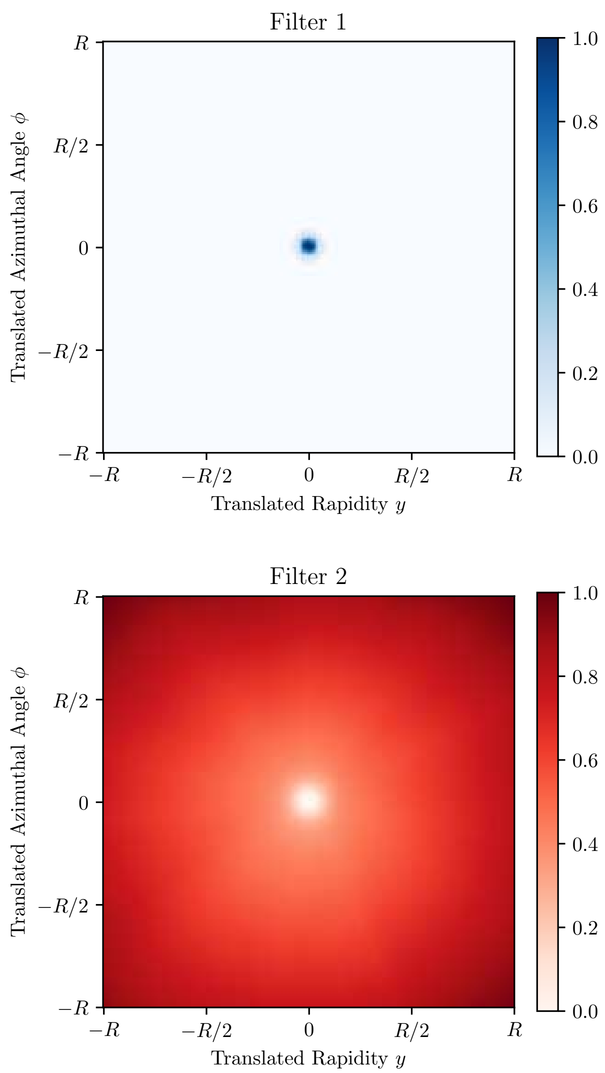


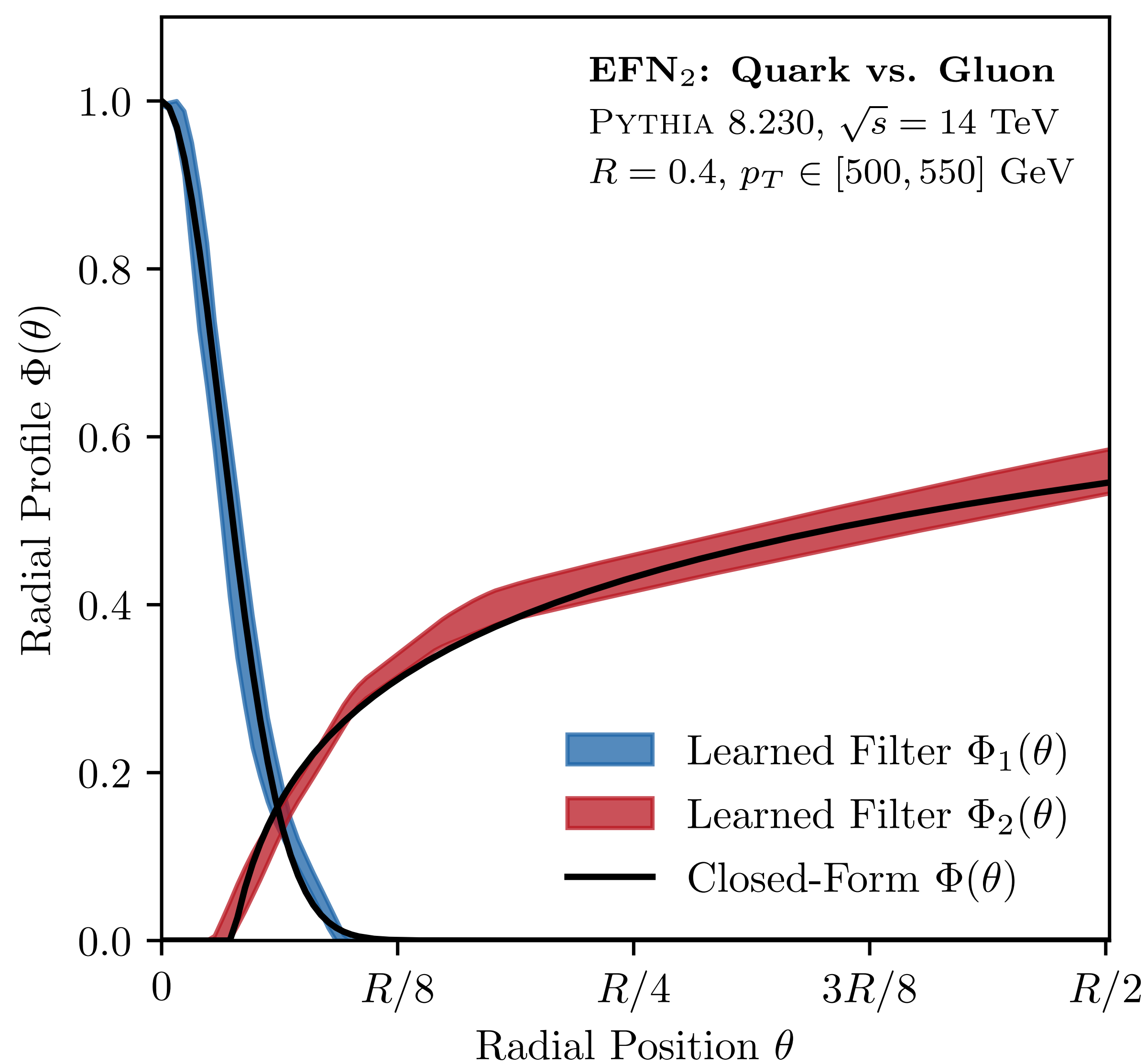
[Komiske, Metodiev, JDT, 1810.05165]

“What is the Machine Learning?”

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

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





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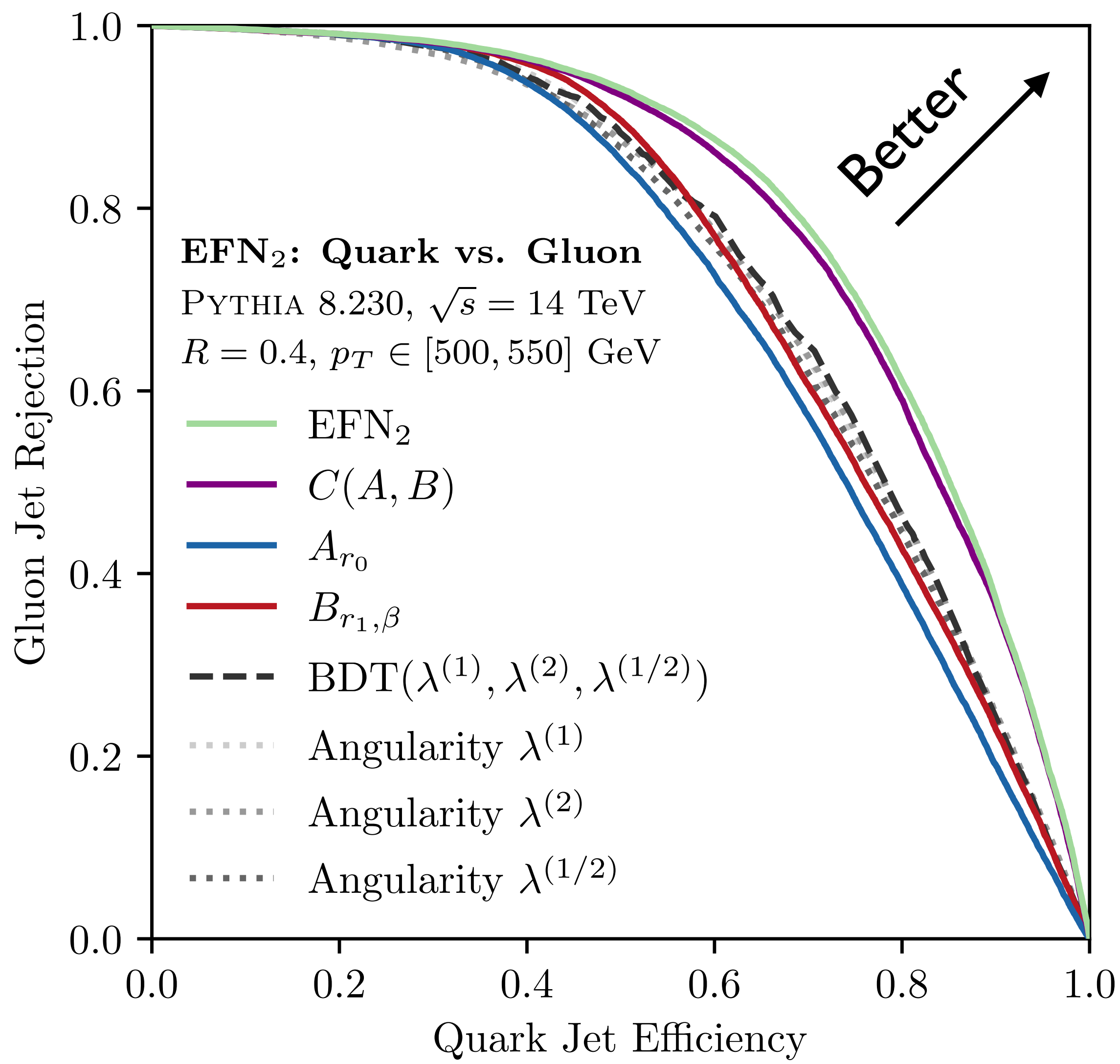


EFN outperformed a domain expert (i.e. me)

But we successfully reverse engineered the machine

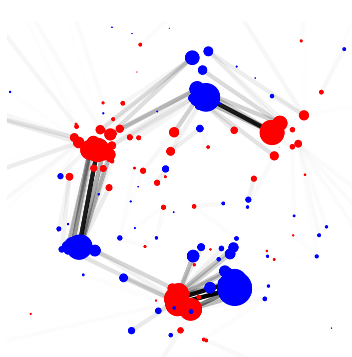
The Broader Lesson

Advances in hep-th, -ph, -ex	$\Leftrightarrow$	*Advances in cs.LG, stat.ML (& astro-ph.CO?)*
Particle Flow Networks	$\longleftarrow$ Point Clouds $\longleftarrow$	Deep Sets
Energy Flow Networks	$\longrightarrow$ Weighted Point Clouds $\longrightarrow$	??

Particle physics is a fascinating domain with rich data sets, established algorithms, and strong theory priors

Particle Physics Primer

Point Clouds & Energy Flow Networks



(The Metric Space of Collider Events)

Relevance for the Dark Universe

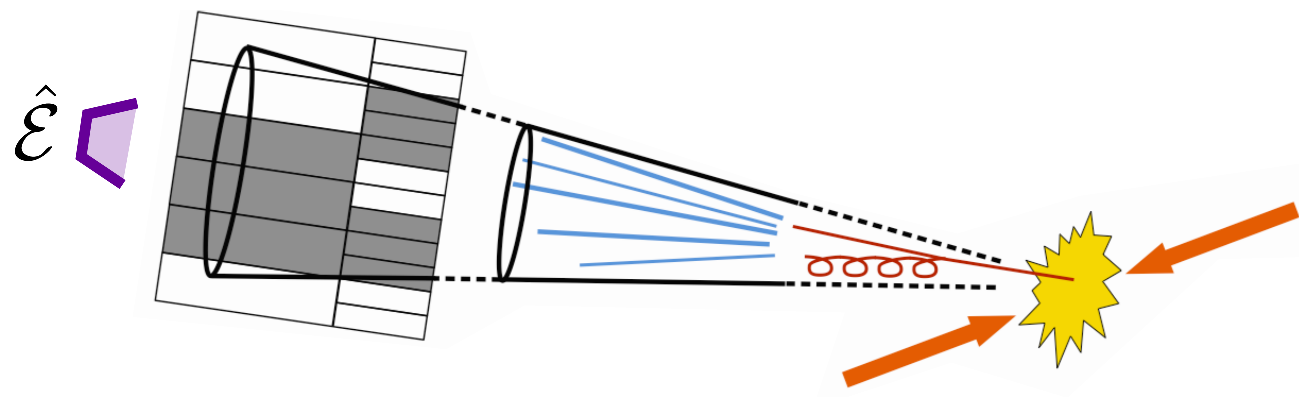
Can ML enhance the search for dark matter (and other BSM physics) at colliders?

Yes, almost every LHC analysis uses ML in some way
Today: Focus on jet classification tasks

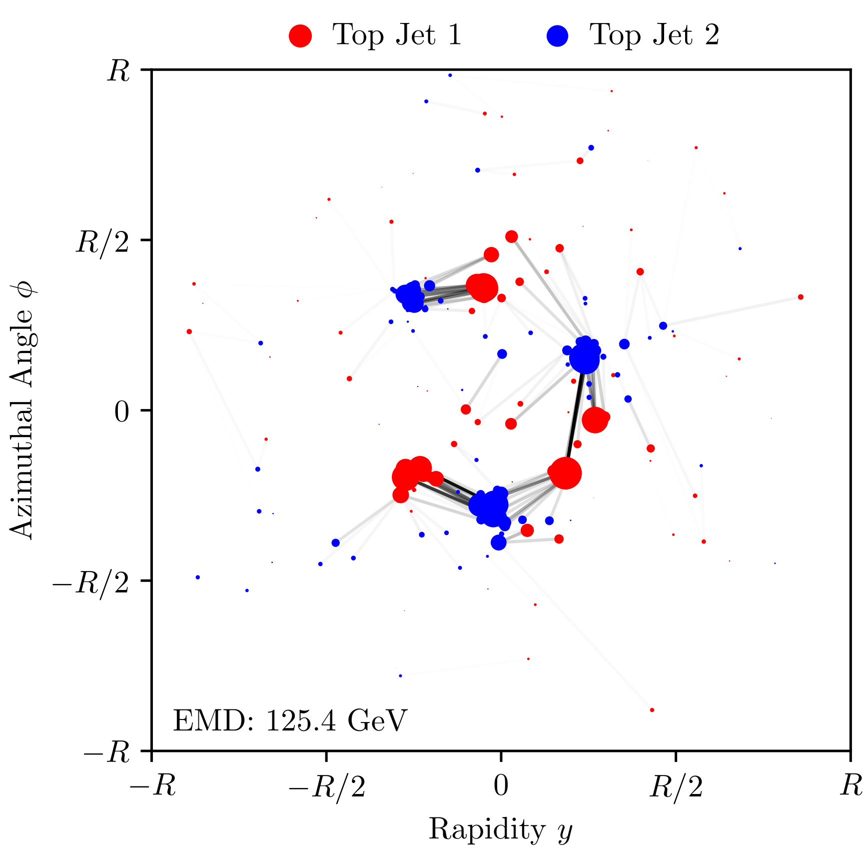
Can the collider approach to ML inform astrophysical/cosmological investigations?

Yes, with two broad lessons:
Match ML architecture to symmetry of dataset
Pursue ML alternatives when data has meta-structures

Theory Prior: Keep a "Safe" Distance



Difference in energy flow $\leftrightarrow$ *IRC-safe similarity measure*



e.g. Earth Mover's Distance

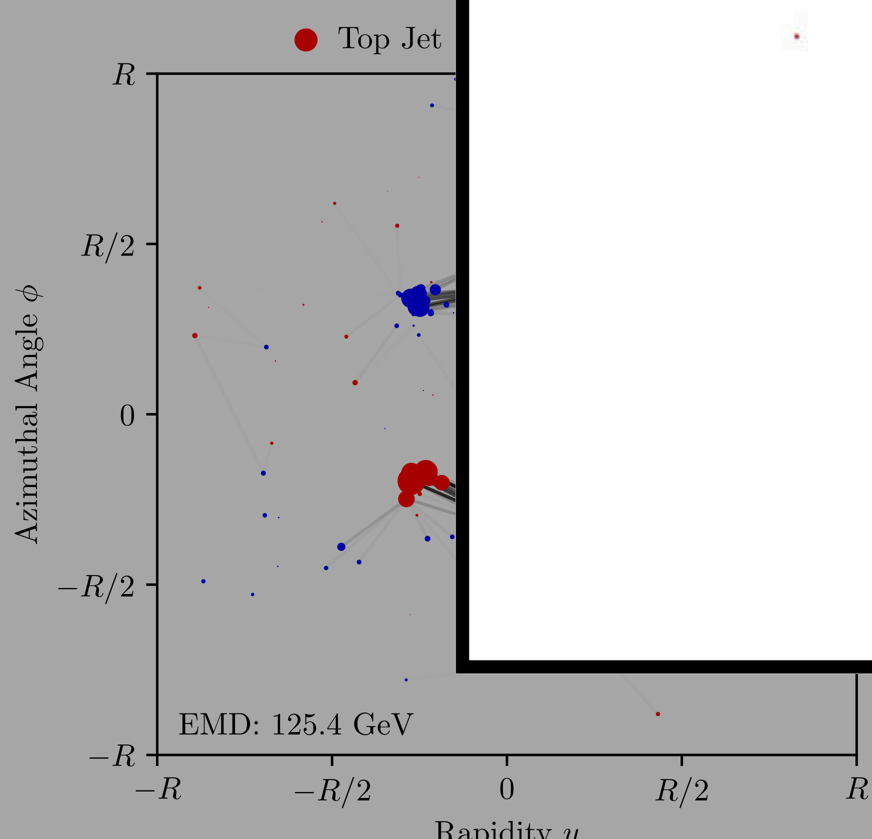
$$\mathrm{EMD}(\mathcal{E}_1, \mathcal{E}_2) = \min_{\{f_{ij}\}} \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} f_{ij} \frac{\theta_{ij}}{R} + \left| E_{\mathrm{tot}}^{(1)} - E_{\mathrm{tot}}^{(2)} \right|$$

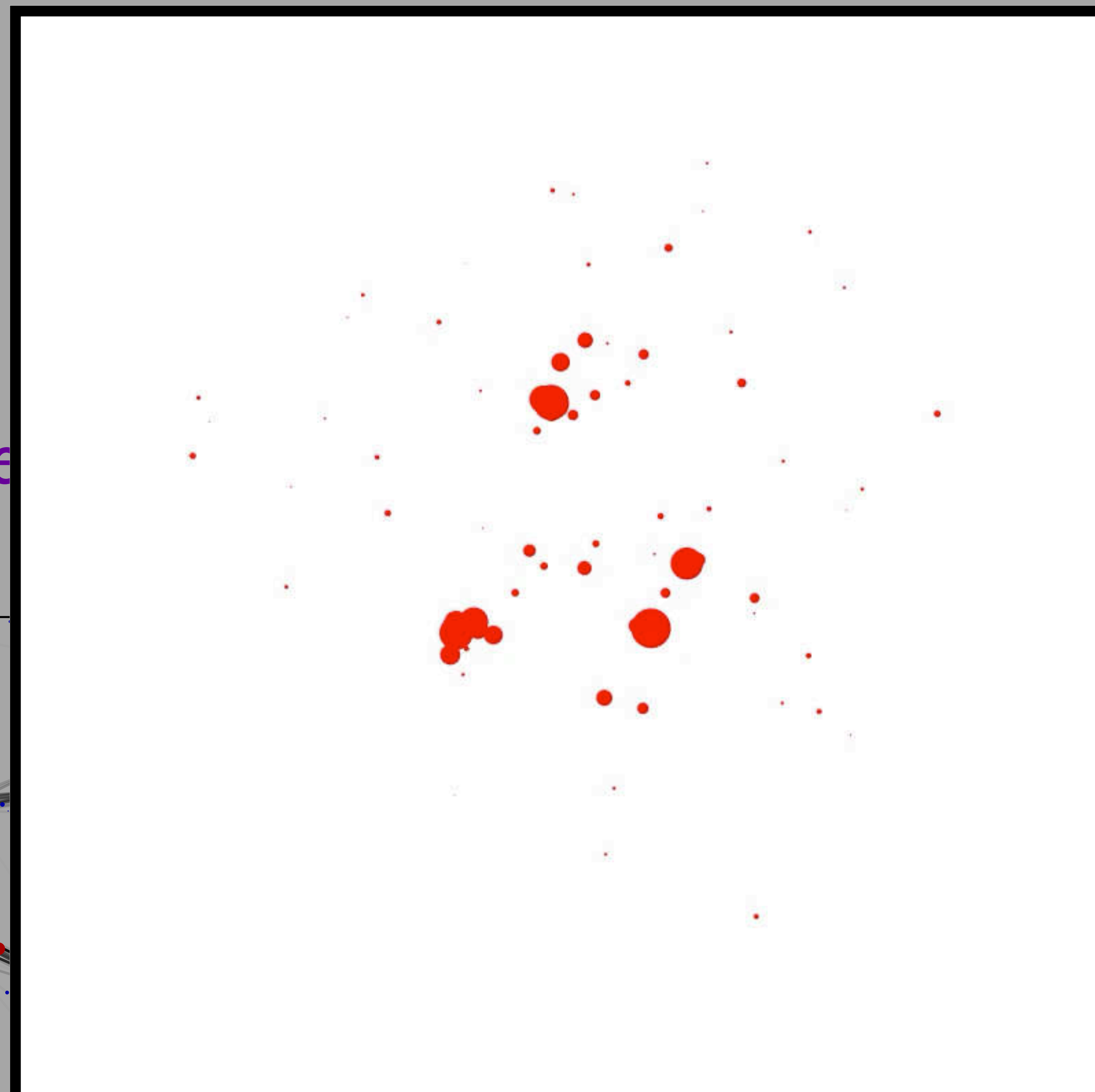
A metric for weighted point clouds

[Komiske, Metodiev, JDT, 1902.02346;
see also Rubner, Tomasi, Guibas, ICJV 2000; Pele, Werman, ECCV 2008]

Theory Prior: Keep a "Safe" Distance

Differenc… …*y measure*





…tance

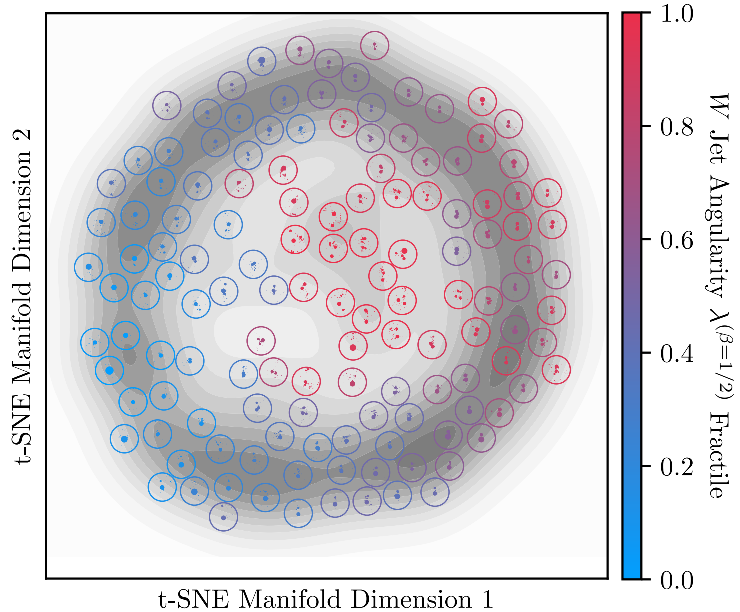
$$\ldots \frac{\ldots ij}{R} + \left| E_{\mathrm{tot}}^{(1)} - E_{\mathrm{tot}}^{(2)} \right|$$

…uds

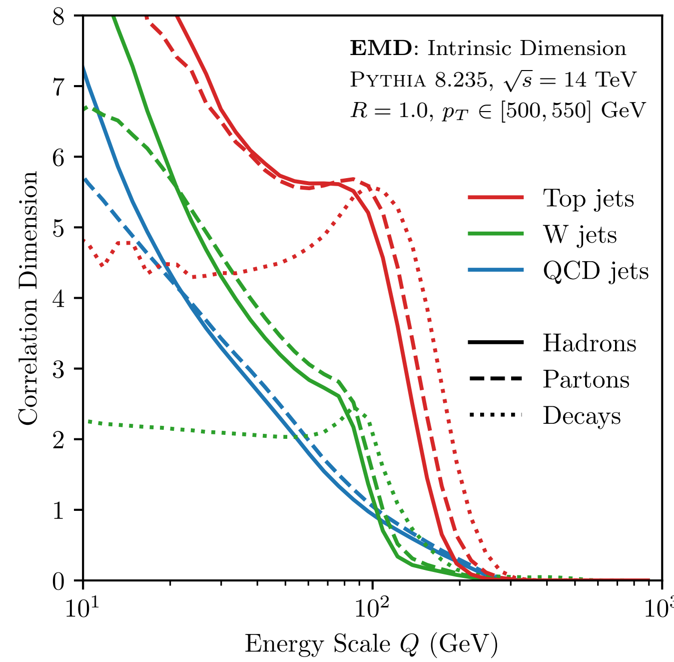
[Komiske, Metodiev, JDT, 1902.02346;
see also Rubner, Tomasi, Guibas, ICJV 2000; Pele, Werman, ECCV 2008]

Rich Opportunities for Data Exploration

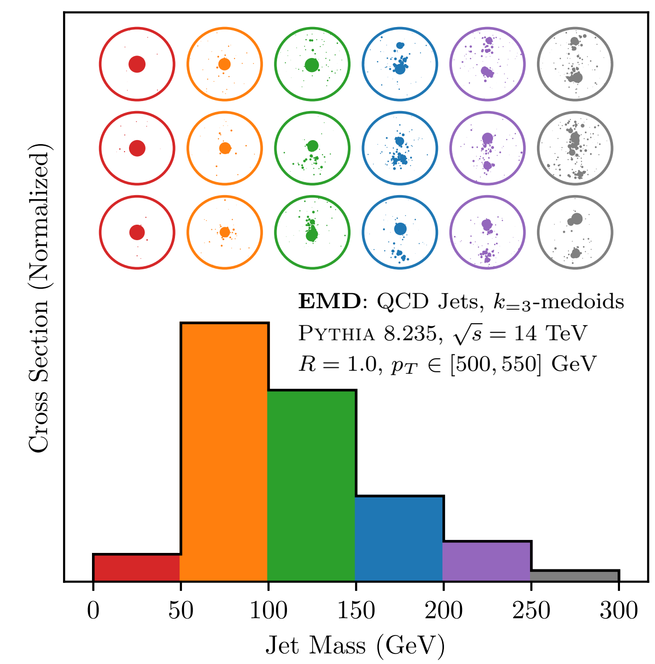
t-SNE



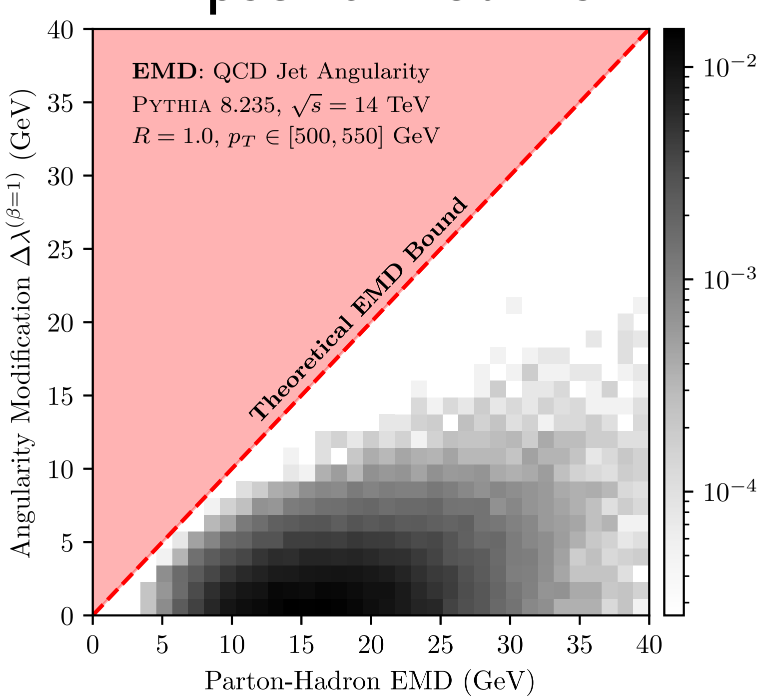
Fractal Dimensions



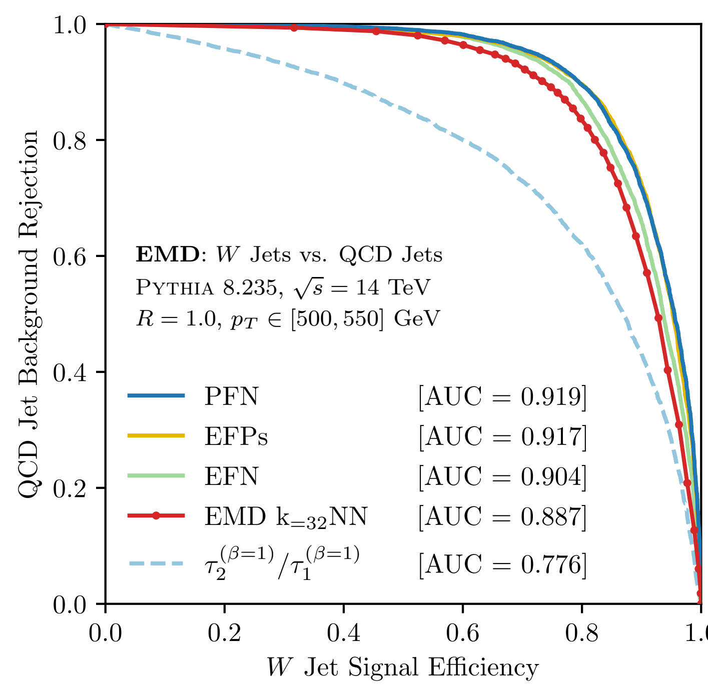
k-medoid Visualization



Lipschitz Bounds



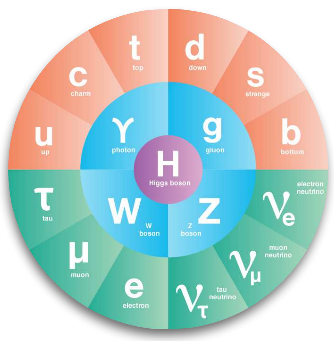
kNN Classification



Plus non-parametric density estimation, anomaly detection, autoencoders, …

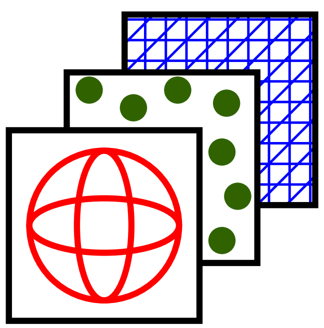
[Komiske, Metodiev, JDT, 1902.02346]

Summary



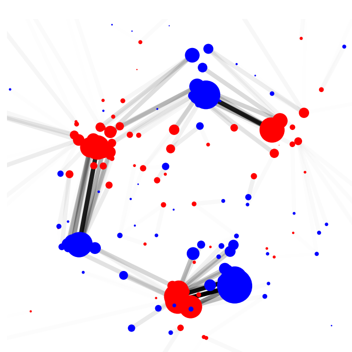
Particle Physics Primer

A rich domain with many machine learning opportunities



Point Clouds & Energy Flow Networks

A new architecture for weighted point clouds



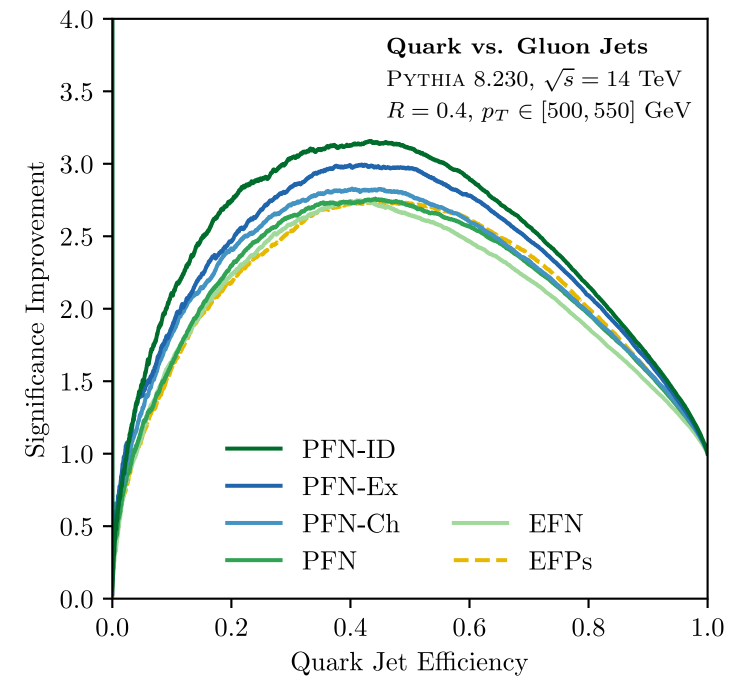
(The Metric Space of Collider Events)

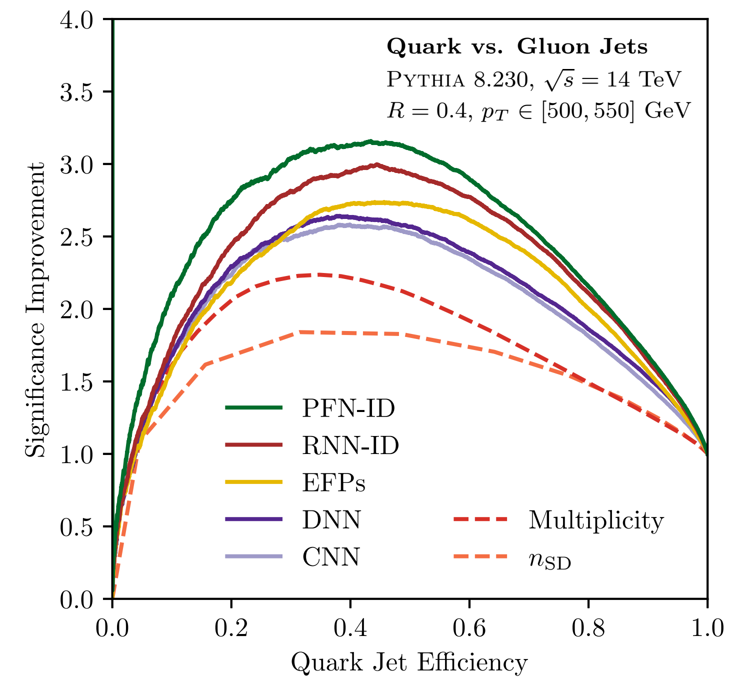
Using geometry for data exploration in particle physics and beyond

Backup Slides

More Quark/Gluon Performance

Model	AUC	$1/\varepsilon_g$ at $\varepsilon_q = 50\%$
PFN-ID	$\mathbf{0.9052} \pm 0.0007$	$\mathbf{37.4} \pm 0.7$
PFN-Ex	0.9005 ± 0.0003	34.7 ± 0.4
PFN-Ch	0.8924 ± 0.0001	31.2 ± 0.3
PFN	0.8911 ± 0.0008	30.8 ± 0.4
EFN	0.8824 ± 0.0005	28.6 ± 0.3
RNN-ID	0.9010	34.4
RNN	0.8899	30.5
EFP	0.8919	29.7
DNN	0.8849	26.4
CNN	0.8781	25.5
M	0.8401	19.0
n_{SD}	0.8297	14.2
m	0.7401	7.2



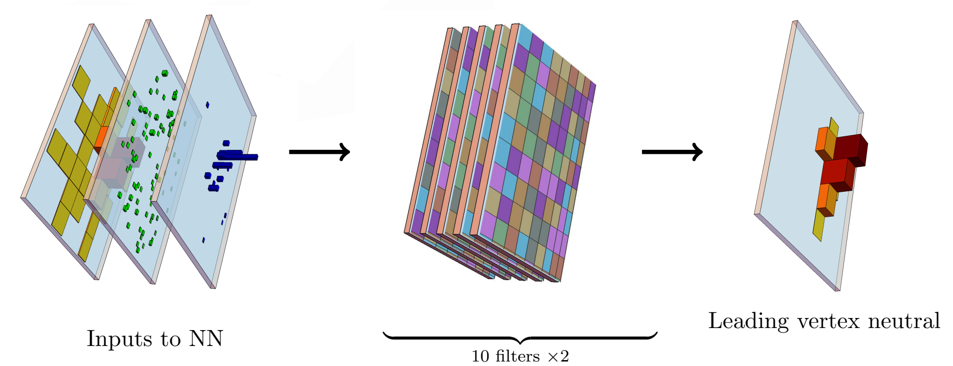


Beyond Classification

PUMML

Pileup Mitigation

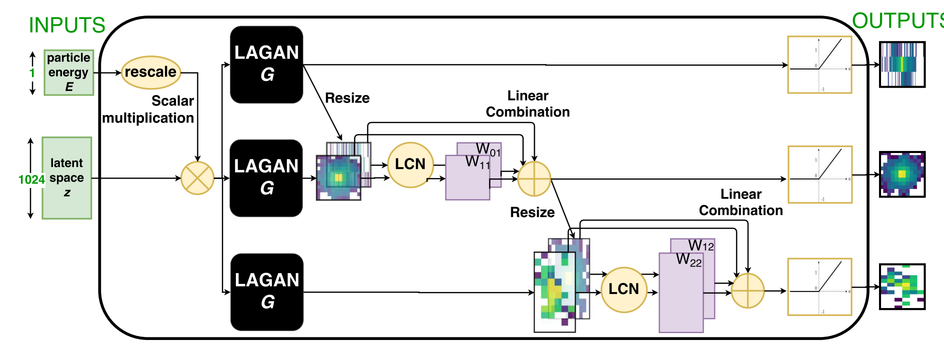
[Komiske, Metodiev, Nachman, Schwartz, 1707.08600]



CaloGAN

Fast Detector Simulation

Paganini, de Oliveira, Nachman, 1705.02355, 1712.10321;
see also de Oliveira, Michela Paganini, Nachman, 1701.05927]



JUNIPR

Probability Modeling

[Andreassen, Feige, Frye, Schwartz, 1804.09720;
see also Monk, 1807.03685]