

# Machine Learning for Fundamental Physics

Jesse Thaler



HKUST Jockey Club Institute for Advanced Study, HEP 2021 — January 21, 2021

# The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI)

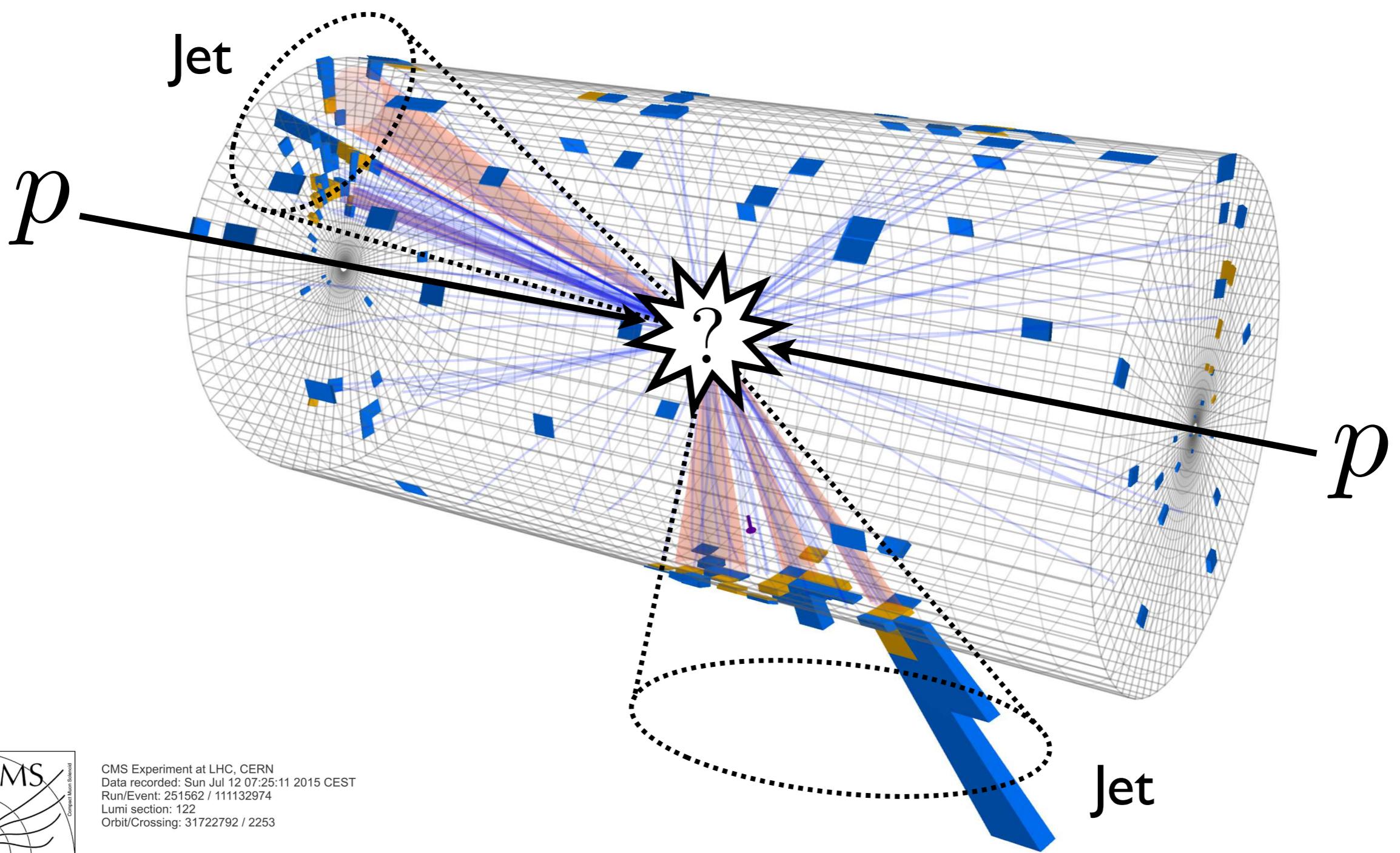
“eye-phi”



*Advance physics knowledge — from the smallest building blocks of nature  
to the largest structures in the universe — and galvanize AI research innovation*

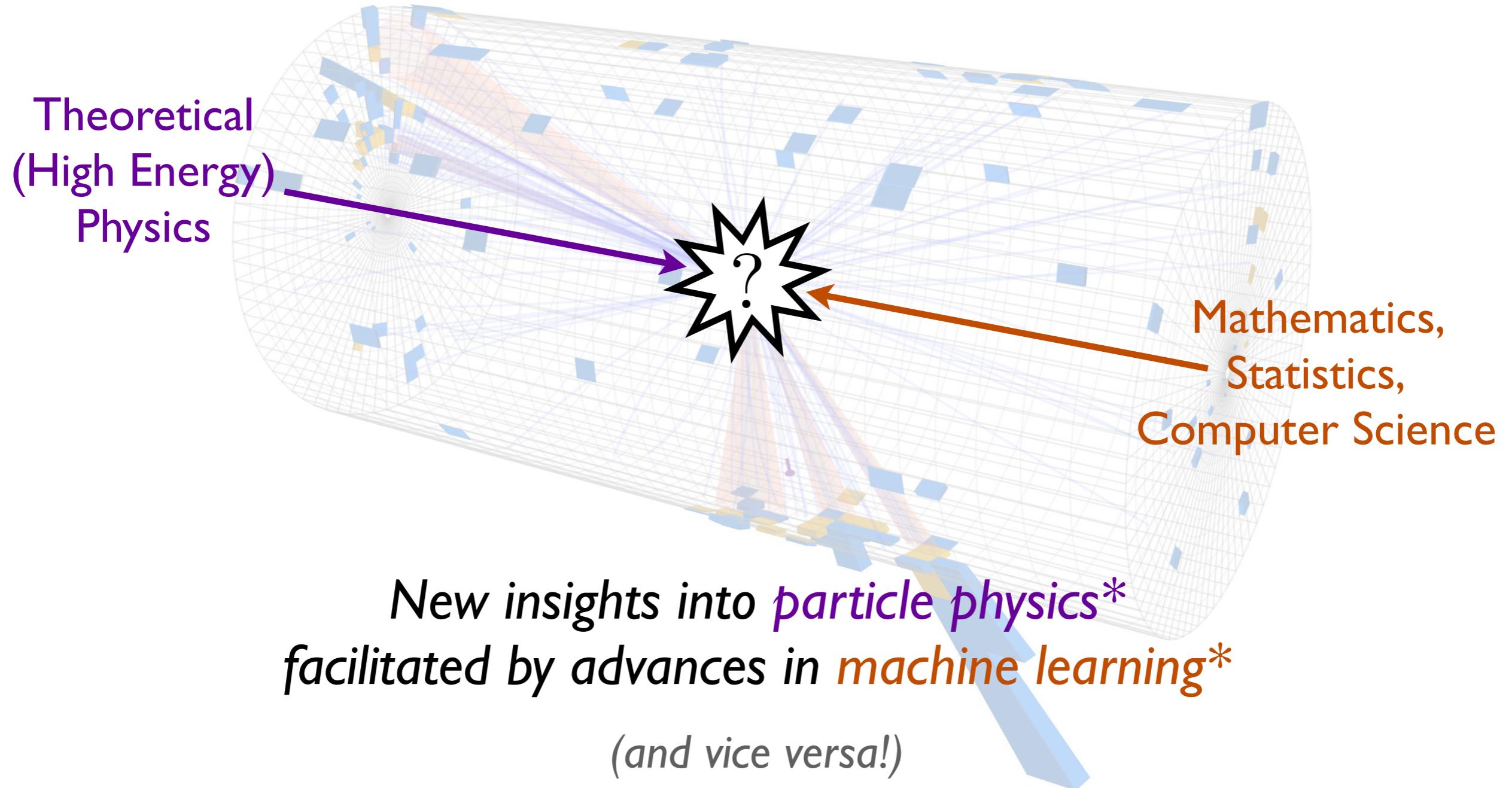


[<http://iaifi.org>, MIT News Announcement]



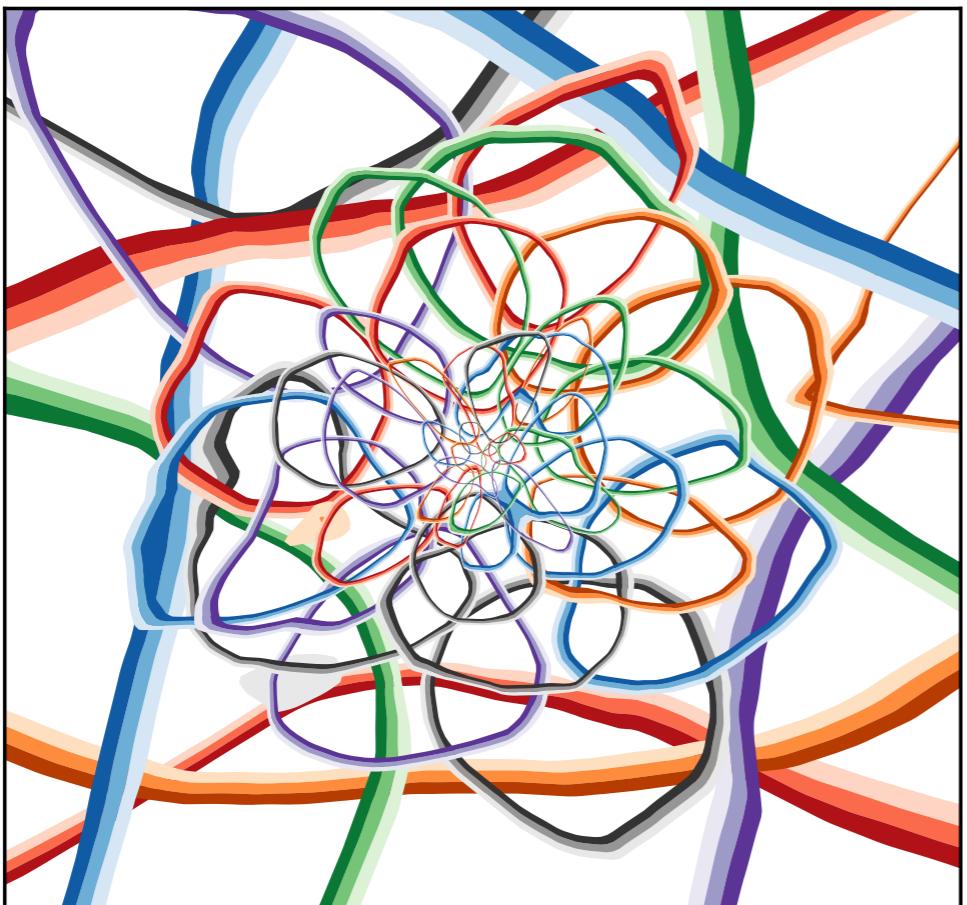
# “Collision Course”

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



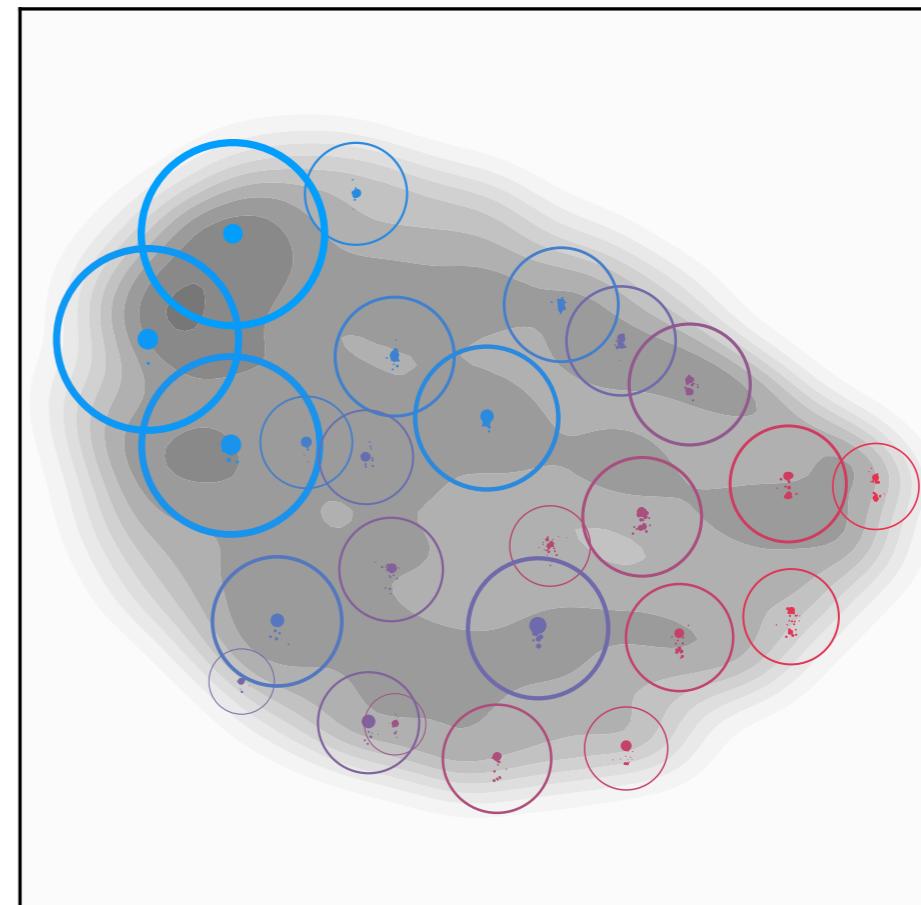
# Two Anecdotes

Teaching a Machine to  
“Think Like a Physicist”



[Komiske, Metodiev, JDT, JHEP 2019]

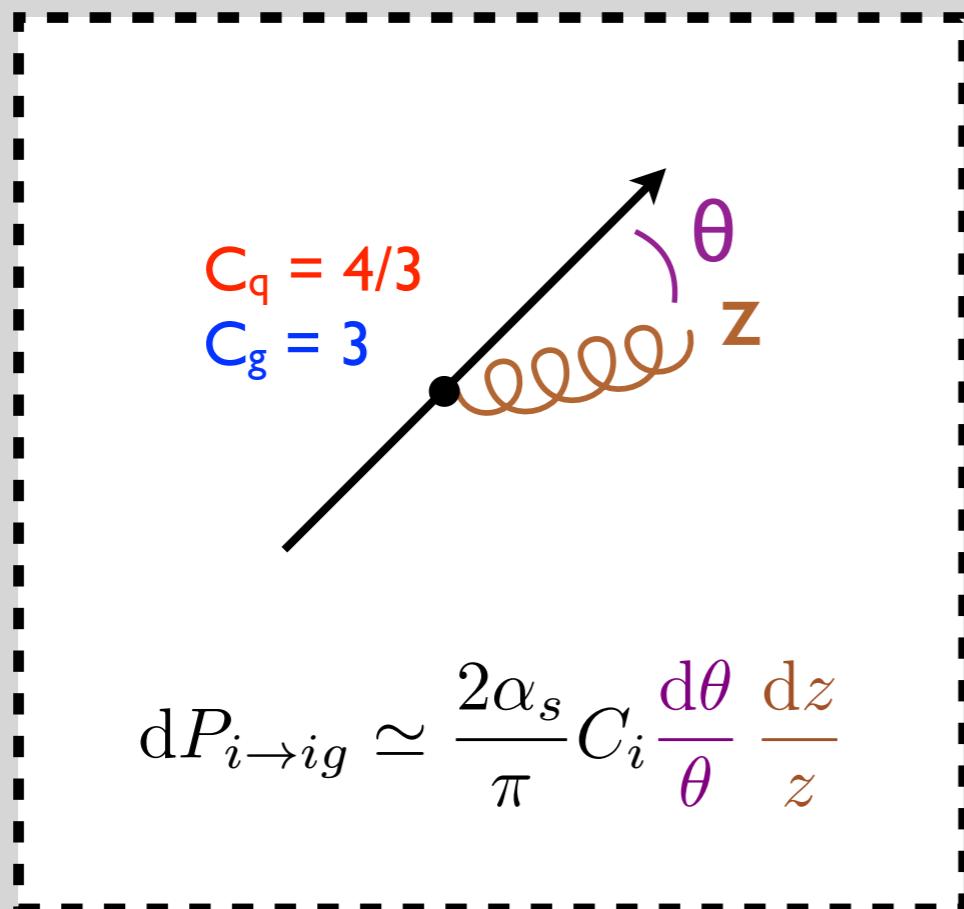
Letting Collider Data  
Speak for Itself



[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;  
based on Komiske, Metodiev, JDT, PRL 2019]

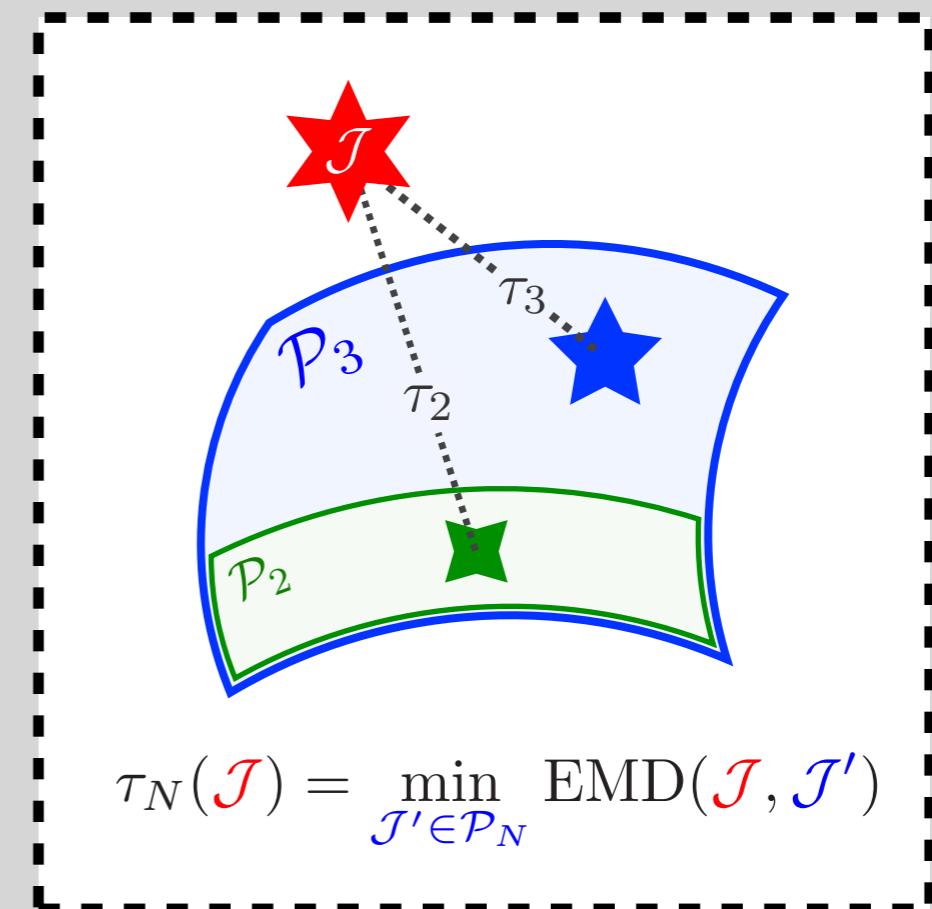
*Data analysis strategies motivated by the  
symmetries and structures of particle physics*

## Exploiting a Core Prediction of QCD



[Altarelli, Parisi, [NPB 1977](#)]

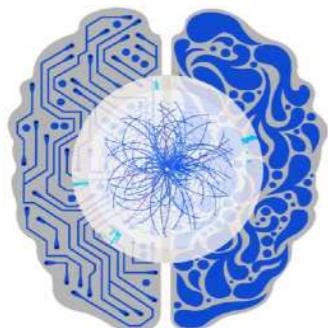
## Nested Singularities of Gauge Theories



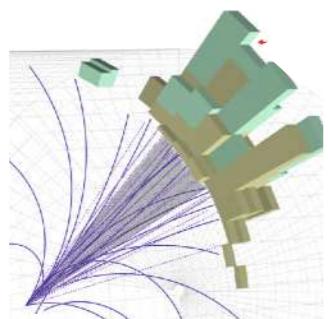
[Stewart, Tackmann, Waalewijn, [PRL 2010](#);  
JDT, Van Tilburg, [JHEP 2011](#), [JHEP 2012](#);  
rephrased via Komiske, Metodiev, JDT, [JHEP 2020](#)]

New perspectives on key theoretical concepts

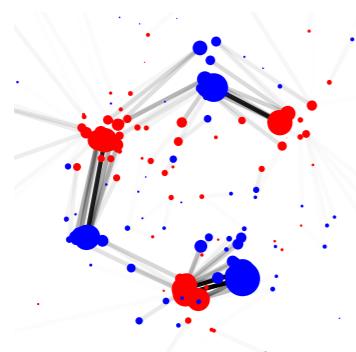
# Outline



Rise of the Machines?



What is a Collider Event?



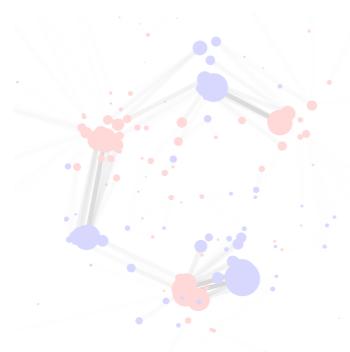
When are Collider Events Similar?



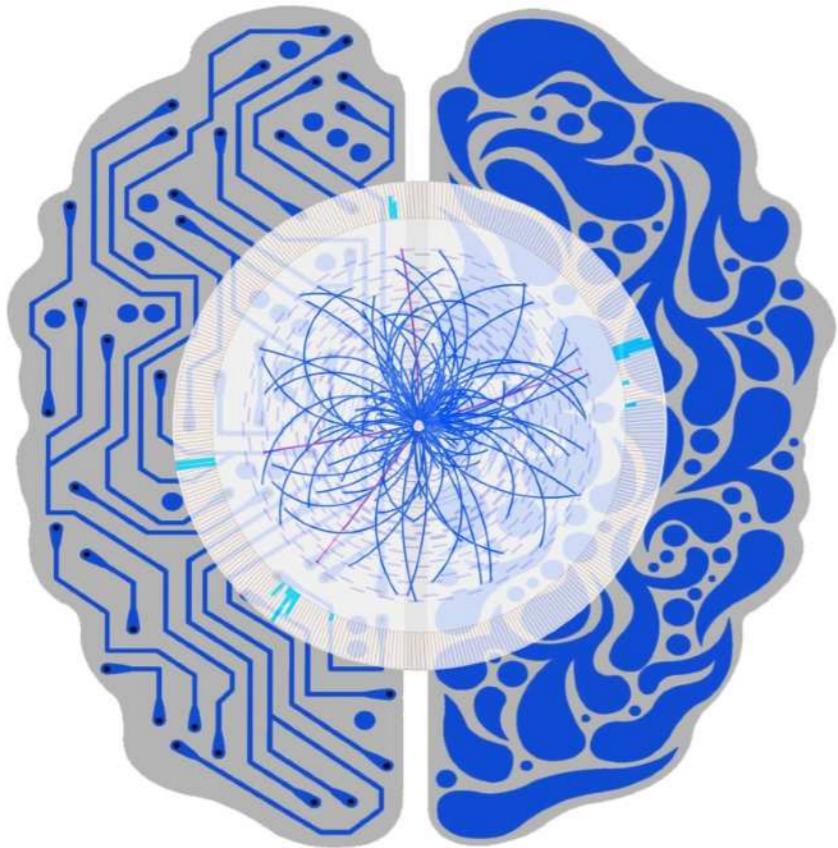
## Rise of the Machines?



What is a Collider Event?



When are Collider Events Similar?



*Can we teach a machine  
to “think” like a physicist?*

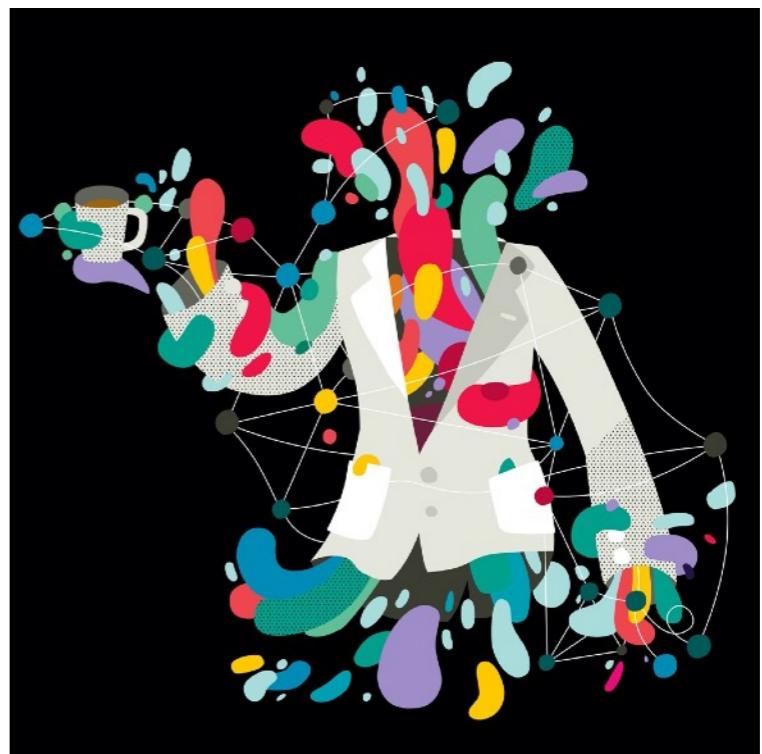
The New York Times



By Dennis Overbye

Nov. 23, 2020

Can a Computer Devise a Theory of Everything?



# AI<sup>2</sup>: Ab Initio Artificial Intelligence

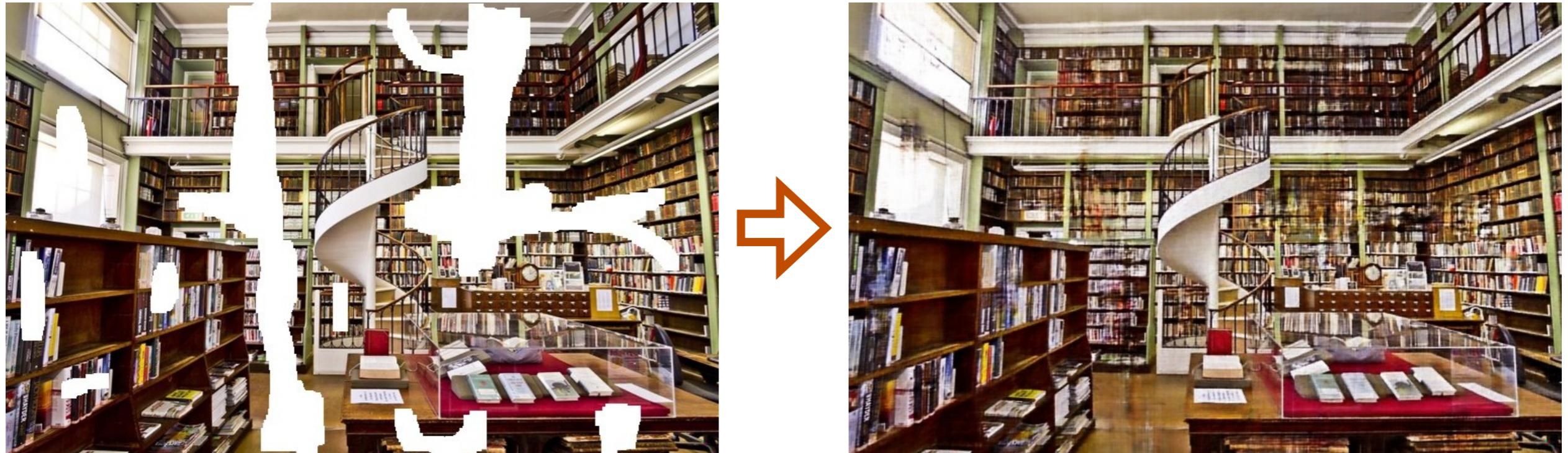


*Machine learning that incorporates  
first principles, best practices, and domain knowledge  
from fundamental physics*

*Symmetries, conservation laws, scaling relations, limiting behaviors, locality, causality,  
unitarity, gauge invariance, entropy, least action, factorization, unit tests,  
exactness, systematic uncertainties, reproducibility, verifiability, ...*

# Deep Learning

*E.g. Inpainting*

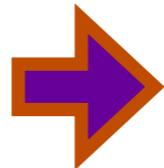


increased computational power and large data sets

[Ulyanov, Vedaldi, Lempitsky, CVPR 2018]

# Deep Learning meets Deep Thinking

E.g. *Inpainting*



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, CVPR 2018]

# ML Targets for Collider Theory

Master formula  
for colliders:

$$\sigma_{\text{obs}} \simeq \frac{1}{2E_{\text{CM}}^2} \sum_{n=2}^{\infty} \int d\Phi_n |\mathcal{M}_{AB \rightarrow 12\dots n}|^2 f_{\text{obs}}(\Phi_n)$$

cross sectionphase spaceamplitudeobservable

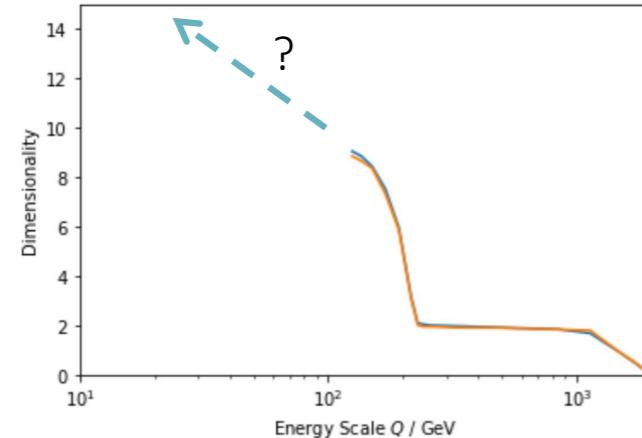
*Exciting progress on multiple fronts from  
theoretical (and experimental) HEP communities!*

Progress in other areas of fundamental physics as well,  
e.g. cosmology, dark matter, string theory, nuclear theory, ...

[apologies for focus on research from my group in this talk; see [HEPML-LivingReview](#) for extensive bibliography]

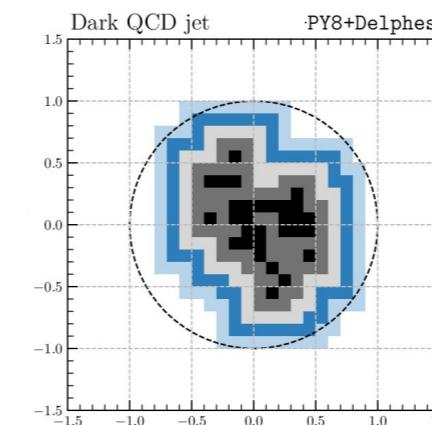
# Mini-Workshop: Machine Learning and Open Data

## Dimensionality via Autoencoding



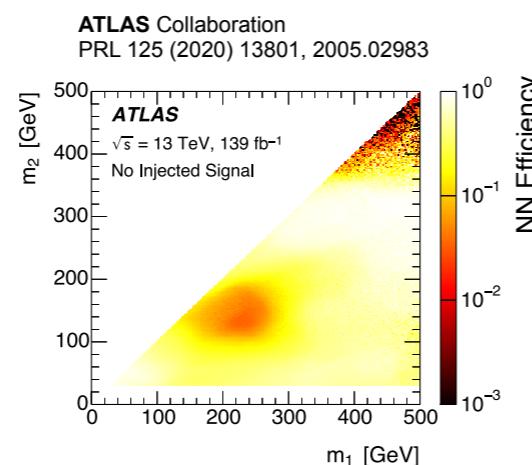
[Talk by Jack Collins]

## Jet Classification via Topology



[Talks by Mihoko Nojiri & Lingfeng Li]

## Anomaly Detection



[Talks by David Shih & Ben Nachman]

## CMS Open Data for BSM Searches

Selection	Data	Signal BM
MET primary	$4.3 \times 10^7$	-
$p_T^{j1} > 150$ GeV, $E_T^{\text{miss}} > 150$ GeV	$1.4 \times 10^6$	830
One displaced vertex ( $N_{vtx,tk} \geq 2$ )	$3.7 \times 10^5$	310
One displaced vertex ( $N_{vtx,tk} \geq 3$ )	$4.7 \times 10^4$	240
One displaced vertex ( $N_{vtx,tk} \geq 4$ , default)	$5.5 \times 10^3$	140
Two displaced vertices	76	9.8
$p_T^{j1} > 300$ GeV, $E_T^{\text{miss}} > 300$ GeV	1	3.0
Two displaced vertices with vertex $H_T < 40$	0	3.0

$$m_{\tilde{t}_1} = 360 \text{ GeV}, \Delta m = 20 \text{ GeV}$$

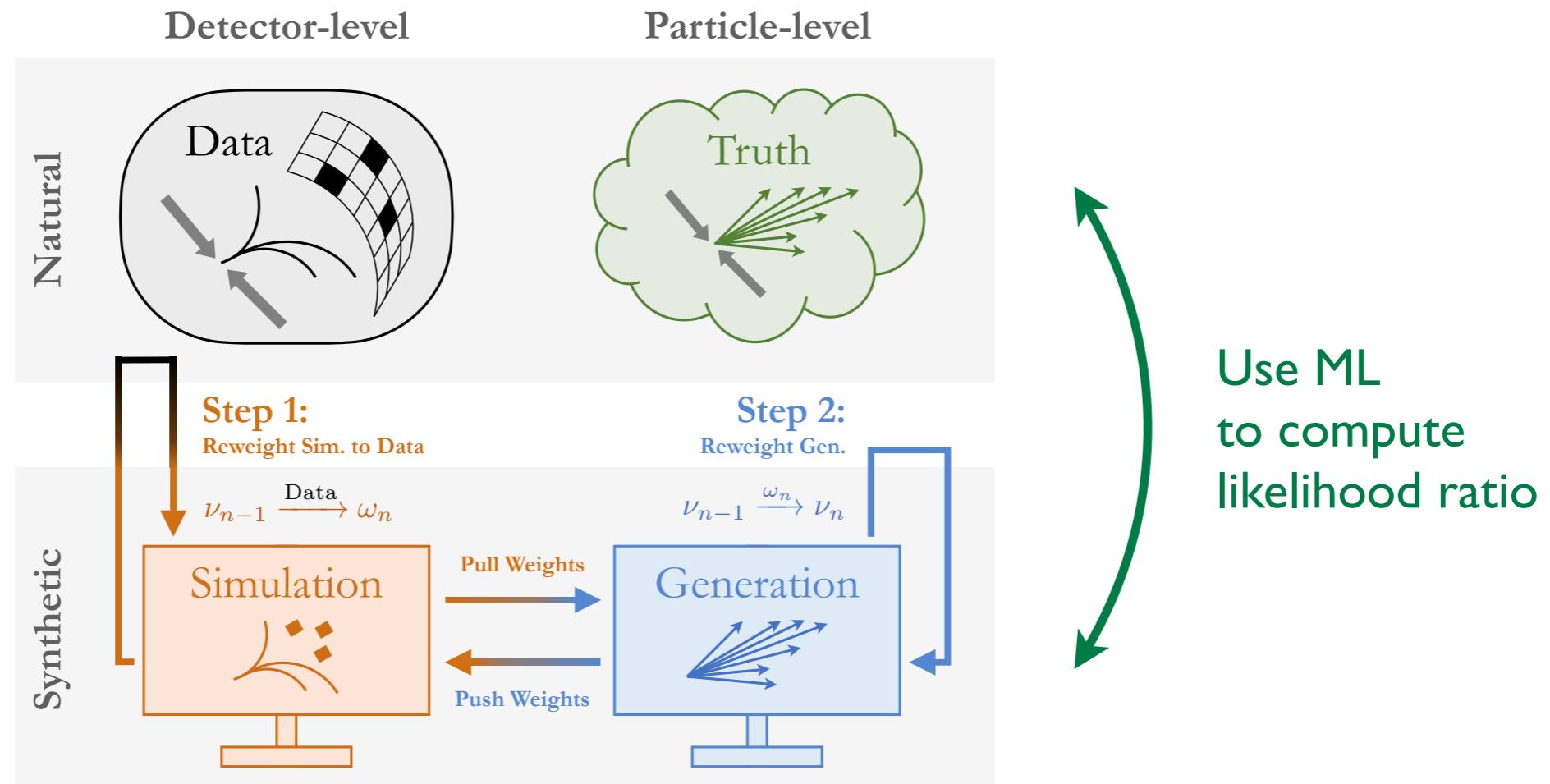
[Talk by Haipeng An]

# Detector Unfolding

OmniFold



*Multi-dimensional unbinned detector corrections  
via iterated binary classification*

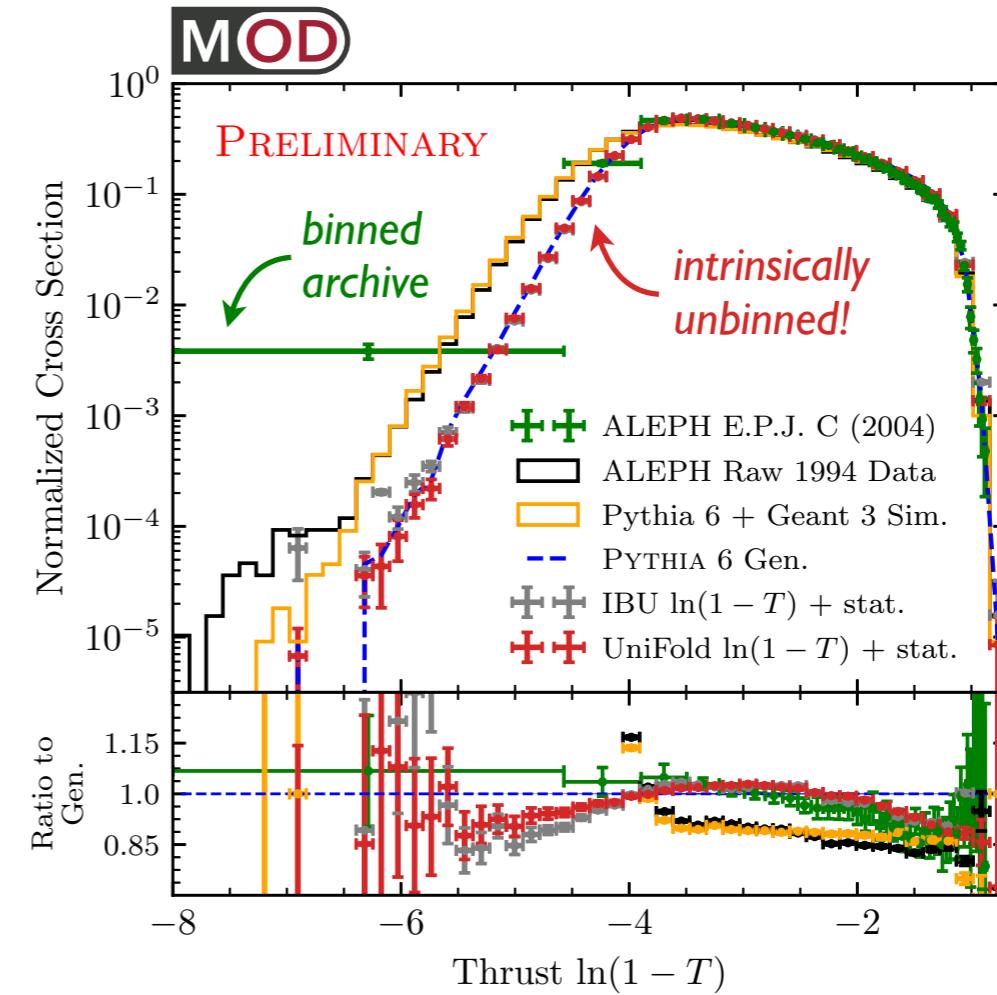
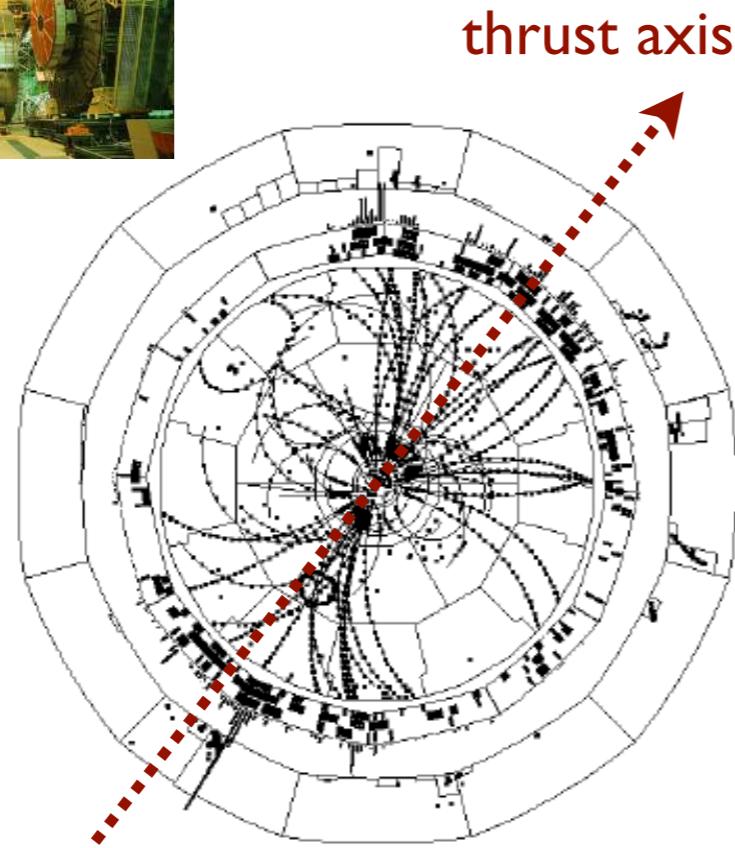


[Andreassen, Komiske, Metodiev, Nachman, JDT, [PRL 2020](#)]



# Detector Unfolding

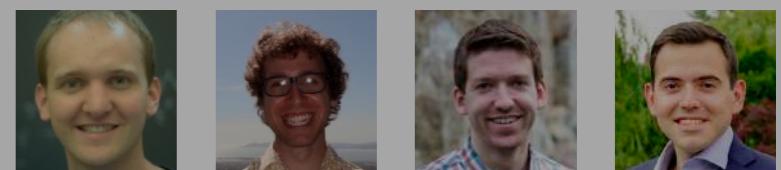
## Back to the Future with ALEPH Archival Data

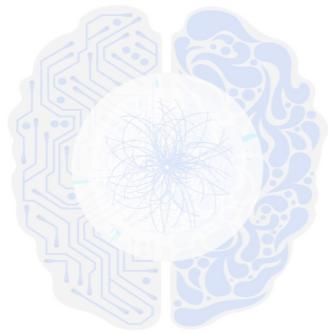


[talk by Badea, [ICHEP 2020](#); cf. ALEPH, [EPJC 2004](#)]  
[see also Badea, Baty, Chang, Innocenti, Maggi, McGinn, Peters, Sheng, JDT, Lee, [PRL 2019](#)]

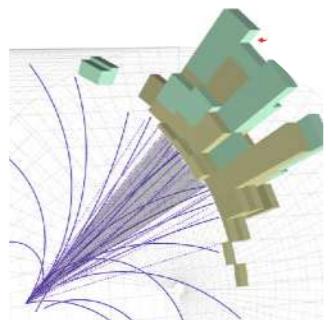


[Andreassen, Komiske, Metodiev, Nachman, JDT, [PRL 2020](#)]

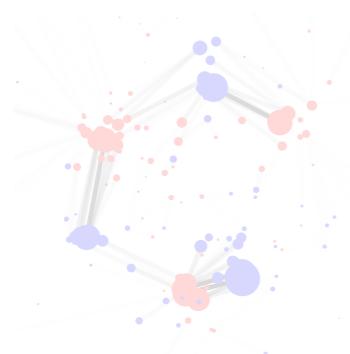




## Rise of the Machines?



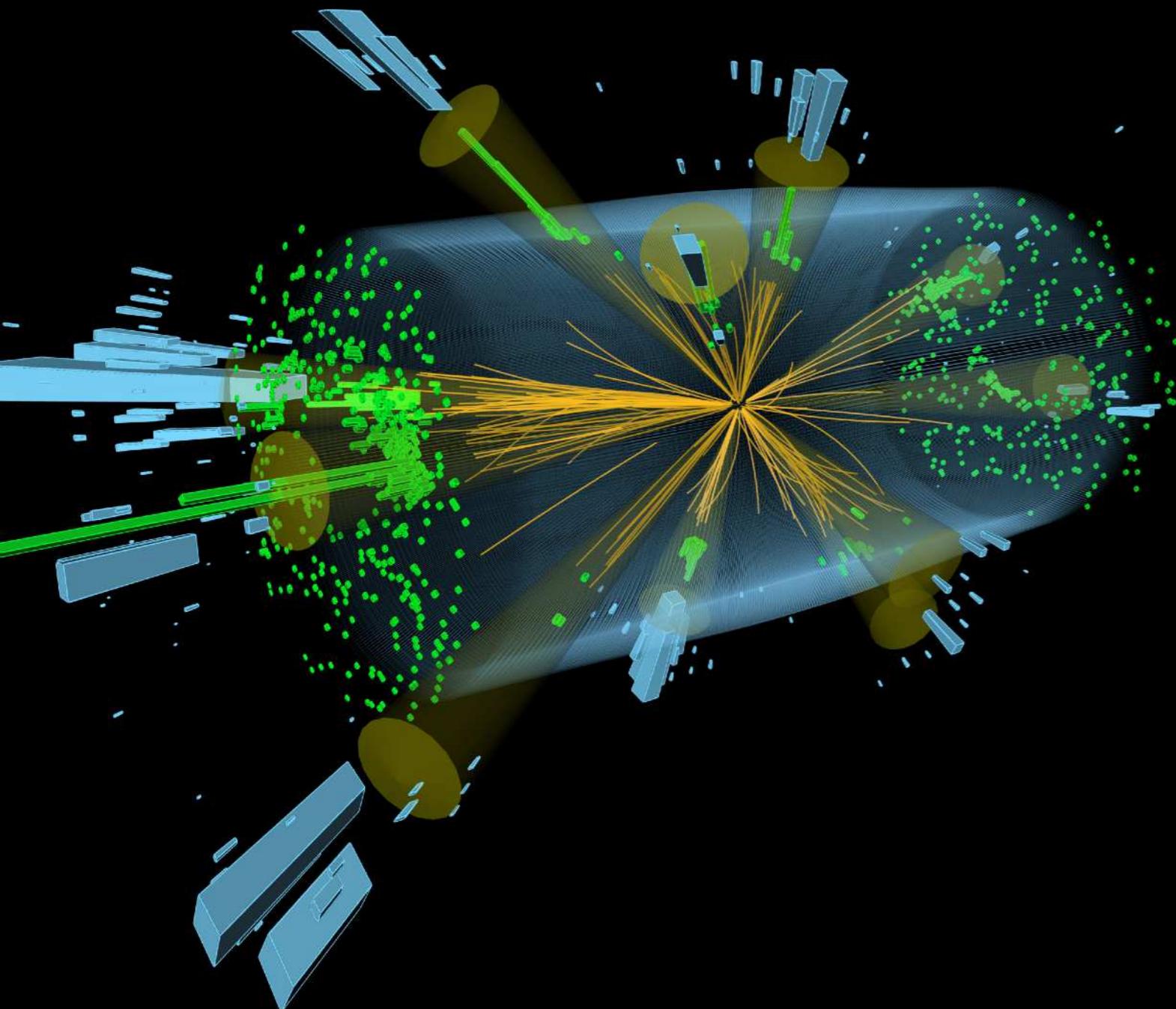
## What is a Collider Event?



## When are Collider Events Similar?

# Collider Event

Collection of points in (momentum) space



T E H M

 $\gamma$ 

photon

 $e^+$ 

electron

 $\mu^+$ 

muon

 $\pi^+$ 

pion

 $K^+$ 

kaon

 $K_L^0$ 

K-long

 $p/\bar{p}$ 

proton

 $n/\bar{n}$ 

neutron

elementary

composite

# Point Cloud

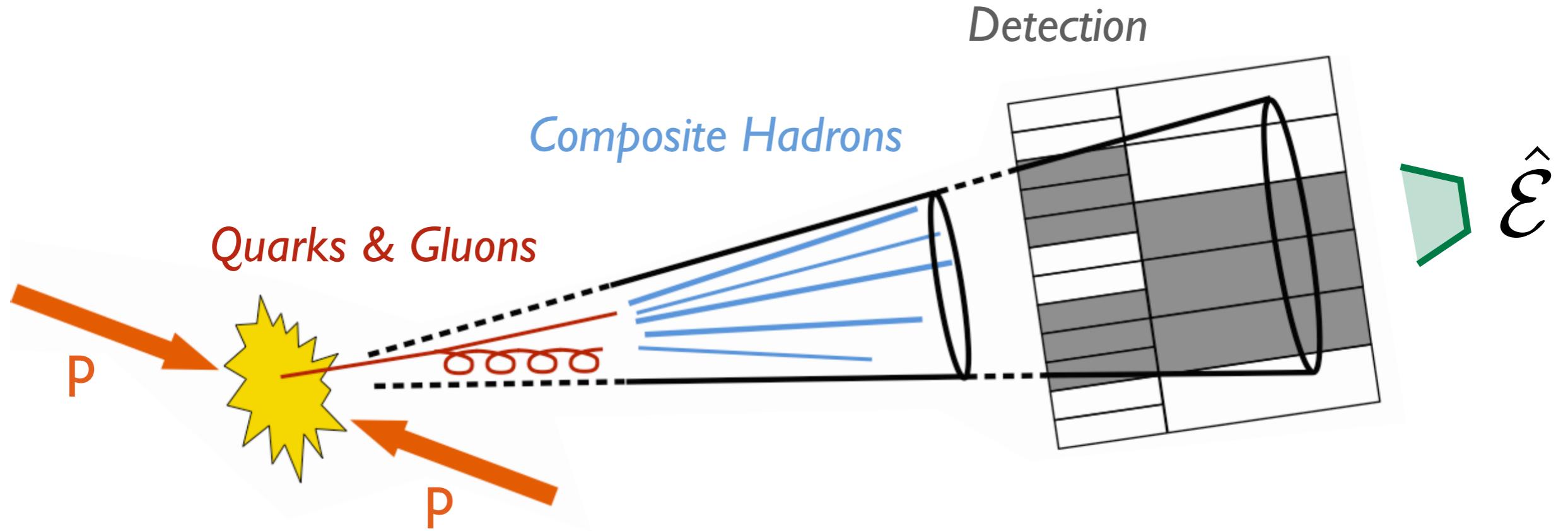
Collection of points in (position) space



[Popular Science, 2013]

# Jet Formation from QCD

Theory



## Energy Flow:

Robust to hadronization and detector effects  
Well-defined for massless gauge theories

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

[see e.g. Sveshnikov, Tkachov, [PLB 1996](#); Hofman, Maldacena, [JHEP 2008](#); Mateu, Stewart, [JDT, PRD 2013](#); Belitsky, Hohenegger, Korchemsky, Sokatchev, Zhiboedov, [PRL 2014](#); Chen, Moult, Zhang, Zhu, [PRD 2020](#)]

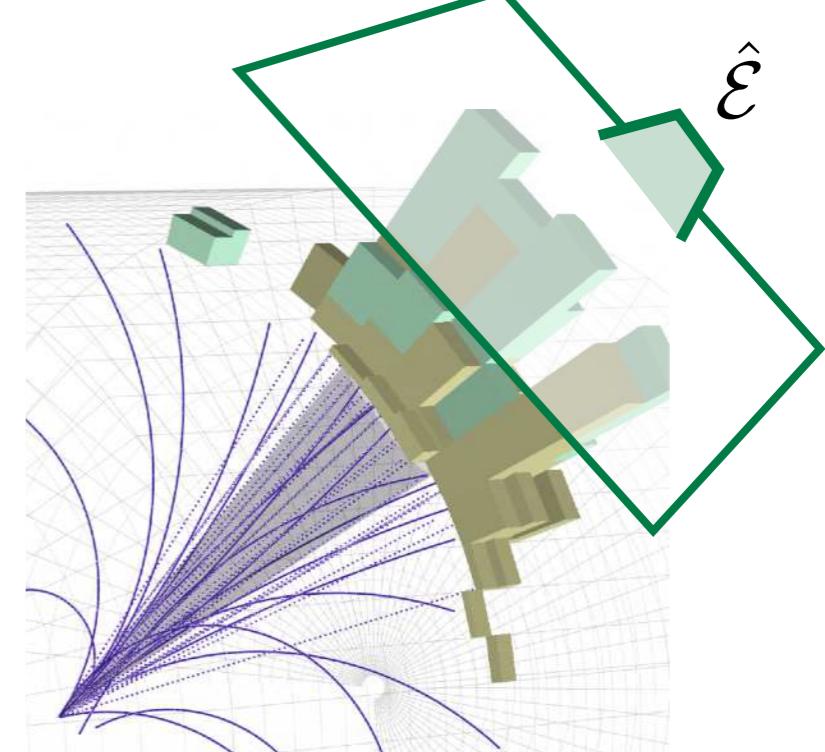
# From Energy Flow to Weighted Point Clouds

- Energy-Weighted Directions

$$\vec{p} = \{E, \hat{n}_x, \hat{n}_y, \hat{n}_z\}$$

↑  
Energy      |  
                Direction

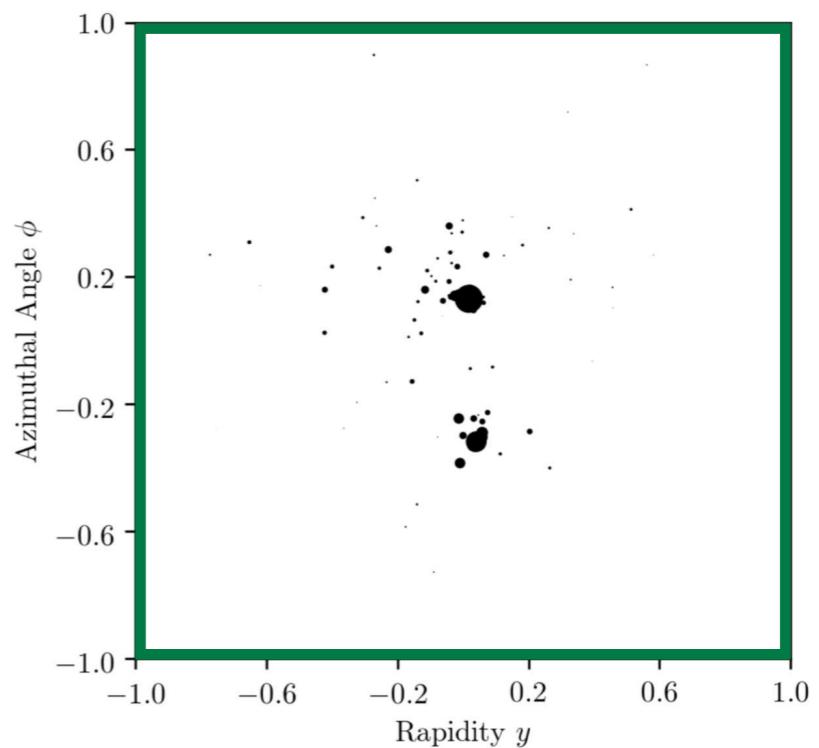
(suppressing “unsafe” charge/flavor information)



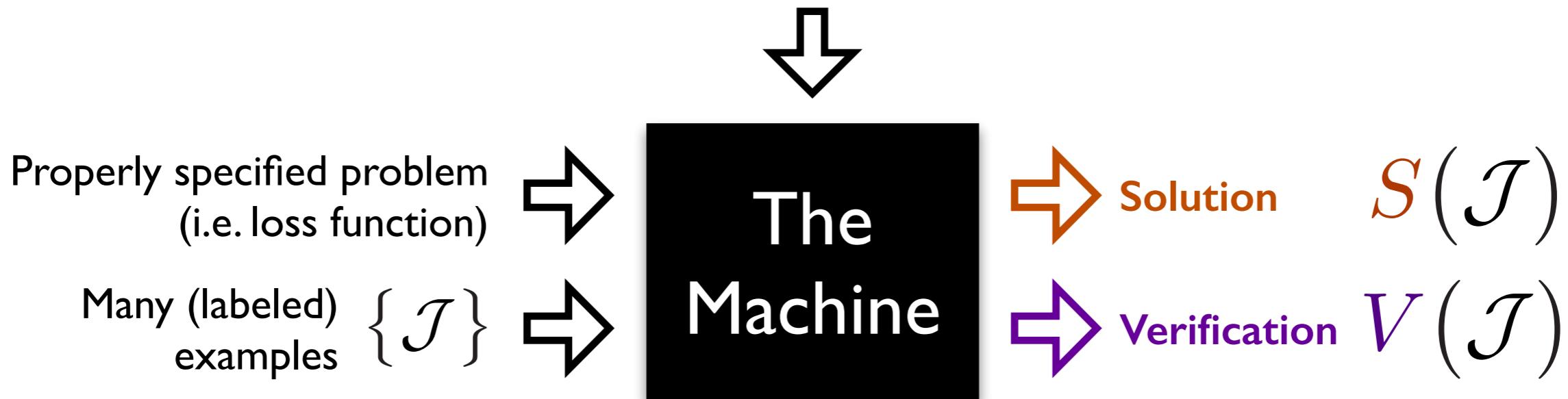
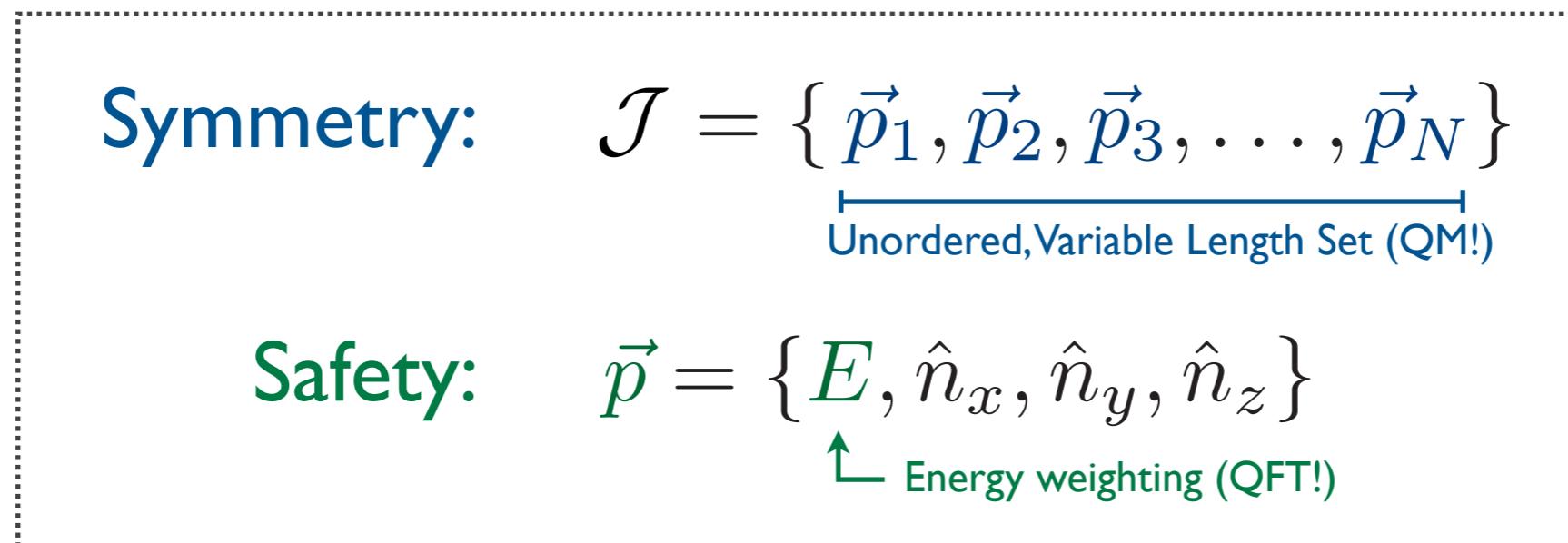
- Equivalently: Energy Density

$$\rho(\hat{n}) = \sum_{i \in \mathcal{J}} E_i \delta^{(2)}(\hat{n} - \hat{n}_i)$$

↑  
Energy      ↑  
                Direction



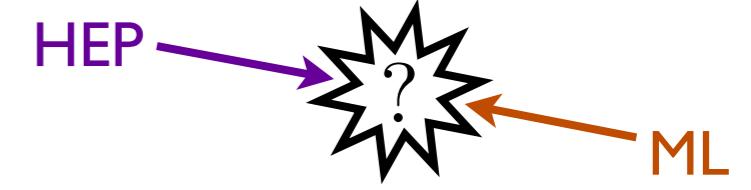
# “Thinking” Like a Physicist



*Check that answer  
is physically sensible*

# Energy Flow Networks

Architecture designed around **symmetries** and **interpretability**



$$S(\mathcal{J}) = F(V_1, V_2, \dots, V_\ell)$$
$$V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} E_i \Phi_a(\hat{n}_i)$$

Permutation invariant  $\downarrow$   $\downarrow$  Linear weights (i.e. safe)  
Parametrized with Neural Networks

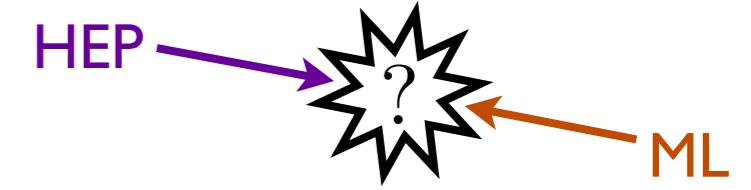
*Provably describes any\* **safe** observable (!)*  
*Excellent jet classification performance*

[Komiske, Metodiev, JDT, [JHEP 2019](#); see also Komiske, Metodiev, JDT, [JHEP 2018](#); code at [energyflow.network](#); special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, [NIPS 2017](#); other set-based architecture in Qu, Gouskos, [PRD 2020](#); Mikuni, Canelli, [EPJP 2020](#); Dolan, Ore, [arXiv 2020](#)]



# Energy Flow Networks

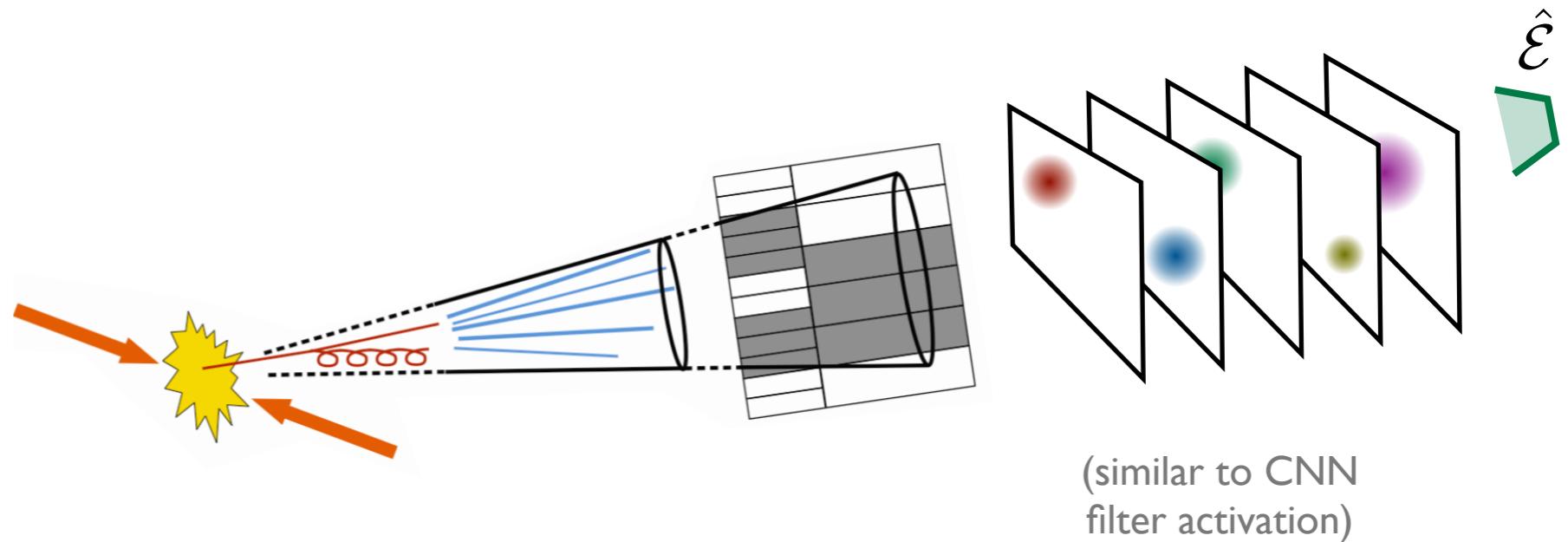
Architecture designed around symmetries and *interpretability*



Latent space of dim  $\ell$

$$S(\mathcal{J}) = F(V_1, V_2, \dots, V_\ell) \quad V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} E_i \Phi_a(\hat{n}_i)$$

*Easy to plot!*

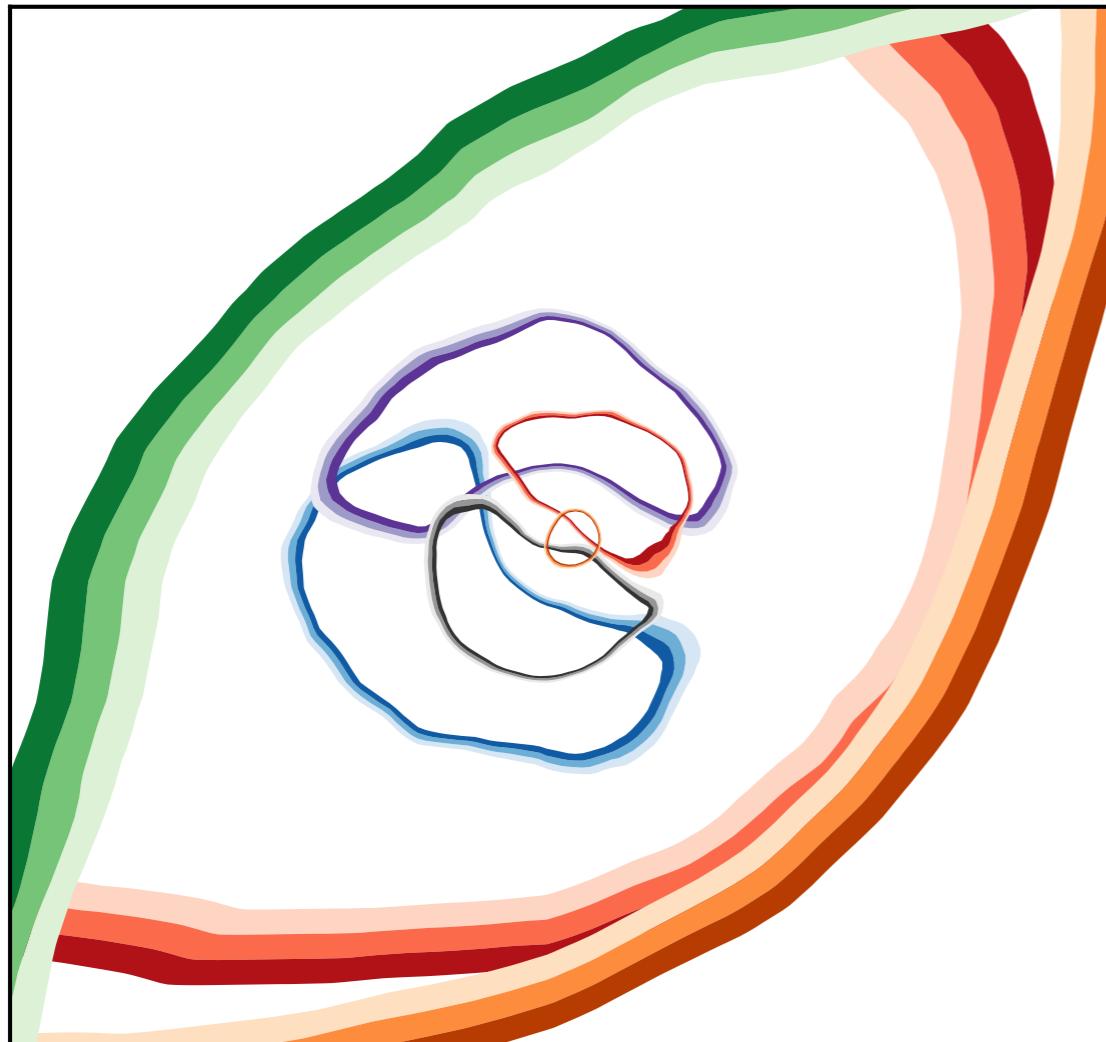


[Komiske, Metodiev, JDT, [JHEP 2019](#); see also Komiske, Metodiev, JDT, [JHEP 2018](#); code at [energyflow.network](#); special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, [NIPS 2017](#); other set-based architecture in Qu, Gouskos, [PRD 2020](#); Mikuni, Canelli, [EPJP 2020](#); Dolan, Ore, [arXiv 2020](#)]

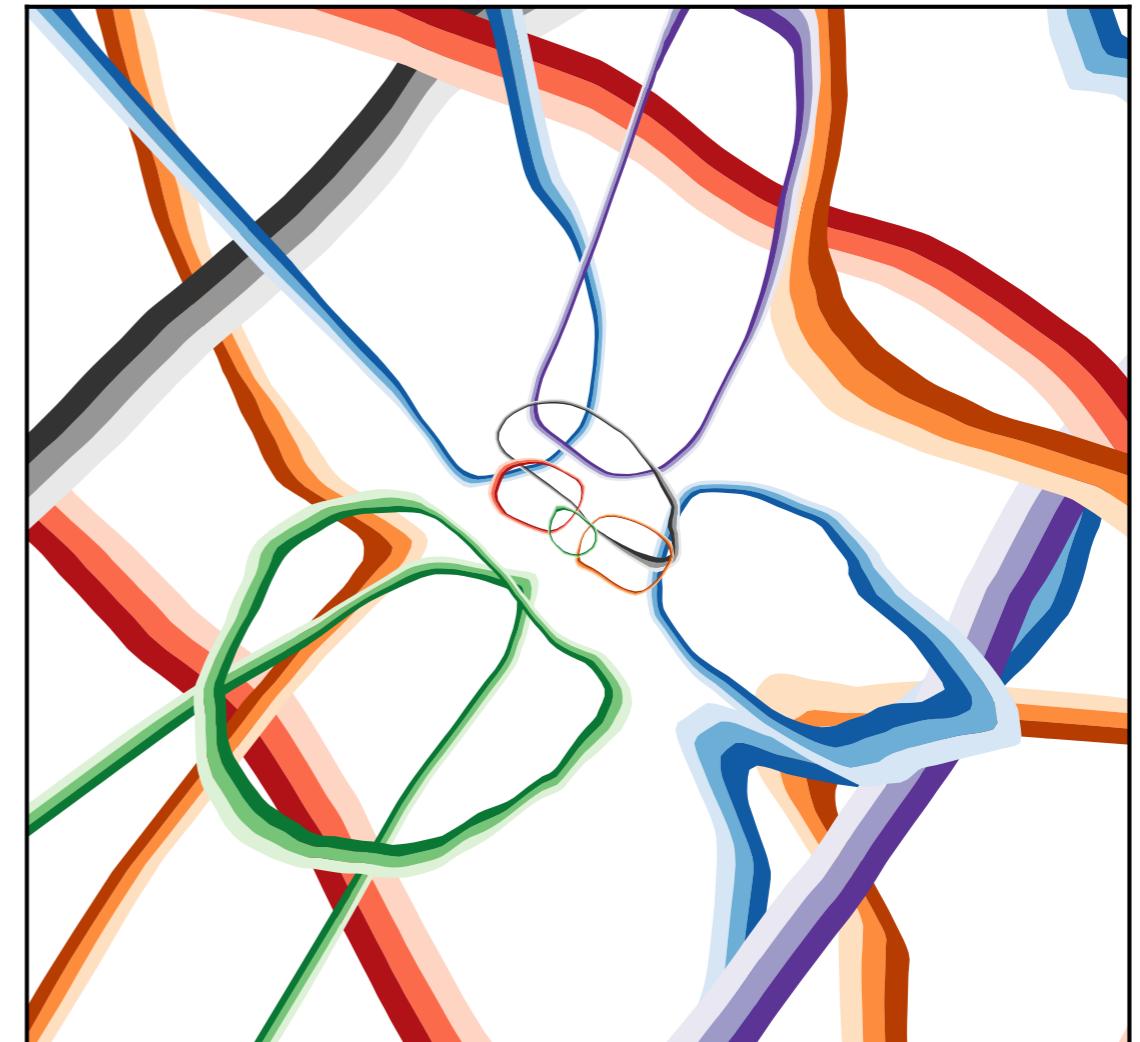


# Psychedelic Network Visualization

Latent Dimension 8



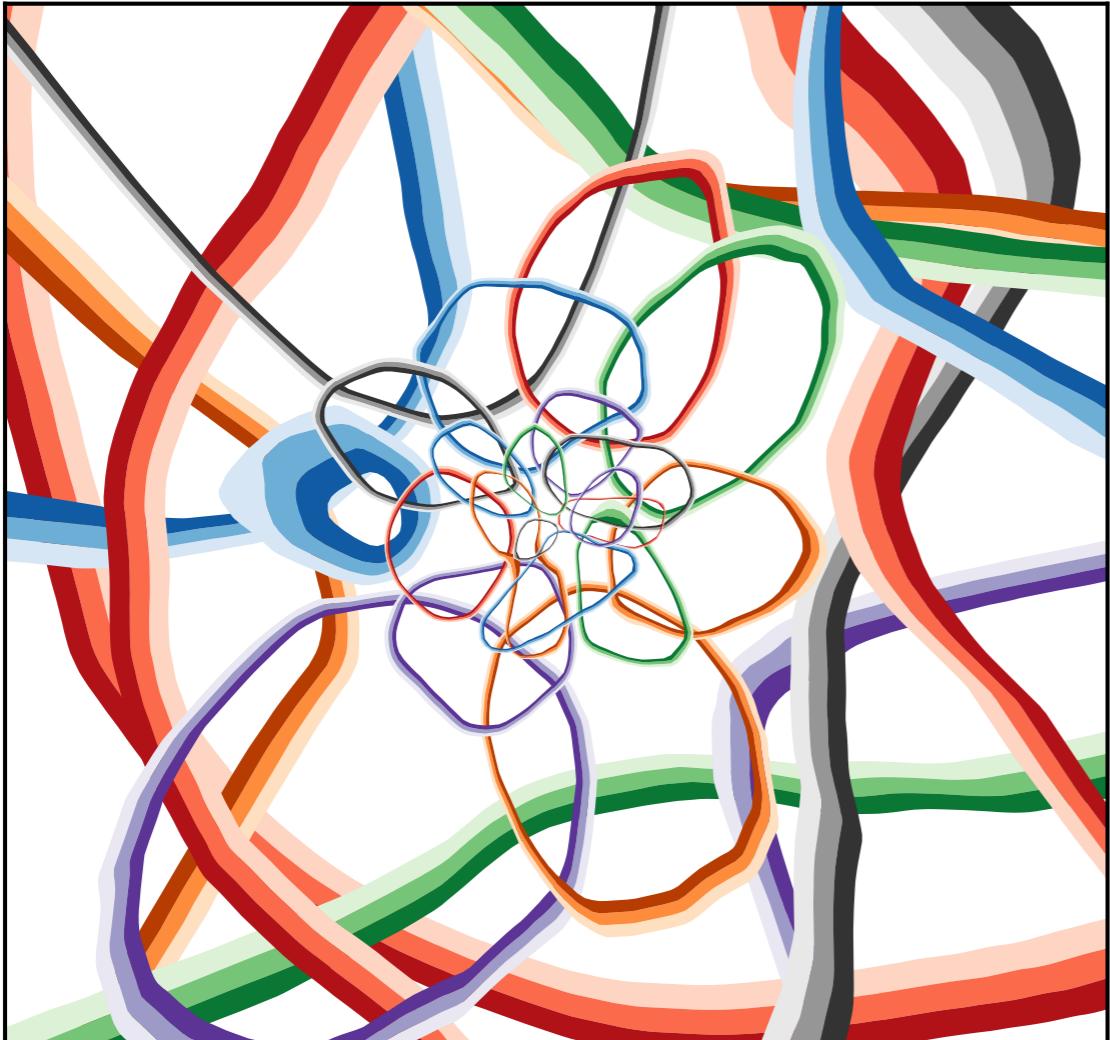
Latent Dimension 16



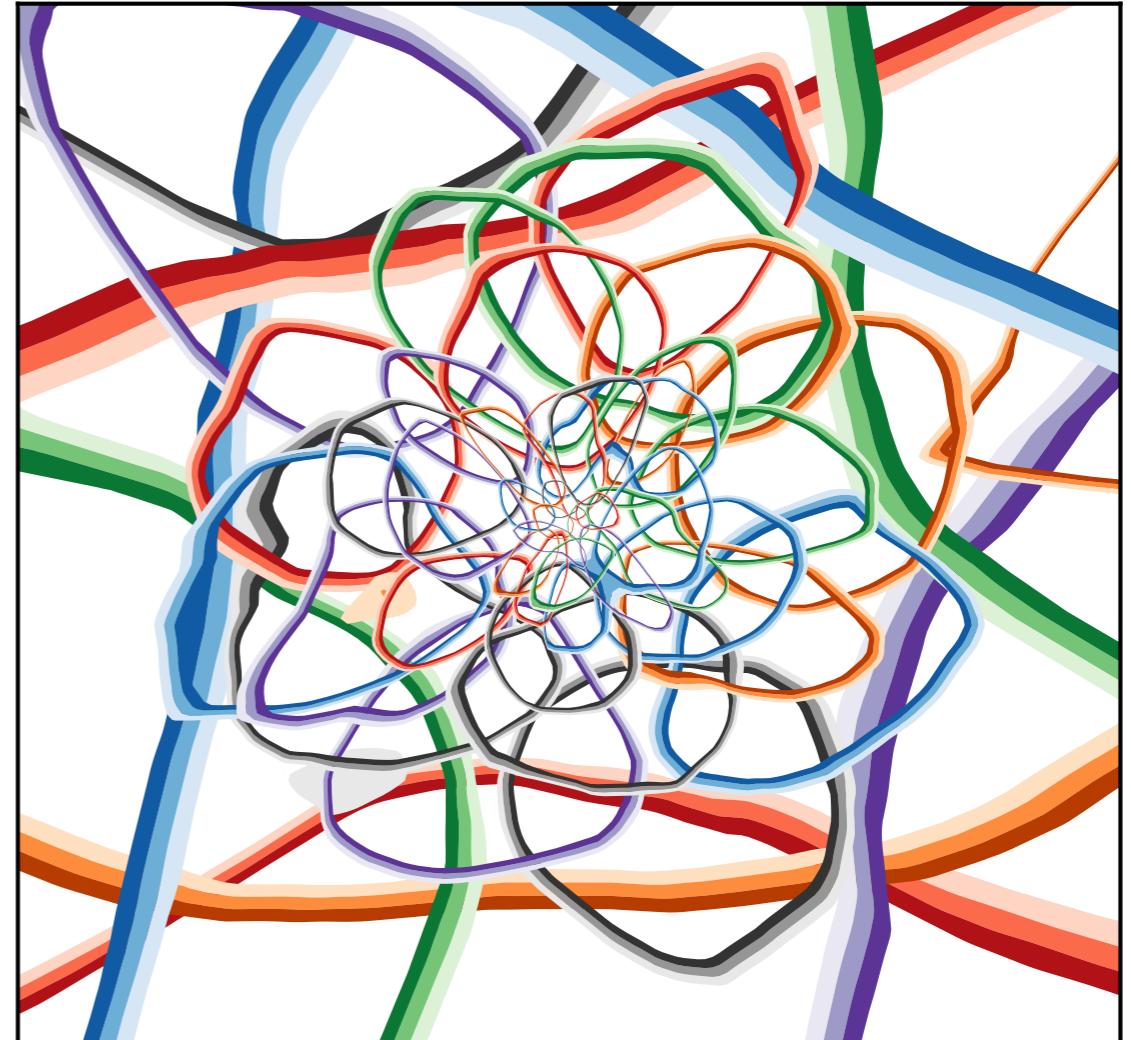
For the case of **quark** vs. **gluon** classification

# Psychedelic Network Visualization

Latent Dimension 32

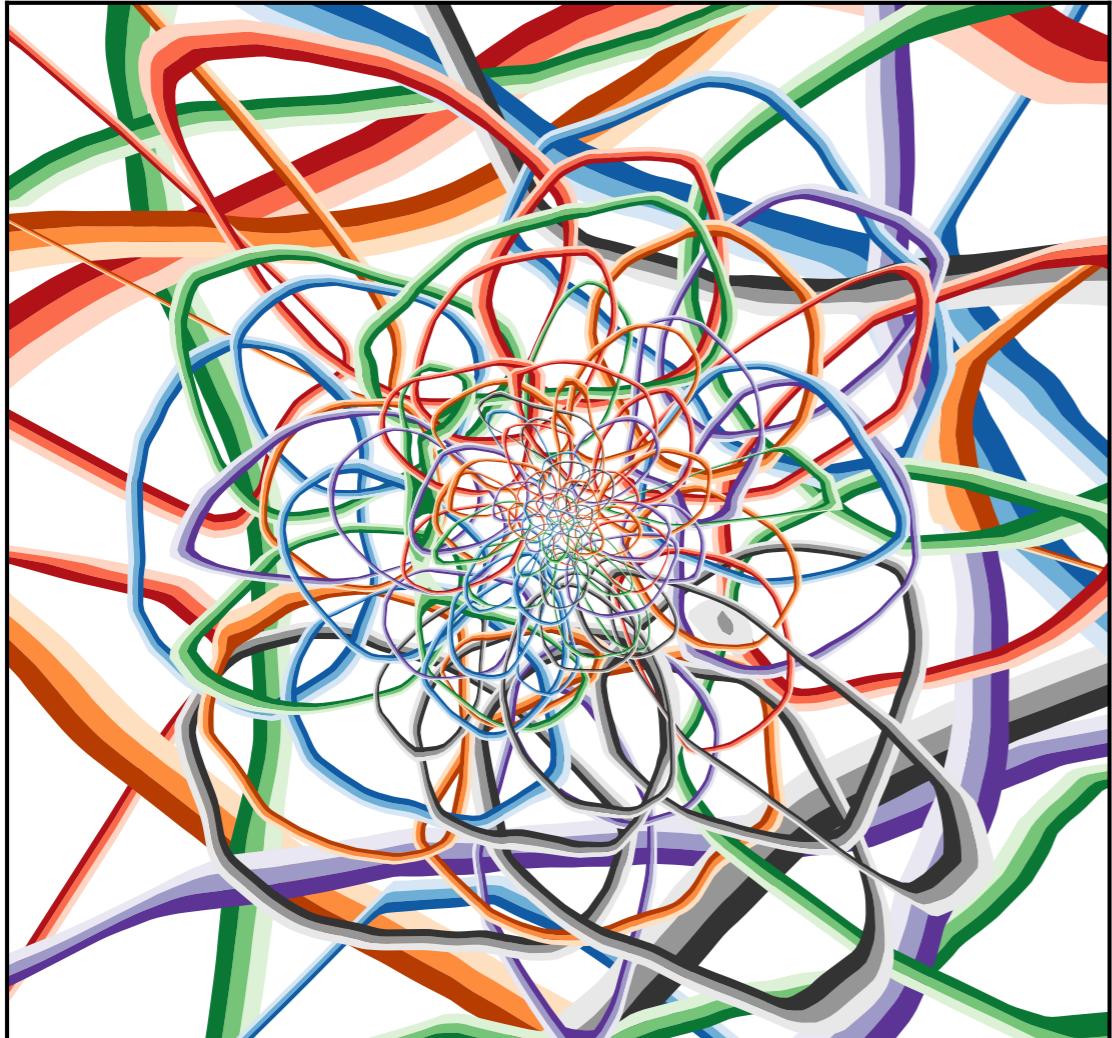


Latent Dimension 64

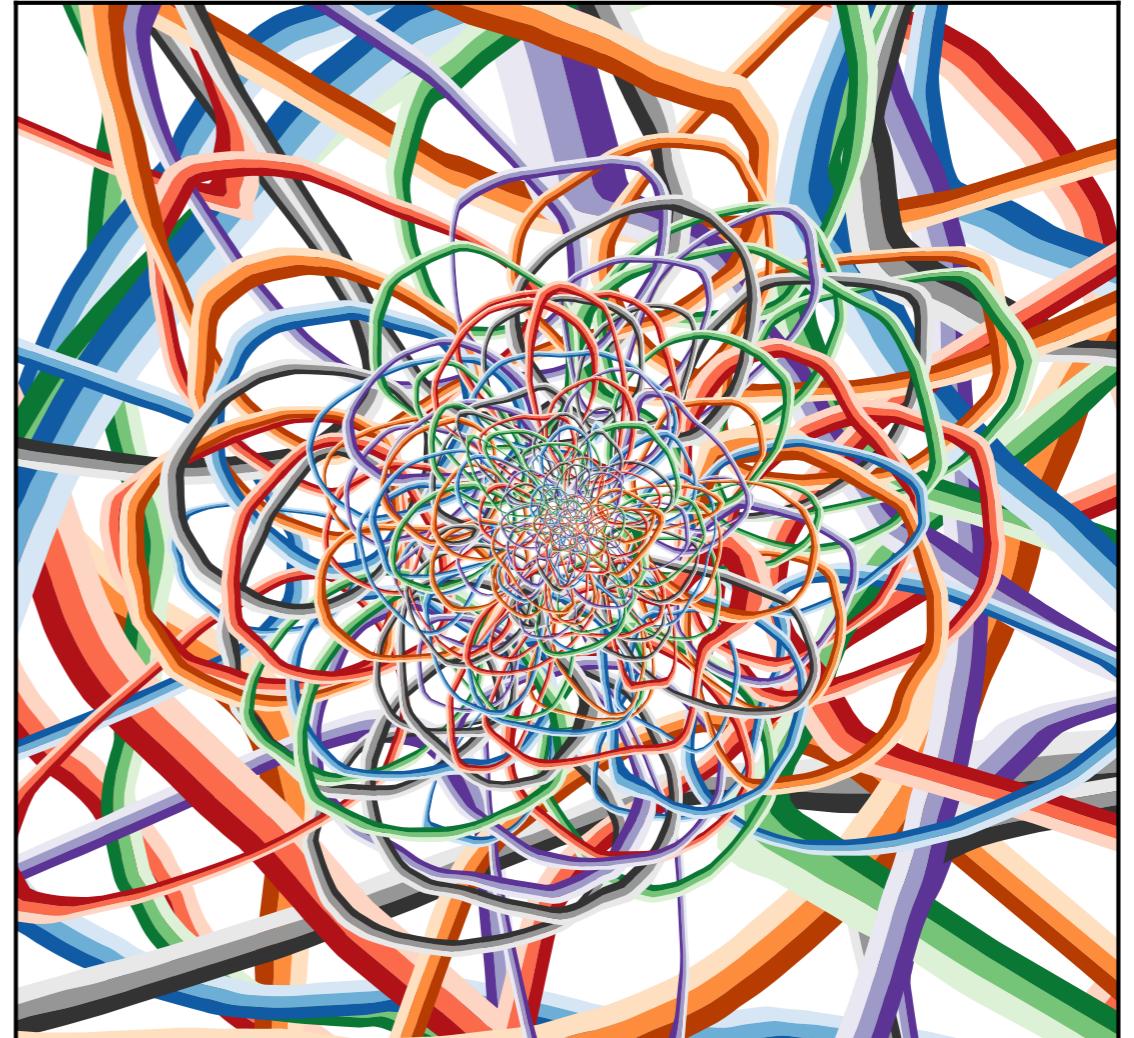


# Psychedelic Network Visualization

Latent Dimension 128

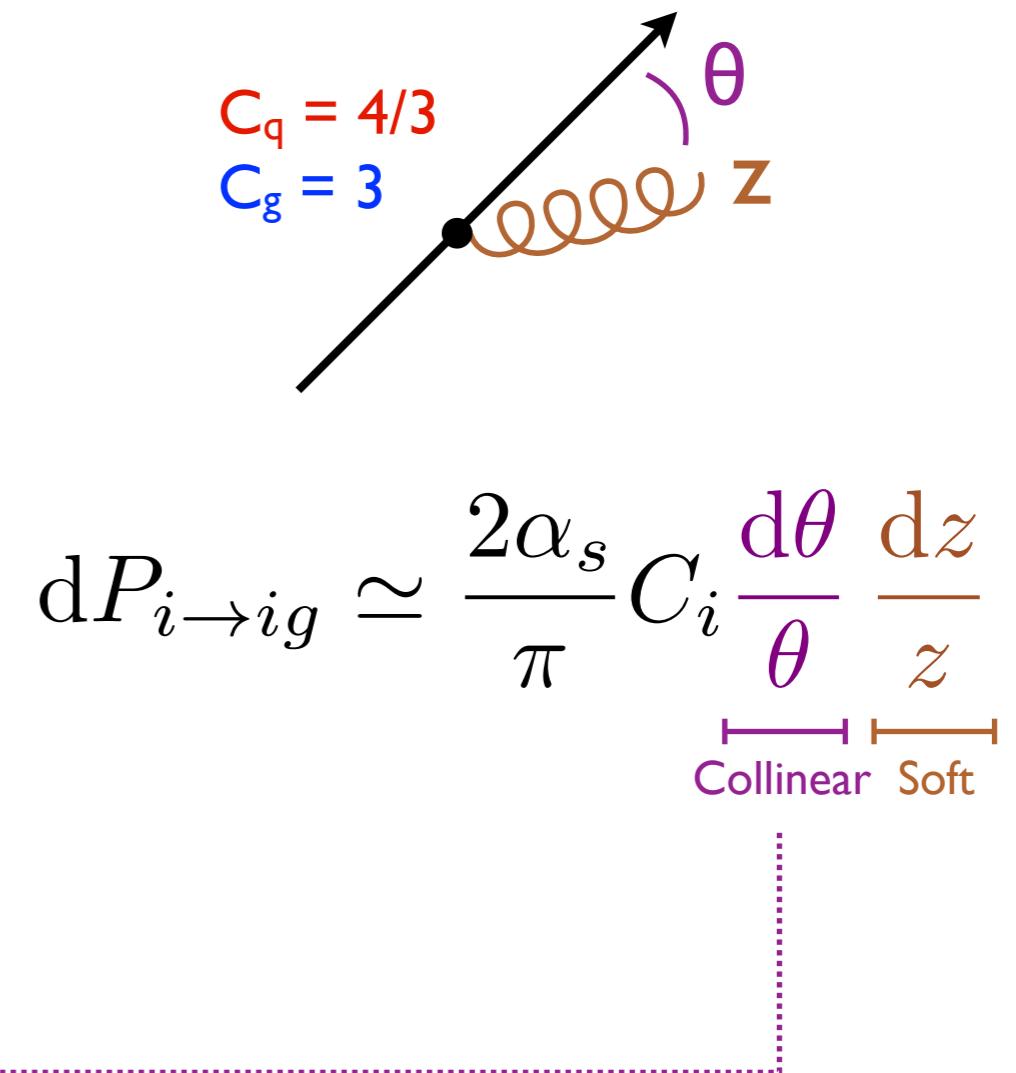
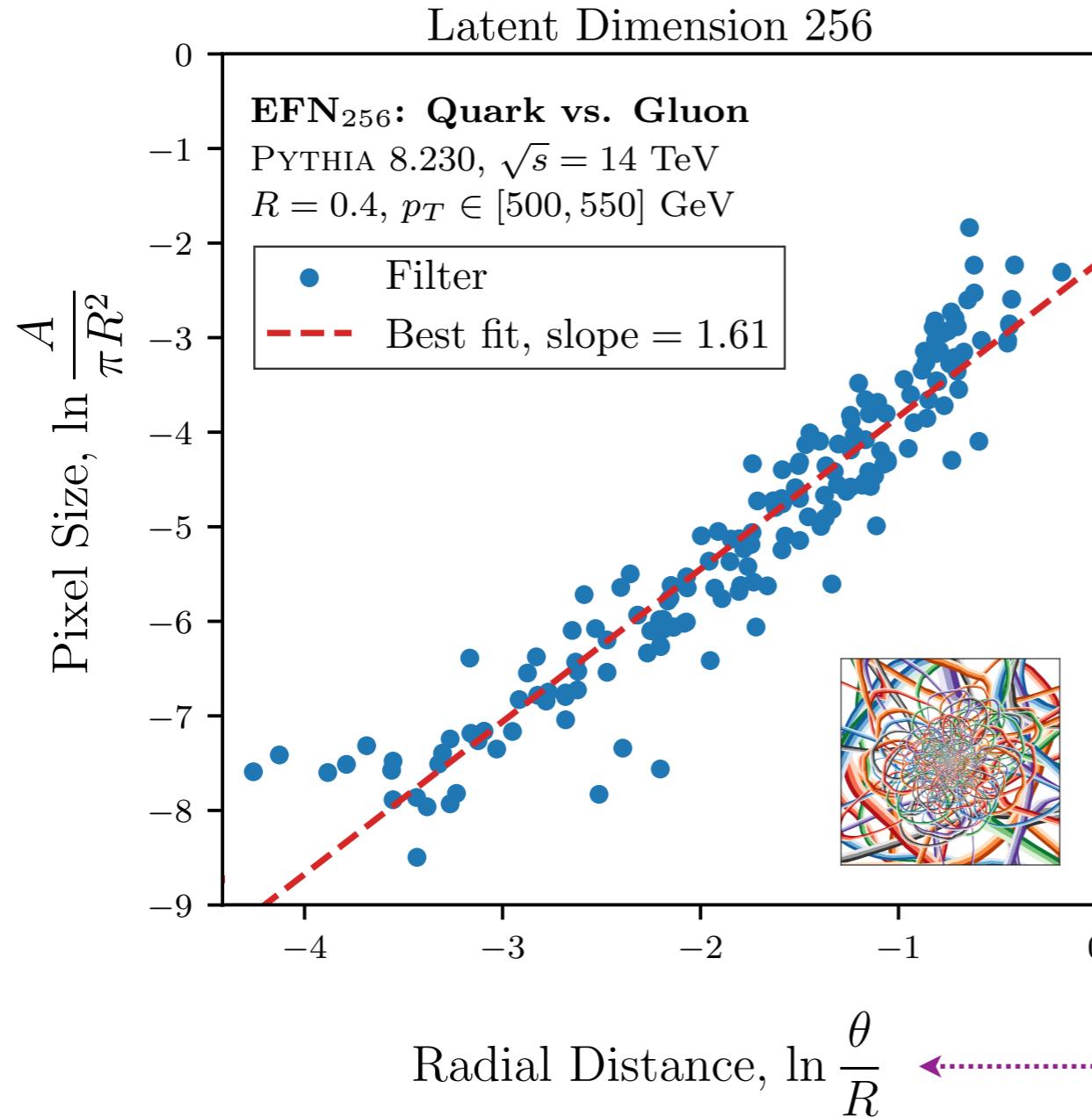


Latent Dimension 256

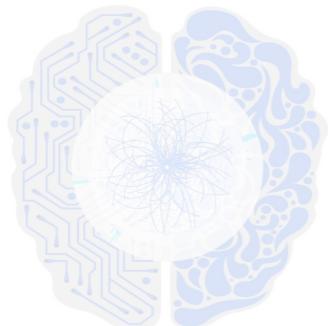


*Singularity structure of QCD!*

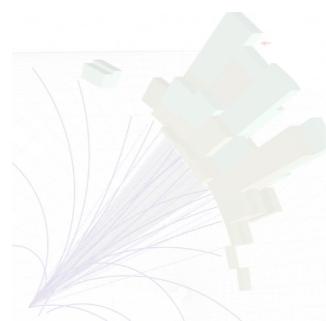
# Machine Learning Collinear QCD



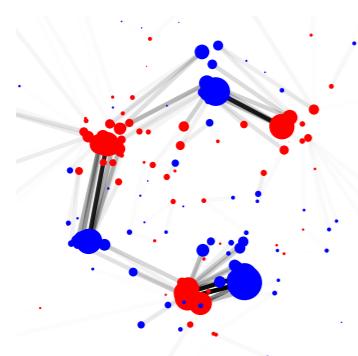
[Komiske, Metodiev, JDT, JHEP 2019]



## Rise of the Machines?



## What is a Collider Event?

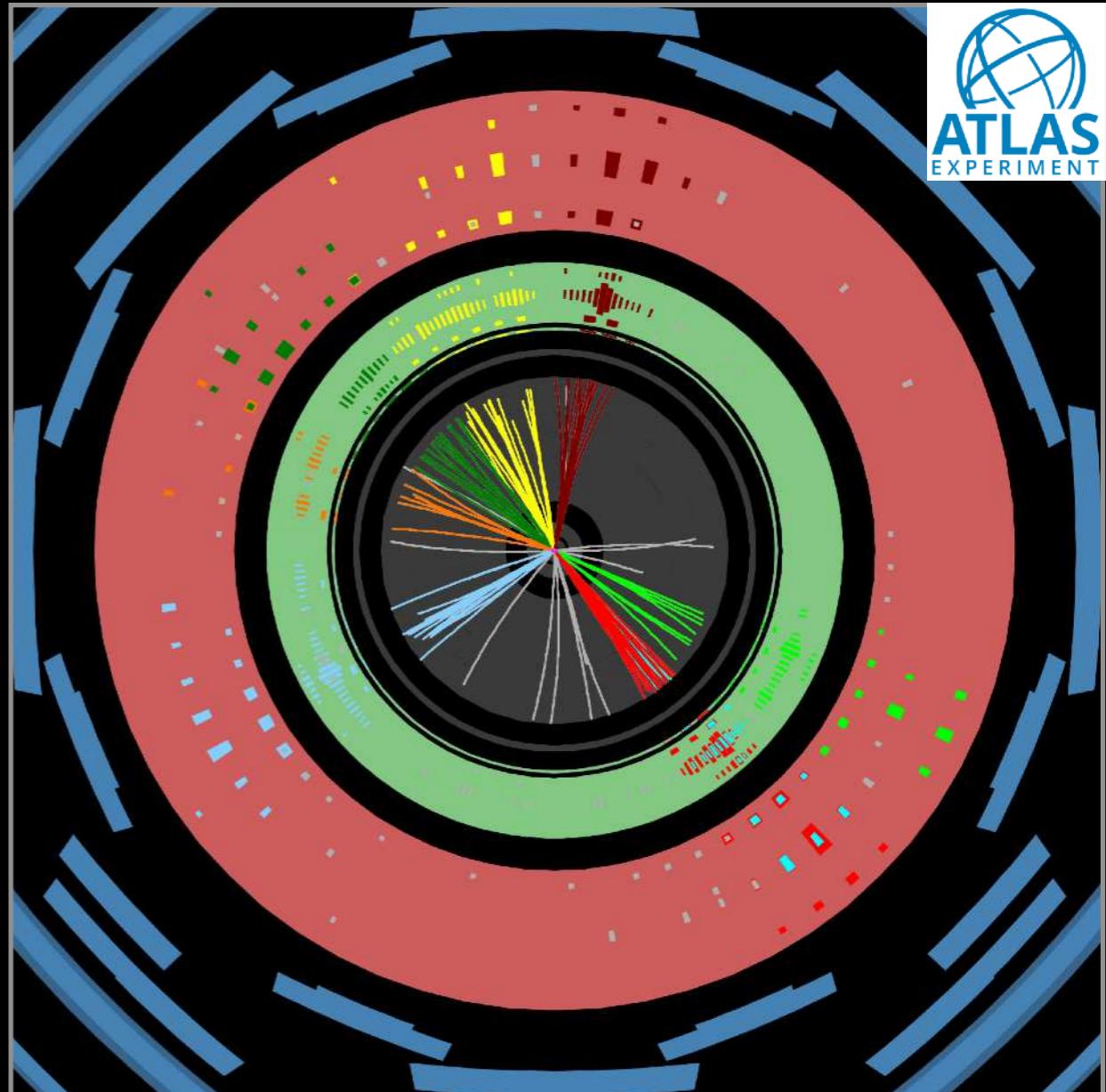
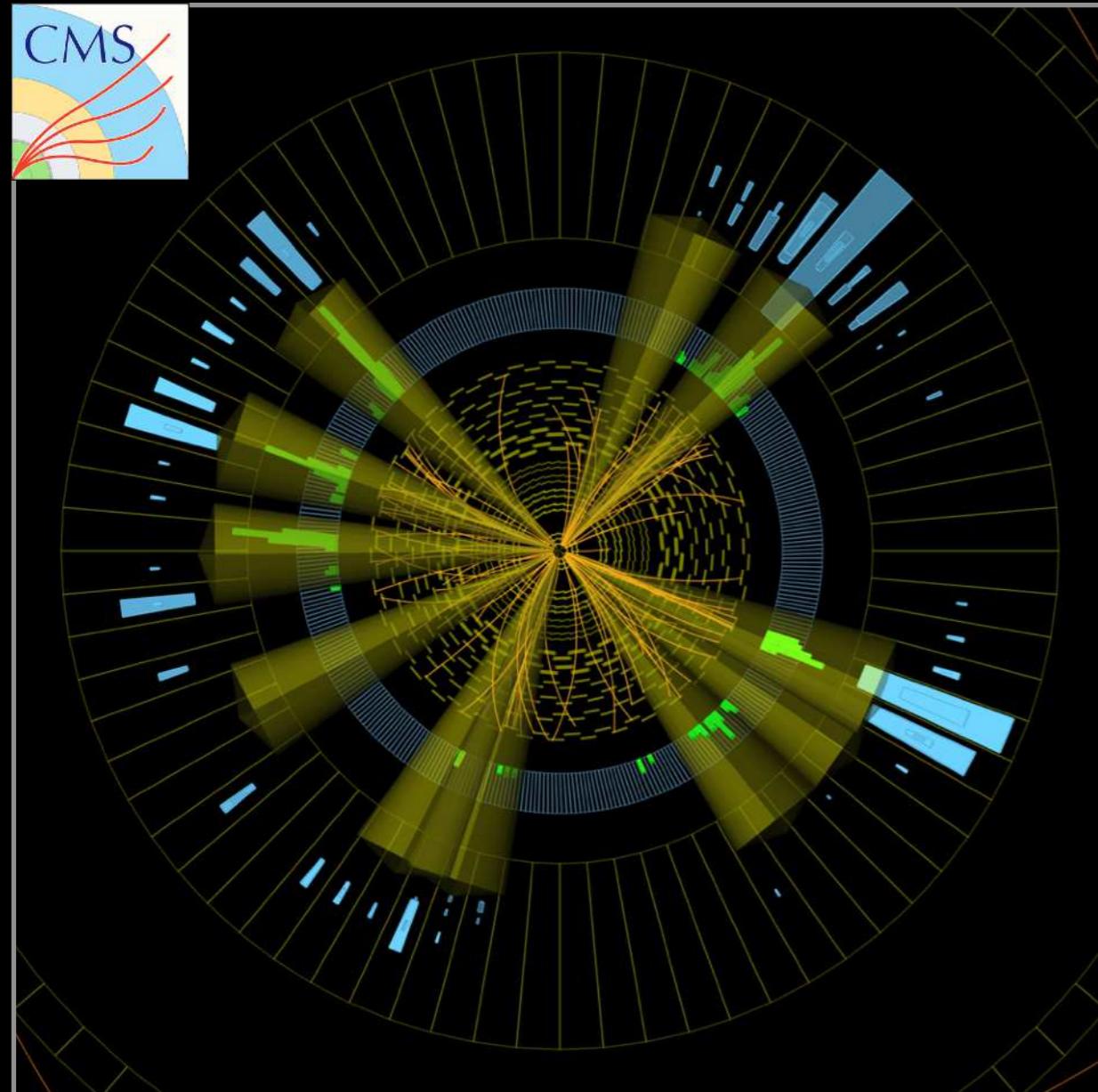


## When are Collider Events Similar?

# Two Collider Events

Two collections of points in (momentum) space

How “close” are these?

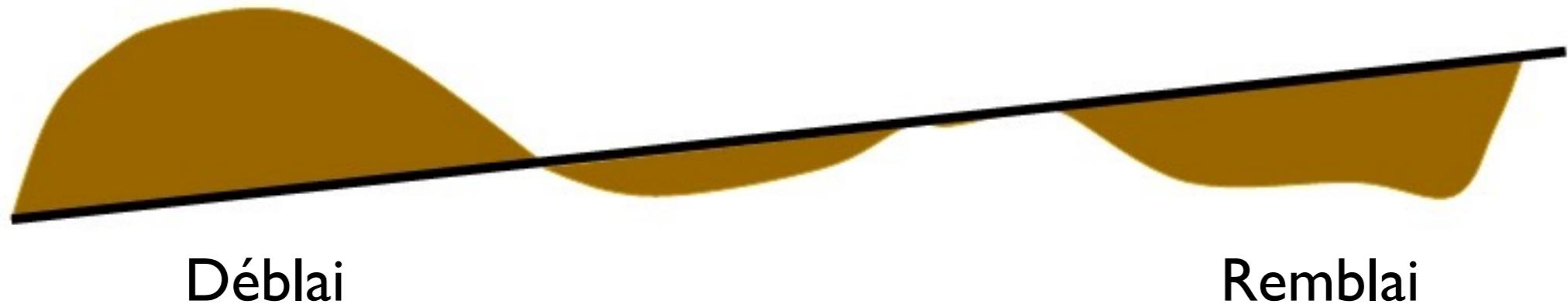


# The Earth Mover's Distance

## Optimal Transport:

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

Minimum “work” (stuff  $\times$  distance) to make one distribution look like another distribution



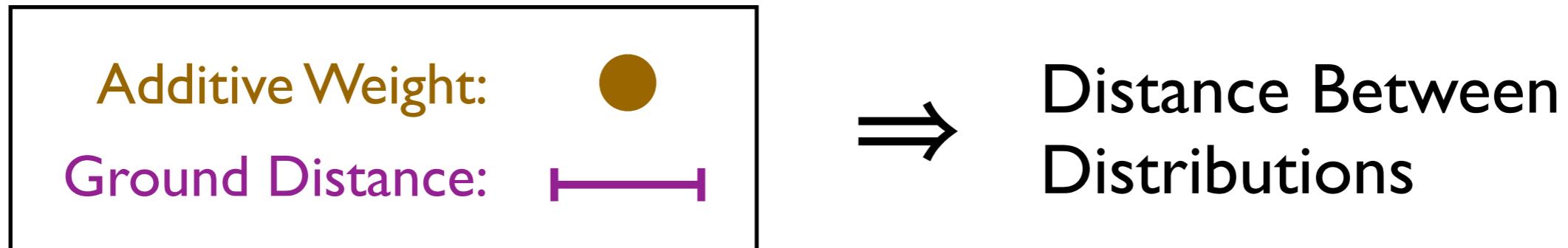
[h/t Niles-Weed, [ML4Jets 2020](#); Monge, 1781; Vaserštejn, 1969; [Wikipedia](#)]

# The Earth Mover's Distance

Optimal Transport:

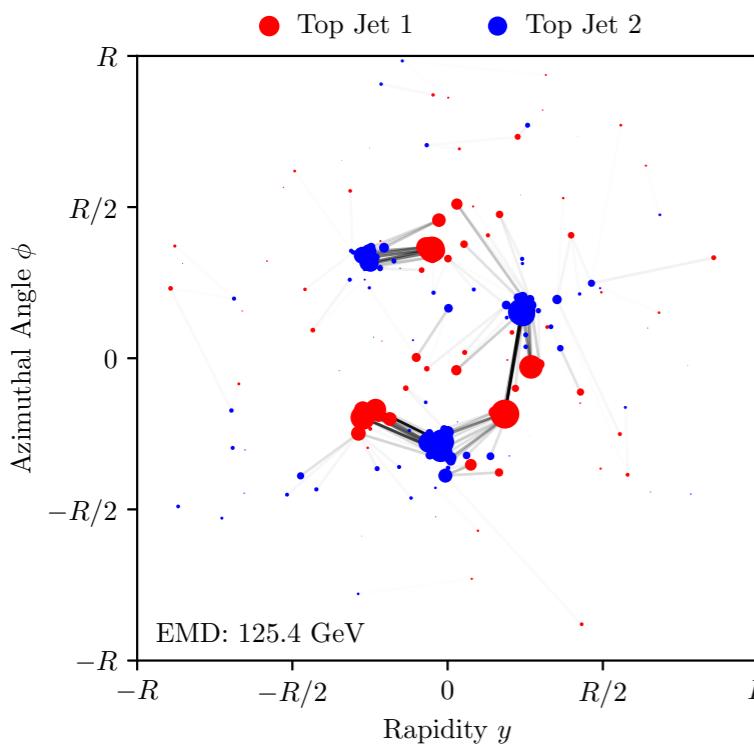
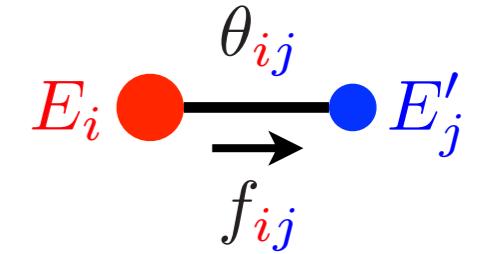
[Peleg, Werman, Rom, [IEEE 1989](#);  
Rubner, Tomasi, Guibas, [ICCV 1998](#), [ICCV 2000](#);  
Pele, Werman, [ECCV 2008](#); Pele Taskar, [GSI 2013](#)]

Minimum “work” (**stuff** × **distance**) to make  
**one distribution** look like **another distribution**



[h/t Niles-Weed, [ML4Jets 2020](#); Monge, 1781; Vaserštejn, 1969; [Wikipedia](#)]

# The Energy Mover's Distance



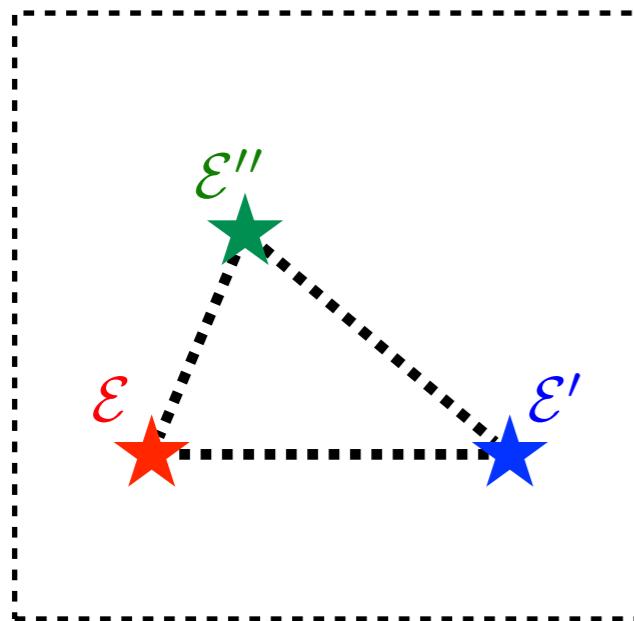
Optimal transport between energy flows...

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

↑  
in GeV

Cost to move energy

Cost to create energy



...defines a metric on the space of events

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

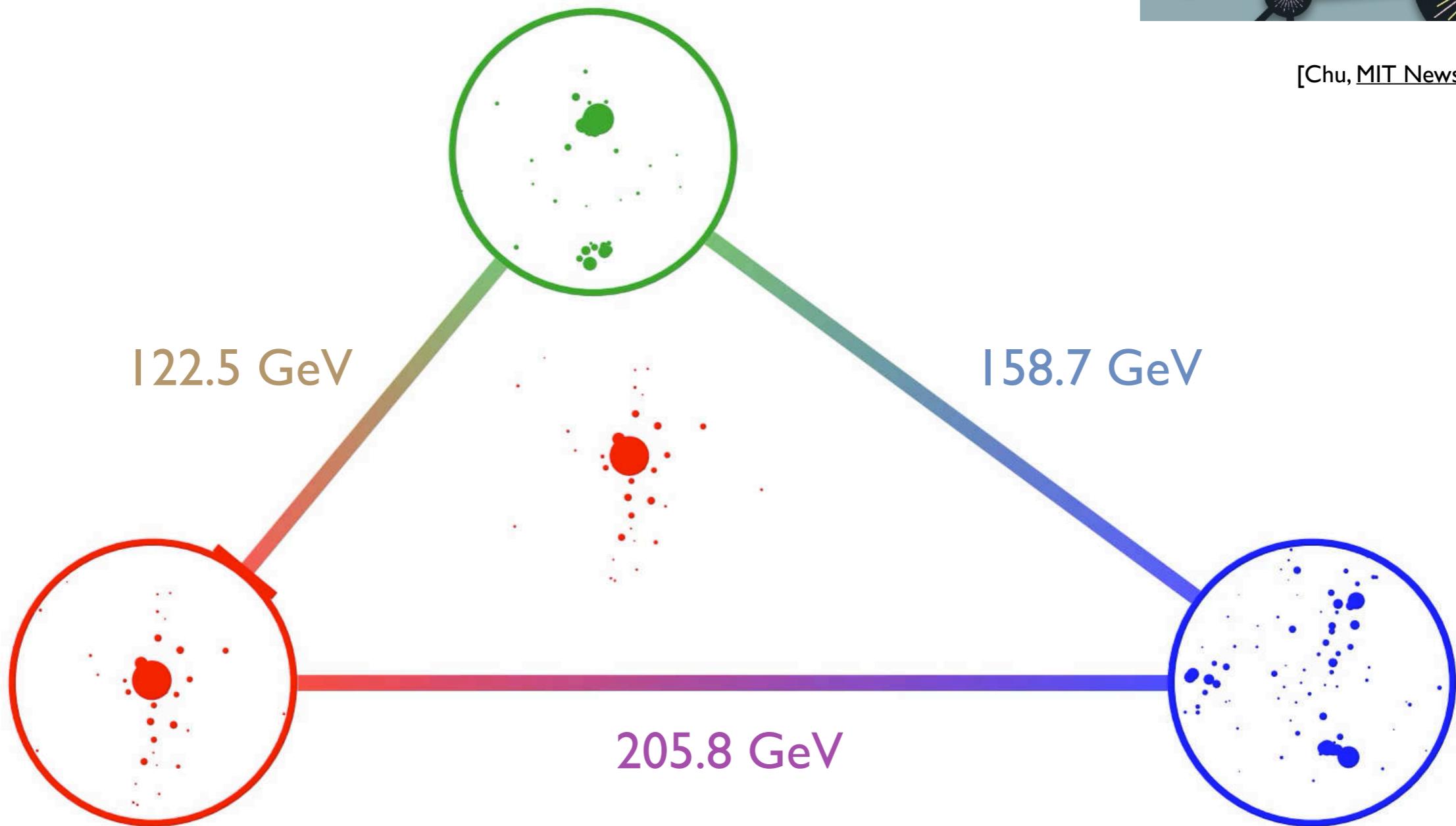
(assuming  $R \geq \theta_{\max}/2$ , i.e.  $R \geq$  jet radius for conical jets)

[Komiske, Metodiev, JDT, [PRL 2019](#);  
 see also Pele, Werman, [ECCV 2008](#); Pele, Taskar, [GSI 2013](#);  
 [see flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, [arXiv 2020](#)]  
 [see computational speed up in Cai, Cheng, Craig, Craig, [arXiv 2020](#)]

# Triangulating the Space of Jets



[Chu, MIT News July 2019]



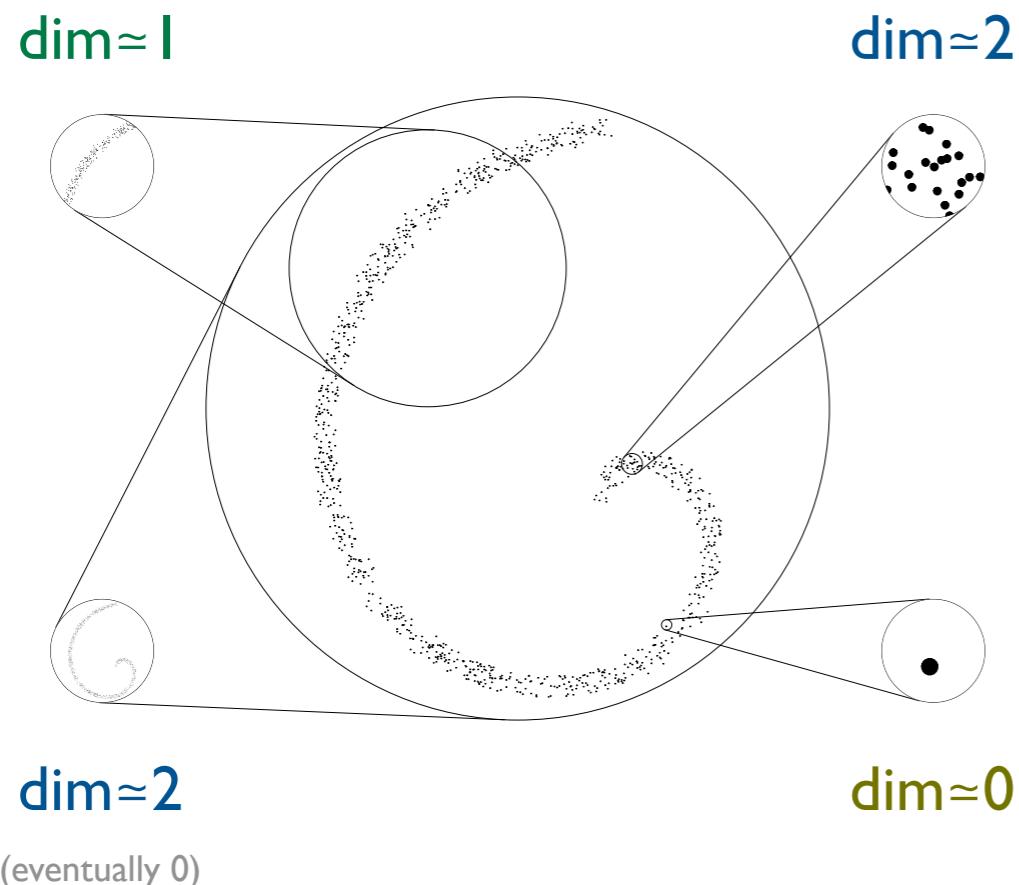
[Komiske, Metodiev, JDT, [PRL 2019](#); code at Komiske, Metodiev, JDT, [energyflow.network](#);  
see alternative graph network approach in Mullin, Pacey, Parker, White, Williams, [arXiv 2019](#)]

# Dimensionality of Space of Jets

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

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

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



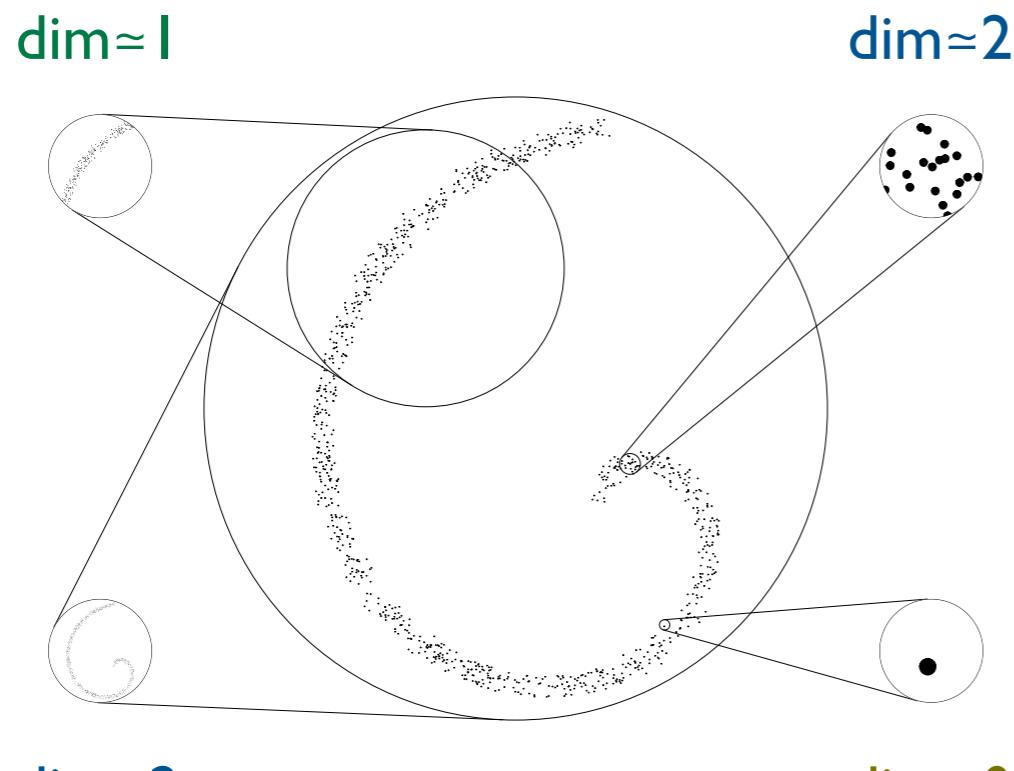
# Dimensionality of Space of Jets



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

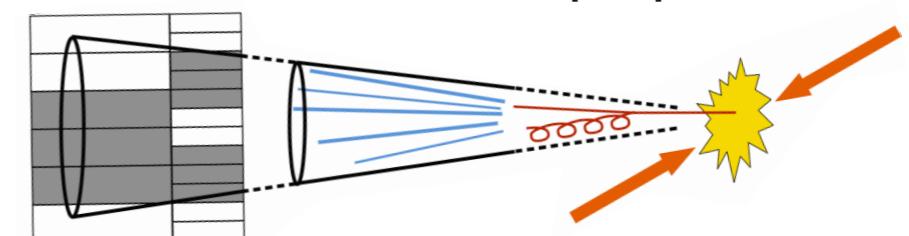
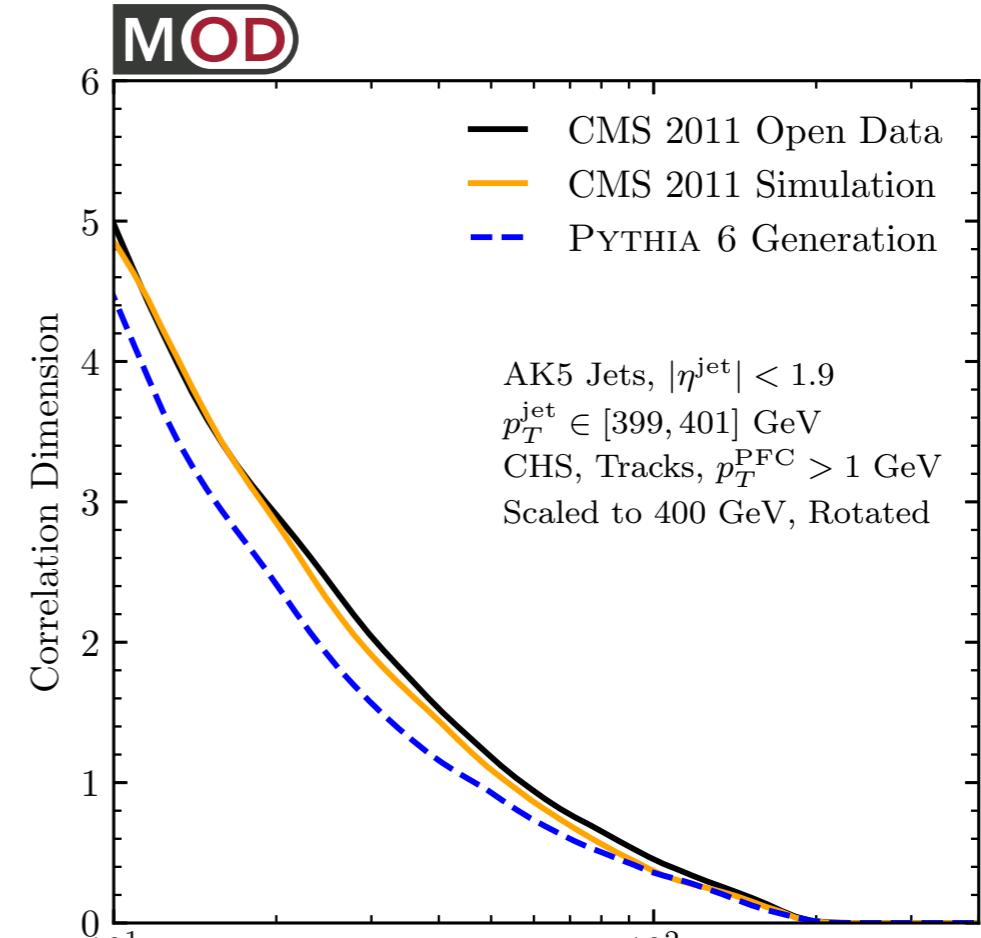
$$\Rightarrow \dim(r) \sim r \frac{\partial}{\partial r} \ln N_{\text{neighbors}}(r)$$

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

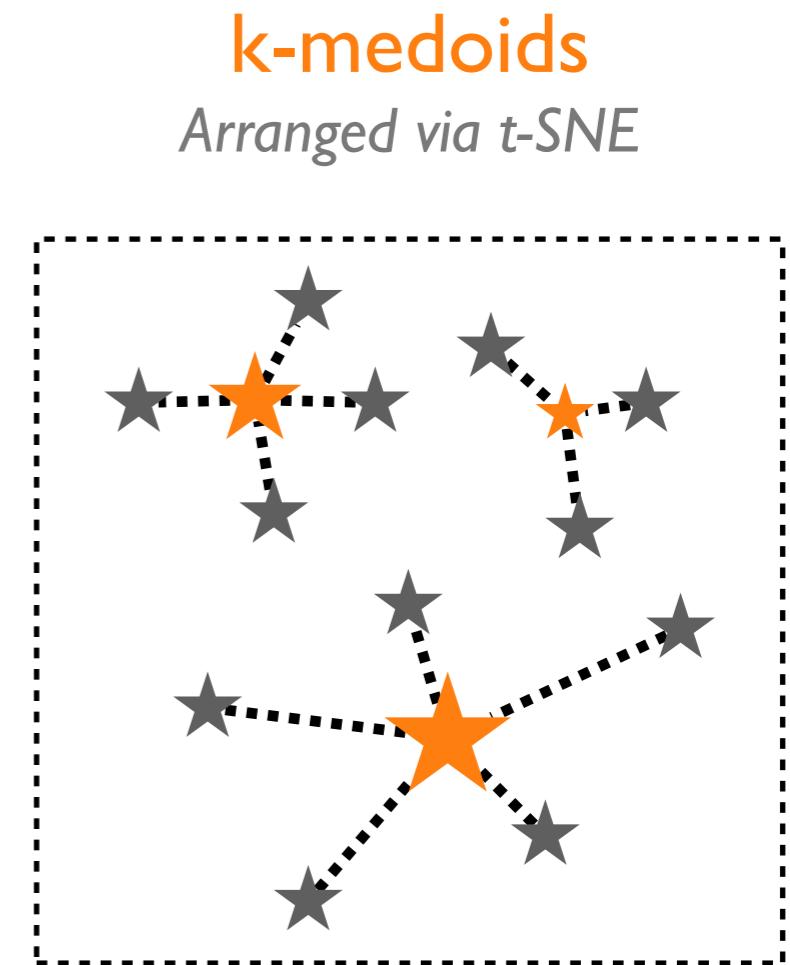
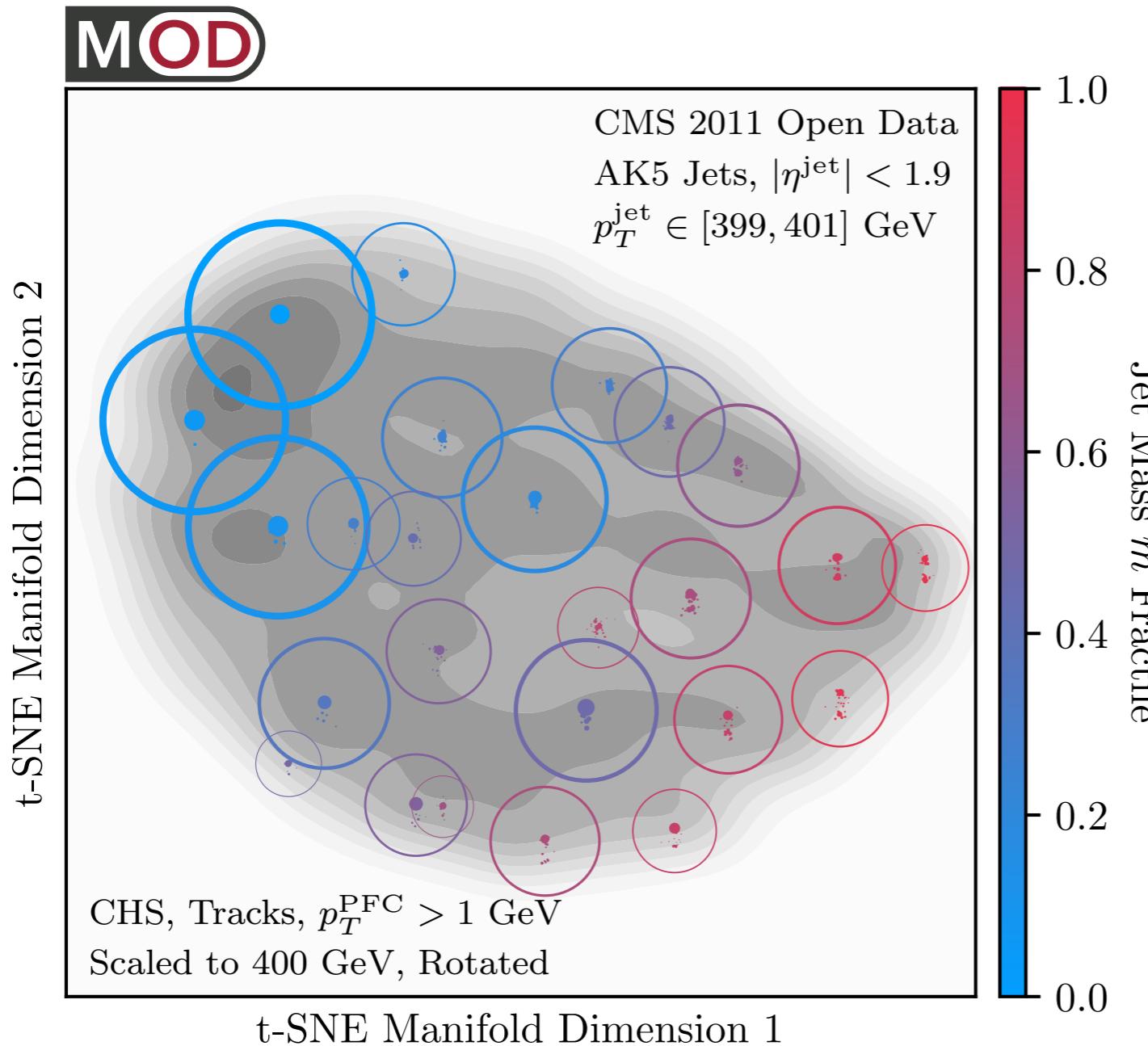


(eventually 0)

[Komiske, Mastandrea, Metodiev, Naik, [JDT, PRD 2020](#);  
using [CMS Open Data](#)]



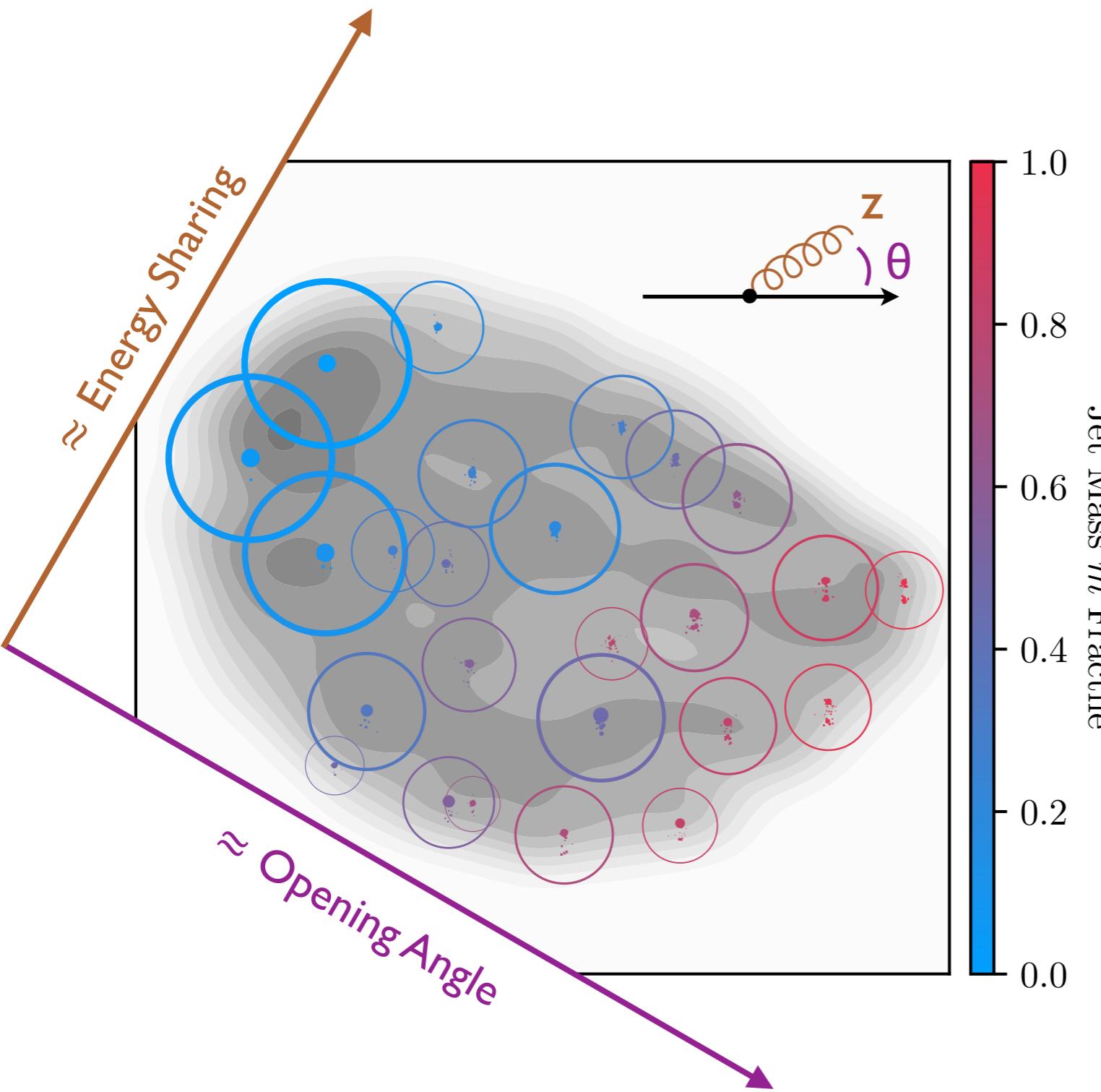
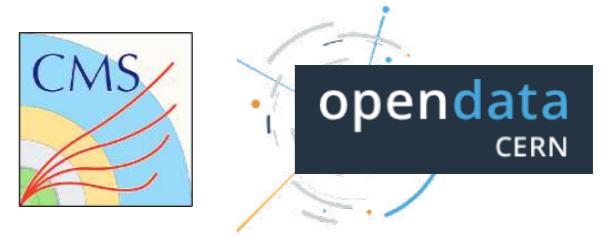
# Most Representative Jets



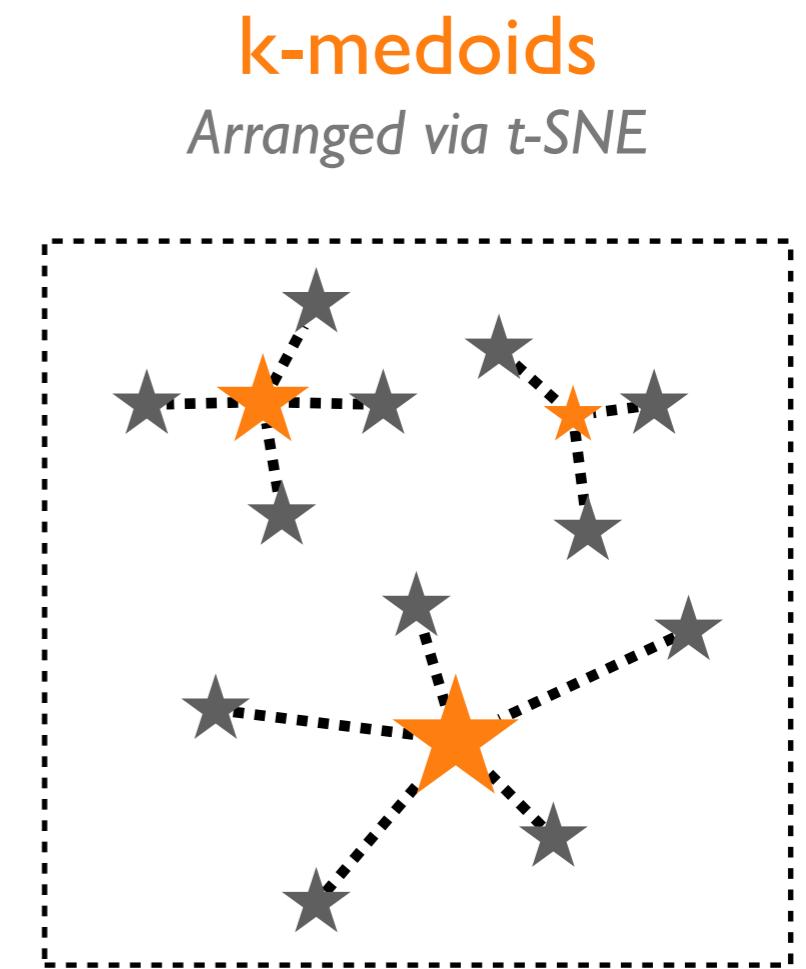
[Komiske, Mastandrea, Metodiev, Naik, JDT, [PRD 2020](#);  
using van der Maaten, Hinton, [JMLR 2008](#)]



# Most Representative Jets



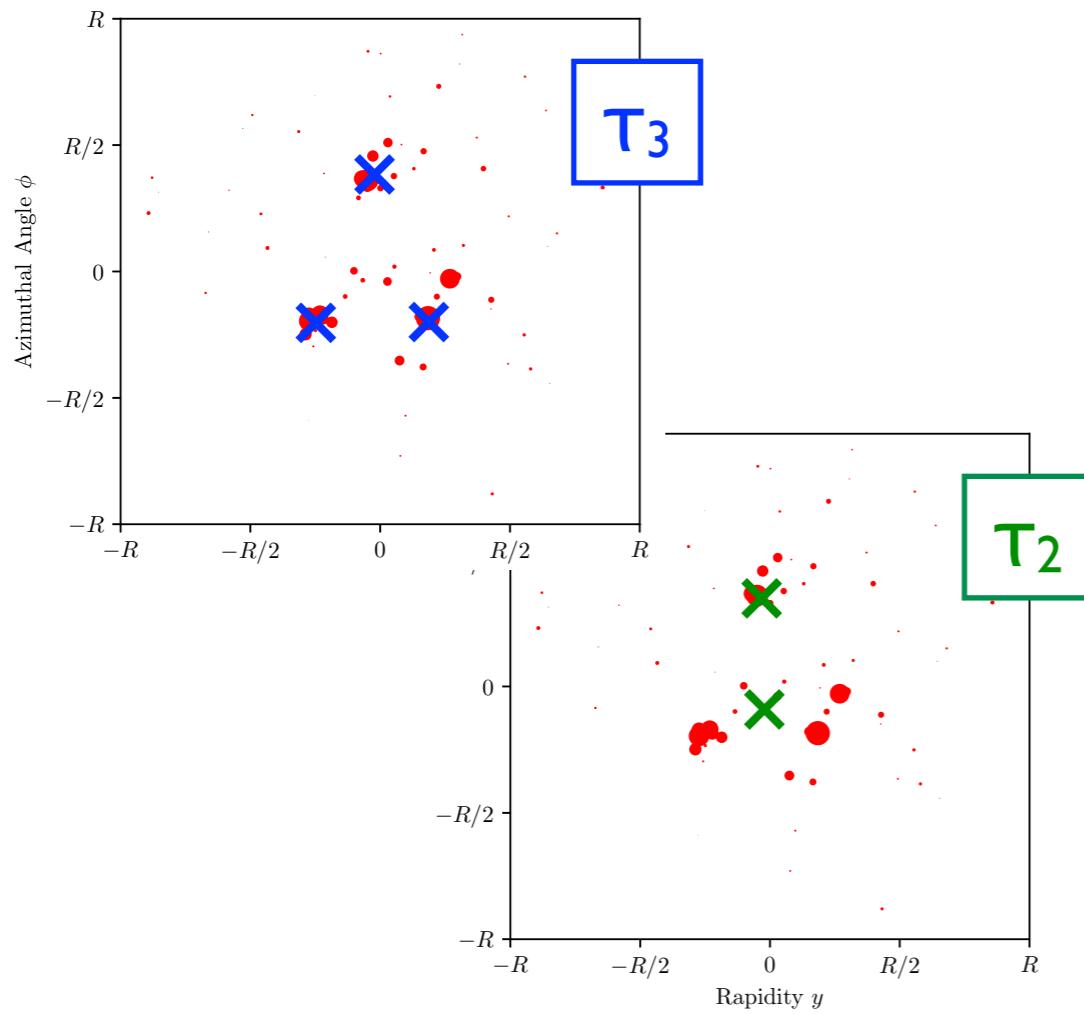
[Komiske, Mastandrea, Metodiev, Naik, JDT, [PRD 2020](#);  
using van der Maaten, Hinton, [JMLR 2008](#)]



# N-subjettiness

*Ubiquitous jet substructure observable used for almost a decade...*

$$\tau_N(\mathcal{J}) = \min_{N \text{ axes}} \sum_i E_i \min \{\theta_{1,i}, \theta_{2,i}, \dots, \theta_{N,i}\}$$

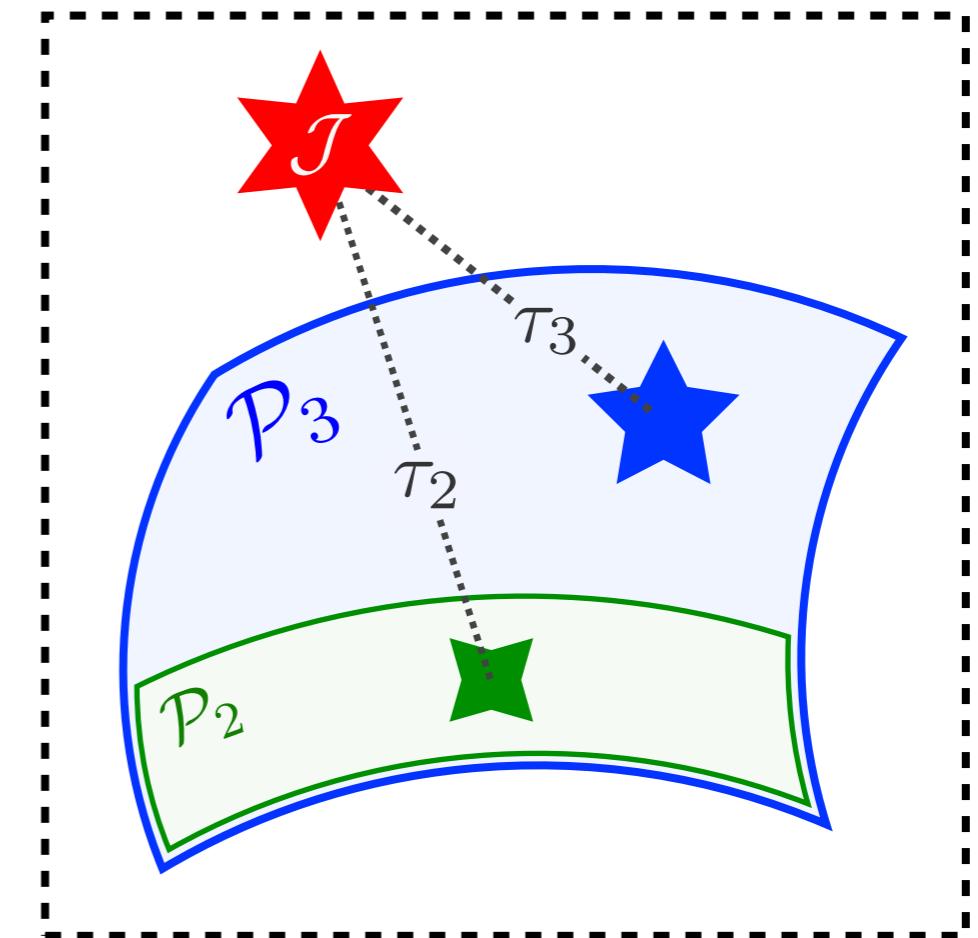
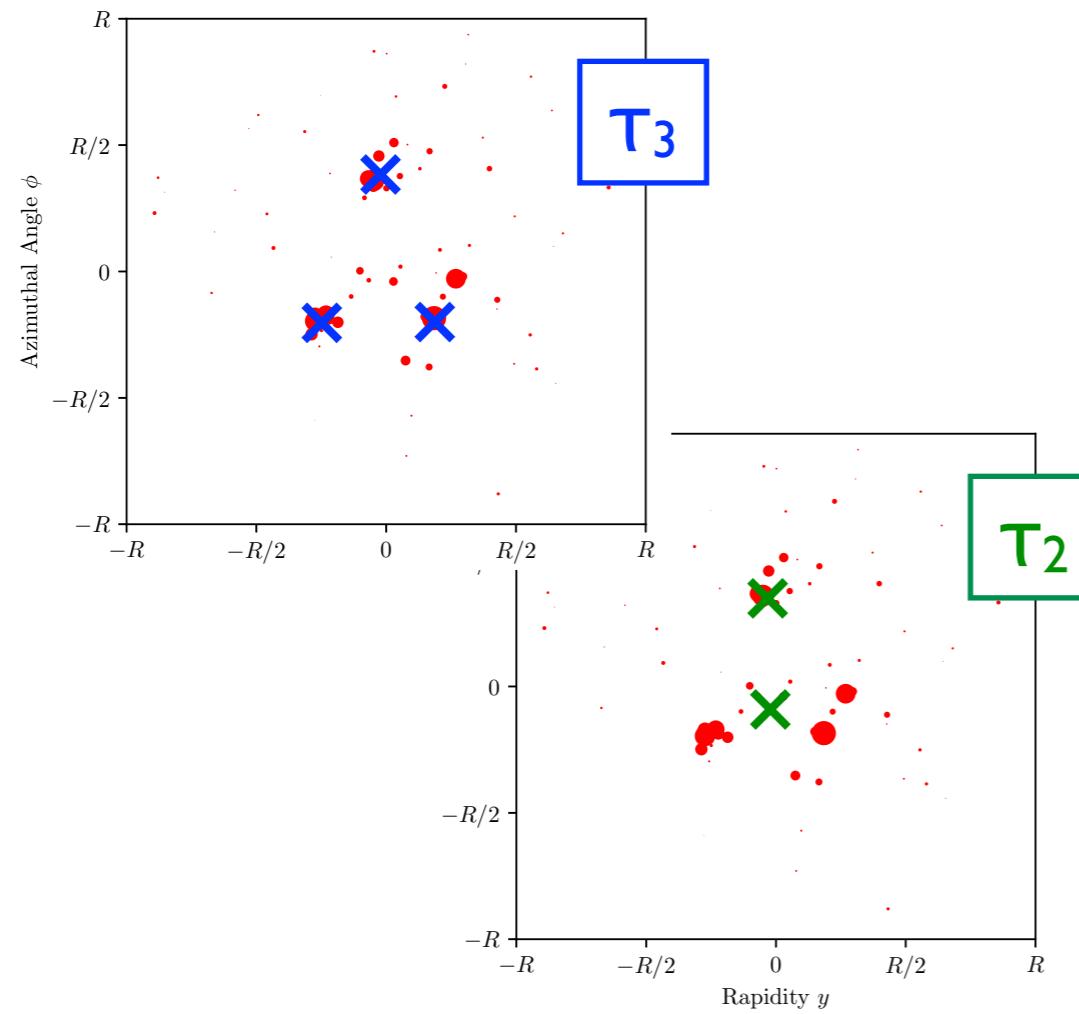


[JDT, Van Tilburg, [JHEP 2011](#), [JHEP 2012](#);  
based on Brandt, Dahmen, [ZPC 1979](#); Stewart, Tackmann, Waalewijn, [PRL 2010](#)]

# N-subjettiness = Point to Manifold EMD

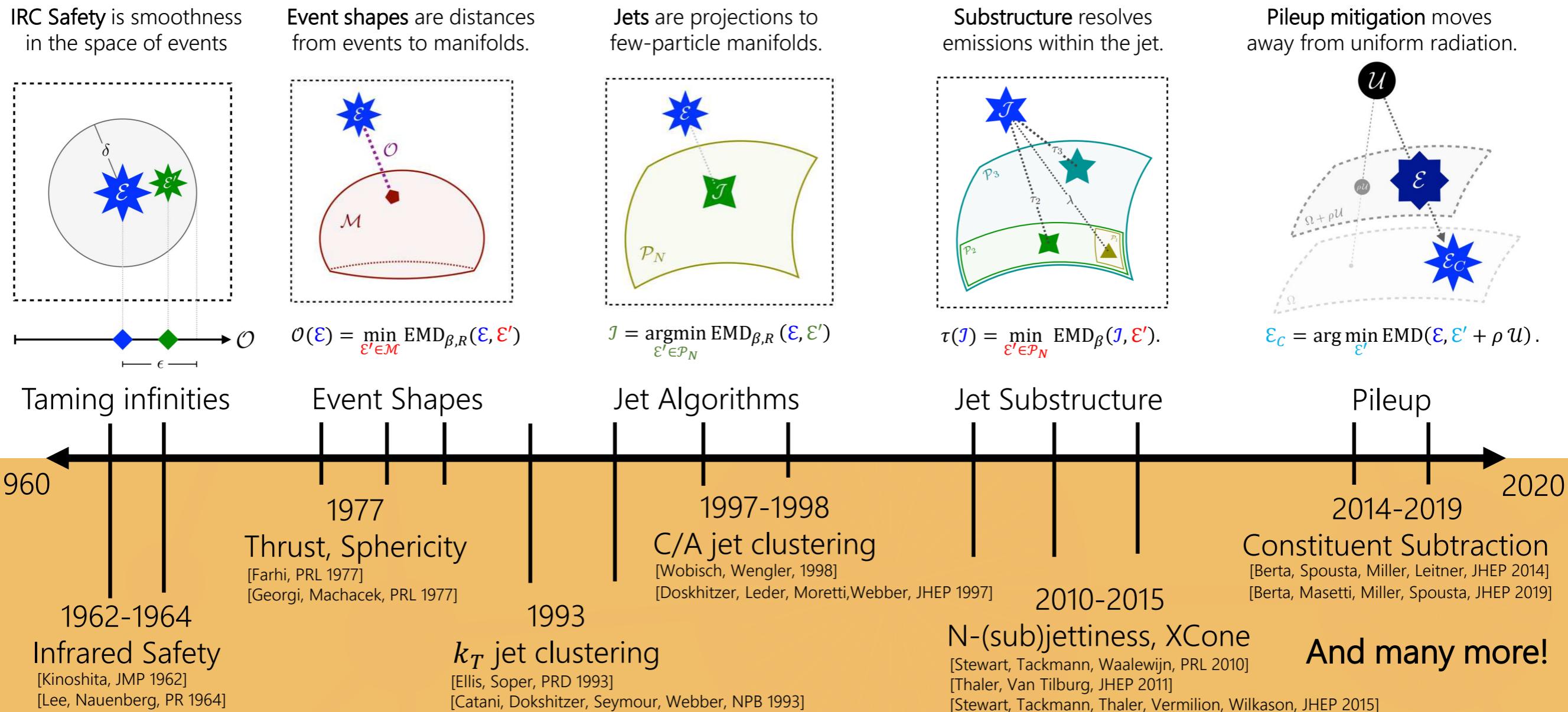
*...is secretly an optimal transport problem*

$$\tau_N(\mathcal{J}) = \min_{\mathcal{J}' \in \mathcal{P}_N} \text{EMD}(\mathcal{J}, \mathcal{J}')$$



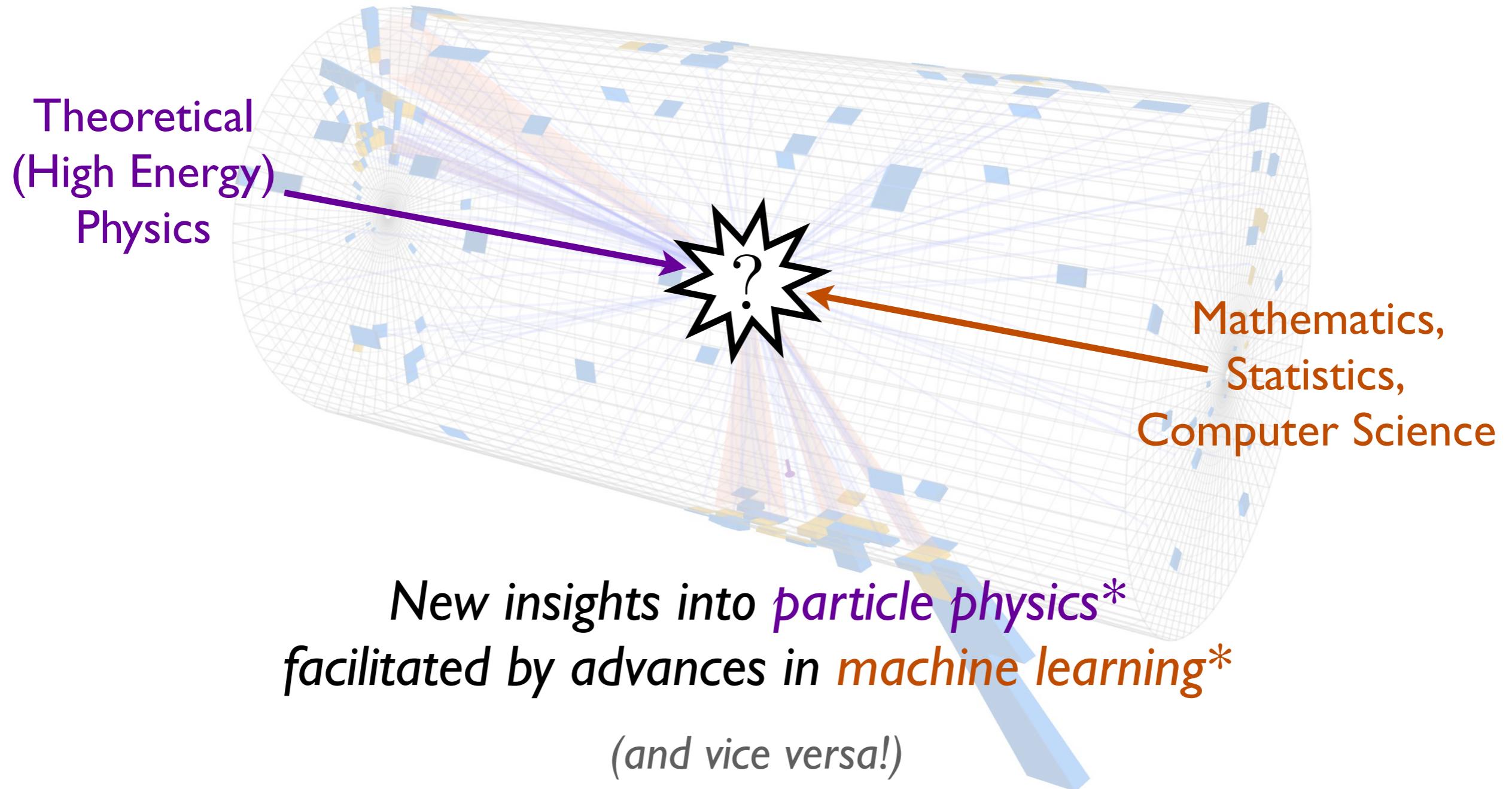
[JDT, Van Tilburg, [JHEP 2011](#), [JHEP 2012](#);  
rephrased via Komiske, Metodiev, JDT, [JHEP 2020](#); see opposite limit in Cesarotti, JDT, [JHEP 2020](#)]

# Six Decades of Collider Physics Translated into a New Geometric Language!



# “Collision Course”

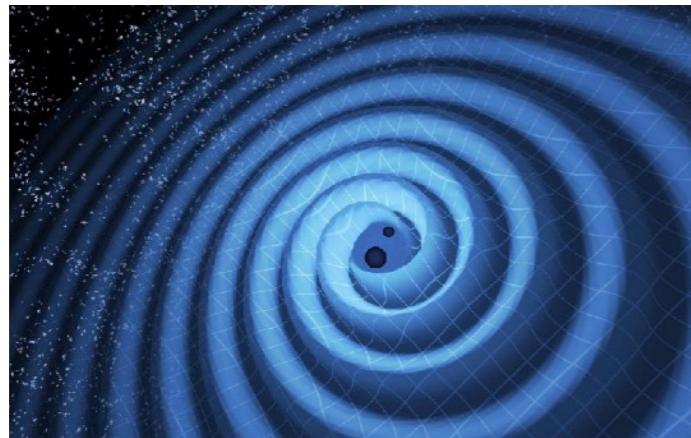
“Theoretical Physics for Machine Learning”  
Aspen Center for Physics, January 2019



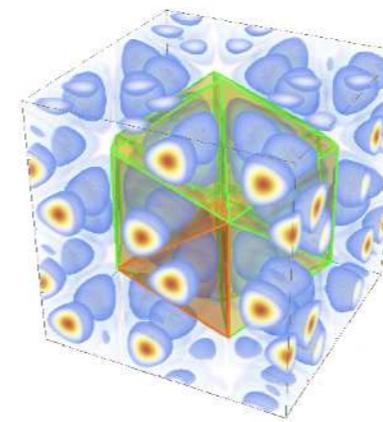
# *Artificial Intelligence $\leftrightarrow$ Fundamental Interactions*



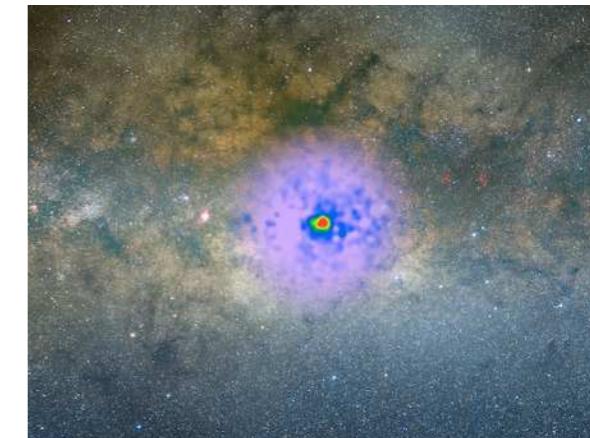
*Gravitational Waves*



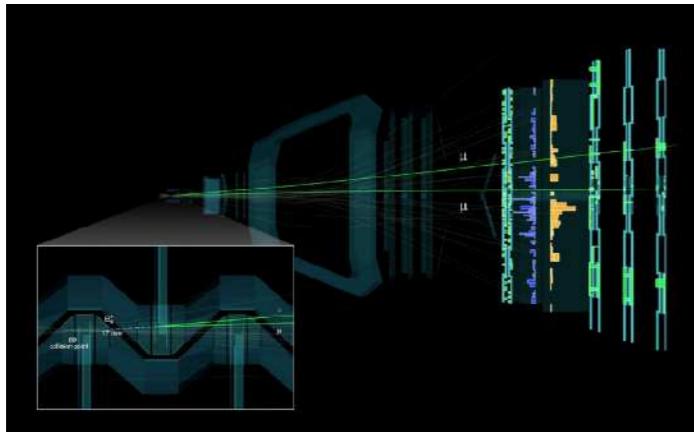
*Nuclear Physics*



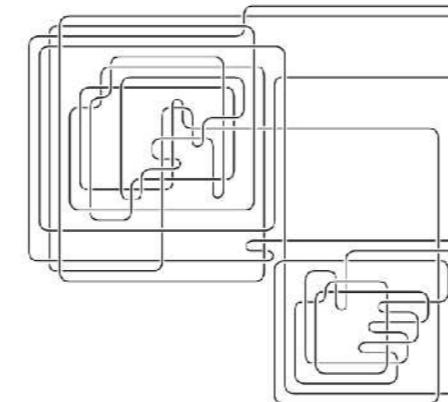
*Astrophysics*



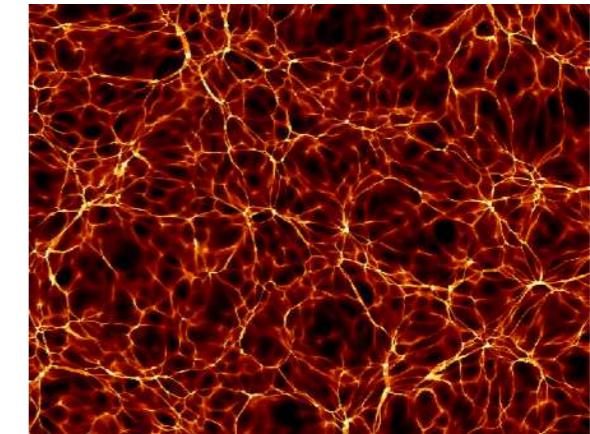
*Particle Colliders*



*Mathematical Physics*



*Dark Matter*

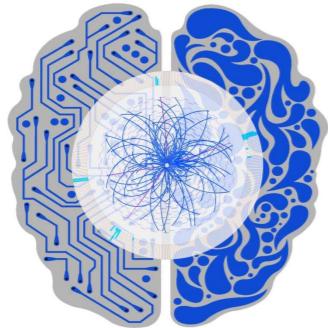


...

*Machine learning that incorporates first principles, best practices, and domain knowledge from fundamental physics*

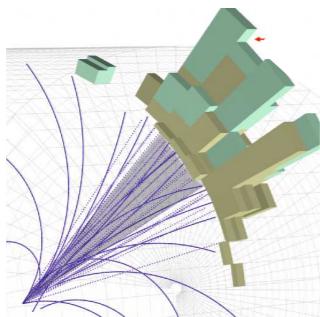
[<http://iaifi.org>]

# Summary



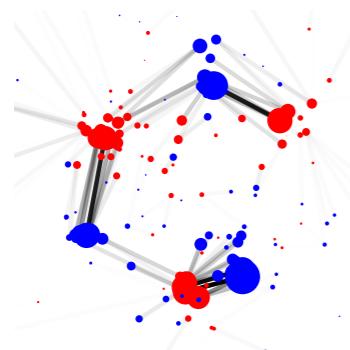
## Rise of the Machines?

*Machine learning offers powerful tools to analyze collision debris  
Progress towards the fusion of deep learning and “deep thinking”*



## What is a Collider Event?

*Unordered set of particles describing energy flow of jets  
Inspires network architectures designed for symmetry and safety*



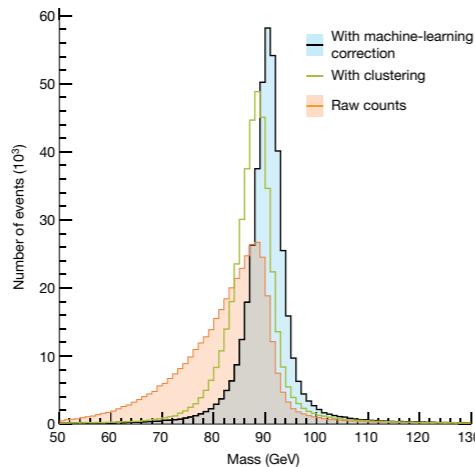
## When are Collider Events Similar?

*When their energy flows are similar  
Inspires unsupervised learning strategies based on event geometry*

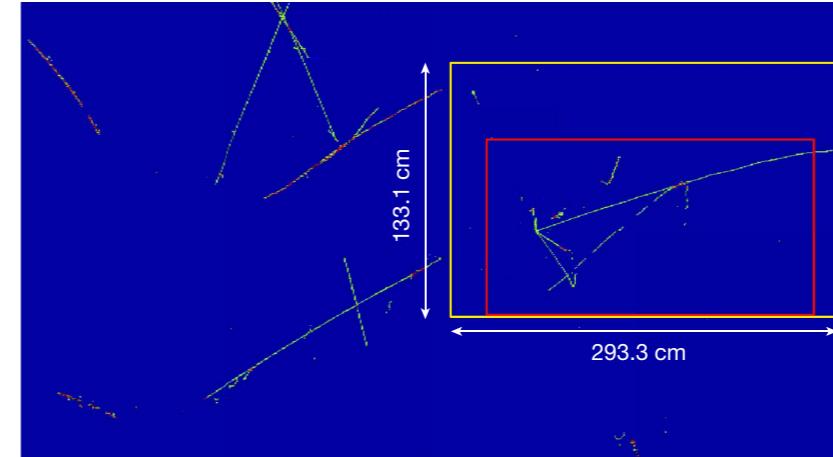
# *Backup Slides*

# Extensive Use of ML in HEP

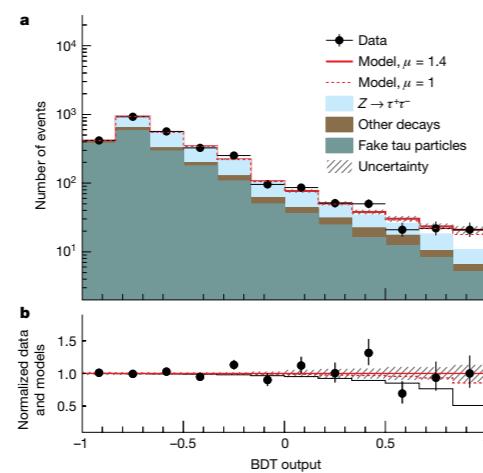
CMS:  $Z \rightarrow e^+e^-$  calibration



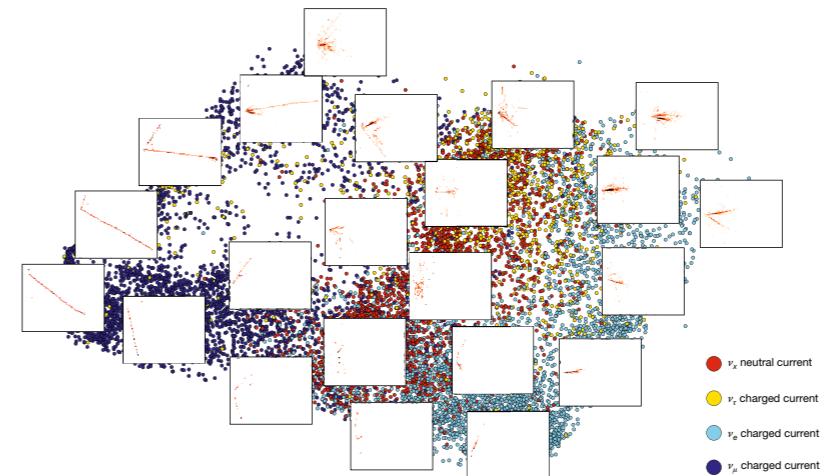
MicroBooNE: Object Identification



ATLAS:  $H \rightarrow \mu^+\mu^-$  search



NOvA: Object Classification



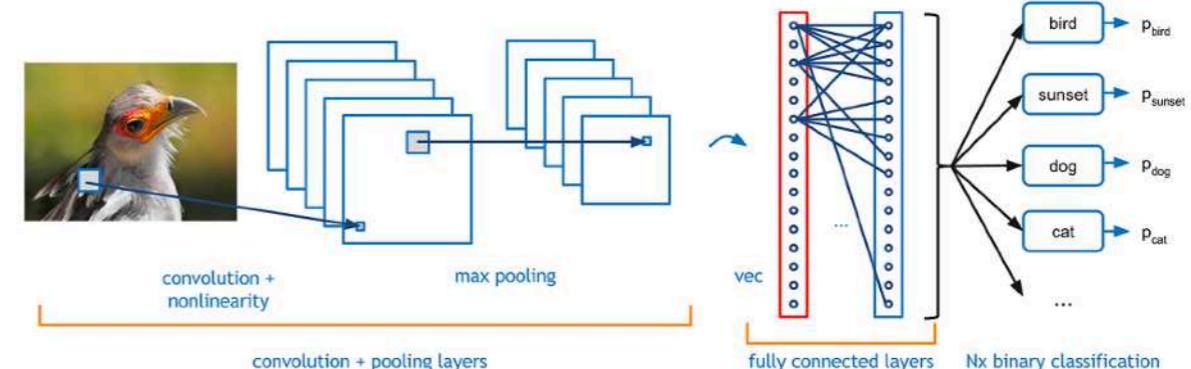
*Machine learning is transforming many aspects of society, including fundamental physics research*

[Radovic, Williams, Rousseau, Kagan, Bonacorsi, Himmel, Aurisano, Terao, Wongjirad, [Nature 2018](#)]

# Off-the-Shelf ML for HEP?

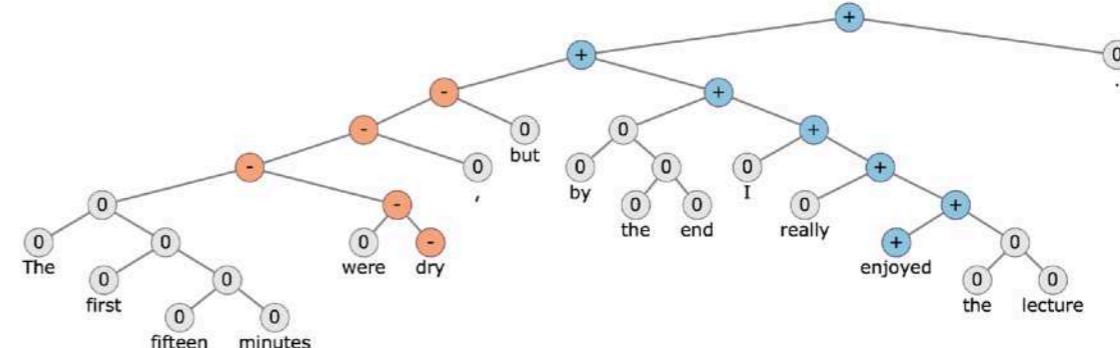
## 2D Images?

Appropriate for fixed-grid calorimeters,  
but less ideal for tracking detectors



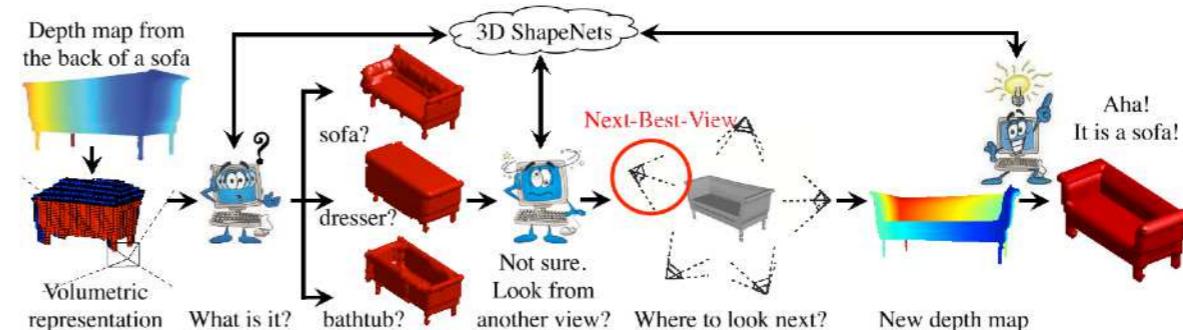
## Natural Language?

Clustering can yield “semantic” structure, but  
identical particles have no intrinsic ordering



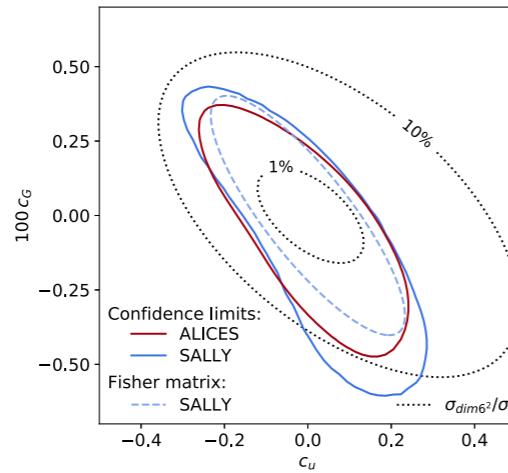
## 3D Objects?

Much closer to particle physics,  
though doesn't capture all symmetries



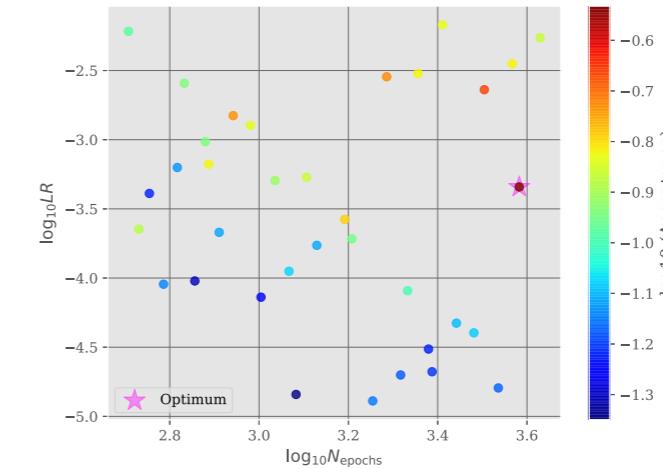
# ML Targets for Collider Theory

e.g. Parameter Inference



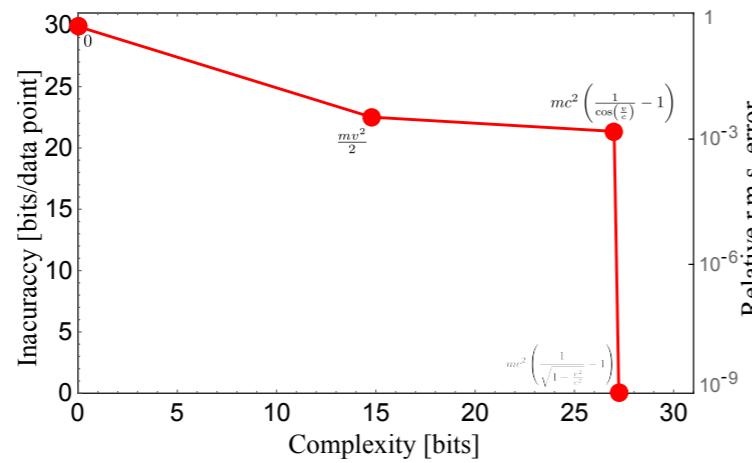
[Brehmer, Kling, Espejo, Cranmer, [CSBS 2020](#)]

e.g. Normalizing Flows



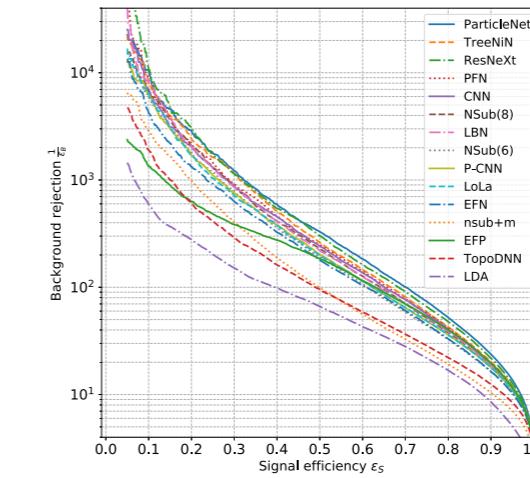
[Gao, Höche, Isaacson, Krause, Schulz, [PRD 2020](#)]

e.g. Symbolic Regression



[Udrescu, Tan, Feng, Neto, Wu, Tegmark, [NeurIPS 2020](#)]

e.g. Jet Classification



[Kasieczka, Plehn, et al., [SciPost 2019](#)]

[apologies for focus on research from my group in this talk; see [HEPML-LivingReview](#) for extensive bibliography]

# Likelihood Ratio Trick

Many HEP problems can be expressed in this form!

Key example of *simulation-based inference*

Goal: Estimate  $p(x)$  /  $q(x)$

Training Data: Finite samples  $P$  and  $Q$

Learnable Function:  $f(x)$  parametrized by, e.g., neural networks

Loss Function(al):  $L = -\langle \log f(x) \rangle_P + \langle f(x) - 1 \rangle_Q$

Asymptotically:  $\arg \min_{f(x)} L = \frac{p(x)}{q(x)}$  *Likelihood ratio*

$-\min_{f(x)} L = \int dx p(x) \log \frac{p(x)}{q(x)}$  *Kullback–Leibler divergence*

[see e.g. D’Agnolo, Wulzer, [PRD 2019](#); simulation-based inference in Cranmer, Brehmer, Louppe, [PNAS 2020](#); relation to f-divergences in Nguyen, Wainwright, Jordan, [AoS 2009](#)]

# Likelihood Ratio Trick

Many HEP problems can be expressed in this form!

Key example of *simulation-based inference*

Asymptotically, same structure as **Lagrangian mechanics!**

Action:  $L = \int dx \mathcal{L}(x)$

Lagrangian:  $\mathcal{L}(x) = -p(x) \log f(x) + q(x)(f(x) - 1)$

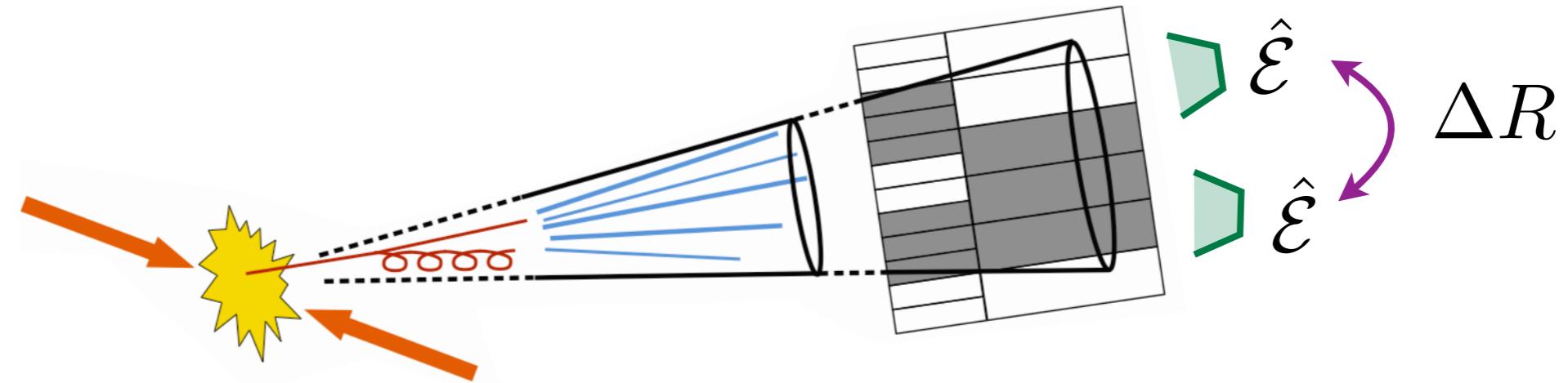
Euler-Lagrange:  $\frac{\partial \mathcal{L}}{\partial f} = 0$

Solution:  $f(x) = \frac{p(x)}{q(x)}$

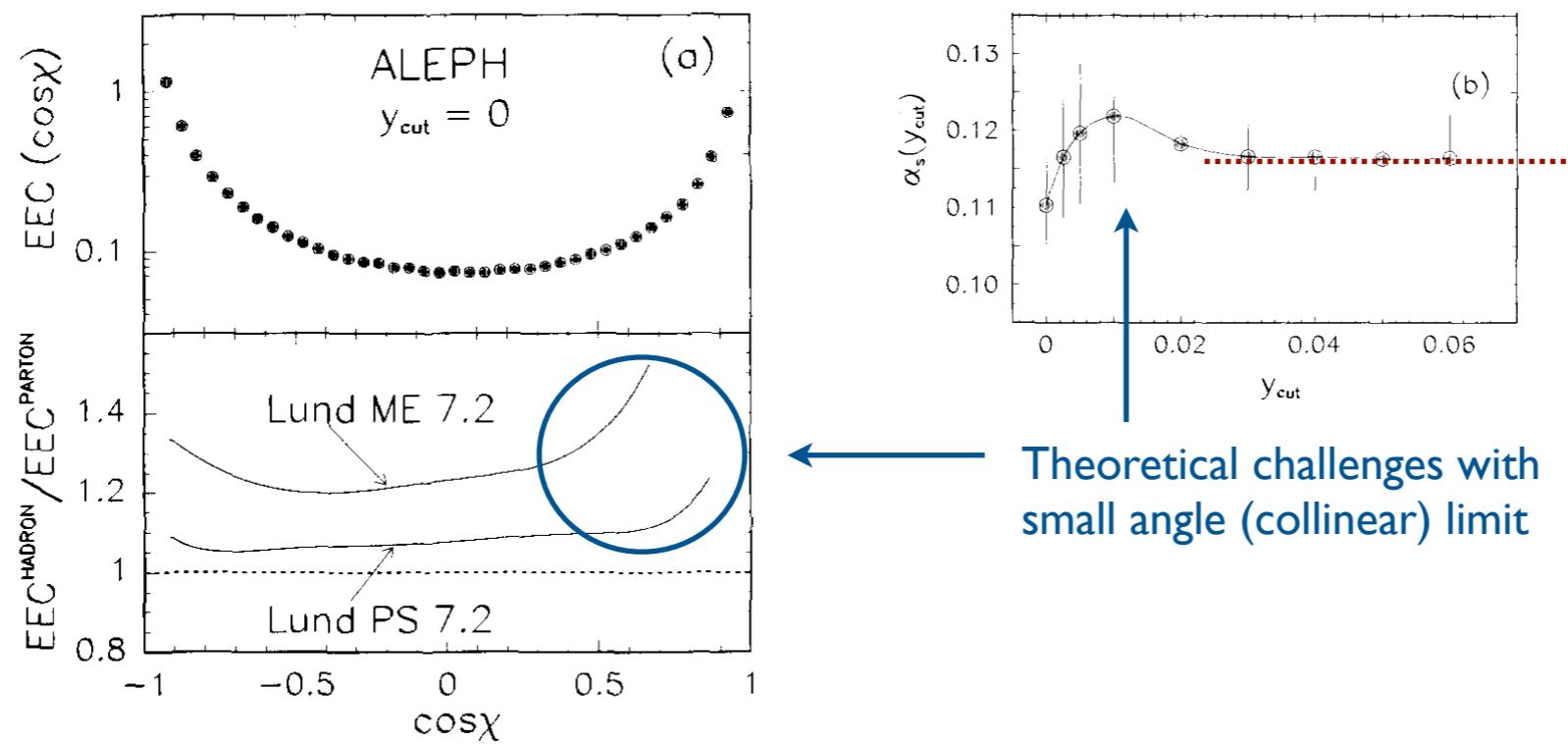
Requires shift in theoretical focus from solving problems to *specifying problems*

[see e.g. D'Agnolo, Wulzer, [PRD 2019](#); simulation-based inference in Cranmer, Brehmer, Louppe, [PNAS 2020](#); relation to f-divergences in Nguyen, Wainwright, Jordan, [AoS 2009](#)]

# Energy-Energy Correlators

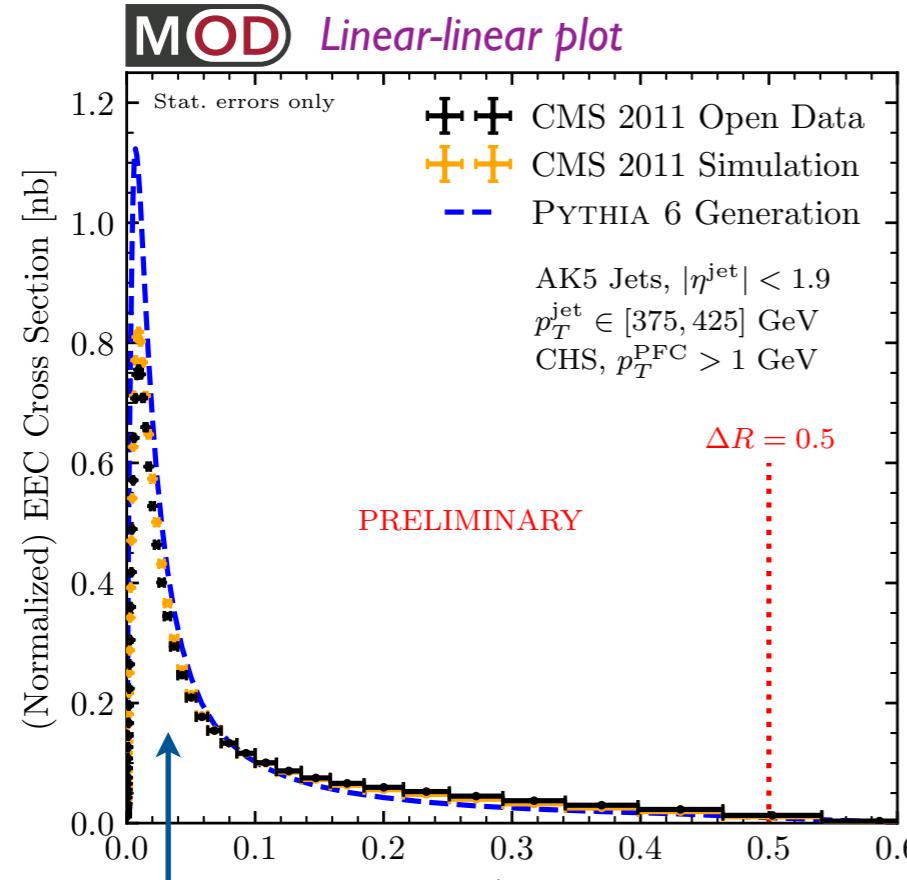


A long history in probing collinear dynamics of QCD



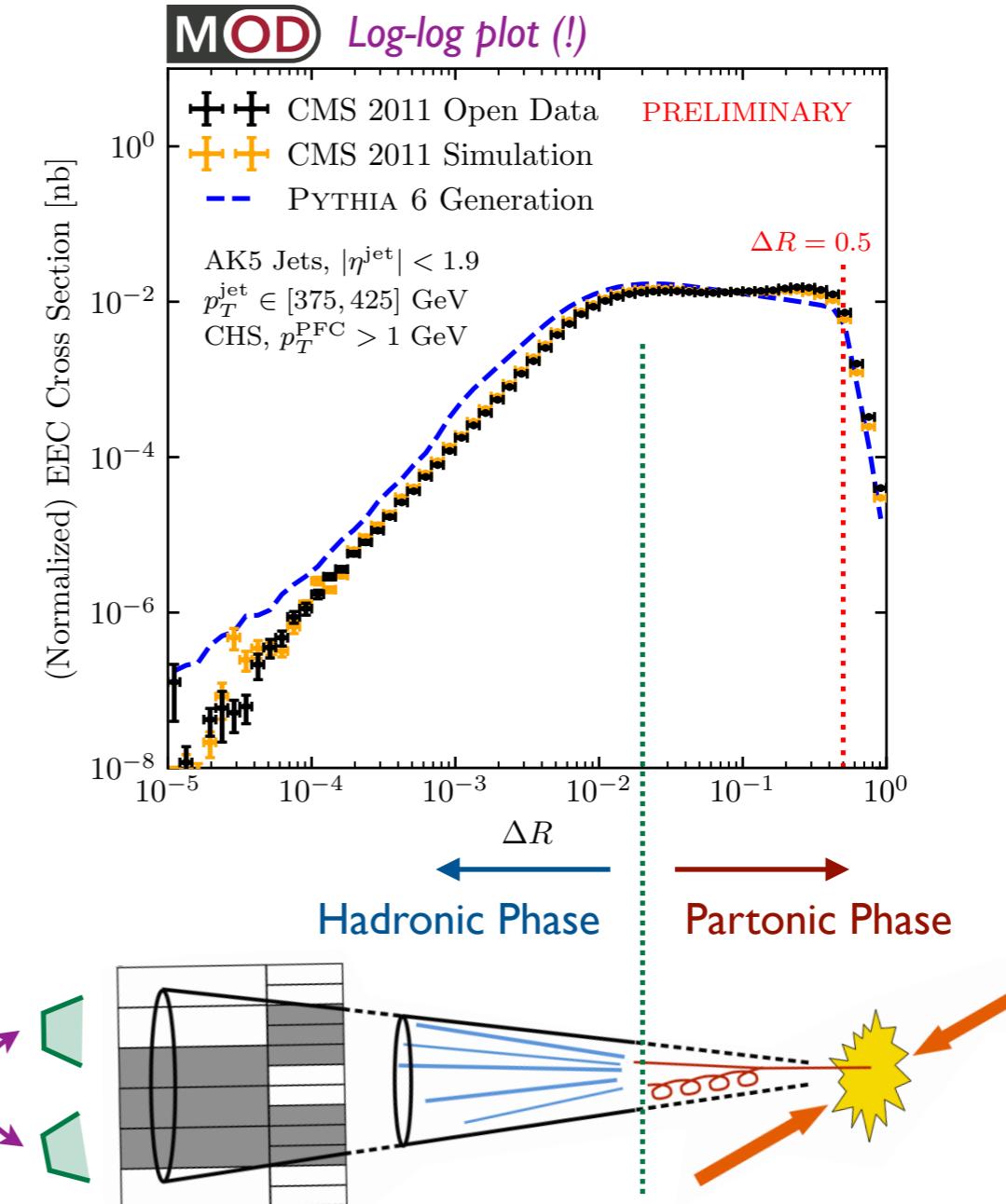
[Basham, Brown, Ellis, Love, [PRL 1978](#); ALEPH, [PLB 1991](#); see Chen, Moult, Zhang, Zhu, [PRD 2020](#)]

# QCD Phase Transition in Jets?



Are we learning something about small angle limit of QCD?

First Jet EEC Plot from the LHC (!)



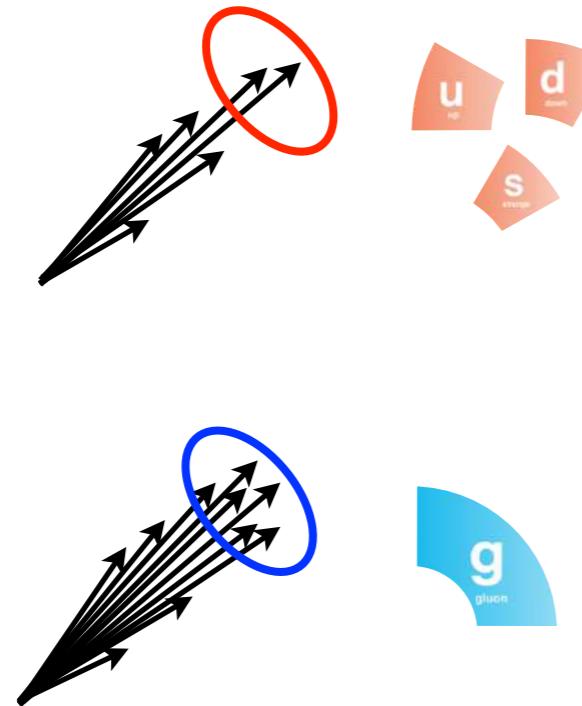
# From Curmudgeon...

*Jet classification via image recognition*

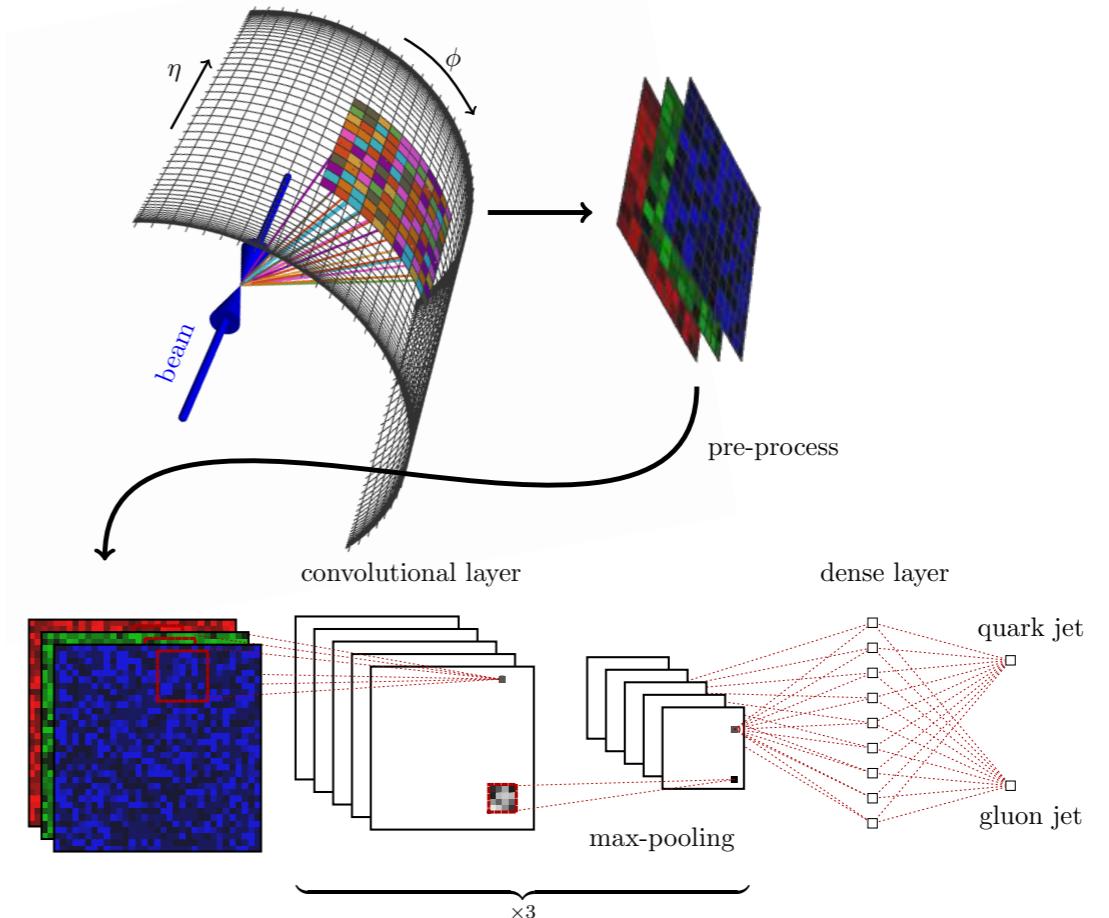
Quark

VS.

Gluon



Multi-channel convolutional neural networks



[e.g. Komiske, Metodiev, Schwartz, [JHEP 2017](#);  
cf. Gras, Höche, Kar, Larkoski, Lönnblad, Plätzer, Siódak, Skands, Soyez, [JHEP 2017](#)]



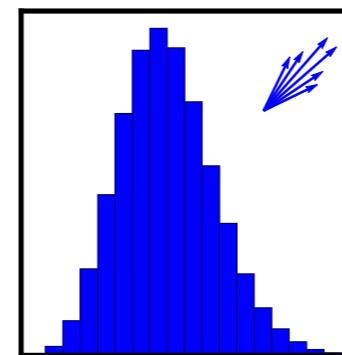
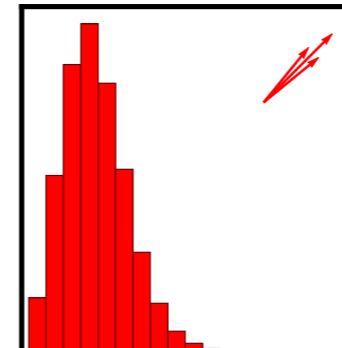
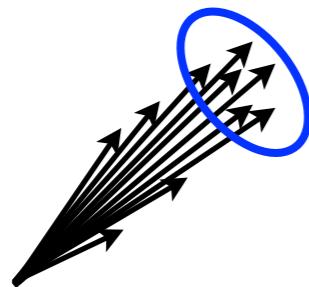
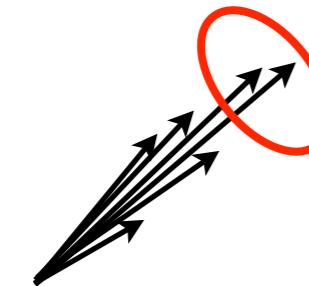
# ...to Evangelist

*Jet flavor definitions via natural language processing*

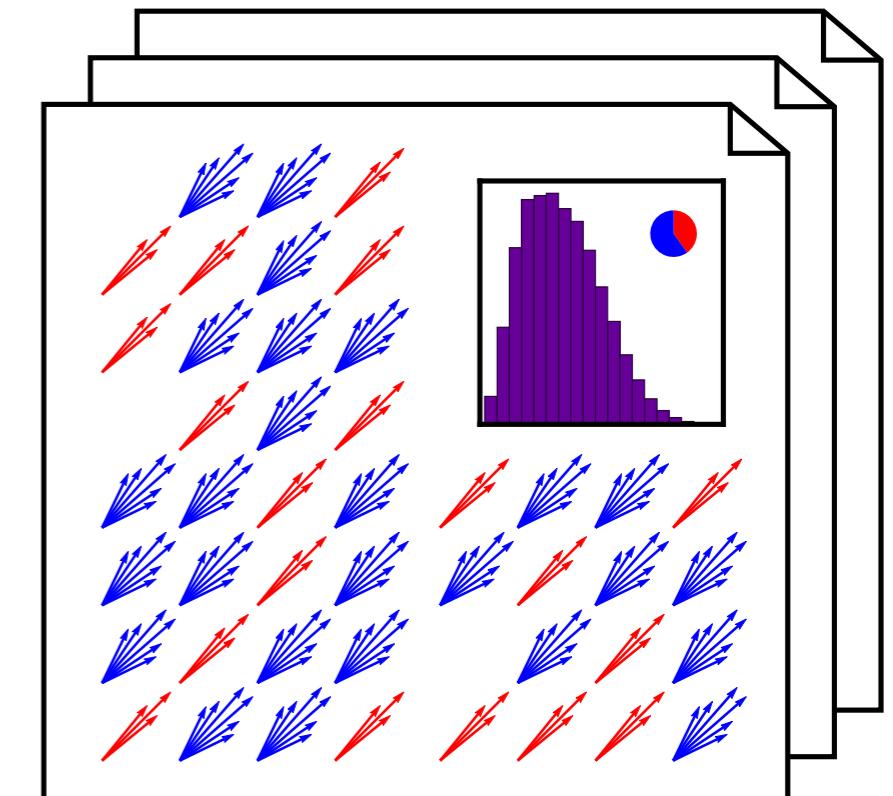
Quark

vs.

Gluon



Topic Modeling / Blind Source Separation

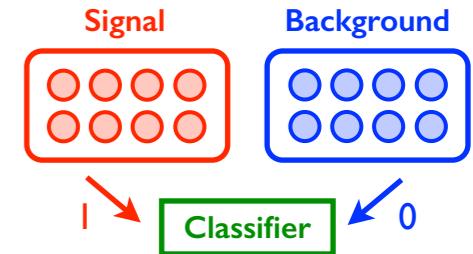


[Komiske, Metodiev, JDT, [JHEP 2018](#); using Metodiev, Nachman, JDT, [JHEP 2017](#); Metodiev, JDT, [PRL 2018](#); Komiske, Metodiev, JDT, [JHEP 2019](#)]



# E.g. Quark/Gluon Classification

“Hello, World!” of Jet Physics



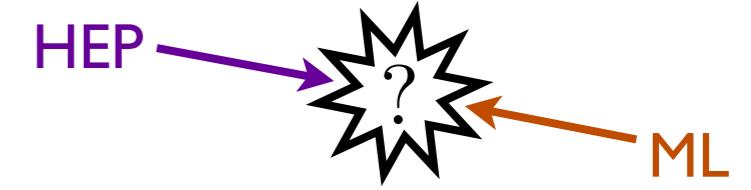
Find  $h\left(\begin{array}{c} \nearrow \\ \nearrow \\ \nearrow \\ \nearrow \end{array}\right)$  such that

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

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

[see e.g. Gras, Höche, Kar, Larkoski, Lönnblad, Plätzer, Siódmok, Skands, Soyez, JDT, [JHEP 2017](#); Komiske, Metodiev, Schwartz, [JHEP 2017](#); Komiske, Metodiev, JDT, [JHEP 2018](#)]

# E.g. Search for Supersymmetry

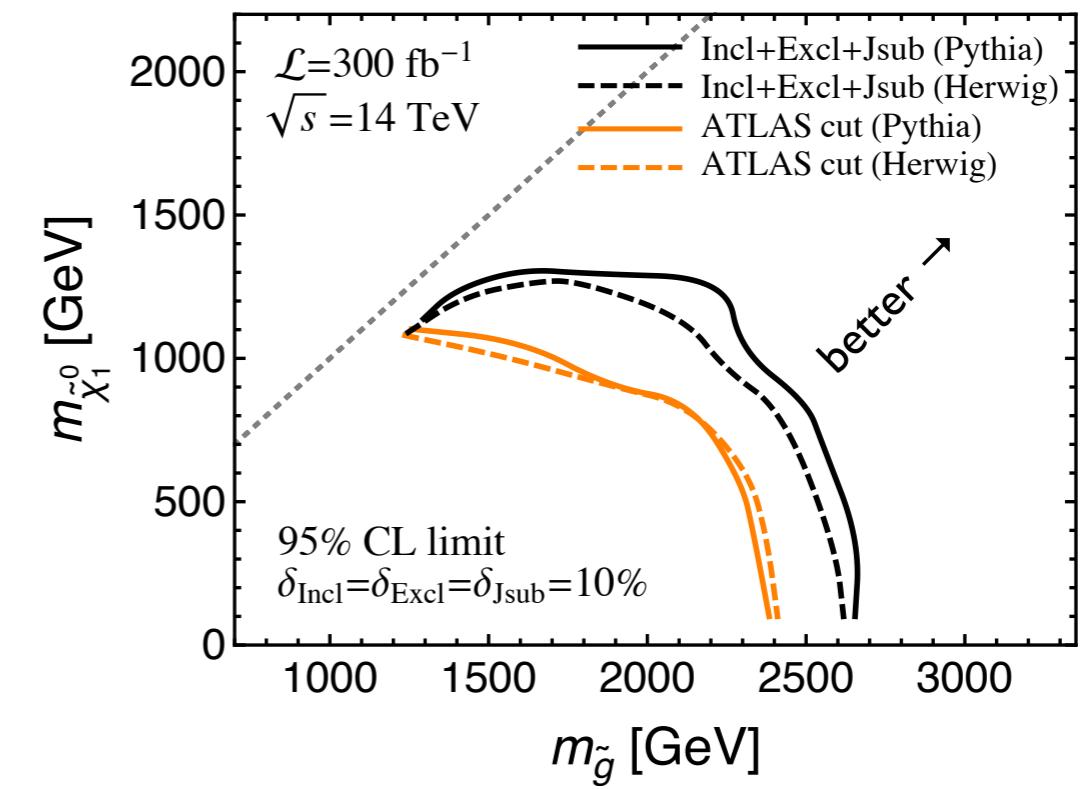
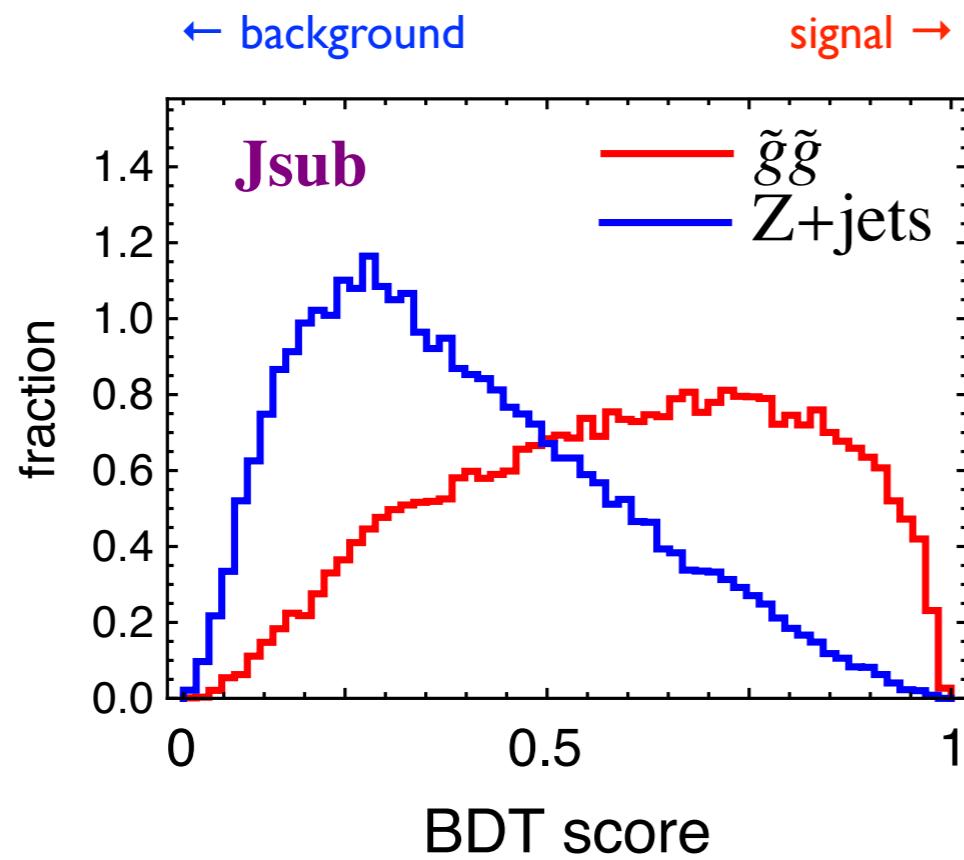
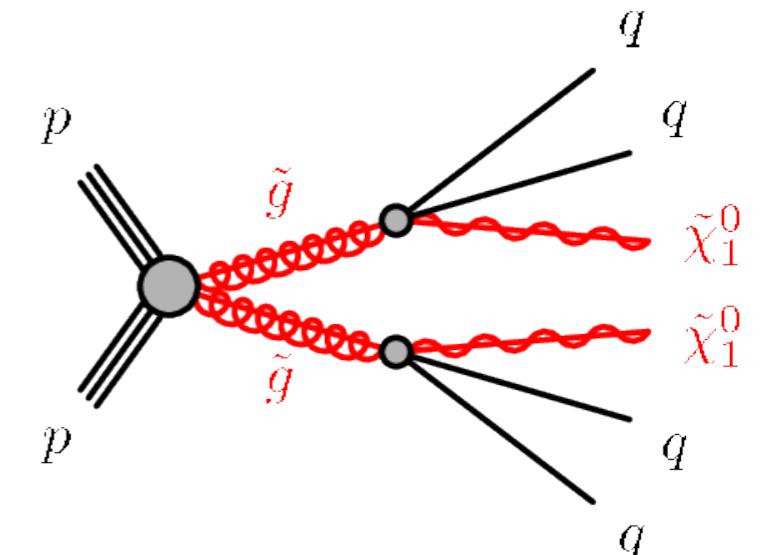


**Classifier:** Boosted decision tree (for each of 4 jets)

**Inputs:** Jet mass, width, track multiplicity

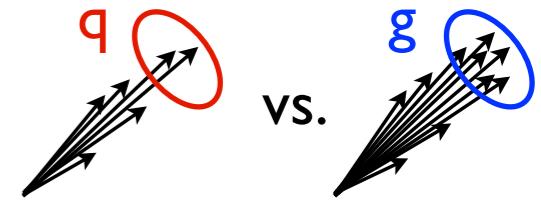
**Signal:** Quark enriched

**Background:** Gluon enriched

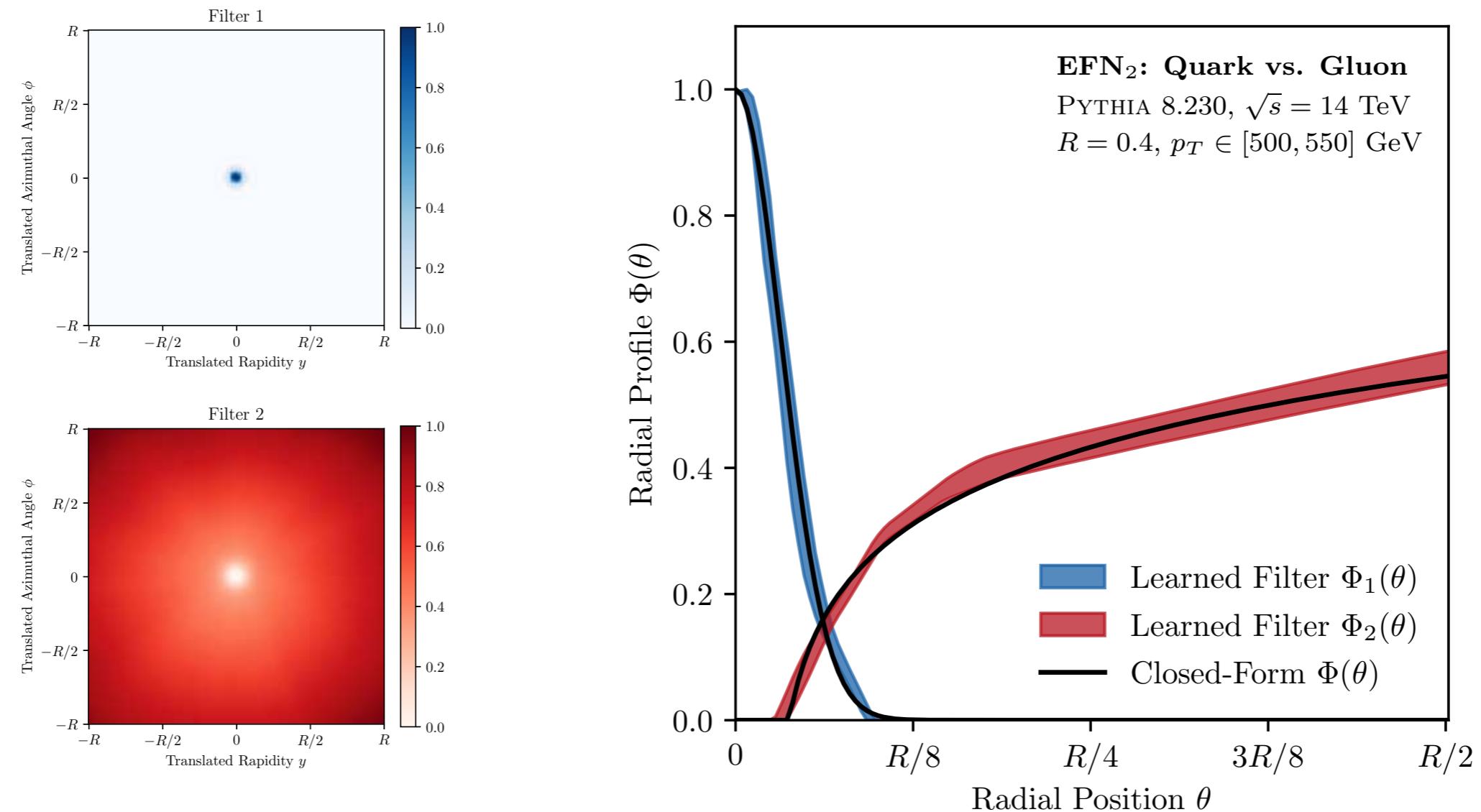


[Bhattacherjee, Mukhopadhyay, Nojiri, Sakakie, Webber, [JHEP 2017](#)]

# 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, JHEP 2019;  
cf. Larkoski, JDT, Waalewijn, JHEP 2014; using Berger, Kucs, Sterman, PRD 2003; Ellis, Vermilion, Walsh, Hornig, Lee, JHEP 2010]

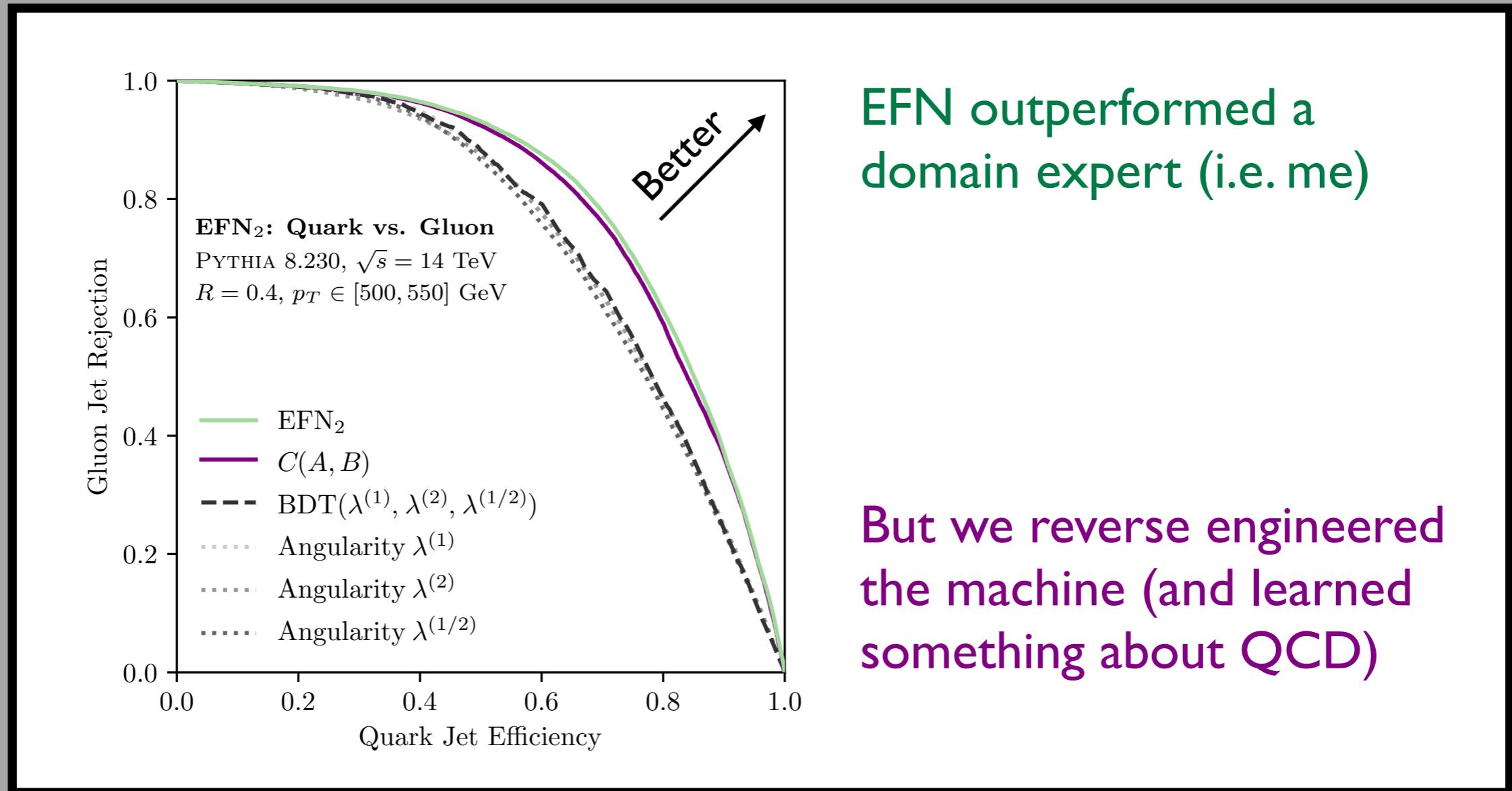
# Learning from the Machine



For  $\ell = 2$  EFN, radial moments:

$$\sum_{i \in \text{jet}} z_i f(\theta_i)$$

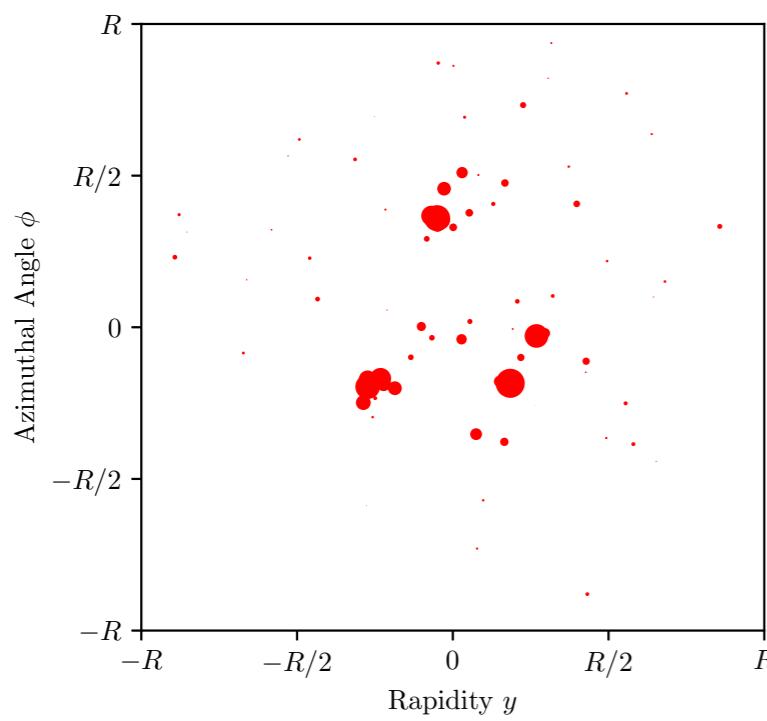
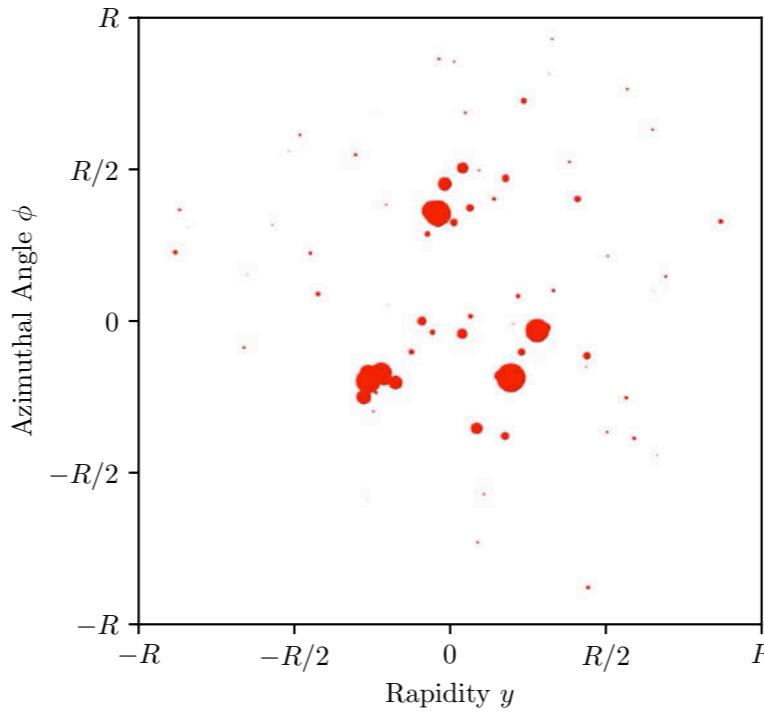
cf. Angularities:  
 $f(\theta) = \theta^\beta$



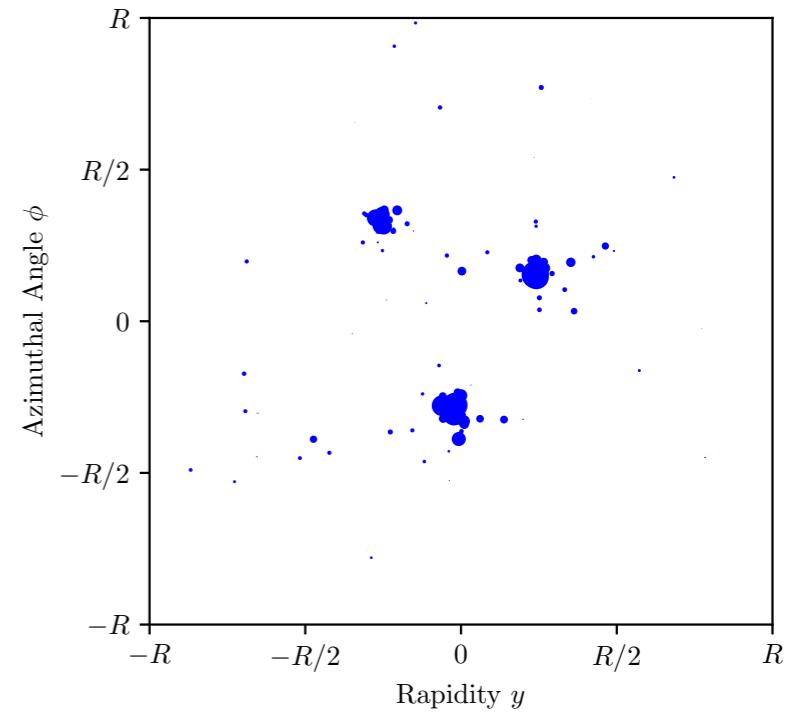
[Komiske, Metodiev, JDT, [JHEP 2019](#);  
cf. Larkoski, JDT, Waalewijn, [JHEP 2014](#); using Berger, Kucs, Sterman, [PRD 2003](#); Ellis, Vermilion, Walsh, Hornig, Lee, [JHEP 2010](#)]

# Similarity of Two Energy Flows?

$$\mathcal{E}(\hat{n}) = \sum_i E_i \delta(\hat{n} - \hat{n}_i)$$



Optimal Transport:  
*Earth Mover's Distance*  
a.k.a. *1-Wasserstein metric*



[Komiske, Metodiev, JDT, PRL 2019; code at Komiske, Metodiev, JDT, [energyflow.network](#)]

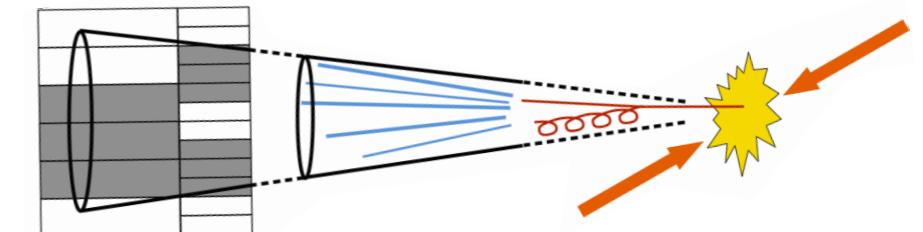
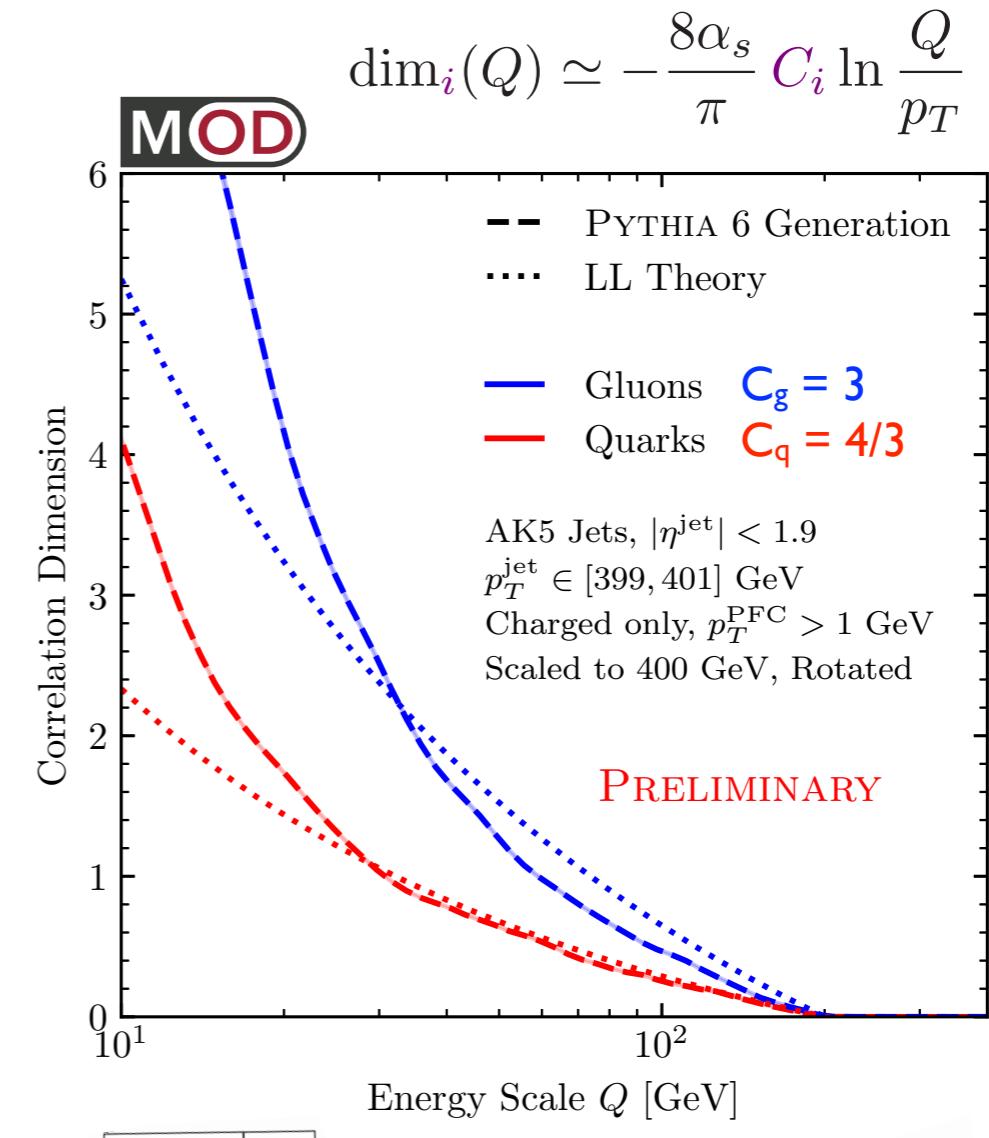
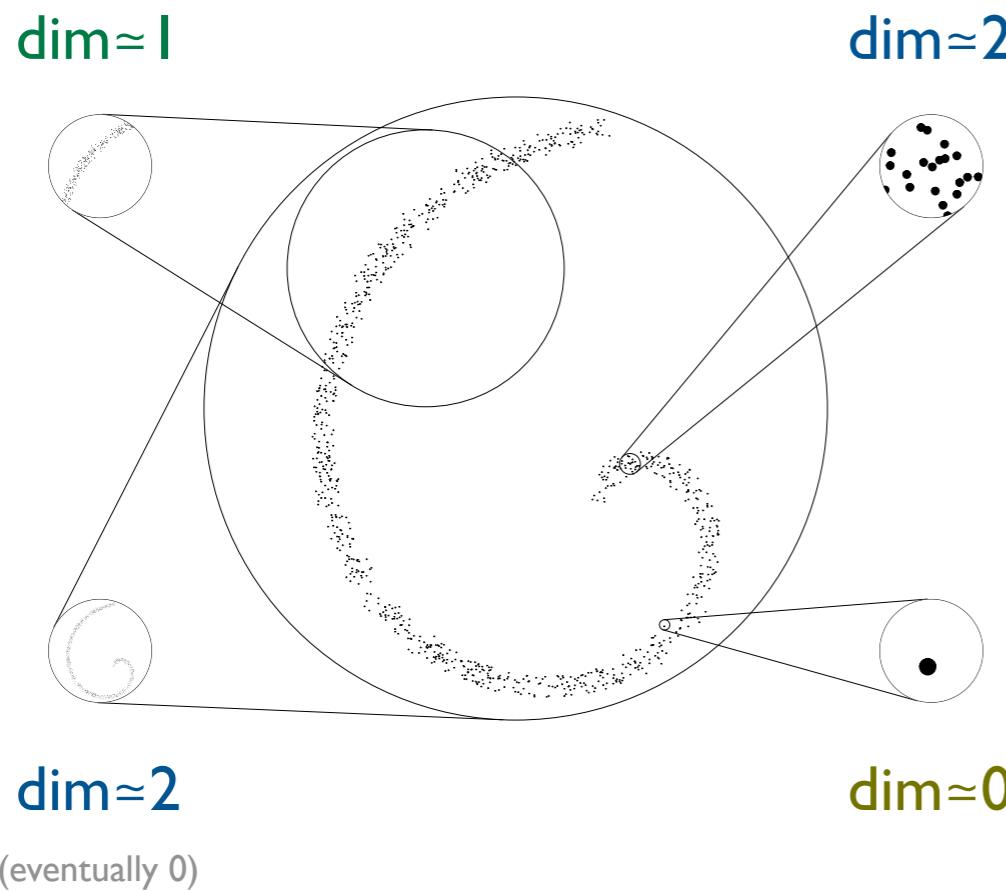
# Dimensionality of Space of Jets



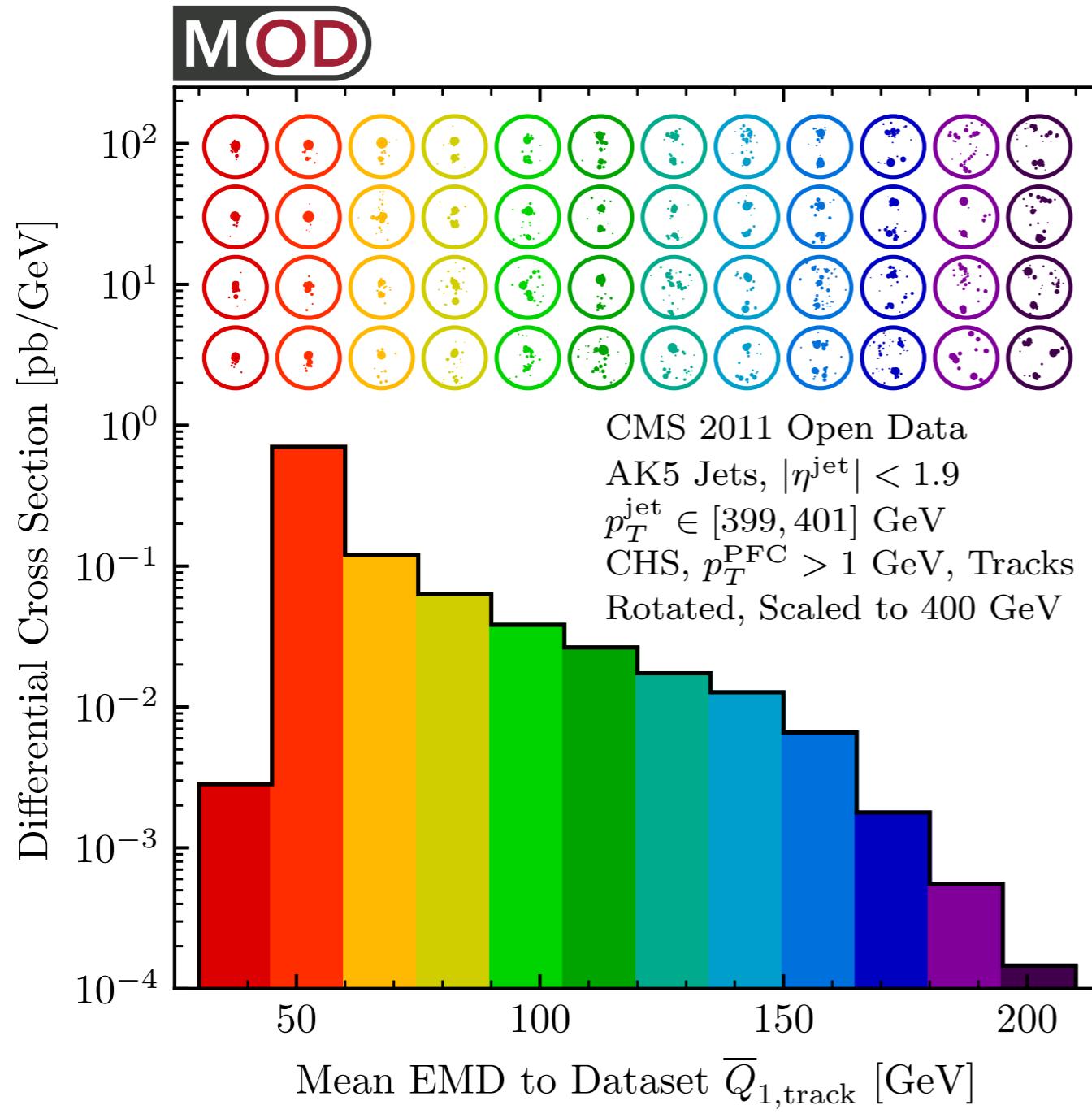
$$N_{\text{neighbors}}(r) \sim r^{\dim}$$

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

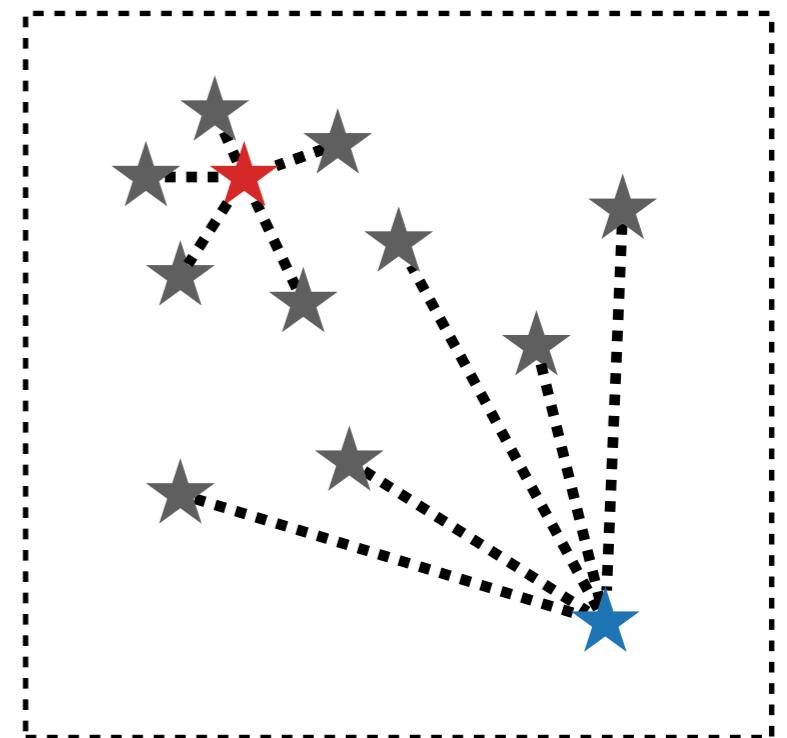
[Grassberger, Procaccia, [PRL 1983](#); Kégl, [NIPS 2002](#)]



# Least Representative Jets



New Physics?  
Or tails of QCD?



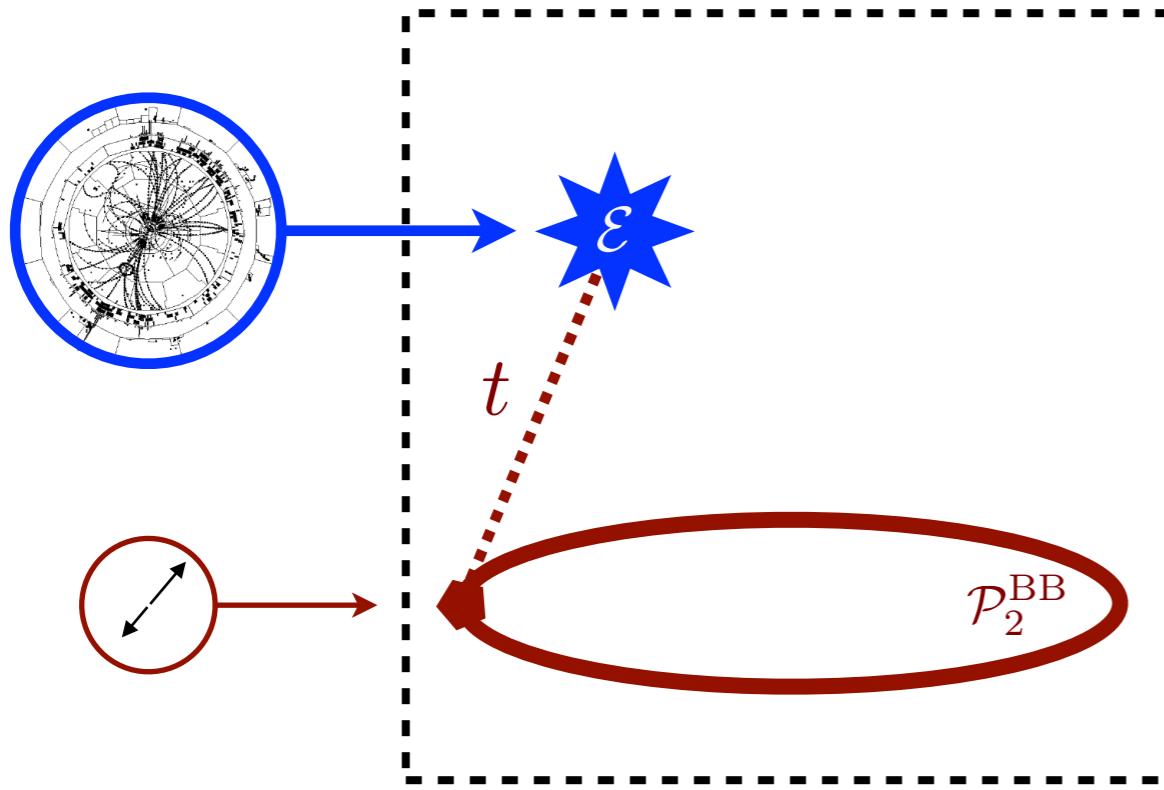
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]



# Back to the Future with Thrust

How dijet-like is an event?

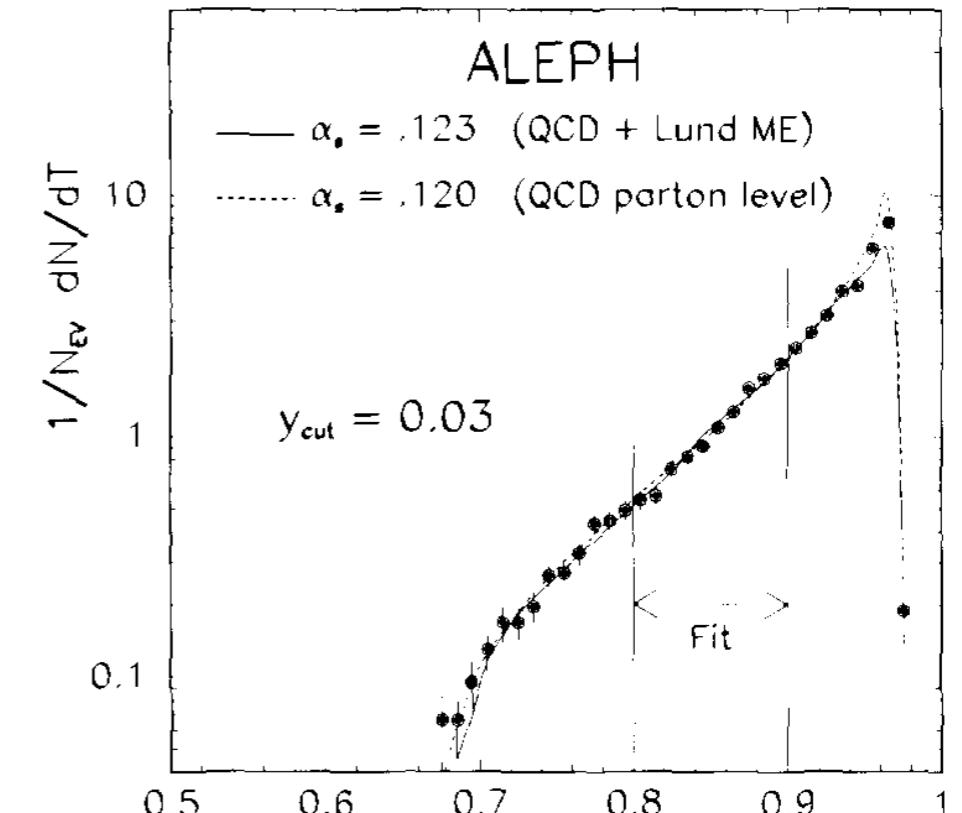
$$t(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_2^{\text{BB}}} \text{EMD}_2(\mathcal{E}, \mathcal{E}')$$



All Back-to-Back Two Particle Configurations

$$\mathcal{P}_2^{\text{BB}} = \left\{ \begin{array}{c} \text{red circles with internal arrows} \\ \dots \end{array} \right\}$$

(using  $\beta=2$  EMD variant)



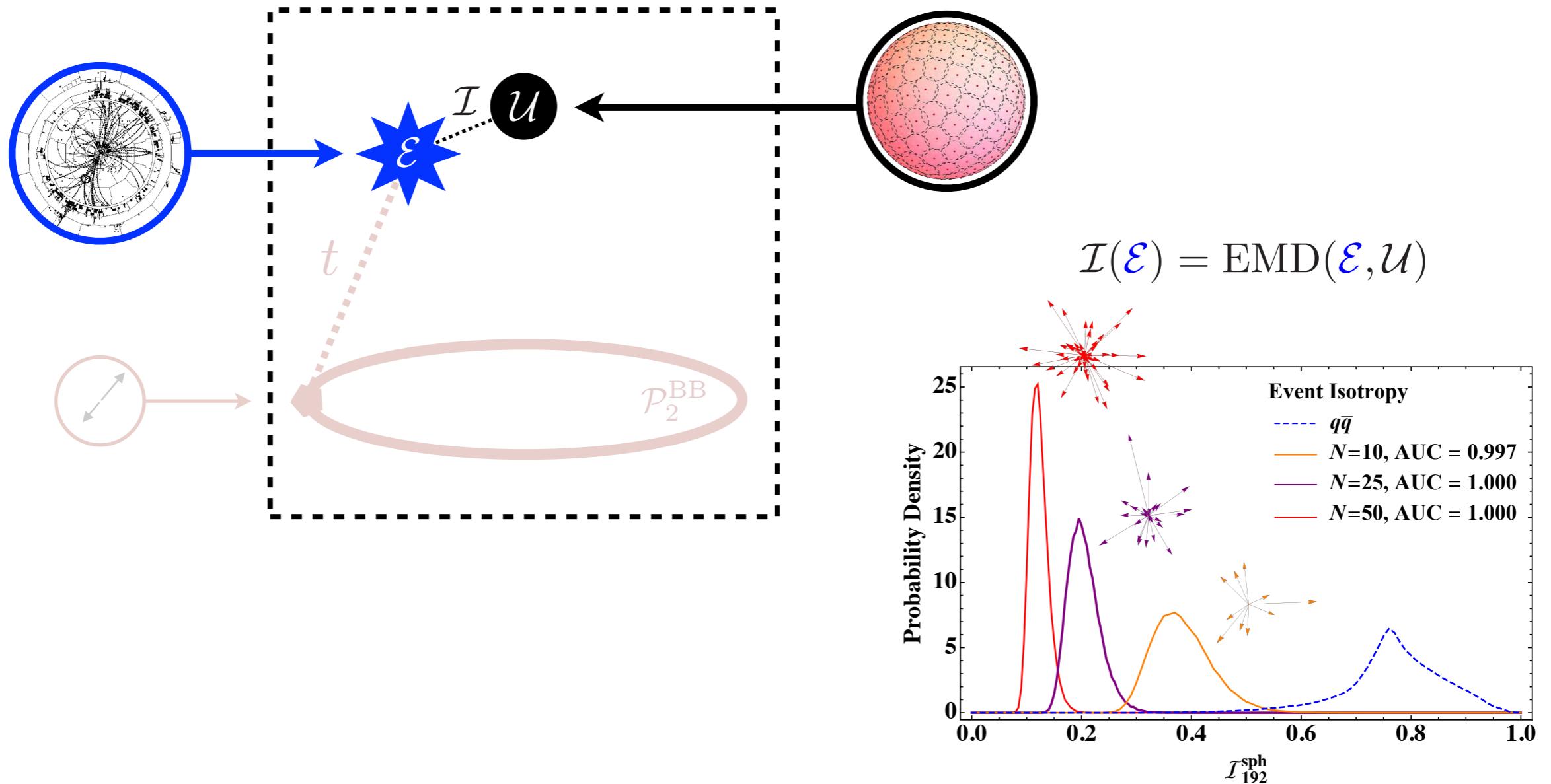
$$1 - \frac{t}{2E_{\text{CM}}}$$

(flipped, linear version of  
ALEPH thrust plot from before)

[Komiske, Metodiev, JDT, JHEP 2020]  
[Brandt, Peyrou, Sosnowski, Wroblewski, PL 1964; Farhi, PRL 1977; ALEPH, PLB 1991]

# Event Isotropy from Collider Geometry

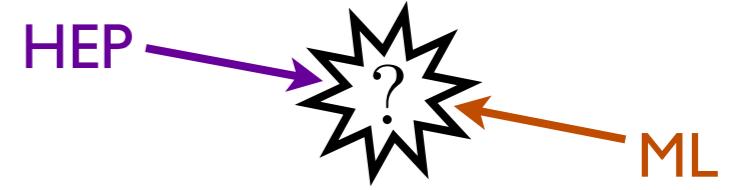
How uniform is an event?



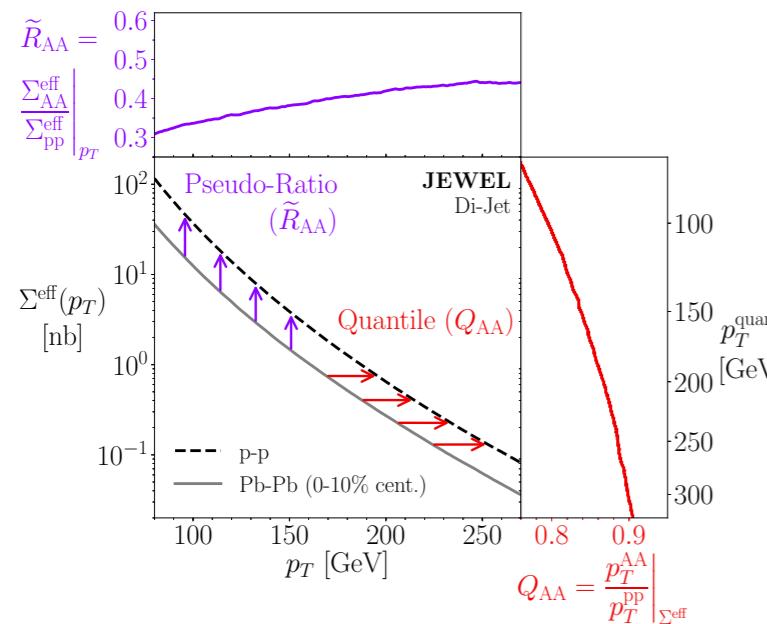
[Cesarotti, JDT, [JHEP 2020](#);  
see also Cesarotti, Reece, Strassler, [arXiv 2020](#)]



# More Collisions

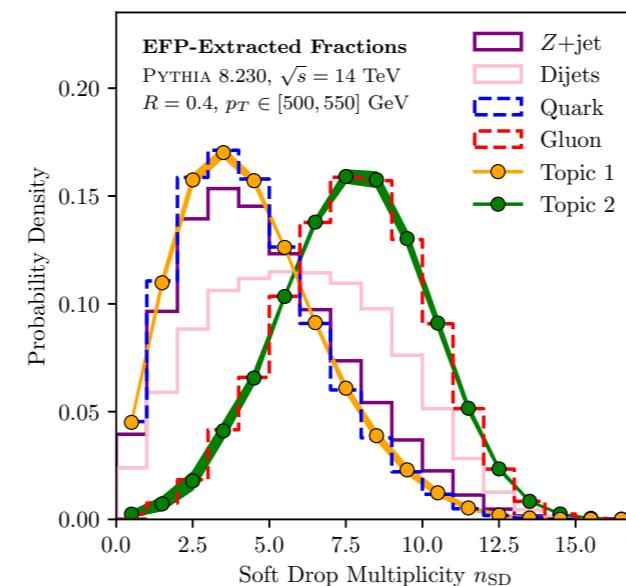


## Jet Quenching via Optimal Transport



[Brewer, Milhano, JDT, PRL 2019]

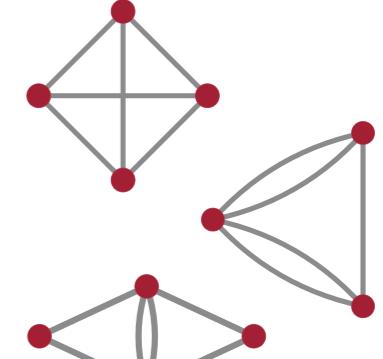
## Quark/Gluon Definitions via Blind Source Separation



[Komiske, Metodiev, JDT, JHEP 2018;  
Brewer, JDT, Turner; arXiv 2020]

## Kinematic Decomposition via Graph Theory

Edges $d$	Leafless Multigraphs		
	Connected	All	A307316
1	0	0	0
2	1	1	1
3	2	2	2
4	4	5	5
5	9	11	11
6	26	34	34
7	68	87	87
8	217	279	279
9	718	897	897
10	2 553	3 129	3 129
11	9 574	11 458	11 458
12	38 005	44 576	44 576
13	157 306	181 071	181 071
14	679 682	770 237	770 237
15	3 047 699	3 407 332	3 407 332
16	14 150 278	15 641 159	15 641 159



[Komiske, Metodiev, JDT, JHEP 2018, PRD 2020]