

Machine Learning for Fundamental Physics

Jesse Thaler



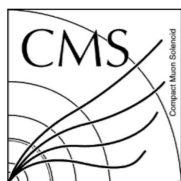
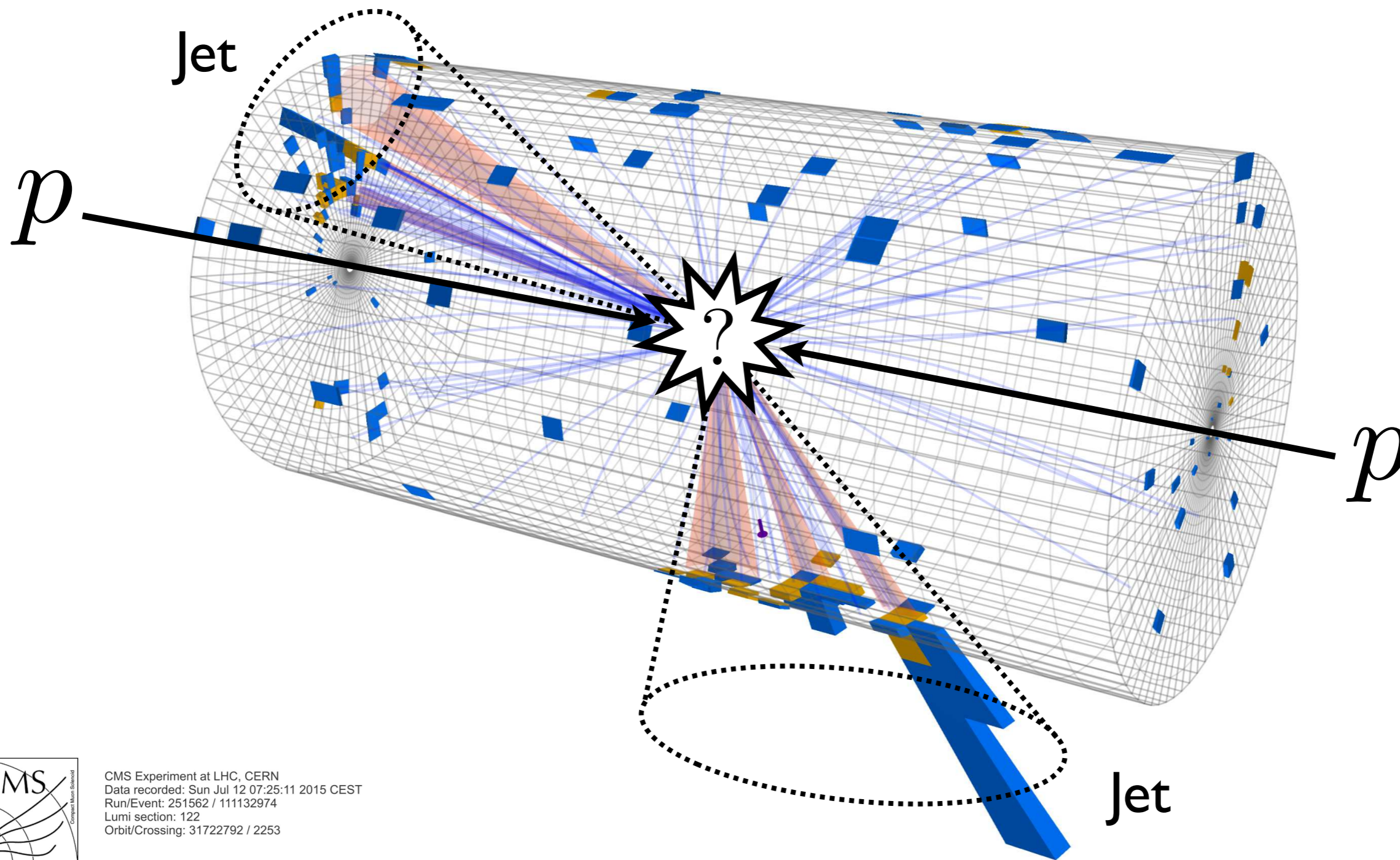
HKUST Jockey Club Institute for Advanced Study, HEP 2021 — January 21, 2021

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



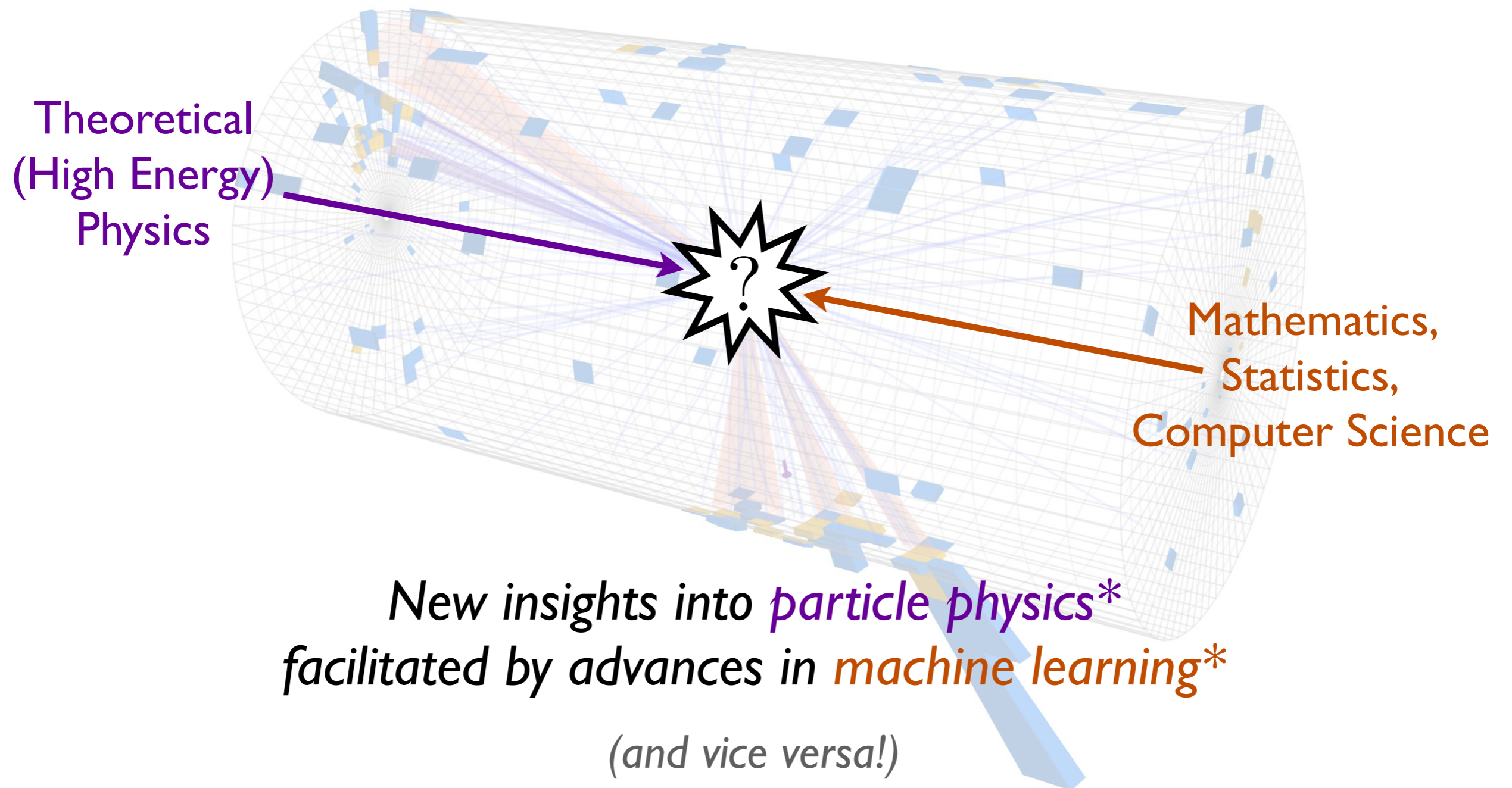
[<http://iaifi.org>, MIT News Announcement]



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

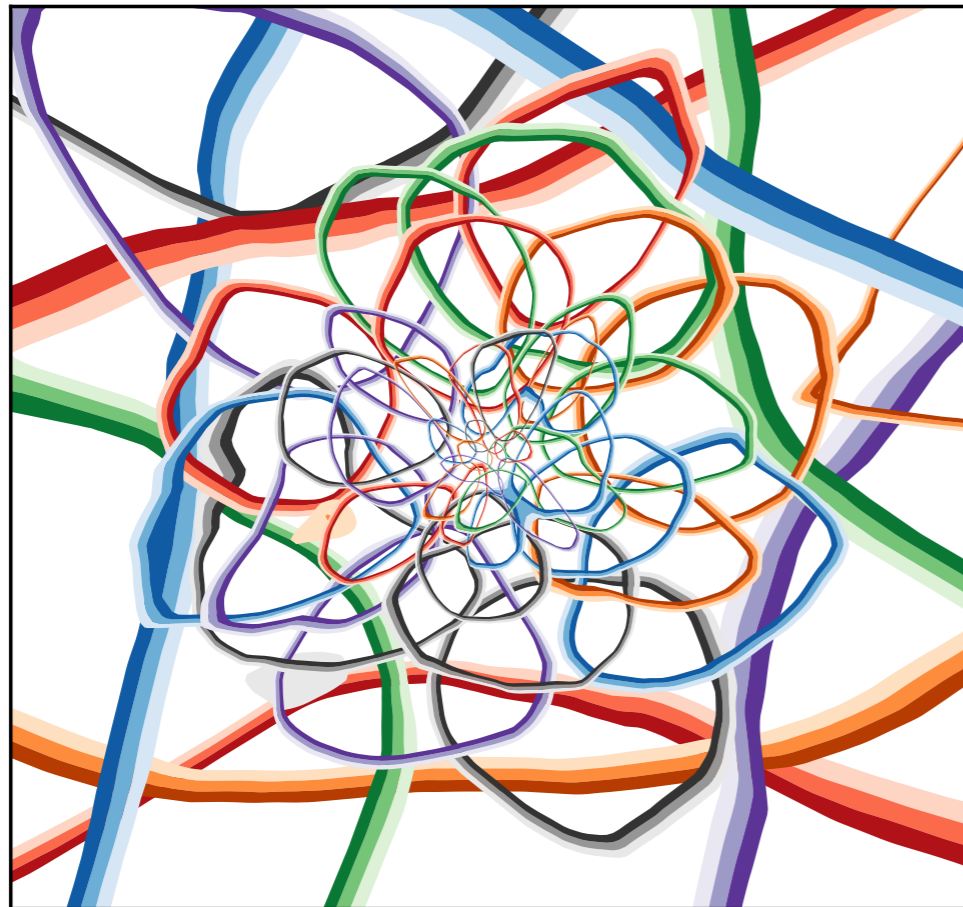
“Collision Course”

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



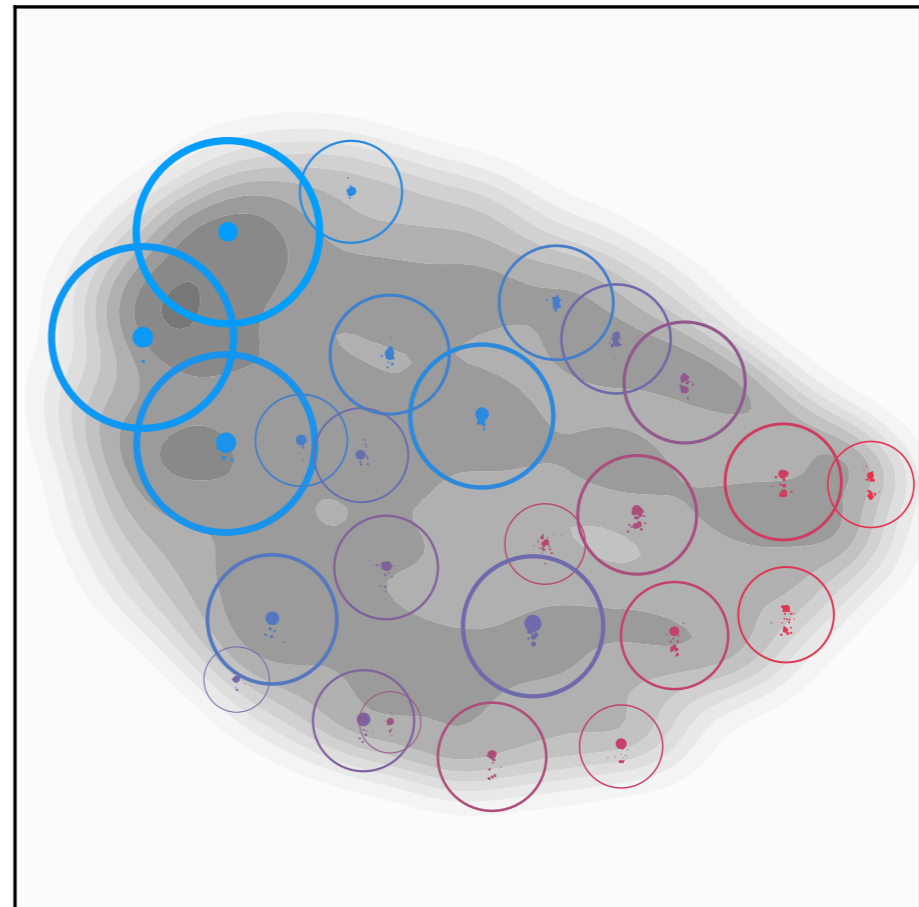
Two Anecdotes

Teaching a Machine to
“Think Like a Physicist”



[Komiske, Metodiev, JDT, [JHEP 2019](#)]

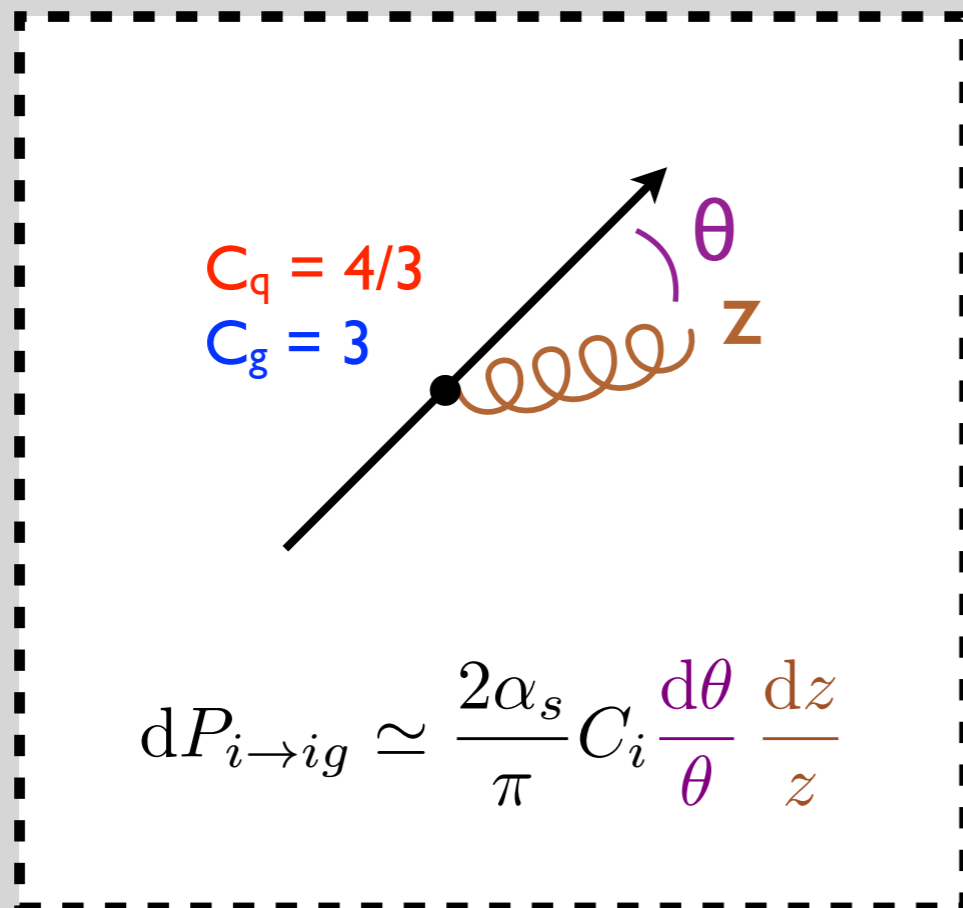
Letting Collider Data
Speak for Itself



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

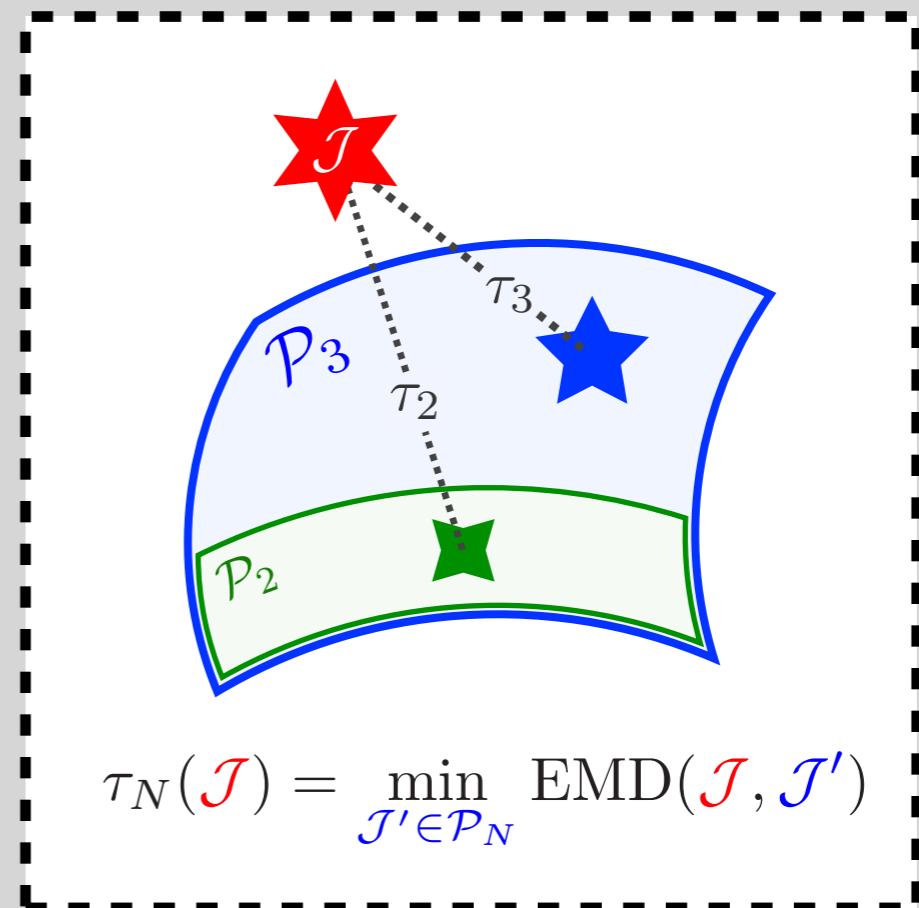
*Data analysis strategies motivated by the
symmetries and structures of particle physics*

Exploiting a Core Prediction of QCD



[Altarelli, Parisi, NPB 1977]

Nested Singularities of Gauge Theories



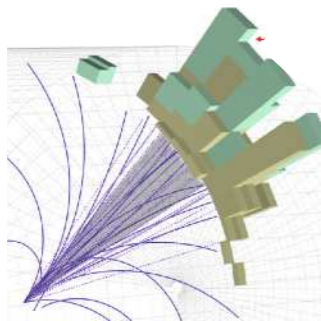
[Stewart, Tackmann, Waalewijn, PRL 2010;
 JDT, Van Tilburg, JHEP 2011, JHEP 2012;
 rephrased via Komiske, Metodiev, JDT, JHEP 2020]

New perspectives on key theoretical concepts

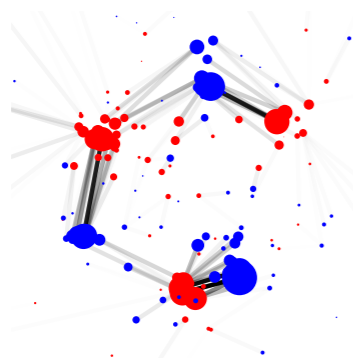
Outline



Rise of the Machines?



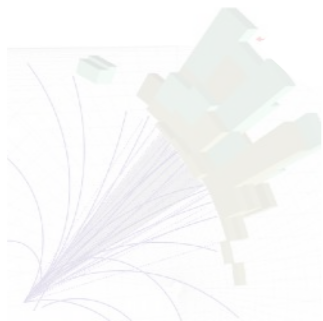
What is a Collider Event?



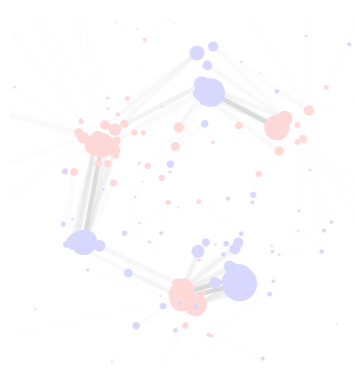
When are Collider Events Similar?



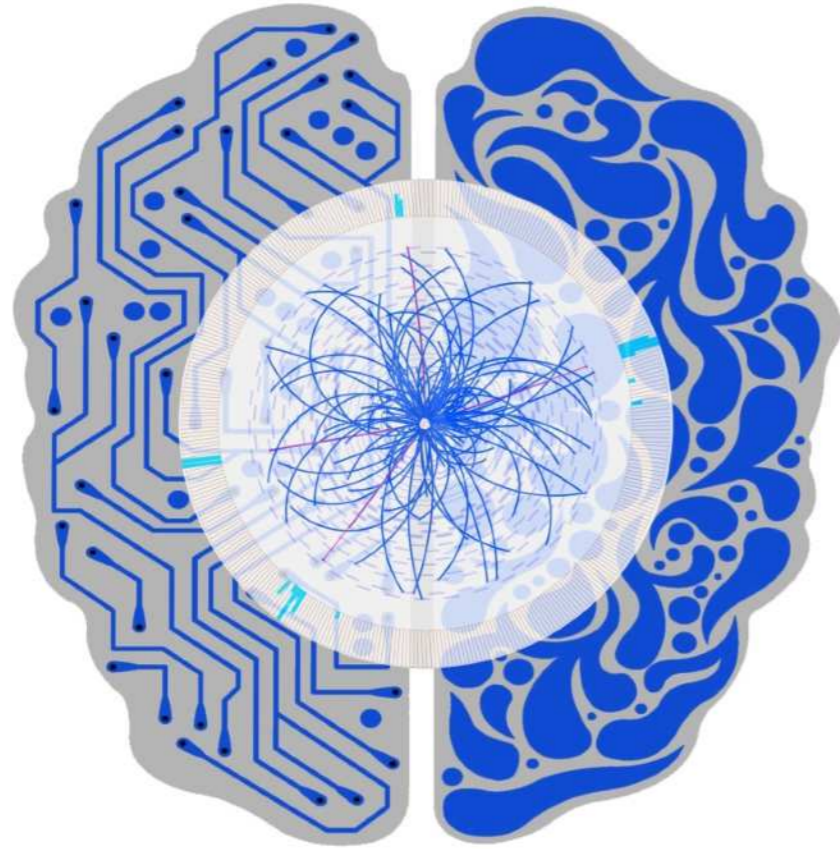
Rise of the Machines?



What is a Collider Event?



When are Collider Events Similar?



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

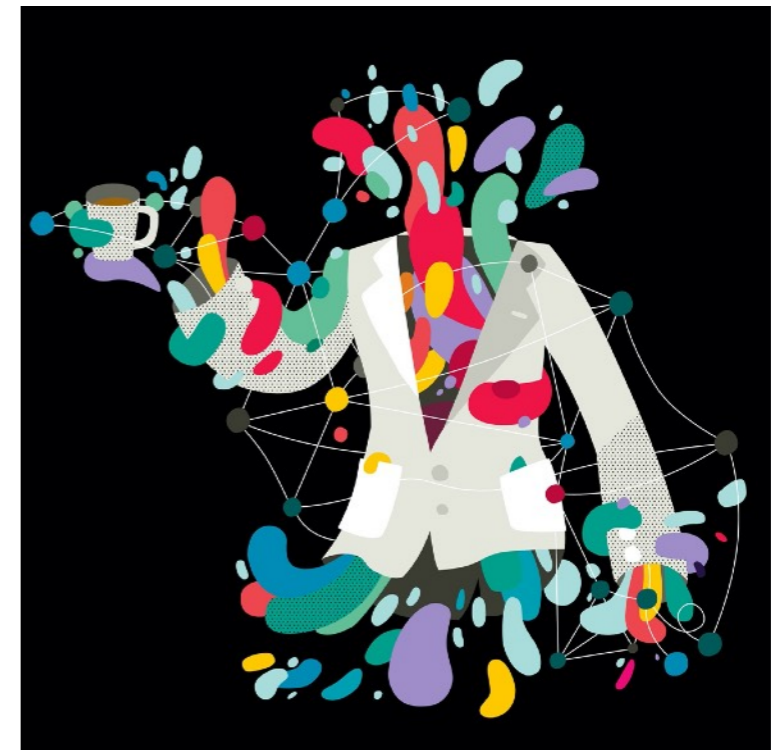
The New York Times



By **Dennis Overbye**

Nov. 23, 2020

Can a Computer Devise a Theory of Everything?



AI²: 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 section phase space amplitude observable

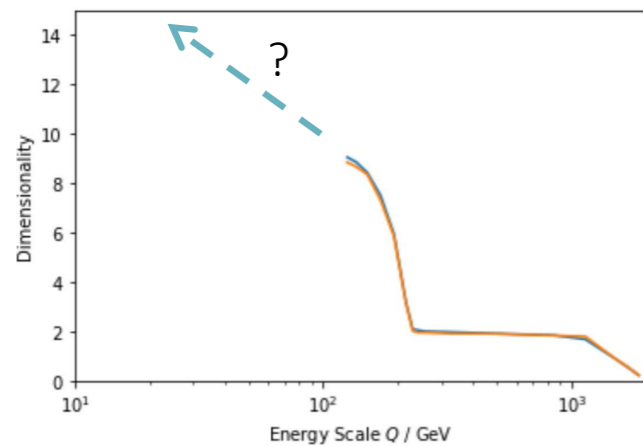
*Exciting progress on multiple fronts from
theoretical (and experimental) HEP communities!*

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]

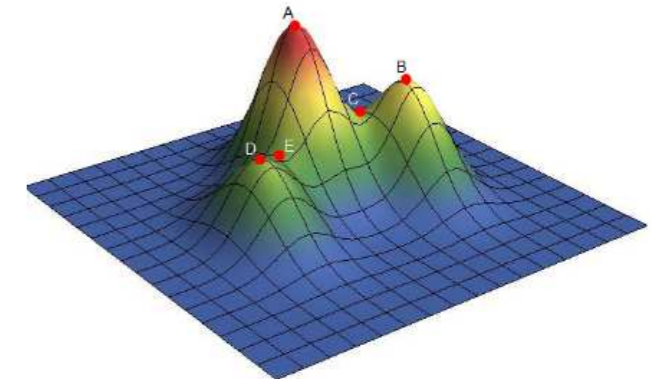
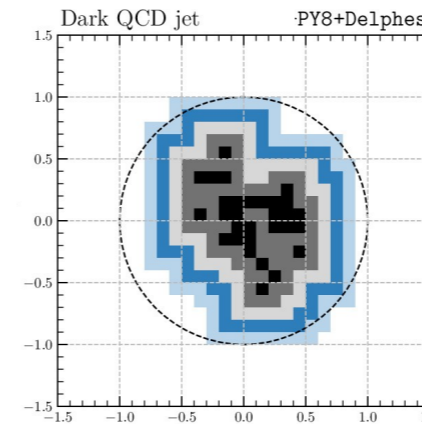
Mini-Workshop: Machine Learning and Open Data

Dimensionality via Autoencoding



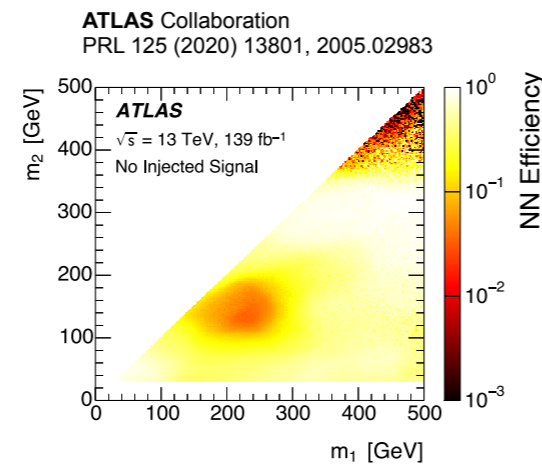
[Talk by [Jack Collins](#)]

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

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

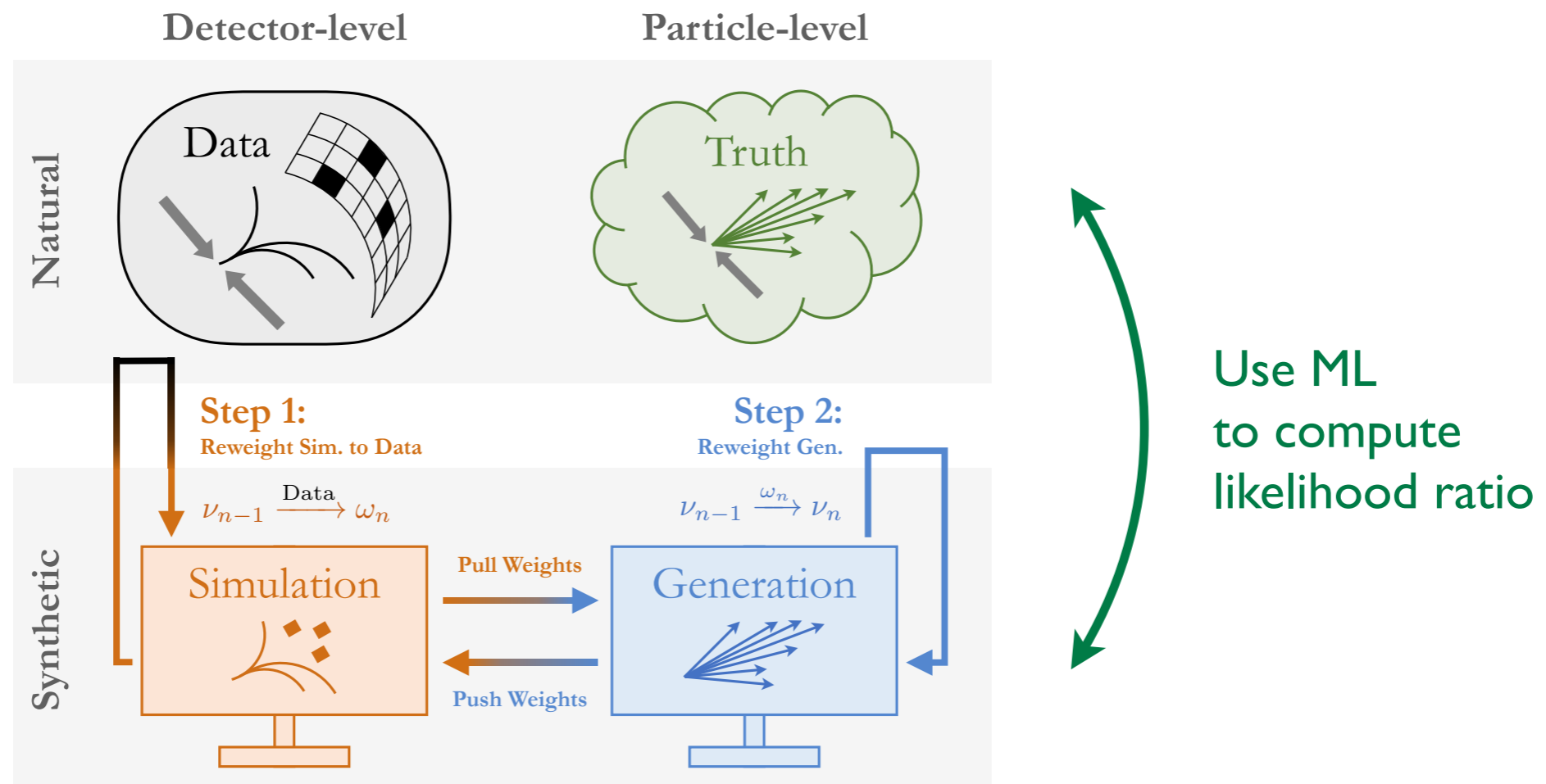
[Talk by [Haipeng An](#)]

Detector Unfolding

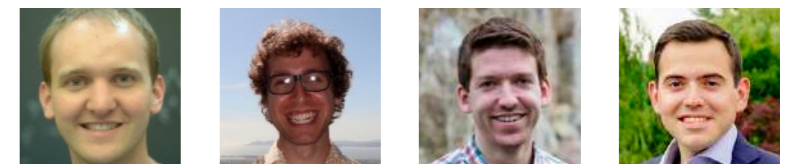
OmniFold



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

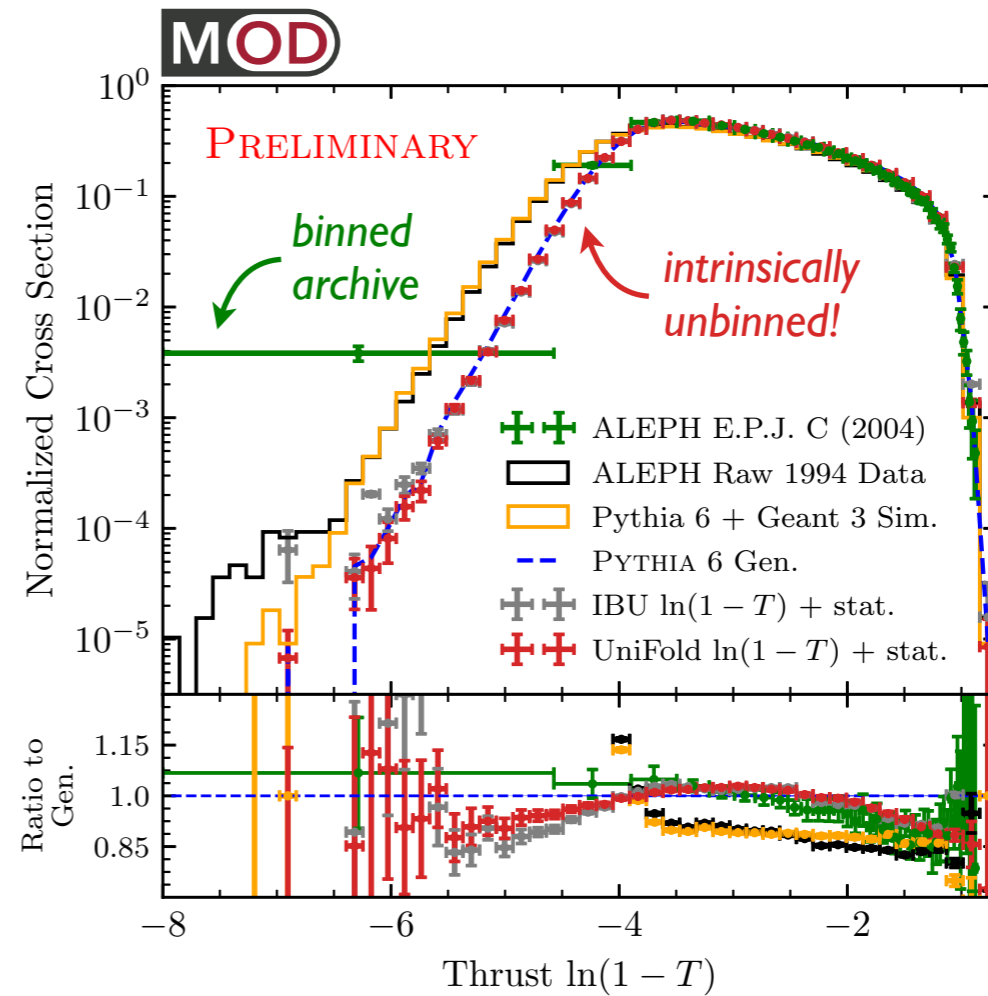
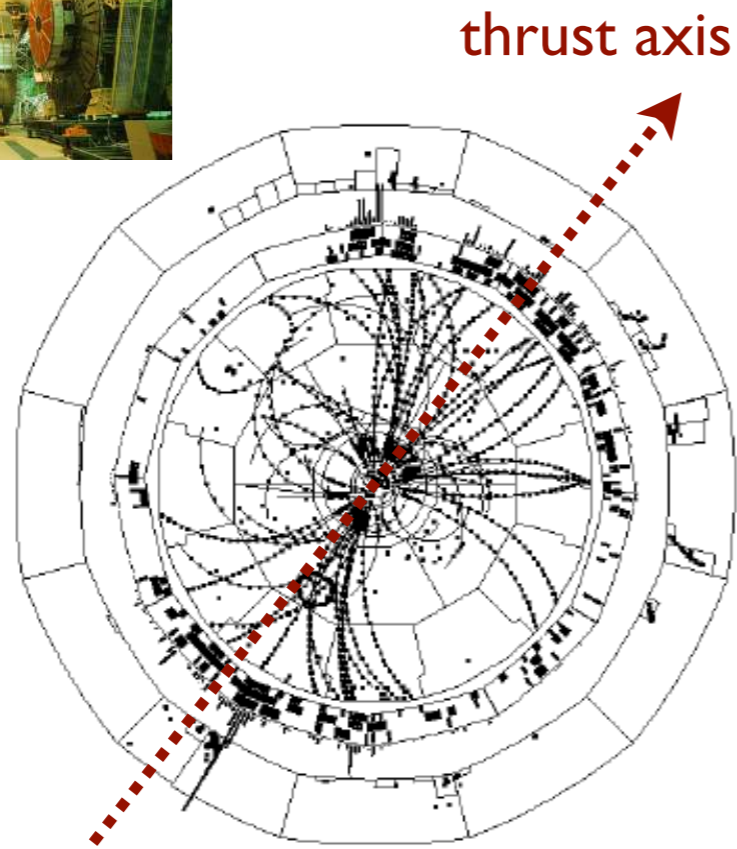


[Andreassen, Komiske, Metodiev, Nachman, JDT, [PRL 2020](#)]



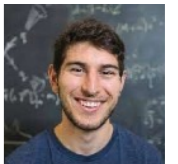
Detector Unfolding

Back to the Future with ALEPH Archival Data

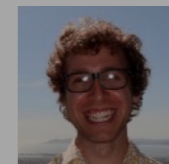


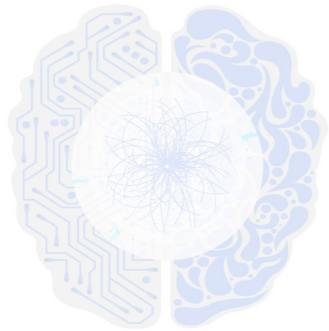
[talk by Badea, ICHEP 2020; cf. ALEPH, EPJ C 2004]

[see also Badea, Baty, Chang, Innocenti, Maggi, McGinn, Peters, Sheng, JDT, Lee, PRL 2019]

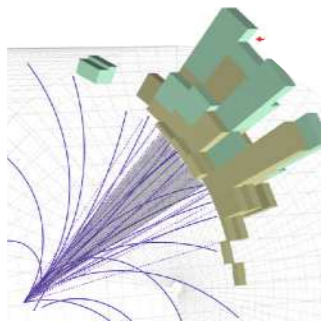


[Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020]

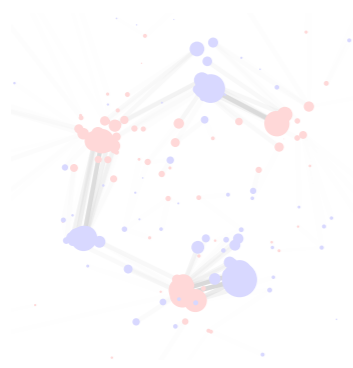




Rise of the Machines?



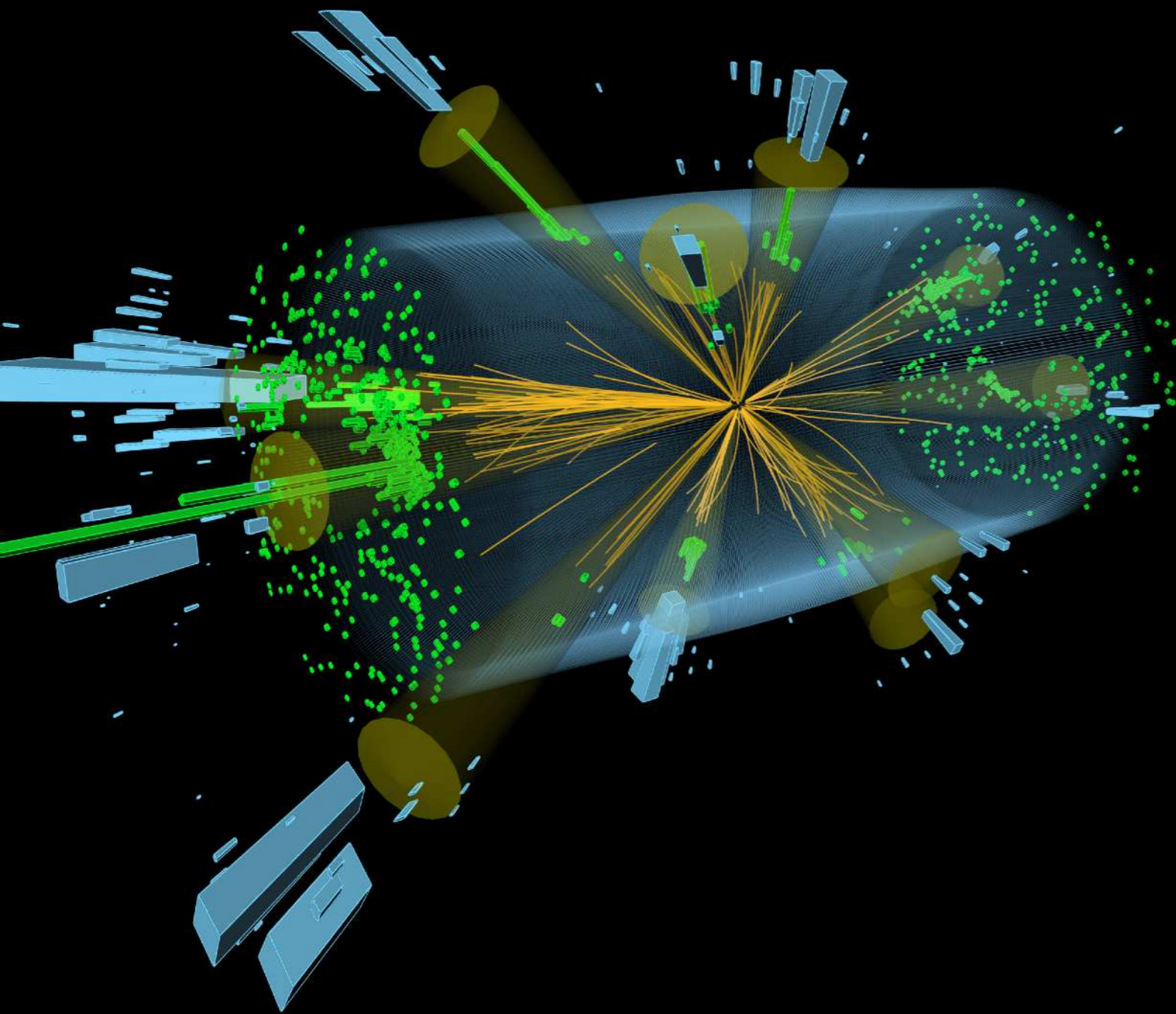
What is a Collider Event?



When are Collider Events Similar?

Collider Event

Collection of points in (momentum) space



T E H M

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

elementary

composite

Point Cloud

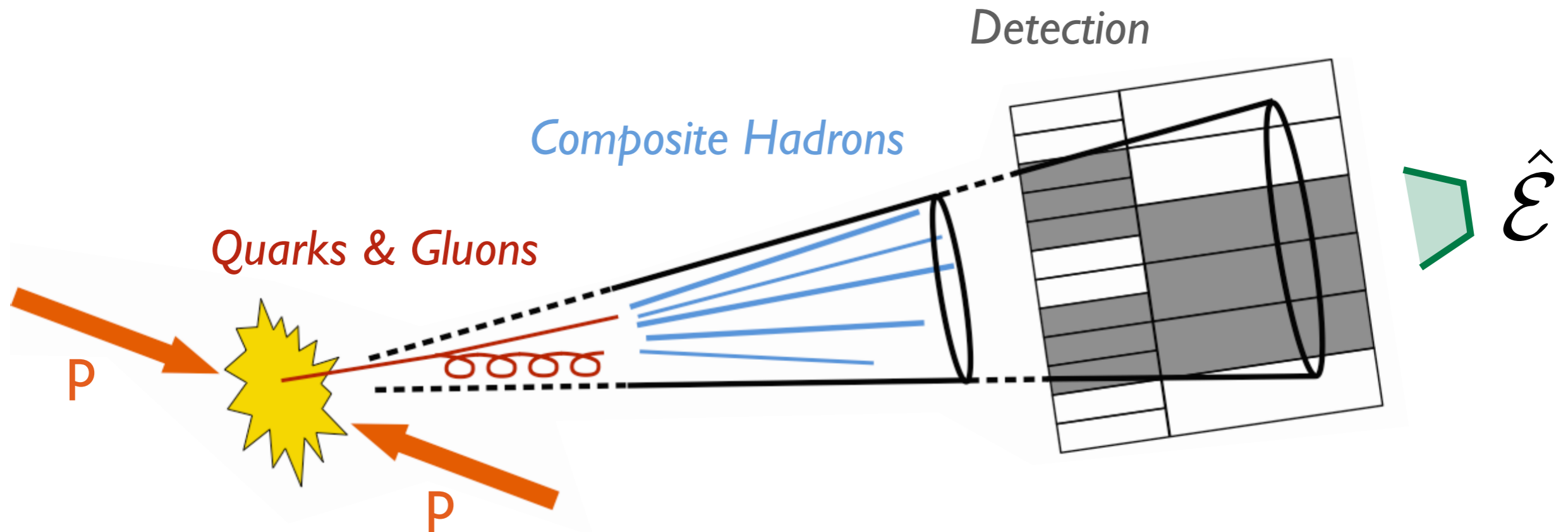
Collection of points in (position) space



[Popular Science, 2013]

Jet Formation from QCD

Theory



Energy Flow:

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

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

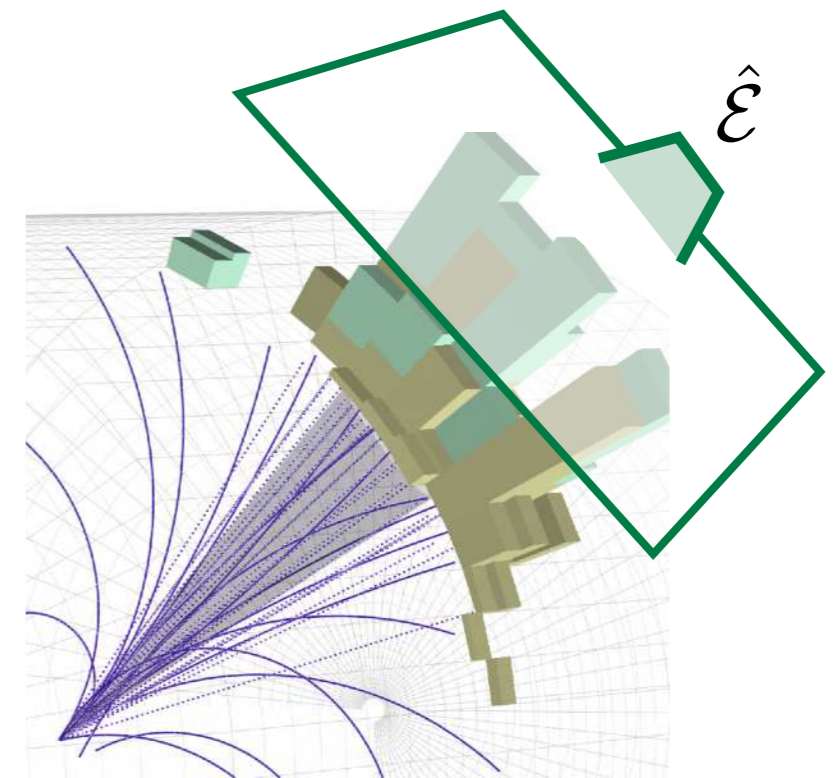
[see e.g. Sveshnikov, Tkachov, [PLB 1996](#); Hofman, Maldacena, [JHEP 2008](#); Mateu, Stewart, [JDT, PRD 2013](#); Belitsky, Hohenegger, Korchemsky, Sokatchev, Zhiboedov, [PRL 2014](#); Chen, Moul, Zhang, Zhu, [PRD 2020](#)]

From Energy Flow to **Weighted** Point Clouds

- **Energy-Weighted Directions**

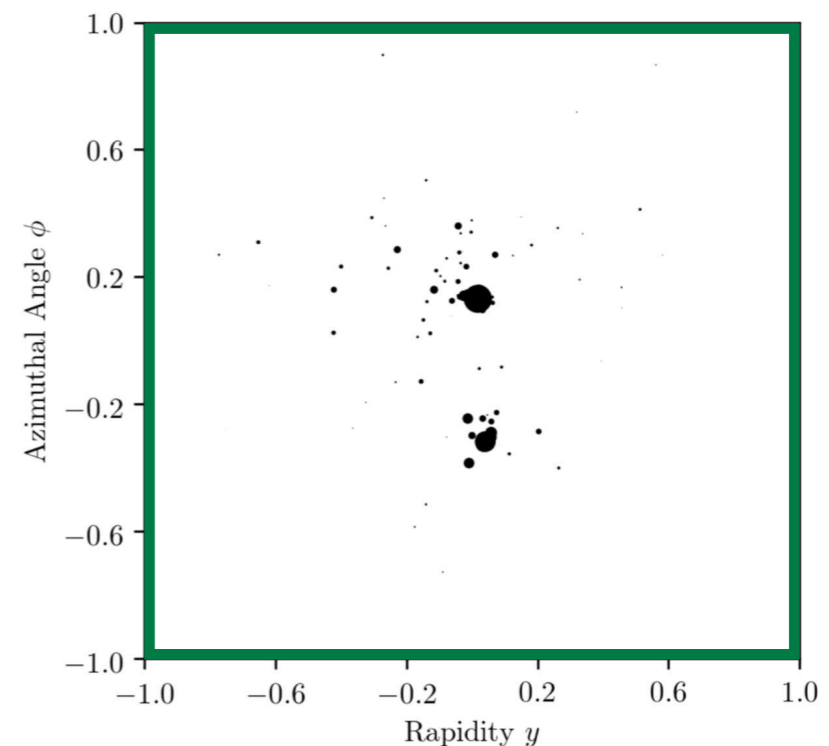
$$\vec{p} = \left\{ \underset{\substack{\uparrow \\ \text{Energy}}}{E}, \underbrace{\hat{n}_x, \hat{n}_y, \hat{n}_z}_{\text{Direction}} \right\}$$

(suppressing “unsafe” charge/flavor information)

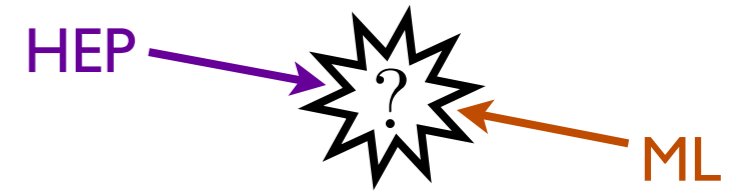


- Equivalently: **Energy Density**

$$\rho(\hat{n}) = \sum_{i \in \mathcal{J}} \underset{\substack{\uparrow \\ \text{Energy}}}{E_i} \delta^{(2)}(\hat{n} - \underset{\substack{\uparrow \\ \text{Direction}}}{\hat{n}_i})$$

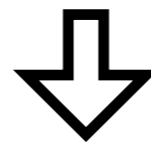


“Thinking” Like a Physicist



Symmetry: $\mathcal{J} = \{ \vec{p}_1, \vec{p}_2, \vec{p}_3, \dots, \vec{p}_N \}$
Unordered, Variable Length Set (QM!)

Safety: $\vec{p} = \{ E, \hat{n}_x, \hat{n}_y, \hat{n}_z \}$
Energy weighting (QFT!)



Properly specified problem
(i.e. loss function)



**The
Machine**



Solution

$$S(\mathcal{J})$$

Many (labeled)
examples $\{ \mathcal{J} \}$



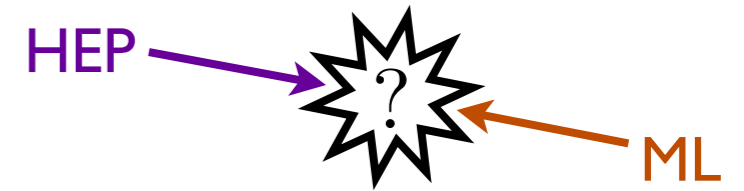
Verification

$$V(\mathcal{J})$$

*Check that answer
is physically sensible*

Energy Flow Networks

Architecture designed around *symmetries* and interpretability



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

Permutation invariant \downarrow Linear weights (i.e. safe) \downarrow

..... Parametrized with **Neural Networks**

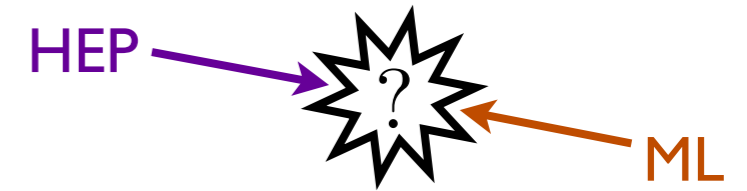
Provably describes any safe observable (!)*
Excellent jet classification performance

[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

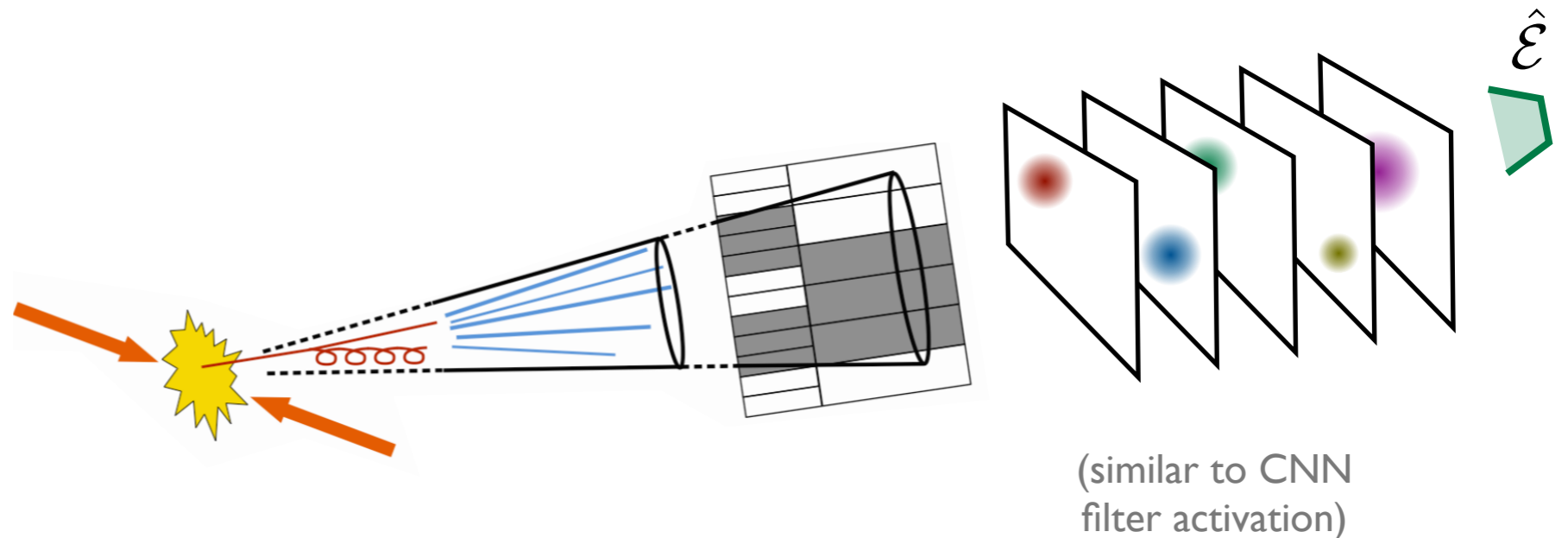
Architecture designed around symmetries and *interpretability*



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

Latent space of dim ℓ

Easy to plot!

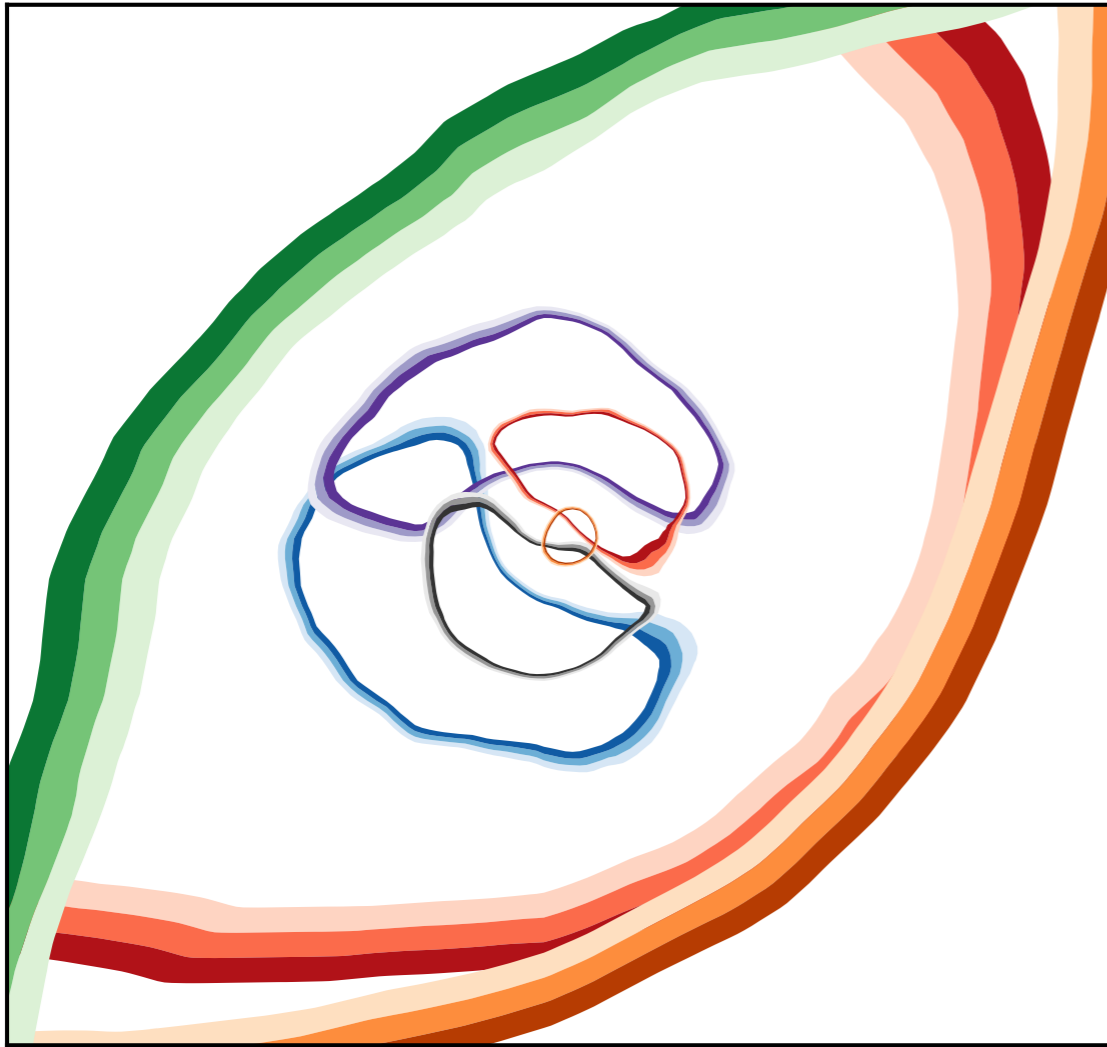


[Komiske, Metodiev, JDT, [JHEP 2019](#); see also Komiske, Metodiev, JDT, [JHEP 2018](#); code at energyflow.network; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, [NIPS 2017](#); other set-based architecture in Qu, Gouskos, [PRD 2020](#); Mikuni, Canelli, [EPJP 2020](#);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

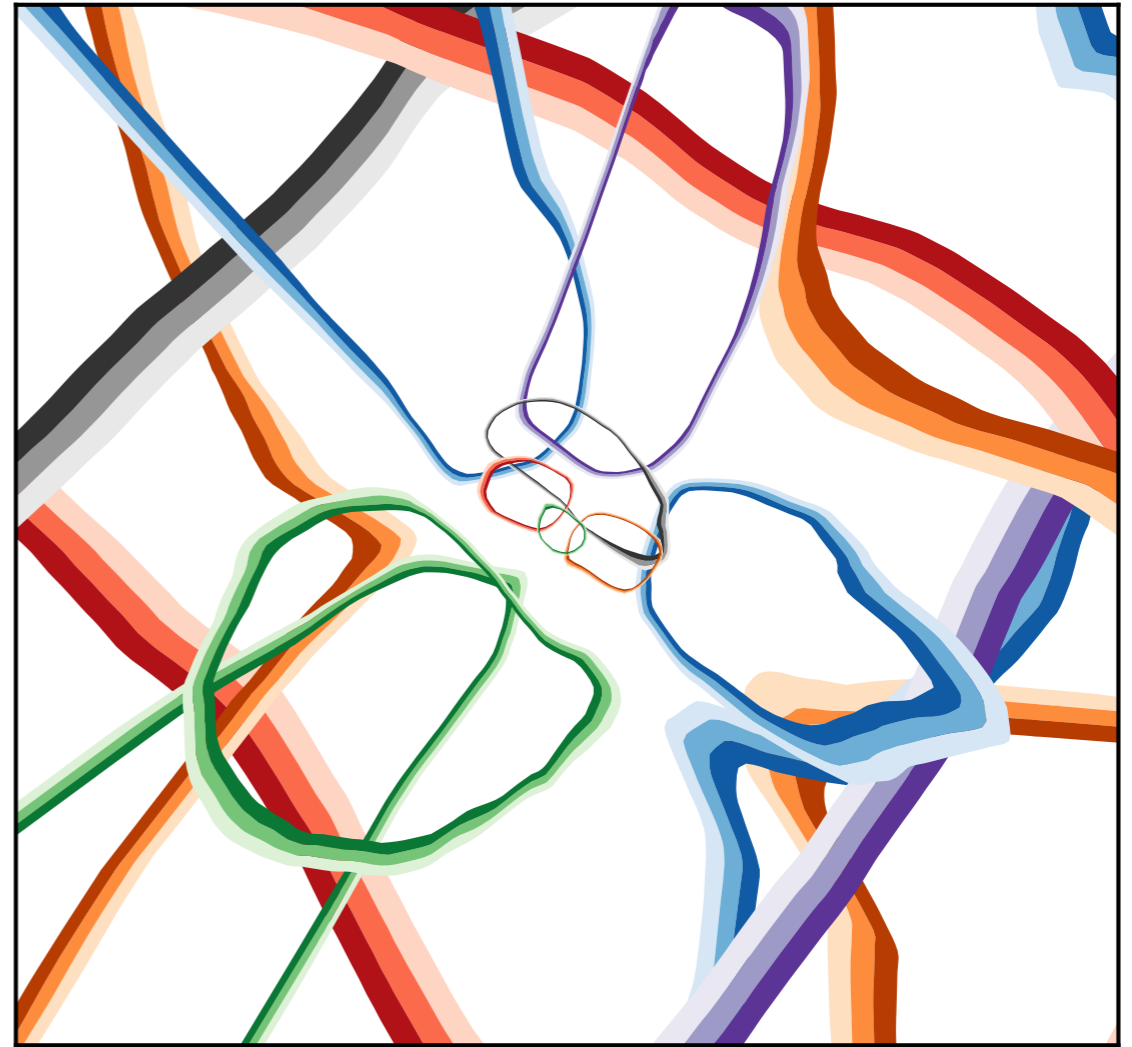


Psychedelic Network Visualization

Latent Dimension 8



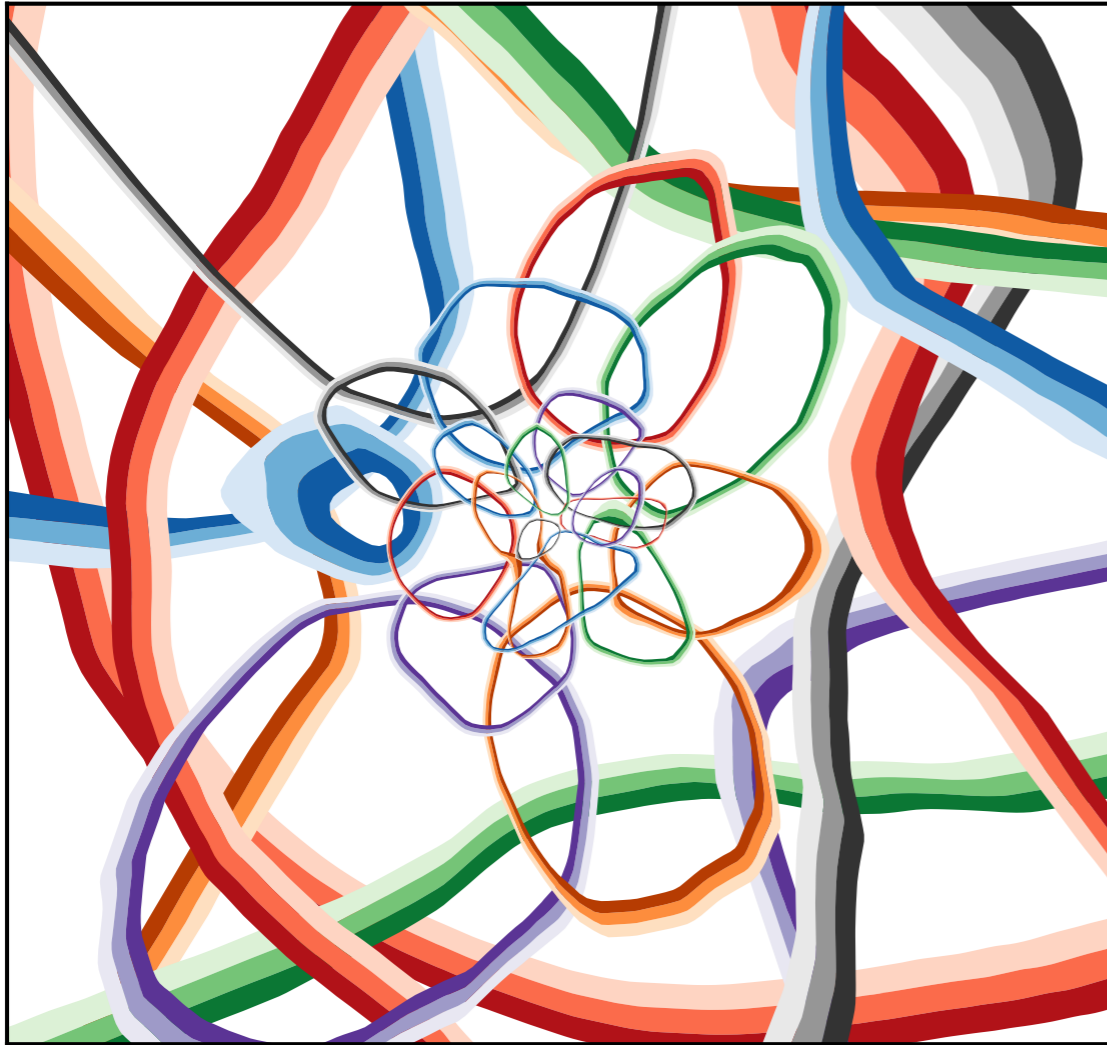
Latent Dimension 16



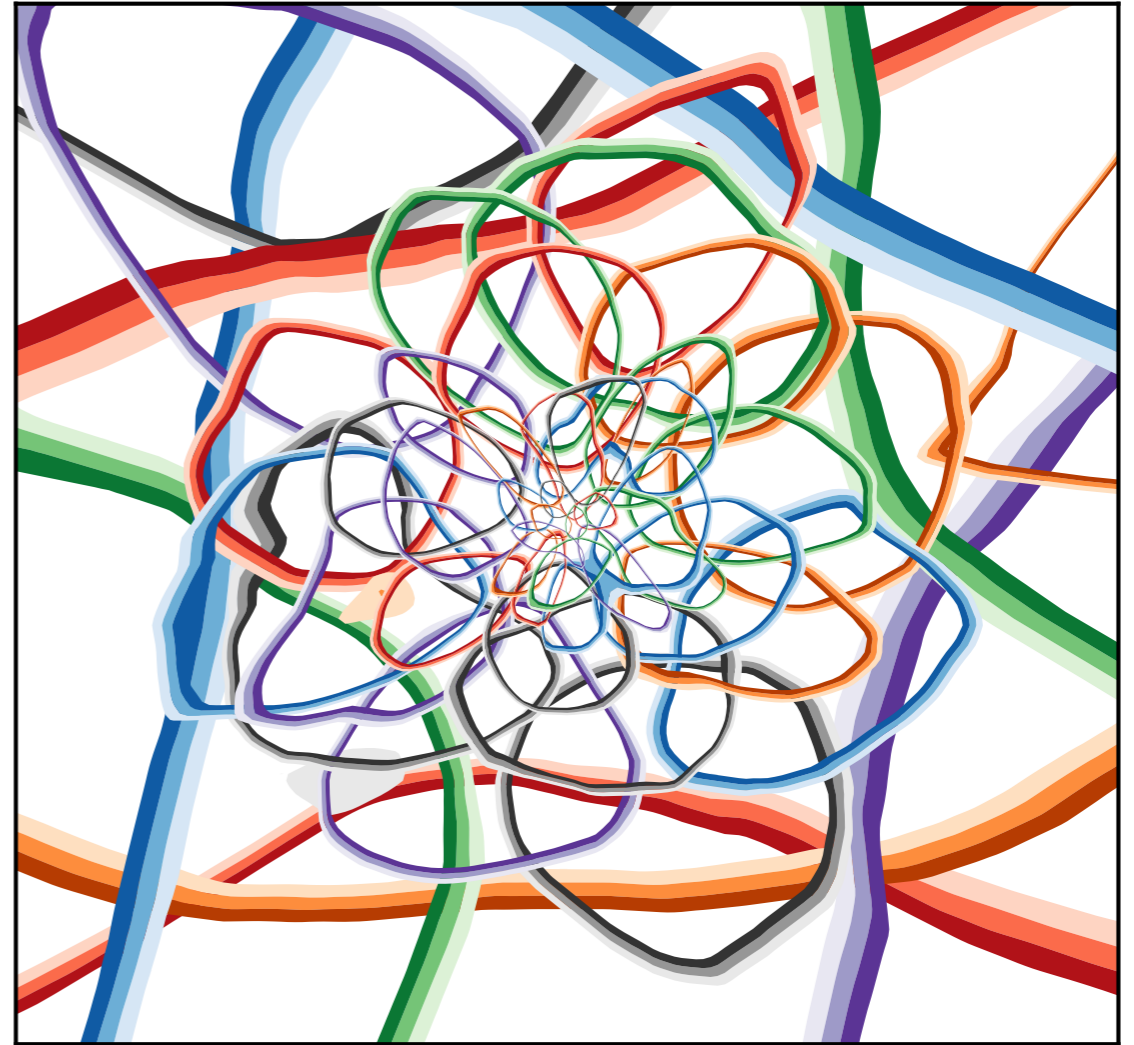
For the case of **quark** vs. **gluon** classification

Psychedelic Network Visualization

Latent Dimension 32

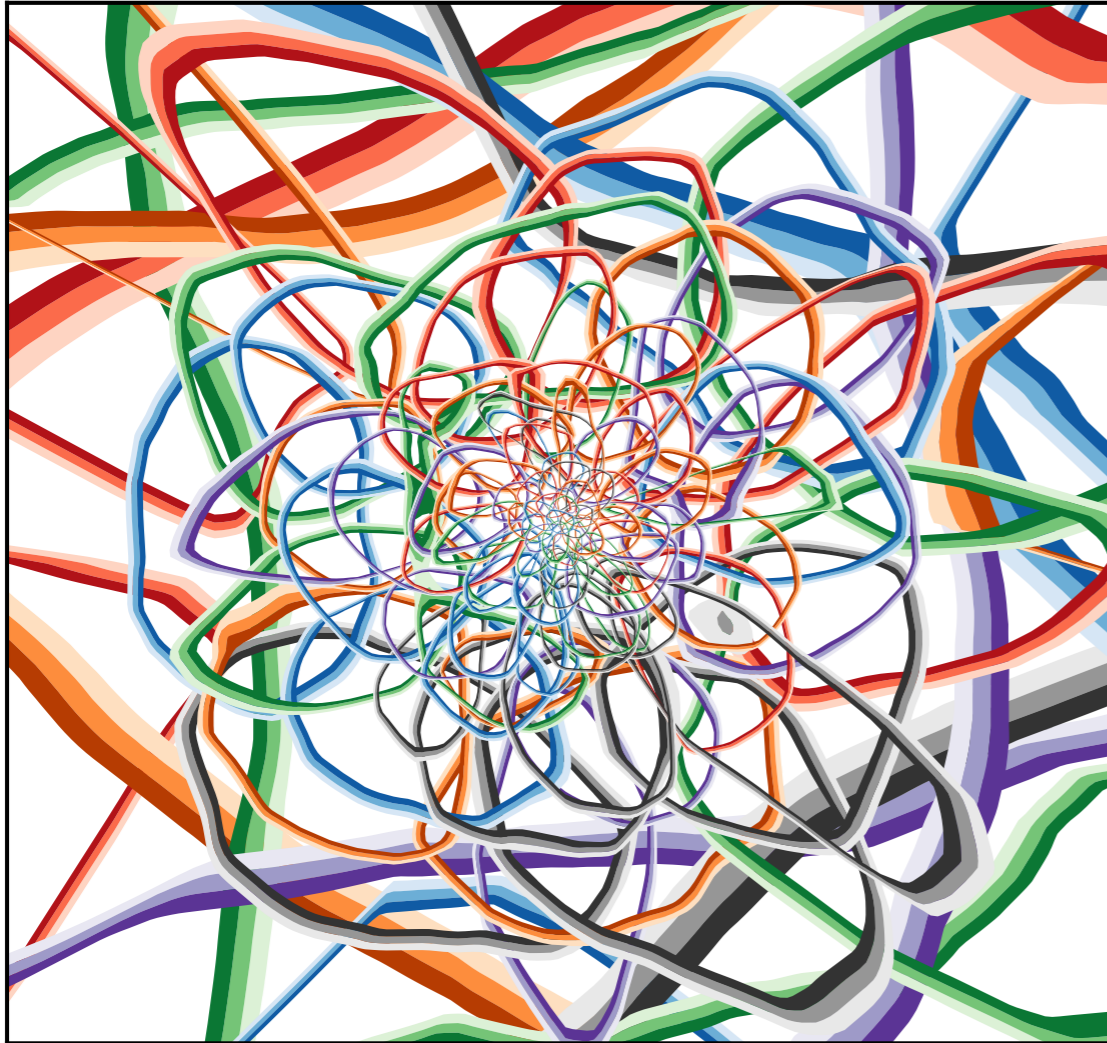


Latent Dimension 64

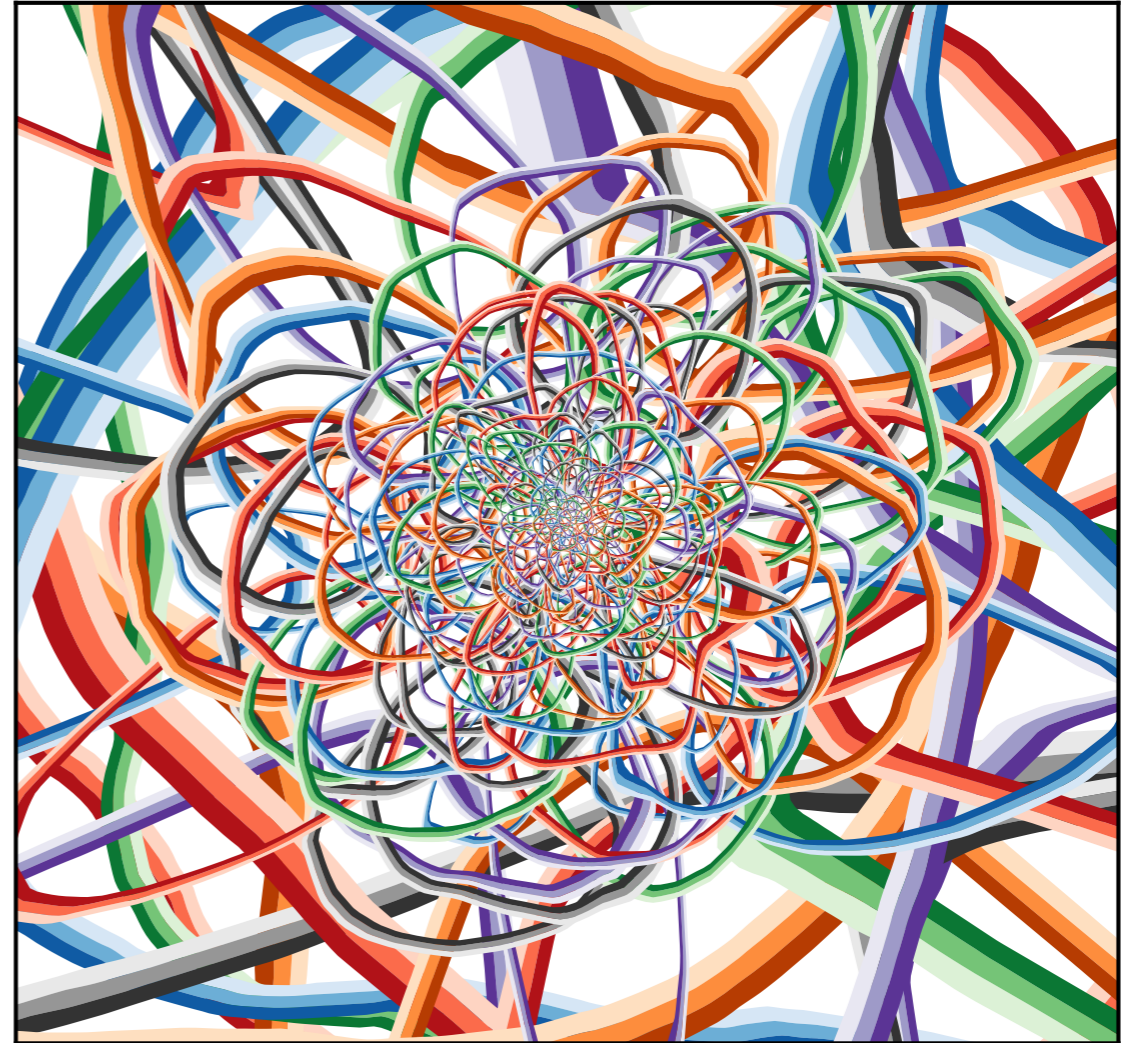


Psychedelic Network Visualization

Latent Dimension 128

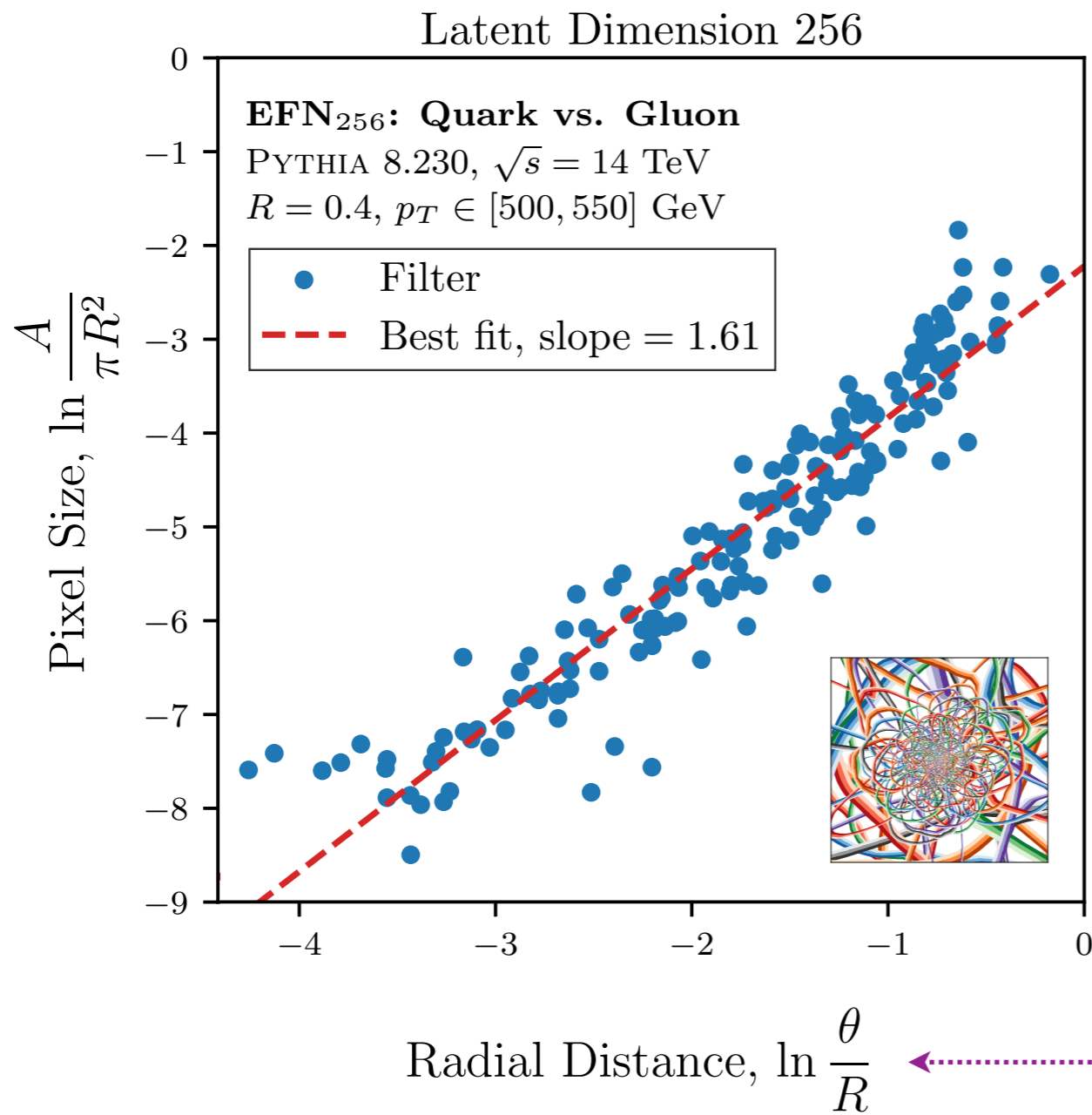
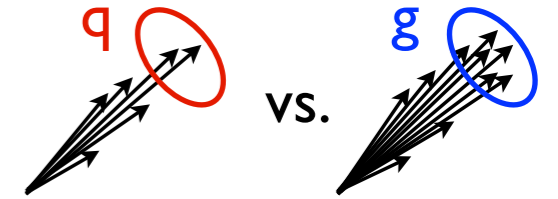


Latent Dimension 256



Singularity structure of QCD!

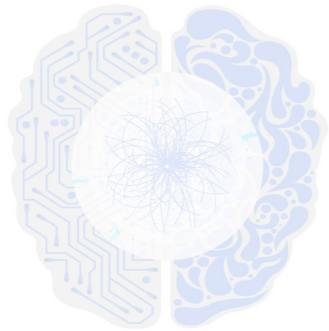
Machine Learning Collinear QCD



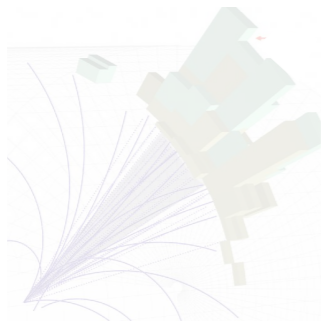
$C_q = 4/3$
 $C_g = 3$

$$dP_{i \rightarrow ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{d\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{dz}{z}}_{\text{Soft}}$$

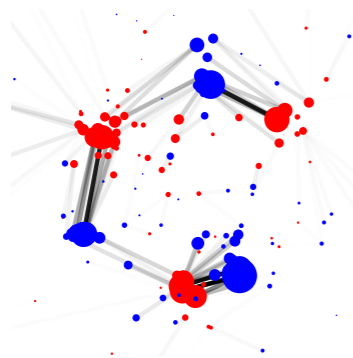
[Komiske, Metodiev, JDT, JHEP 2019]



Rise of the Machines?



What is a Collider Event?

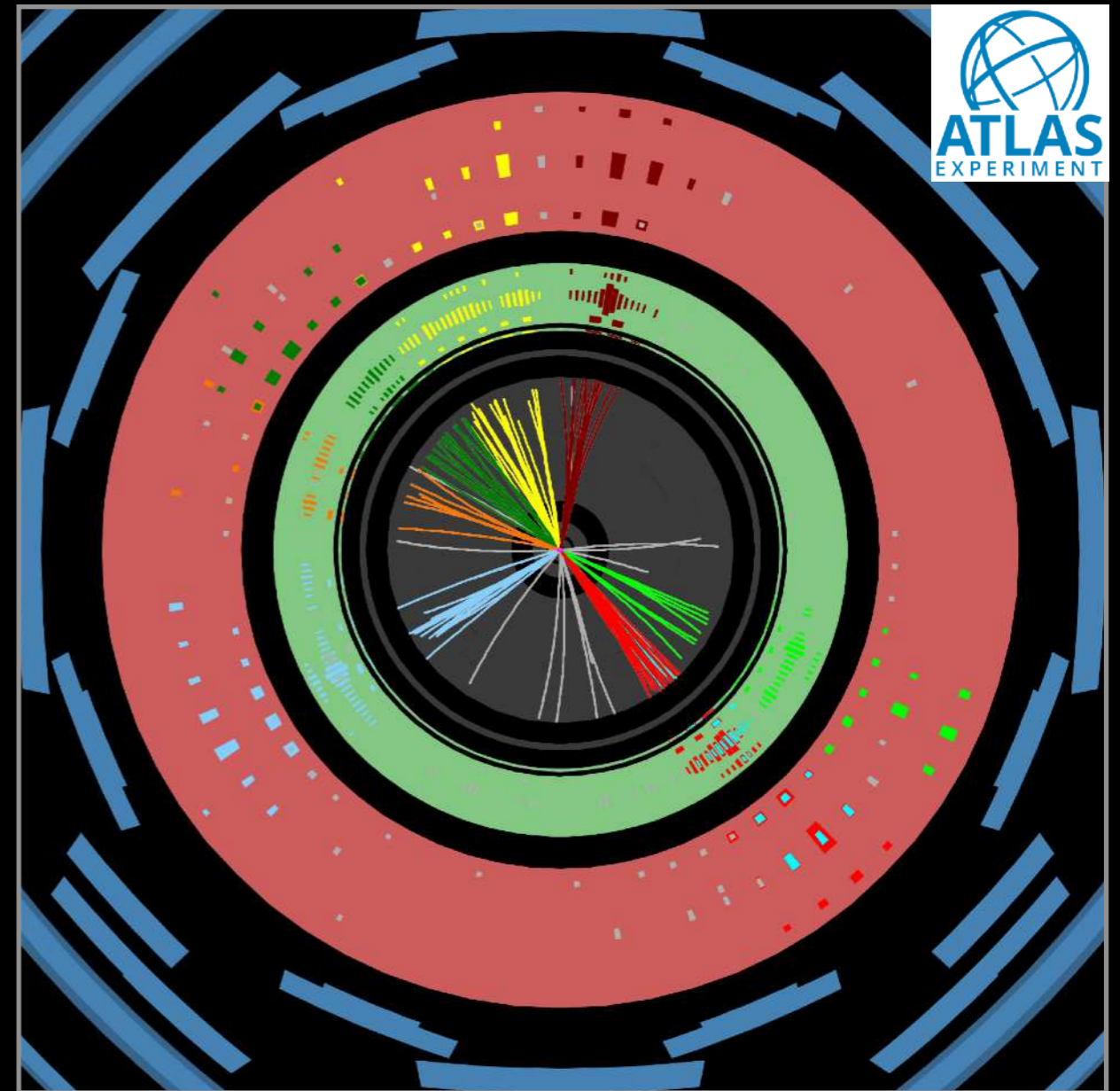
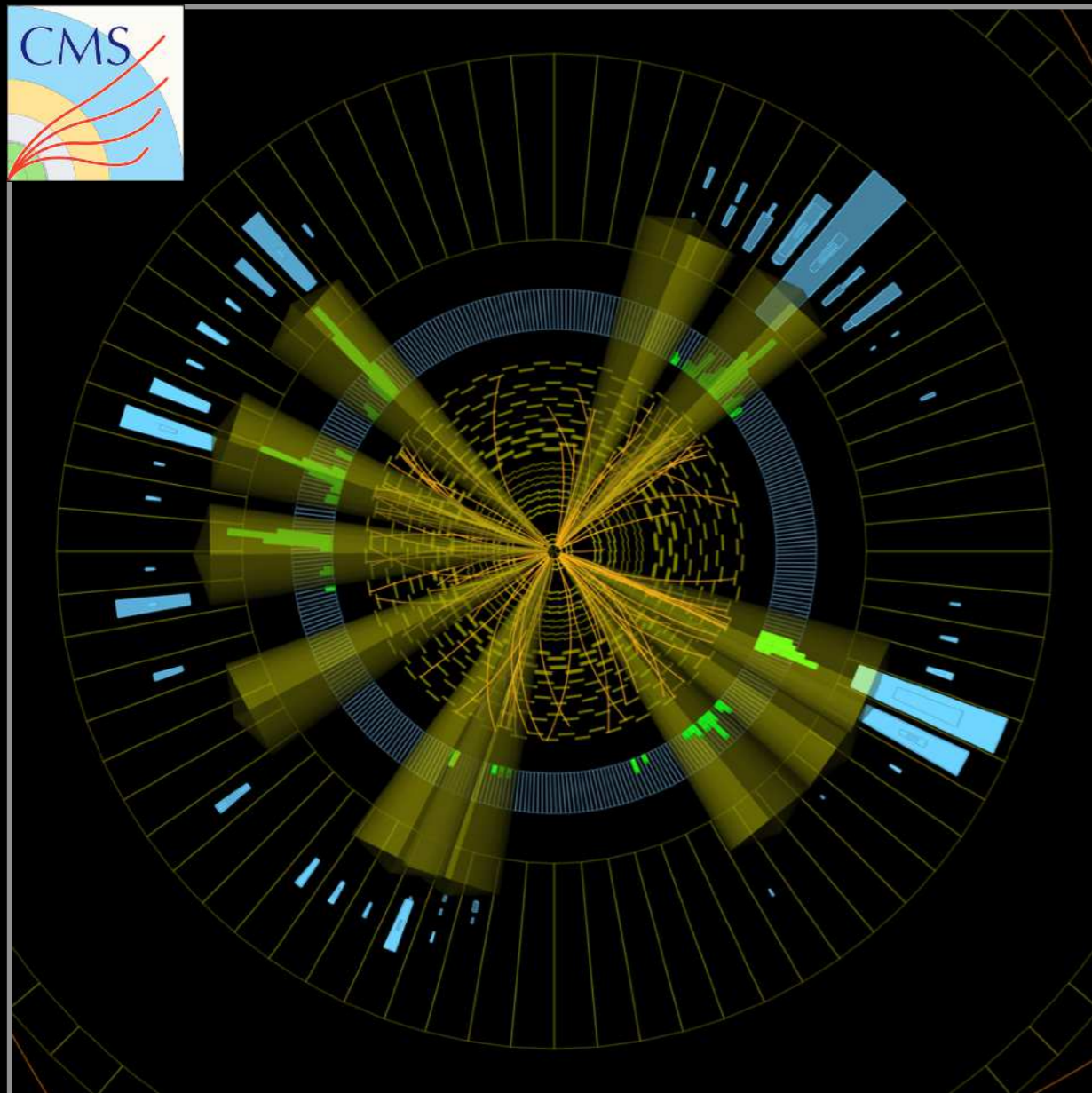
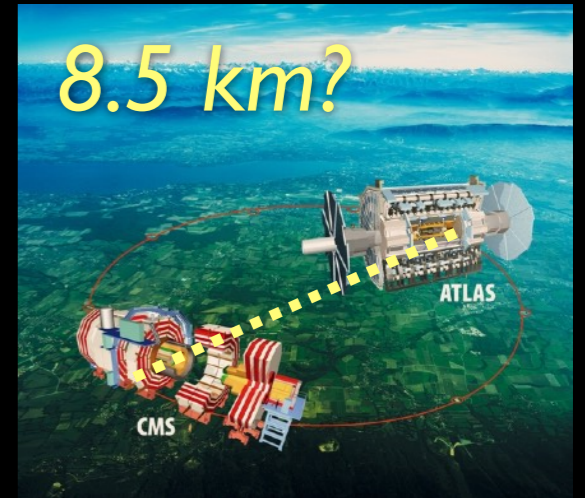


When are Collider Events Similar?

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](#), [ICJV 2000](#);
Pele, Werman, [ECCV 2008](#); Pele Taskar, [GSI 2013](#)]

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



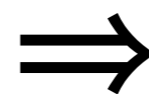
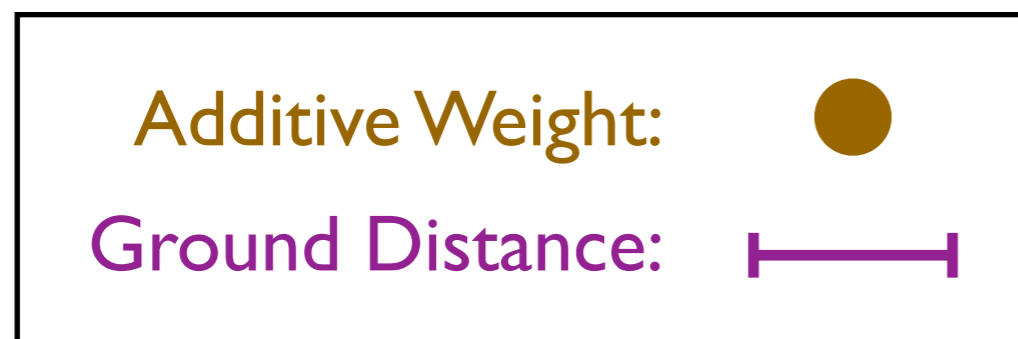
[h/t Niles-Weed, [ML4jets 2020](#); Monge, 1781; Vaserštejn, 1969; [Wikipedia](#)]

The Earth Mover's Distance

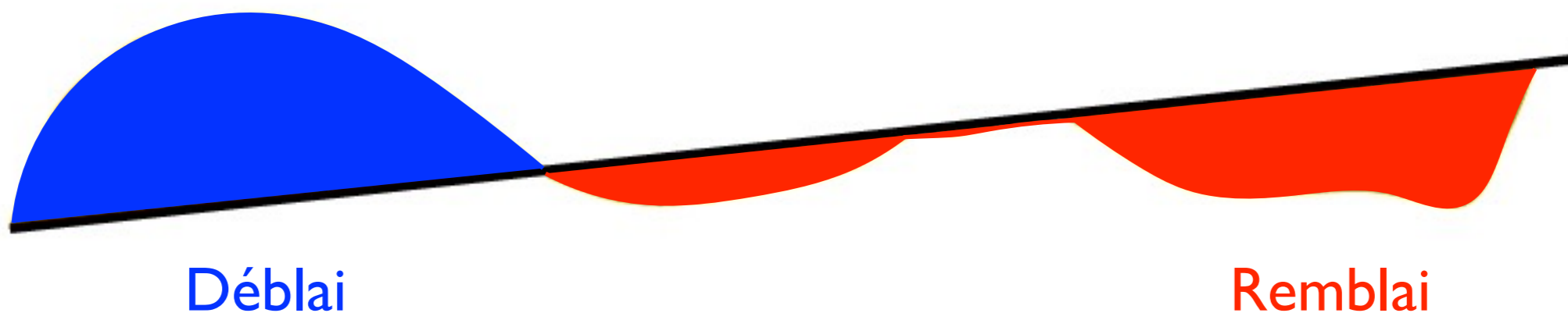
Optimal Transport:

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

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

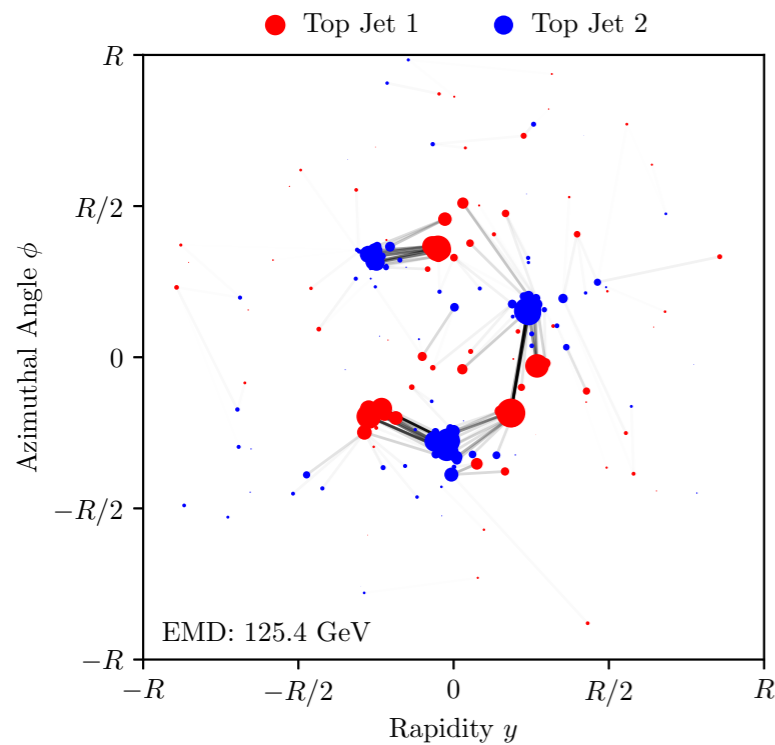
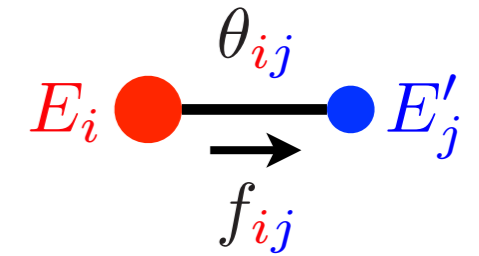


Distance Between
Distributions



[h/t Niles-Weed, [ML4jets 2020](#); Monge, 1781; Vaserštejn, 1969; [Wikipedia](#)]

The Energy Mover's Distance



Optimal transport between energy flows...

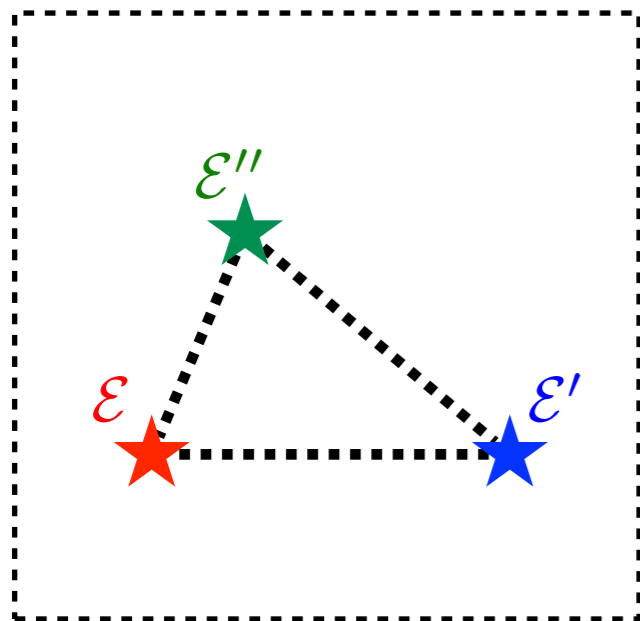
$$\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \underbrace{\sum_i \sum_j f_{ij} \frac{\theta_{ij}}{R}}_{\text{Cost to move energy}} + \underbrace{\left| \sum_i E_i - \sum_j E'_j \right|}_{\text{Cost to create energy}}$$

↑
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, PRL 2019;

see also Pele, Werman, ECCV 2008; Pele, Taskar, GSI 2013;

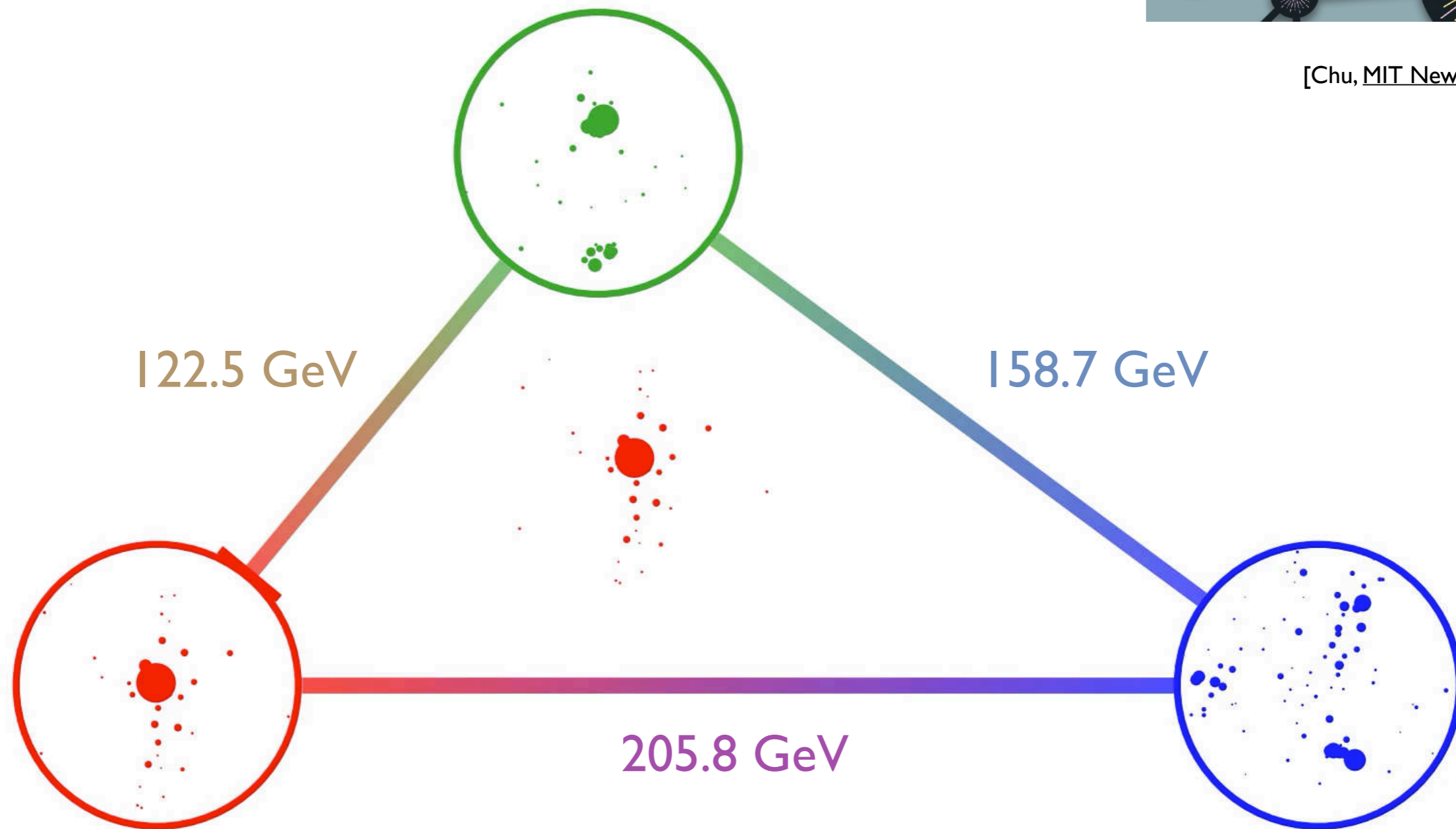
[see flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, arXiv 2020]

[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

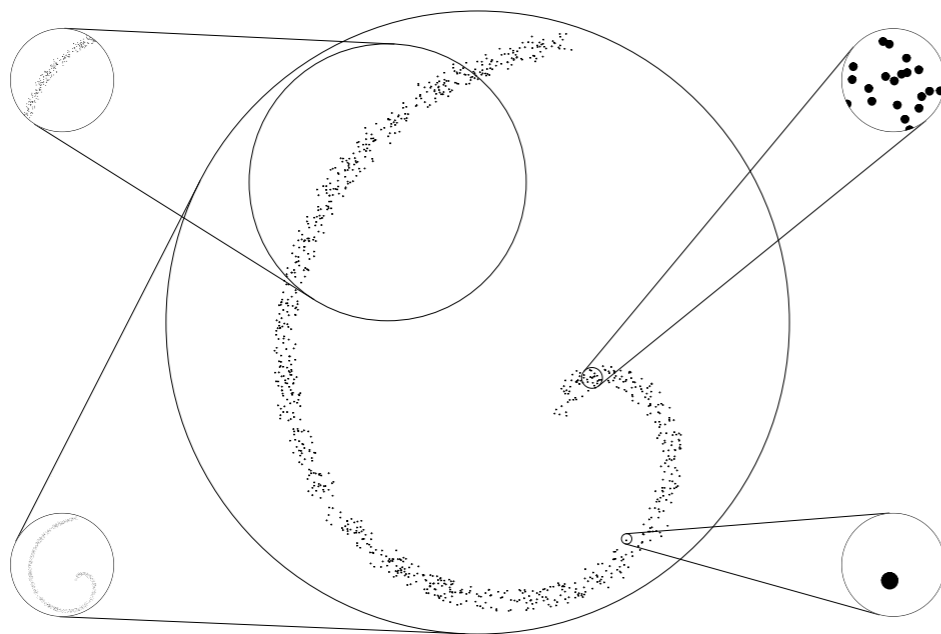
$$N_{\text{neighbors}}(r) \sim r^{\text{dim}}$$

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

[Grassberger, Procaccia, PRL 1983; Kégl, NIPS 2002]

dim ≈ 1

dim ≈ 2



dim ≈ 2

dim ≈ 0

(eventually 0)

Dimensionality of Space of Jets



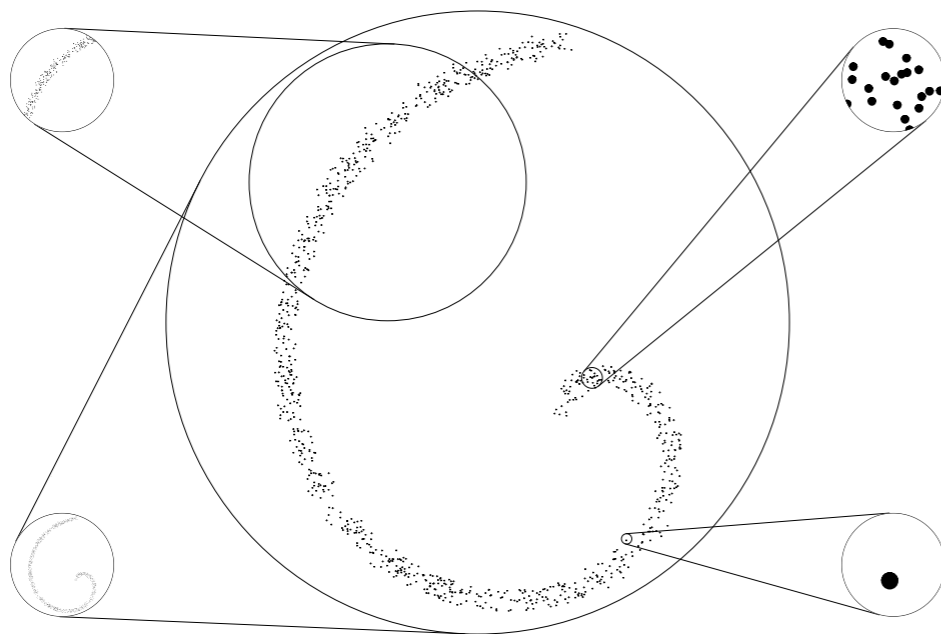
$$N_{\text{neighbors}}(r) \sim r^{\text{dim}}$$

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

[Grassberger, Procaccia, PRL 1983; Kégl, NIPS 2002]

dim ≈ 1

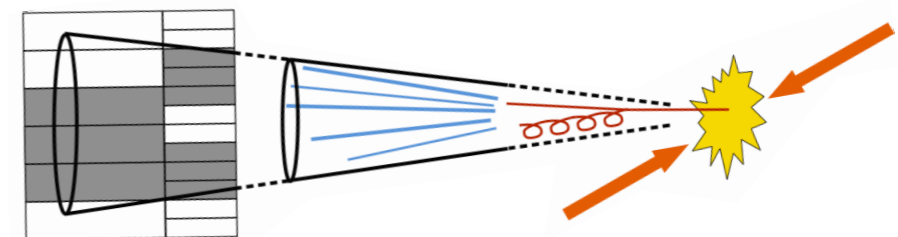
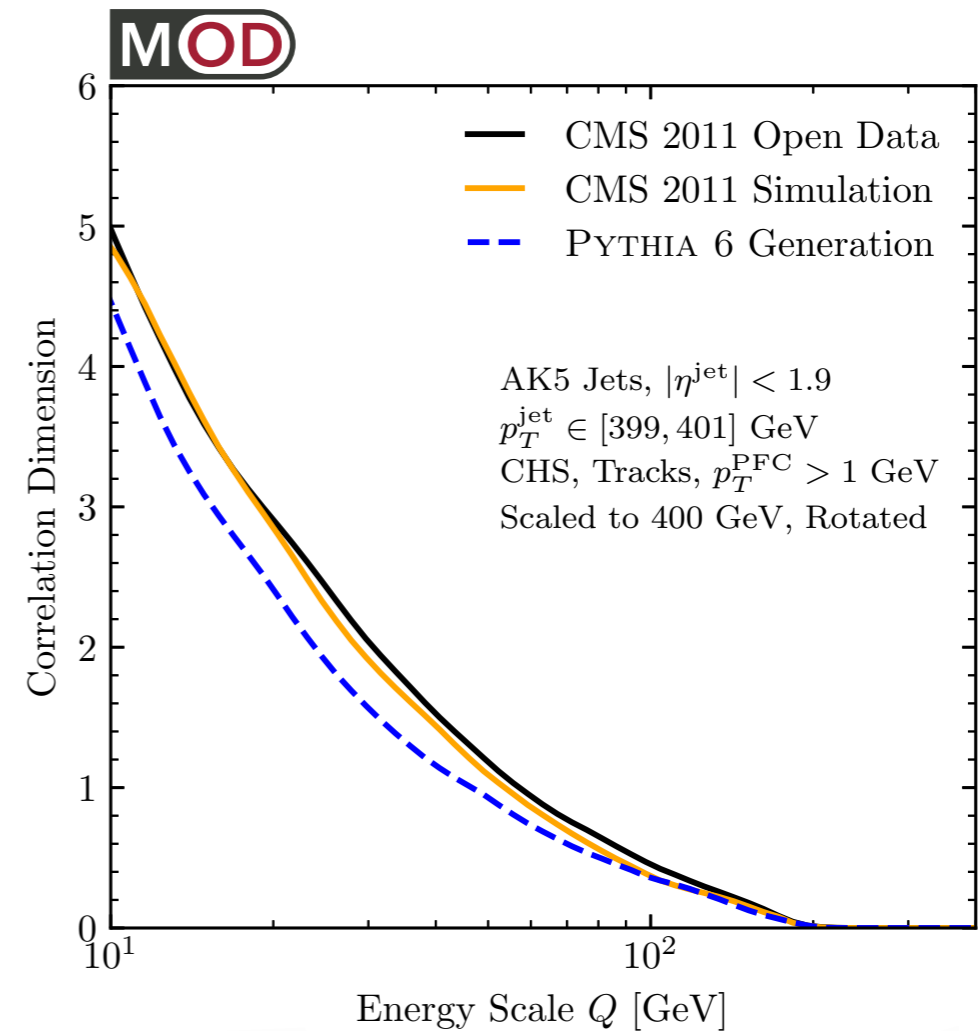
dim ≈ 2



dim ≈ 2

dim ≈ 0

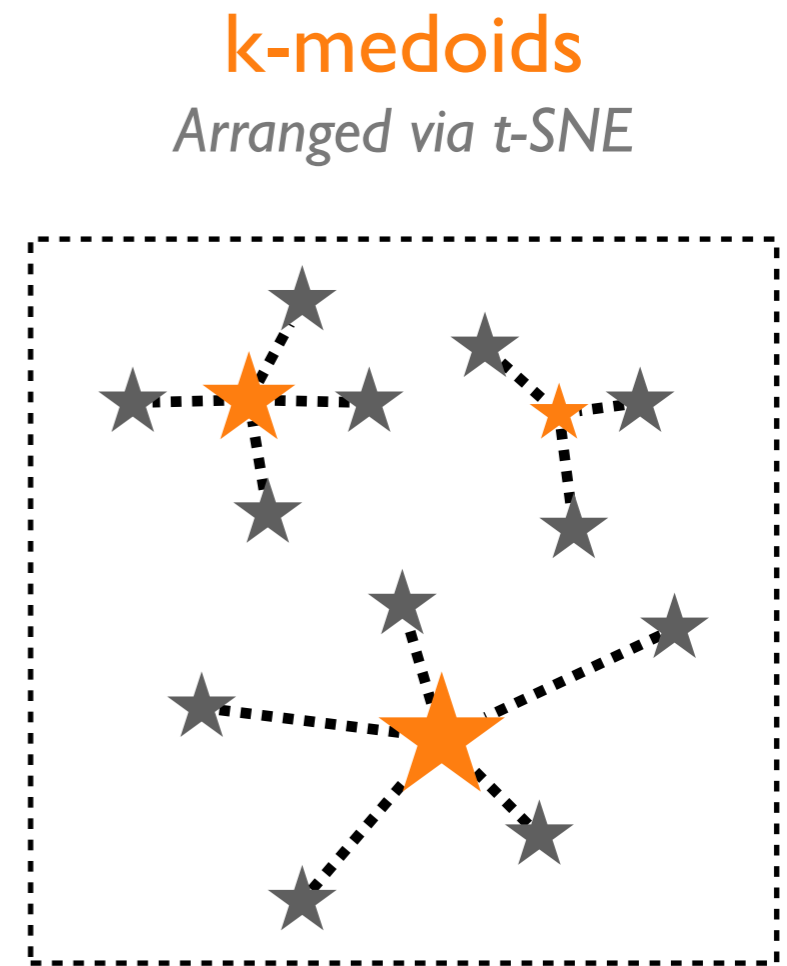
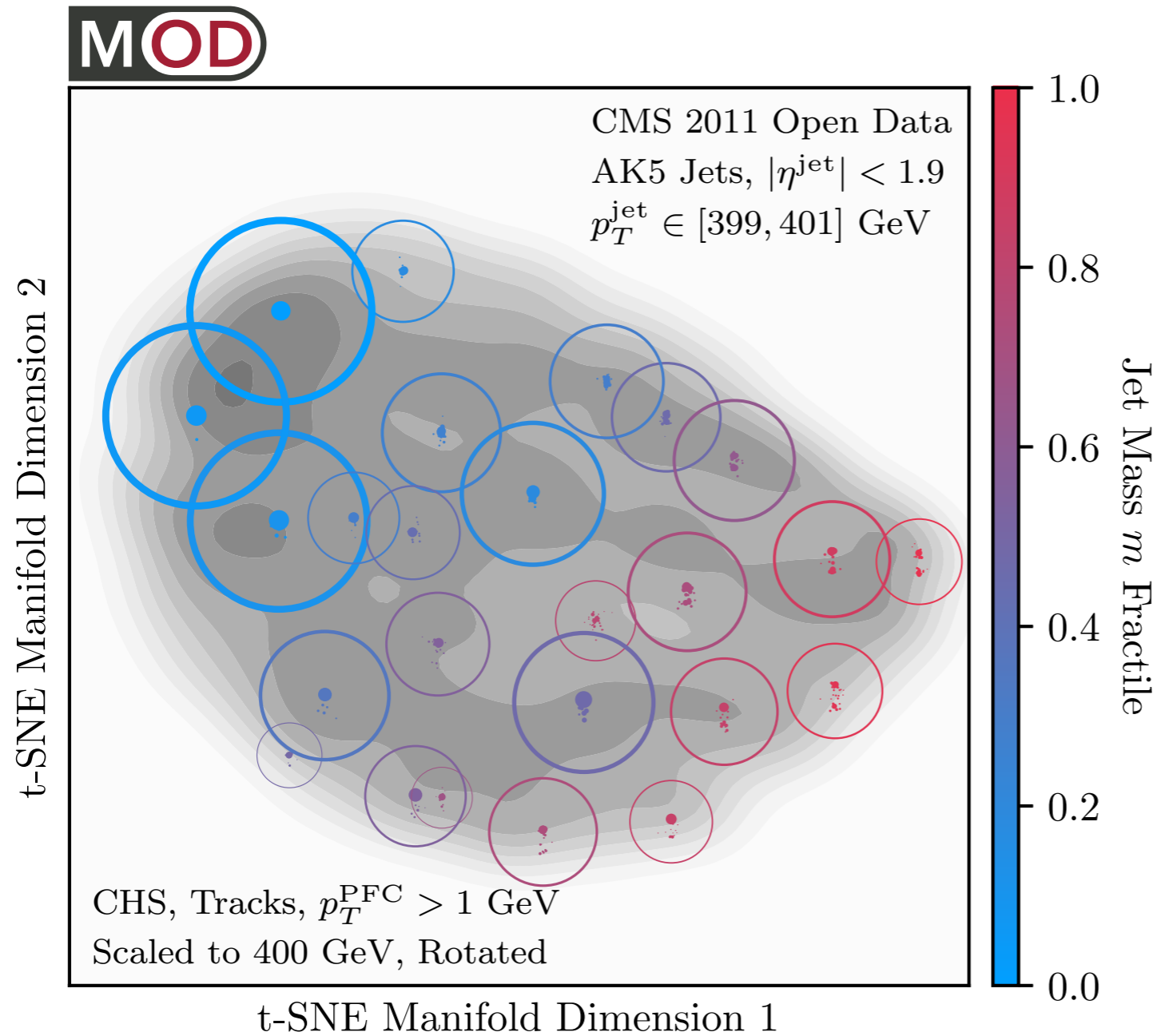
(eventually 0)



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



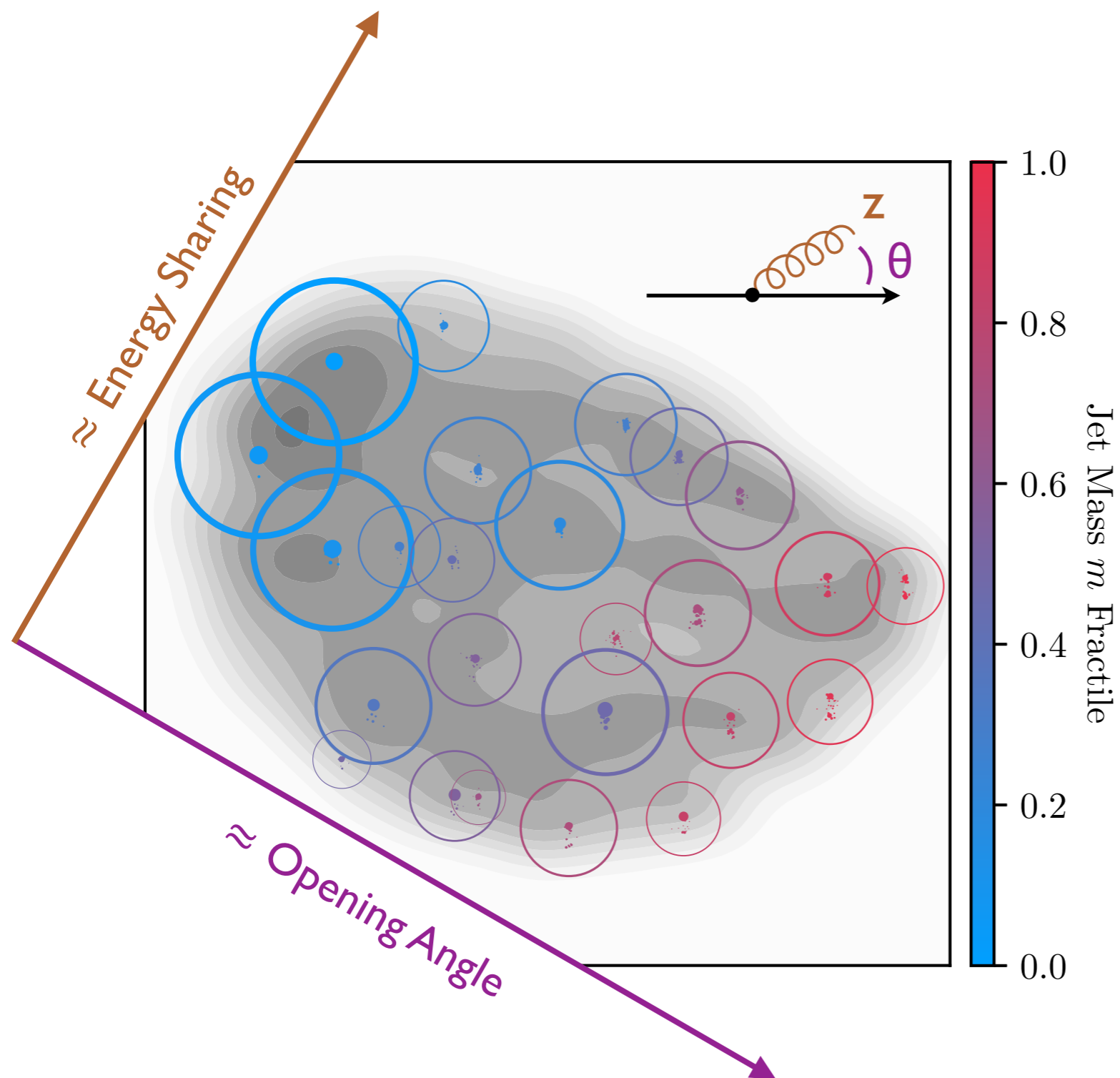
Most Representative Jets



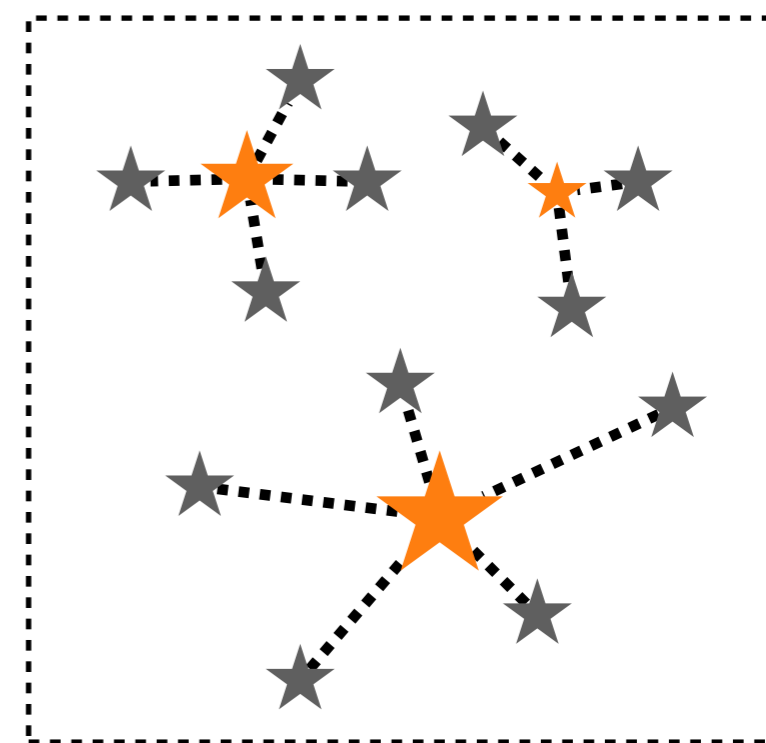
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using van der Maaten, Hinton, JMLR 2008]



Most Representative Jets



k-medoids
Arranged via *t*-SNE



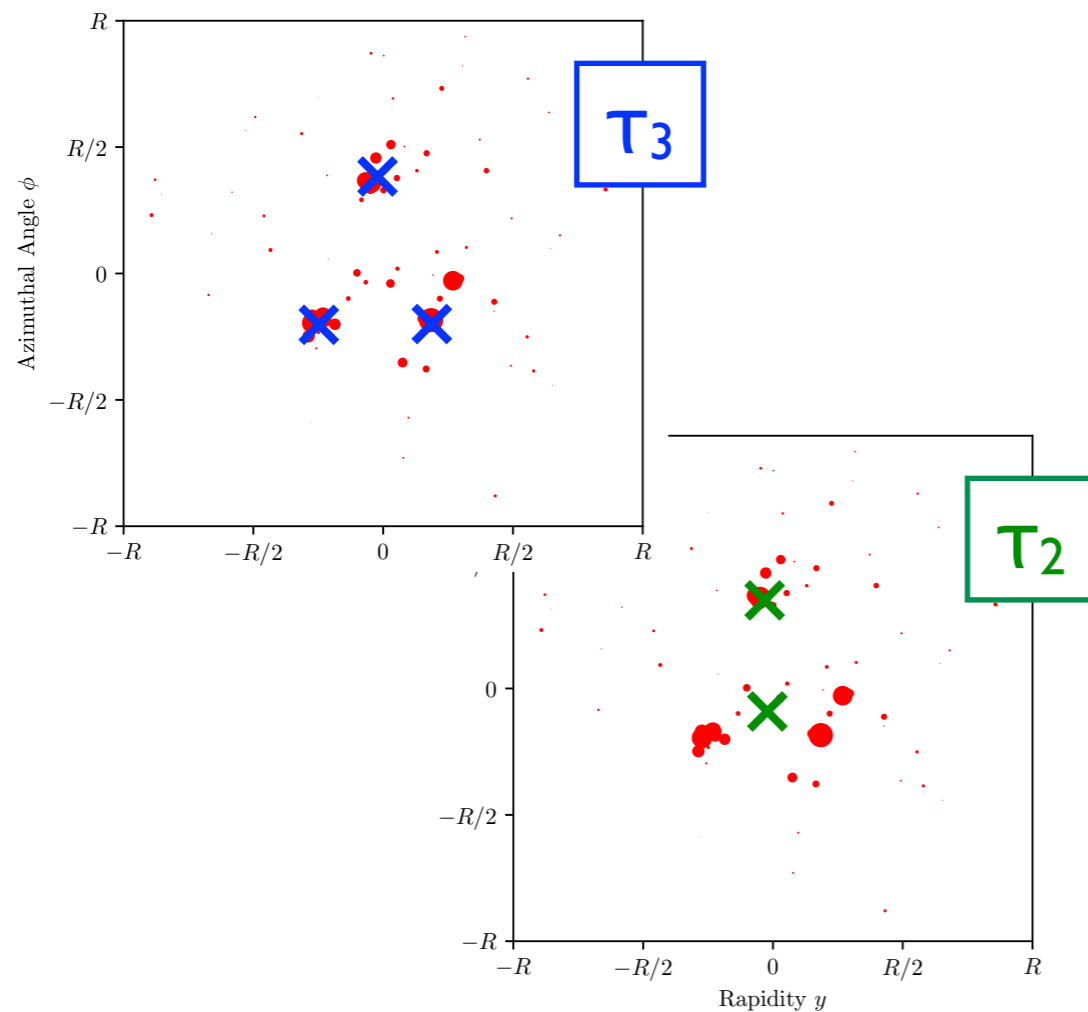
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using van der Maaten, Hinton, JMLR 2008]



N-subjettiness

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

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

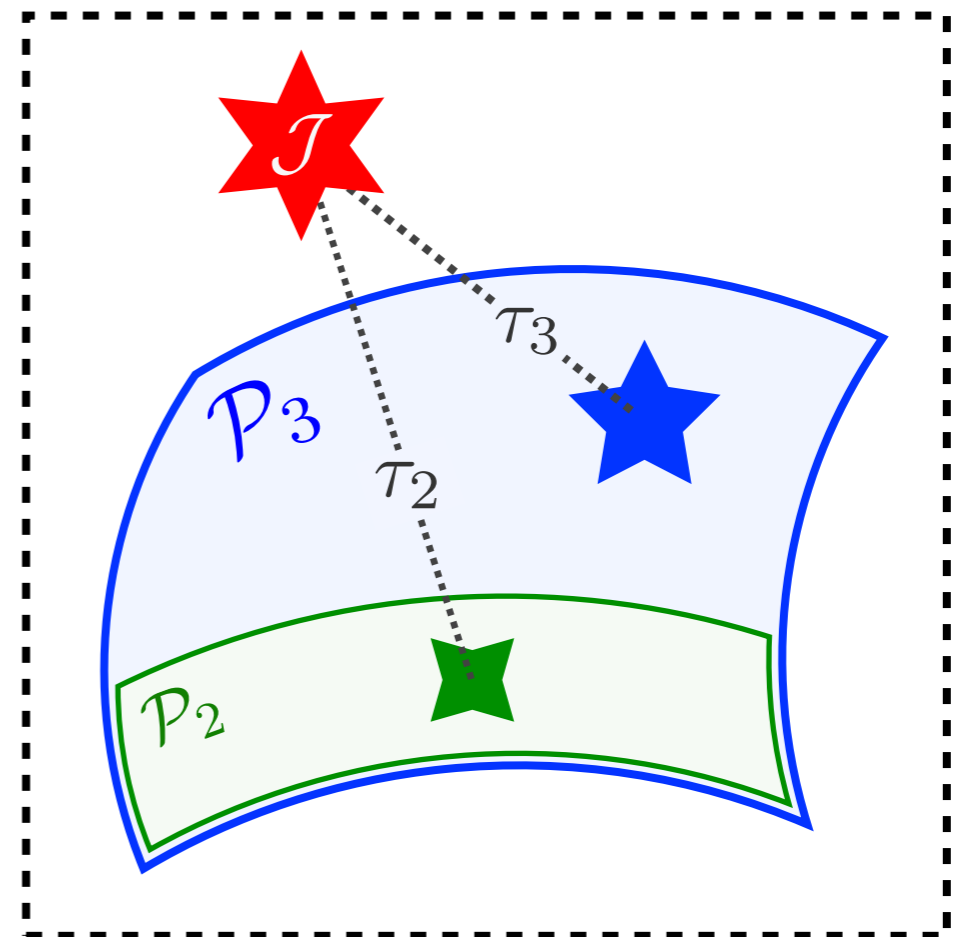
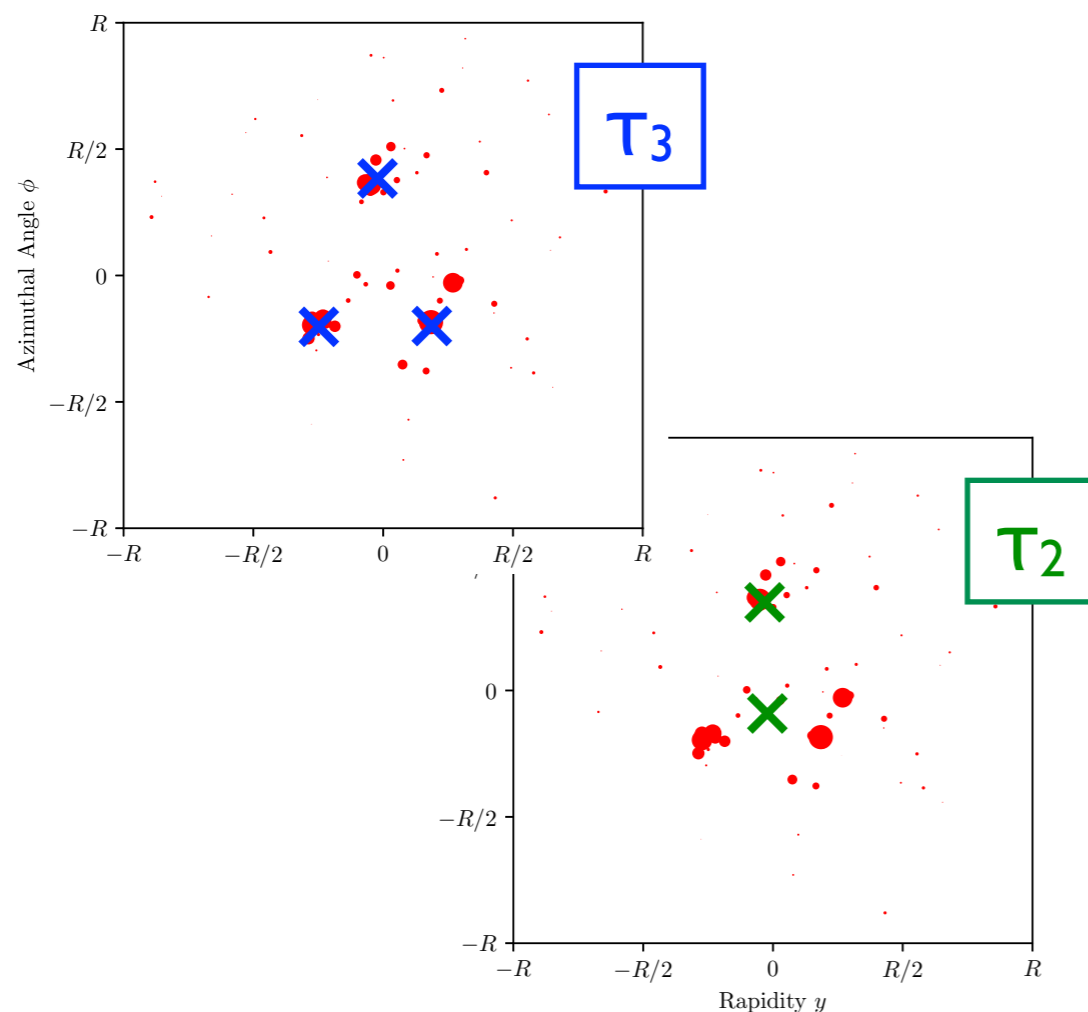


[JDT, Van Tilburg, JHEP 2011, JHEP 2012;
based on Brandt, Dahmen, ZPC 1979; Stewart, Tackmann, Waalewijn, PRL 2010]

N-subjettiness = Point to Manifold EMD

...is secretly an optimal transport problem

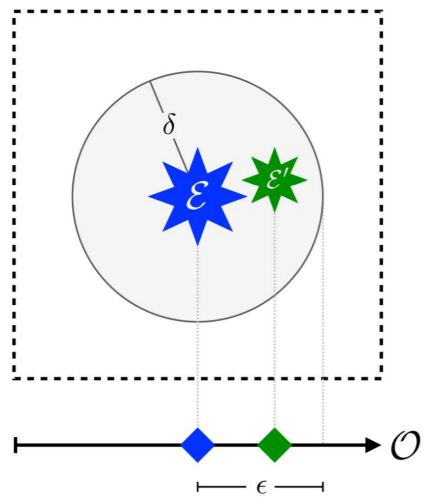
$$\tau_N(\mathcal{J}) = \min_{\mathcal{J}' \in \mathcal{P}_N} \text{EMD}(\mathcal{J}, \mathcal{J}')$$



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

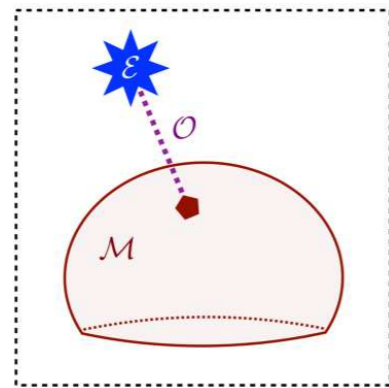
Six Decades of Collider Physics Translated into a New Geometric Language!

IRC Safety is smoothness in the space of events



Taming infinities

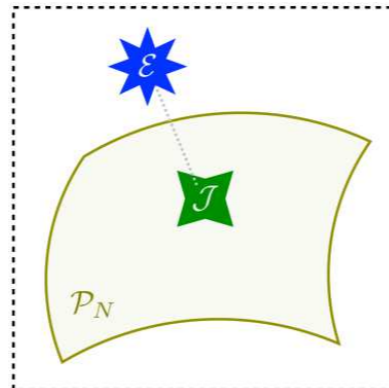
Event shapes are distances from events to manifolds.



$$O(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{M}} \text{EMD}_{\beta, R}(\mathcal{E}, \mathcal{E}')$$

Event Shapes

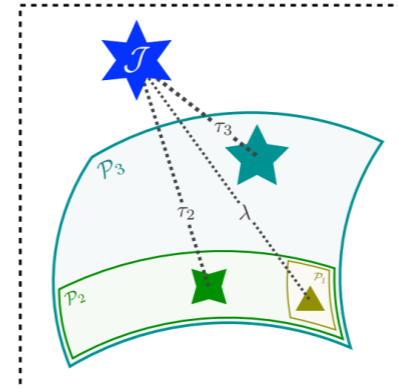
Jets are projections to few-particle manifolds.



$$J = \operatorname{argmin}_{\mathcal{E}' \in \mathcal{P}_N} \text{EMD}_{\beta, R}(\mathcal{E}, \mathcal{E}')$$

Jet Algorithms

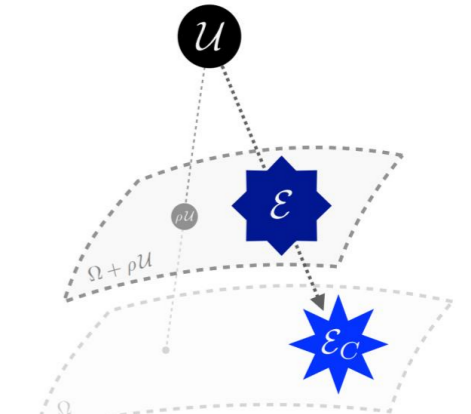
Substructure resolves emissions within the jet.



$$\tau(J) = \min_{\mathcal{E}' \in \mathcal{P}_N} \text{EMD}_{\beta}(\mathcal{J}, \mathcal{E}')$$

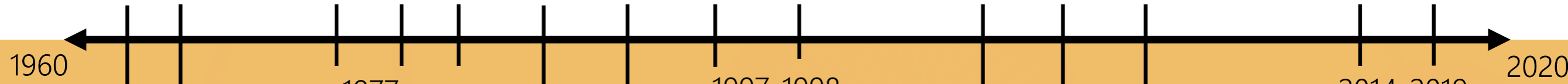
Jet Substructure

Pileup mitigation moves away from uniform radiation.



$$\mathcal{E}_C = \operatorname{argmin}_{\mathcal{E}'} \text{EMD}(\mathcal{E}, \mathcal{E}' + \rho \mathcal{U}).$$

Pileup



1962-1964
Infrared Safety
[Kinoshita, JMP 1962]
[Lee, Nauenberg, PR 1964]

1977
Thrust, Sphericity
[Farhi, PRL 1977]
[Georgi, Machacek, PRL 1977]

1993
 k_T jet clustering
[Ellis, Soper, PRD 1993]
[Catani, Dokshitzer, Seymour, Webber, NPB 1993]

1997-1998
C/A jet clustering
[Wobisch, Wengler, 1998]
[Dokshitzer, Leder, Moretti, Webber, JHEP 1997]

2010-2015
N-(sub)jettiness, XCone
[Stewart, Tackmann, Waalewijn, PRL 2010]
[Thaler, Van Tilburg, JHEP 2011]
[Stewart, Tackmann, Thaler, Vermilion, Wilkason, JHEP 2015]

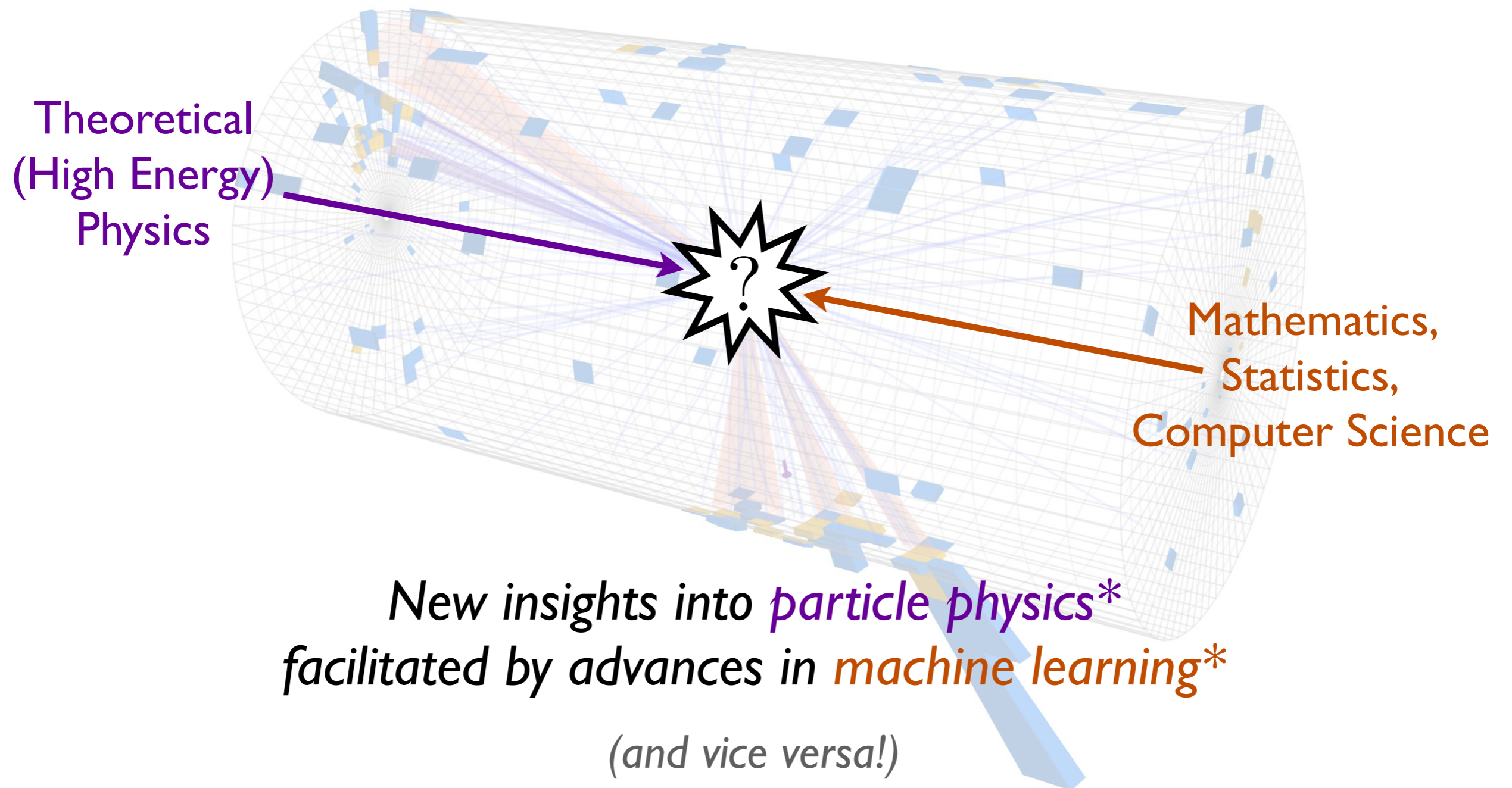
2014-2019
Constituent Subtraction
[Berta, Spousta, Miller, Leitner, JHEP 2014]
[Berta, Masetti, Miller, Spousta, JHEP 2019]

And many more!

[Komiske, Metodiev, JDT, JHEP 2020; timeline by Metodiev]

“Collision Course”

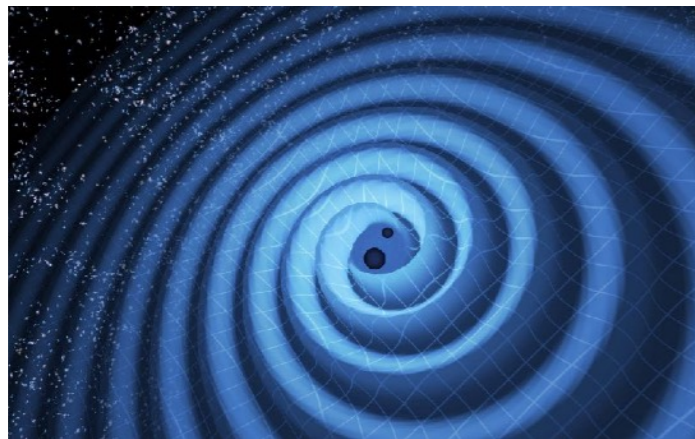
“Theoretical Physics for Machine Learning”
Aspen Center for Physics, January 2019



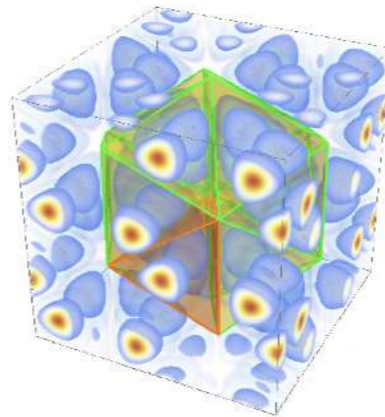
Artificial Intelligence \Leftrightarrow Fundamental Interactions



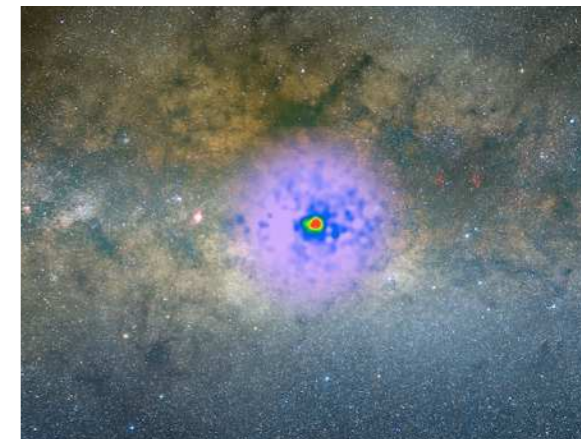
Gravitational Waves



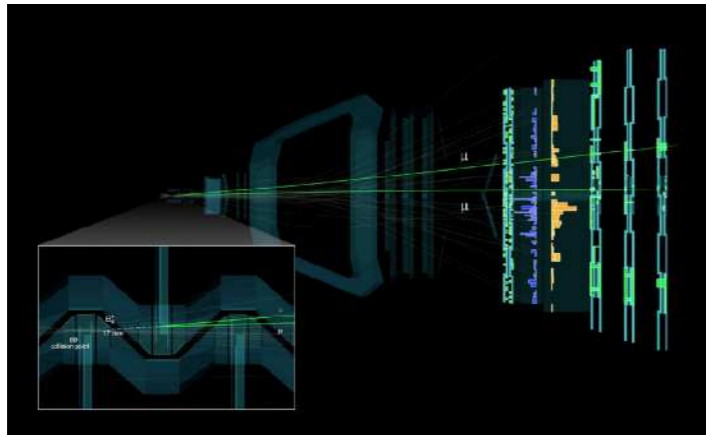
Nuclear Physics



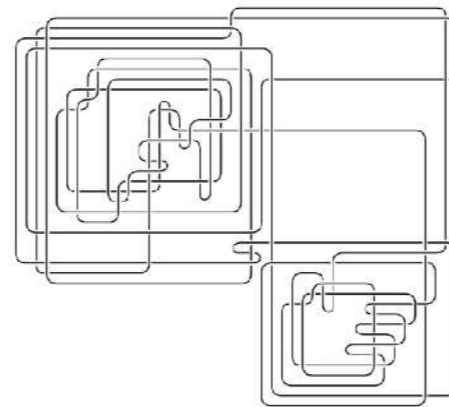
Astrophysics



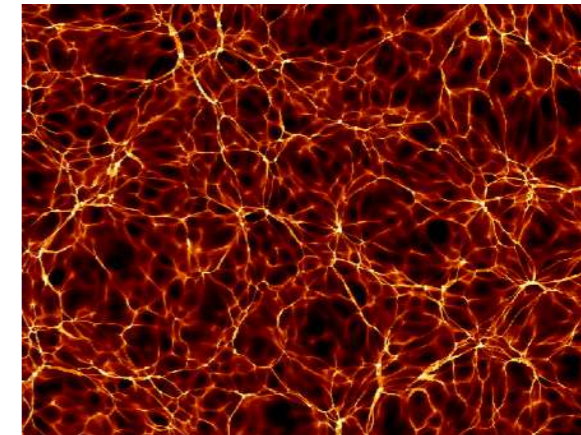
Particle Colliders



Mathematical Physics



Dark Matter

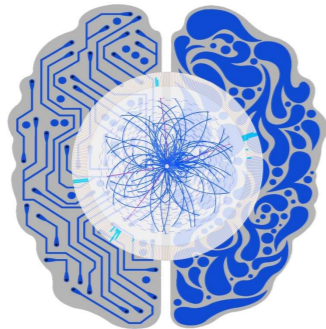


...

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

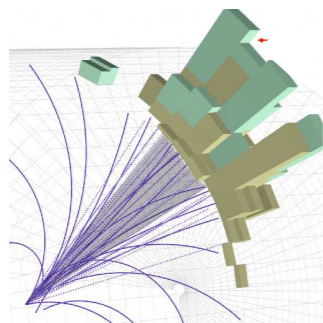
[<http://iaifi.org>]

Summary



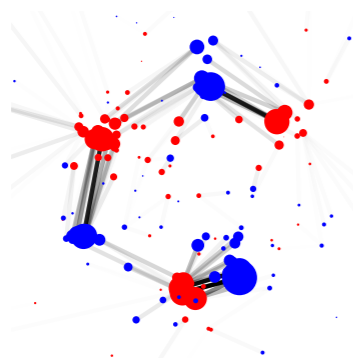
Rise of the Machines?

*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*



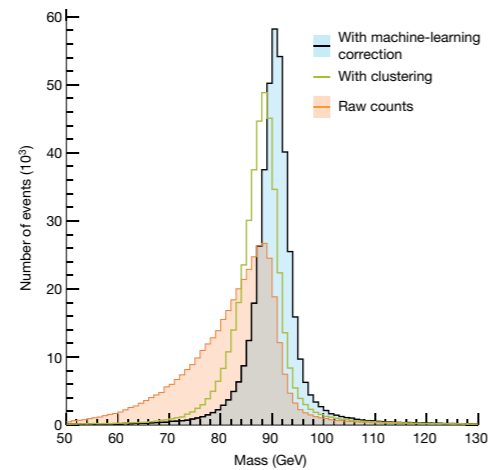
When are Collider Events Similar?

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

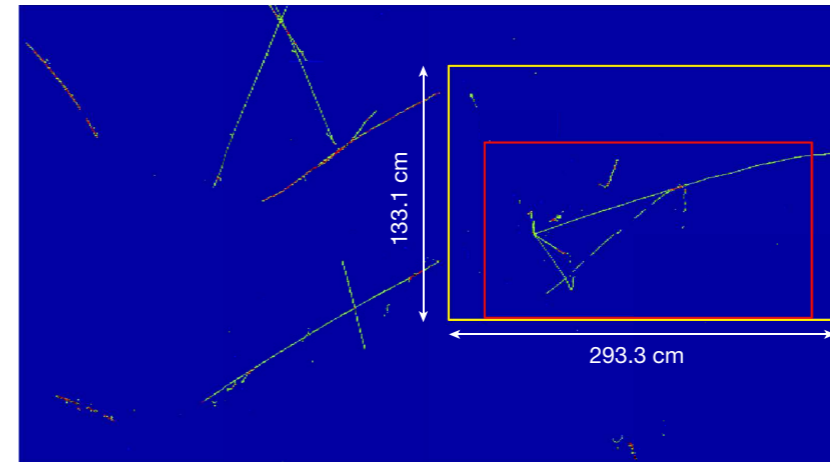
Backup Slides

Extensive Use of ML in HEP

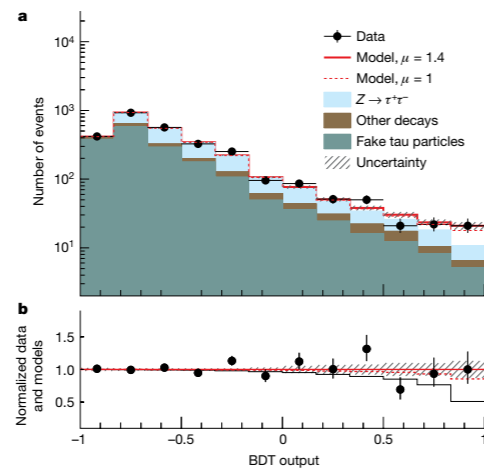
CMS: $Z \rightarrow e^+e^-$ calibration



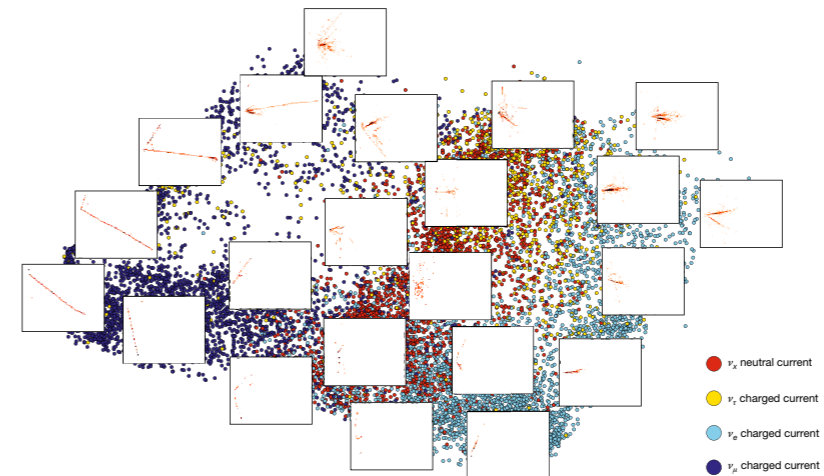
MicroBooNE: Object Identification



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



NOvA: Object Classification



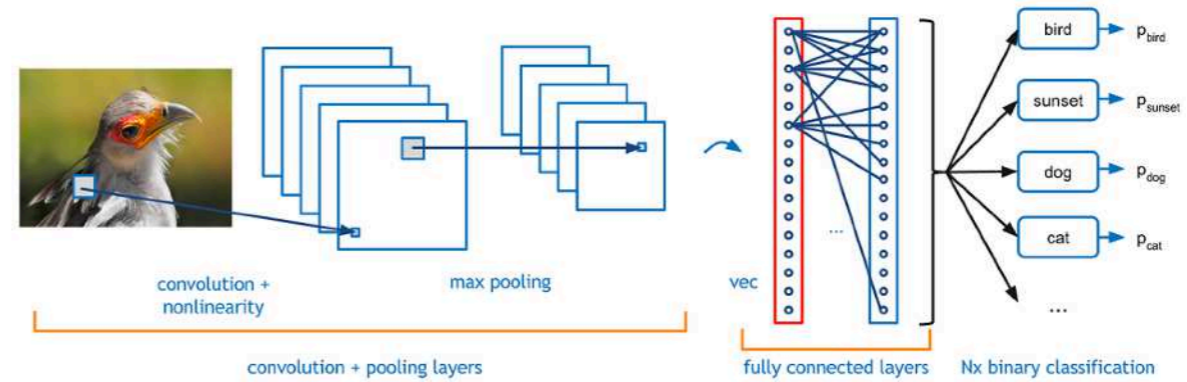
Machine learning is transforming many aspects of society, including fundamental physics research

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

Off-the-Shelf ML for HEP?

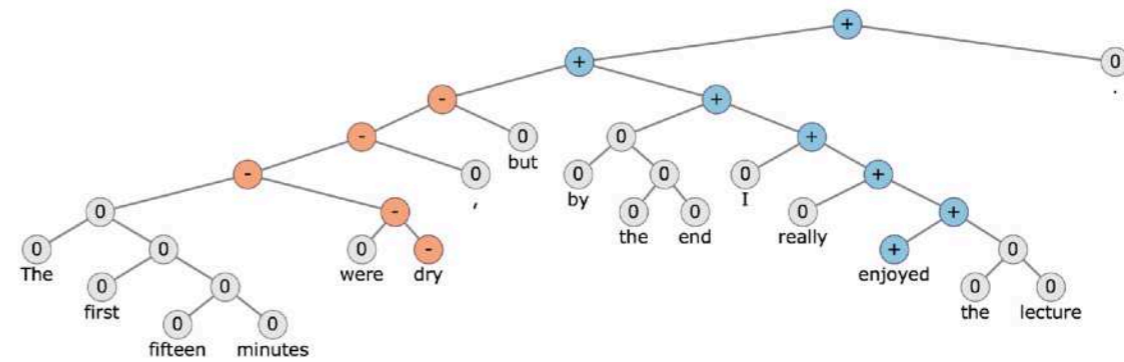
2D Images?

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



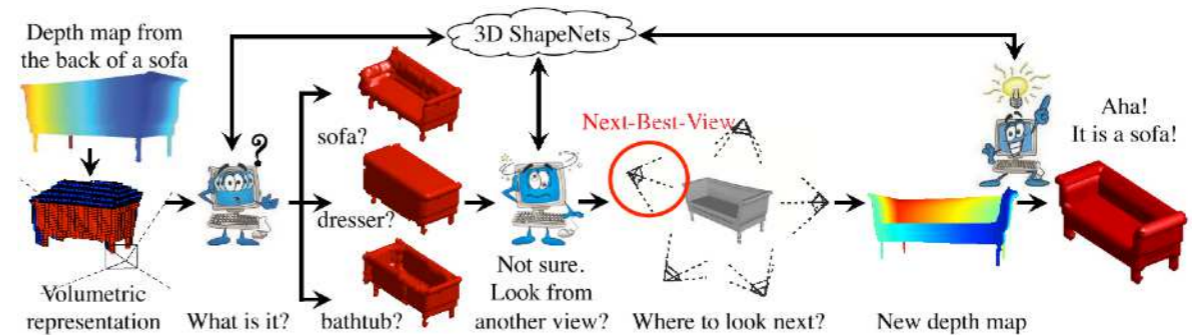
Natural Language?

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



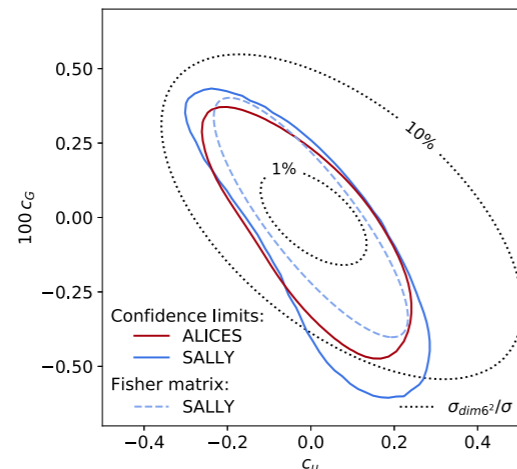
3D Objects?

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



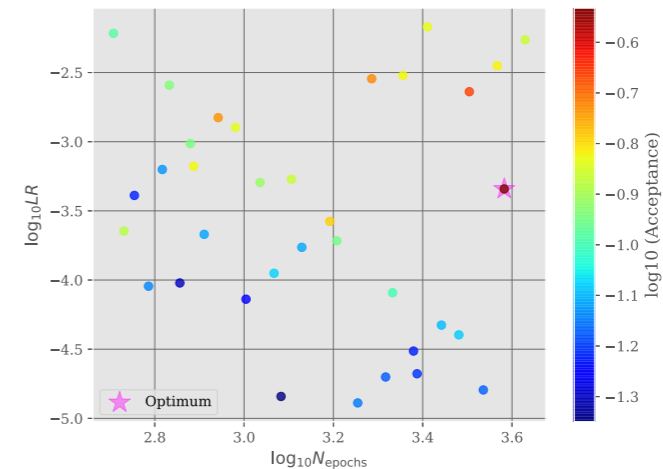
ML Targets for Collider Theory

e.g. Parameter Inference



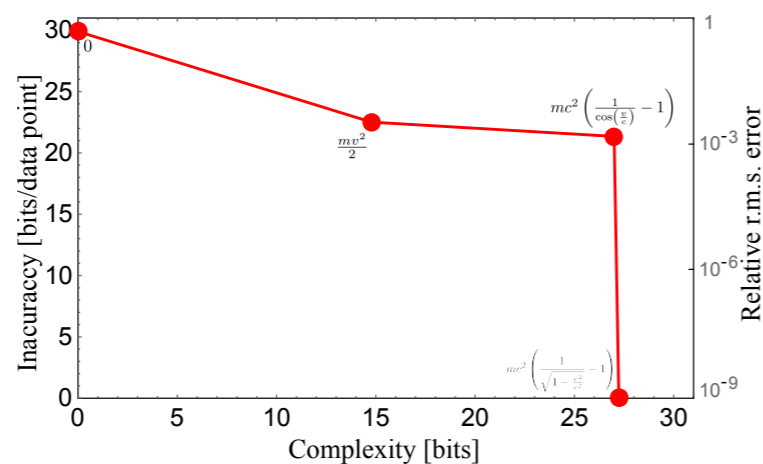
[Brehmer, Kling, Espejo, Cranmer, [CSBS 2020](#)]

e.g. Normalizing Flows



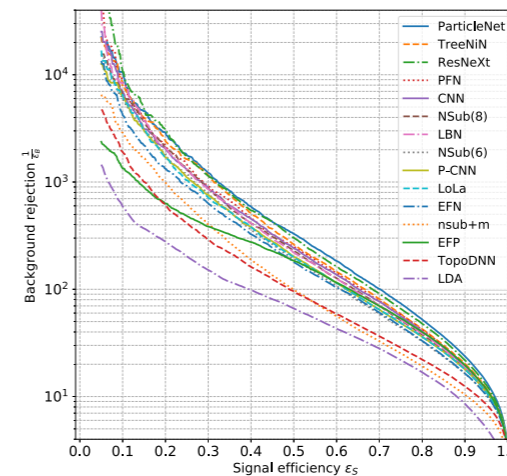
[Gao, Höche, Isaacson, Krause, Schulz, [PRD 2020](#)]

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

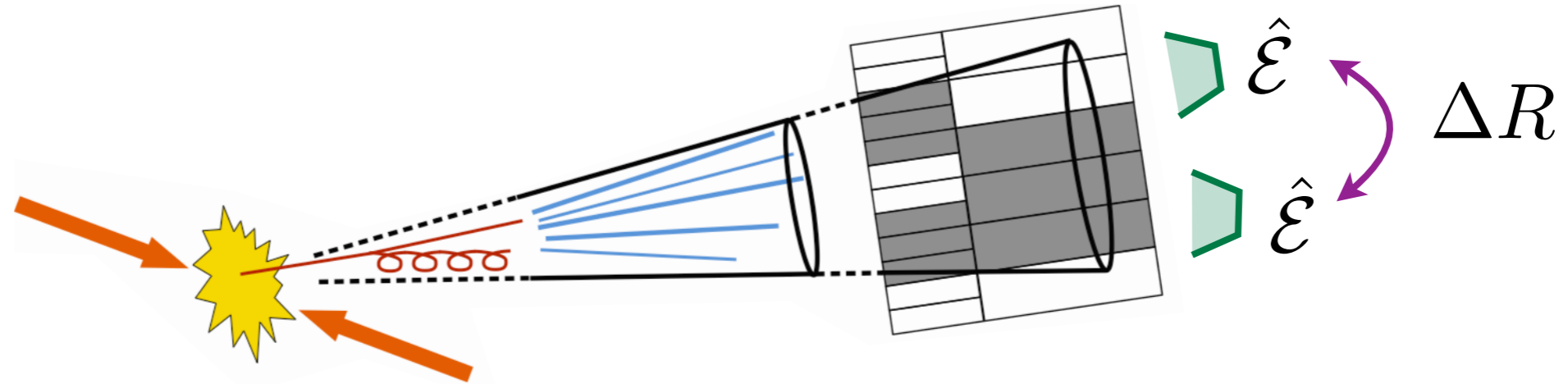
Lagrangian:
$$\mathcal{L}(x) = -p(x) \log f(x) + q(x) (f(x) - 1)$$

Euler-Lagrange:
$$\frac{\partial \mathcal{L}}{\partial f} = 0$$
 Solution:
$$f(x) = \frac{p(x)}{q(x)}$$

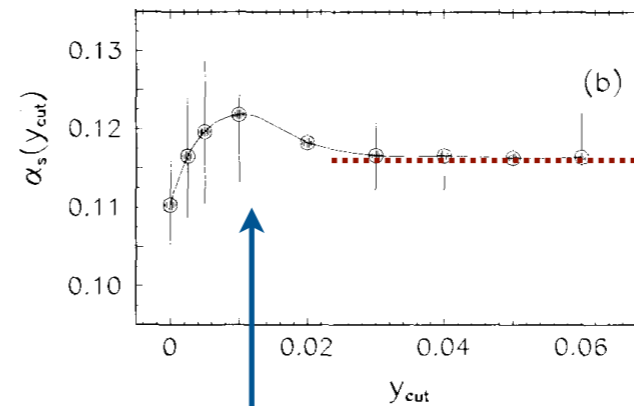
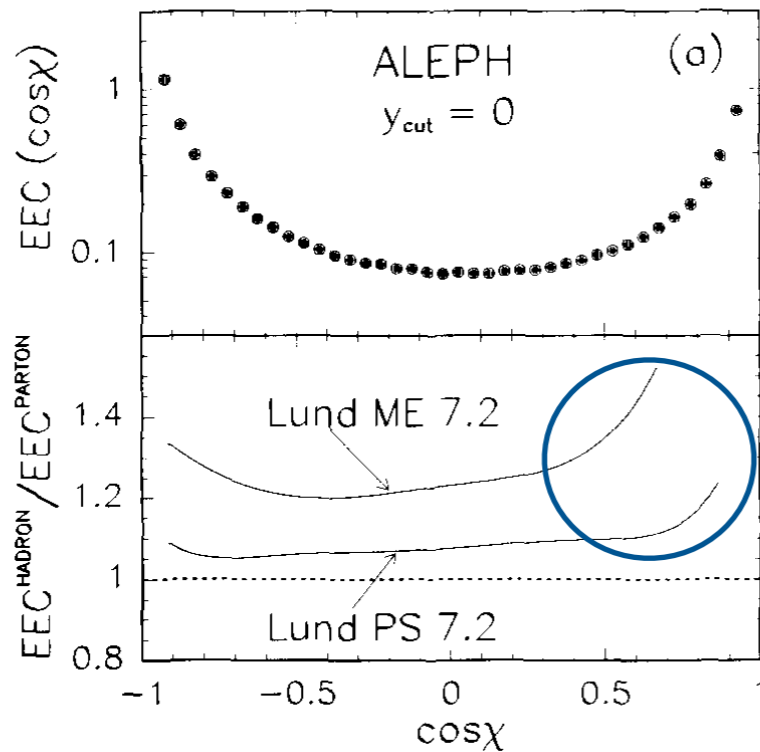
Requires shift in theoretical focus from solving problems to **specifying problems**

[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

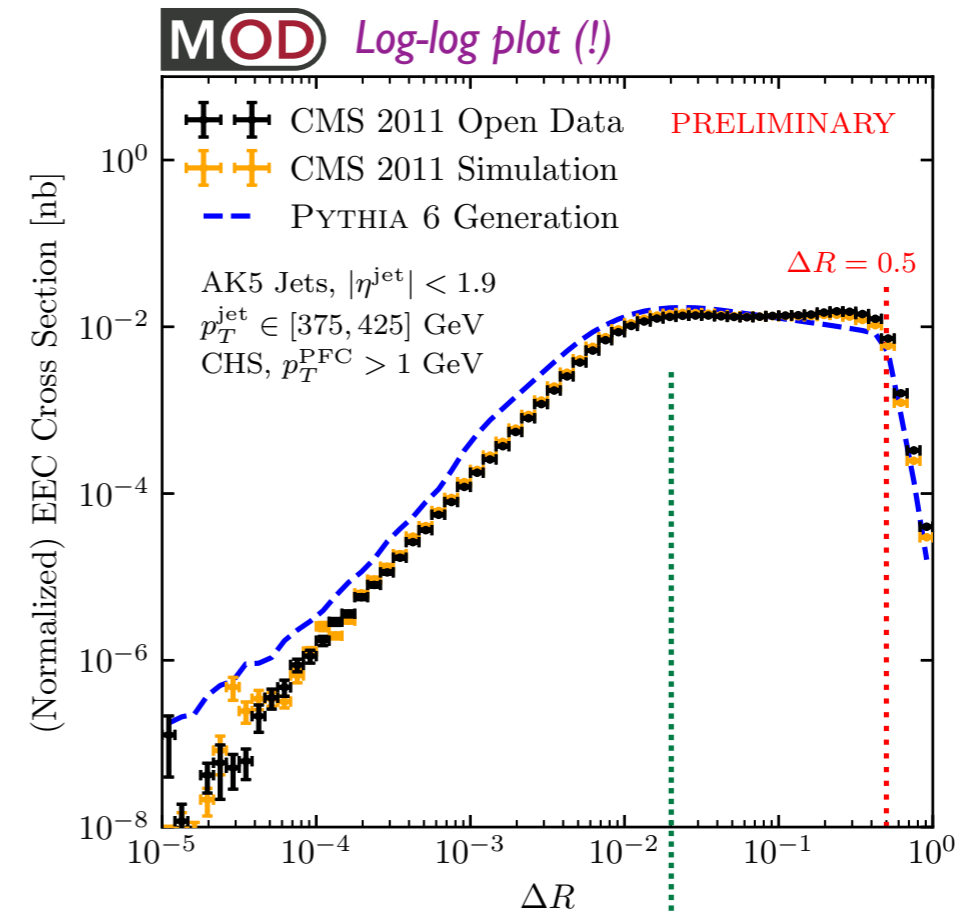
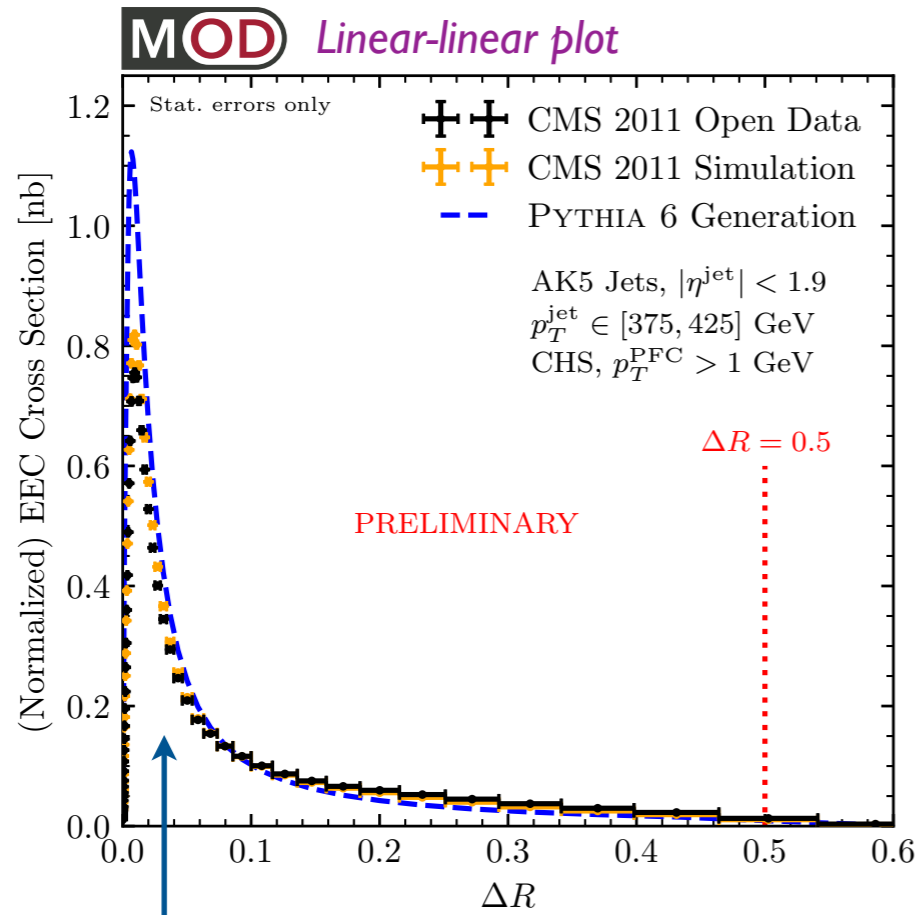


Extracting the strong coupling constant

Theoretical challenges with small angle (collinear) limit

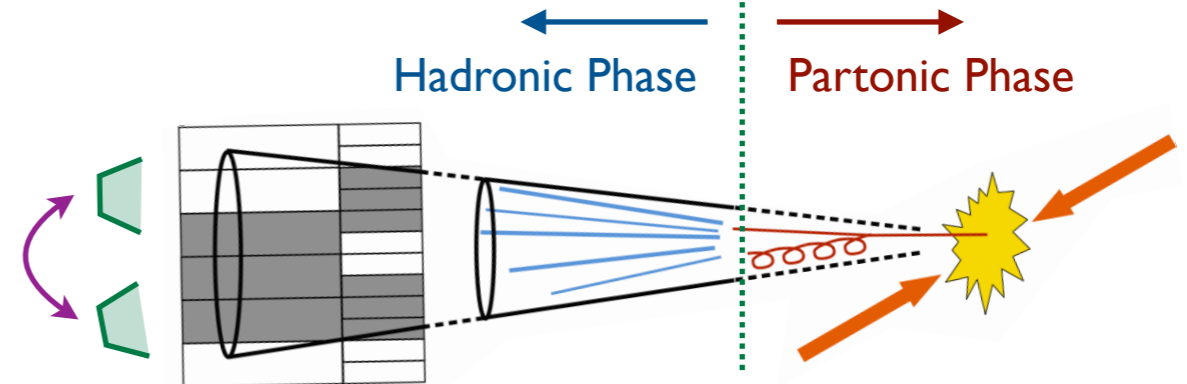
[Basham, Brown, Ellis, Love, PRL 1978; ALEPH, PLB 1991; see Chen, Mout, Zhang, Zhu, PRD 2020]

QCD Phase Transition in Jets?



Are we learning something about small angle limit of QCD?

First Jet EEC Plot from the LHC (!)



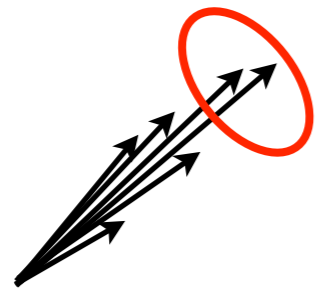
[Komiske, Mout, JDT, Zhu, in progress; see talks by Mout, BOOST 2019, BOOST 2020]



From Curmudgeon...

Jet classification via image recognition

Quark

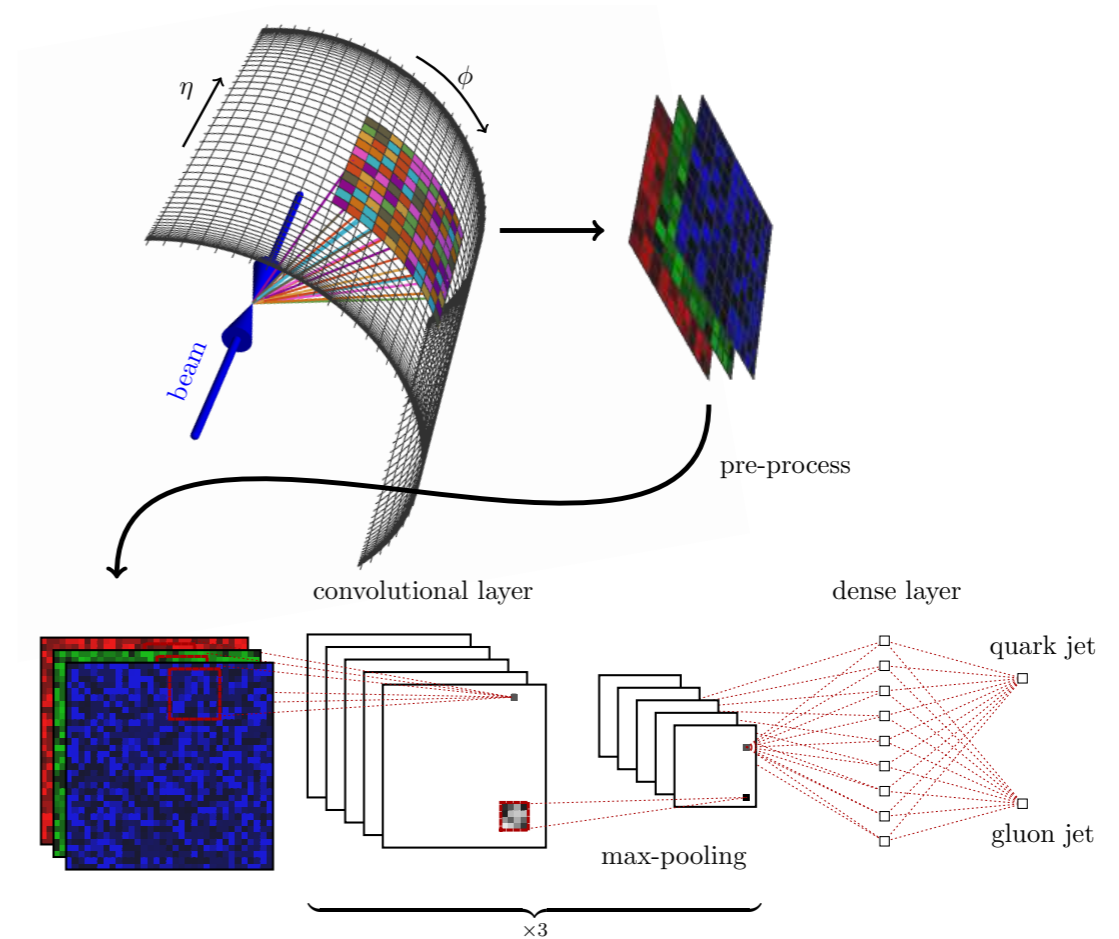


VS.

Gluon



Multi-channel convolutional neural networks



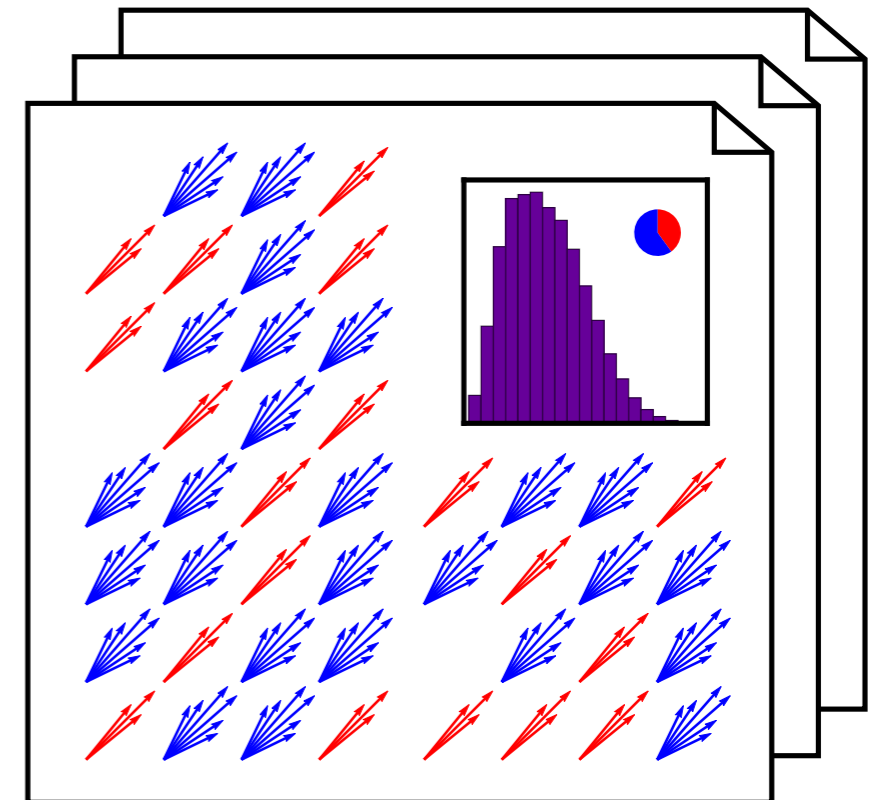
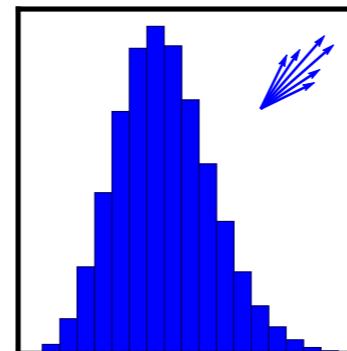
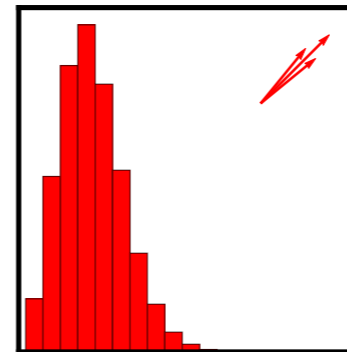
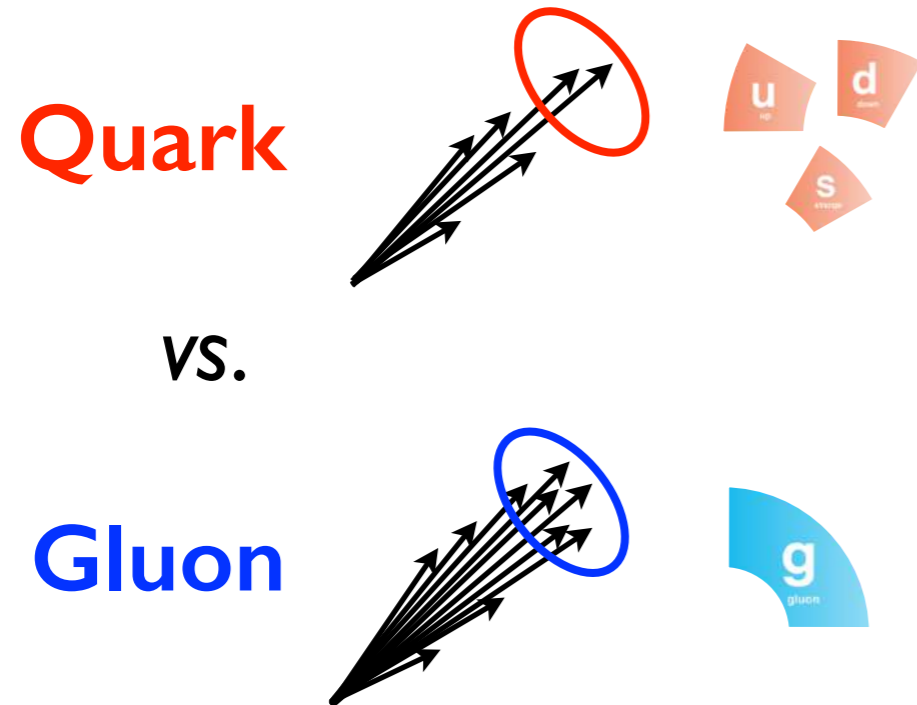
[e.g. Komiske, Metodiev, Schwartz, *JHEP* 2017;
cf. Gras, Höche, Kar, Larkoski, Lönnblad, Plätzer, Siódmok, Skands, Soyez, *JDT, JHEP* 2017]



...to Evangelist

Jet flavor definitions via natural language processing

Topic Modeling / Blind Source Separation

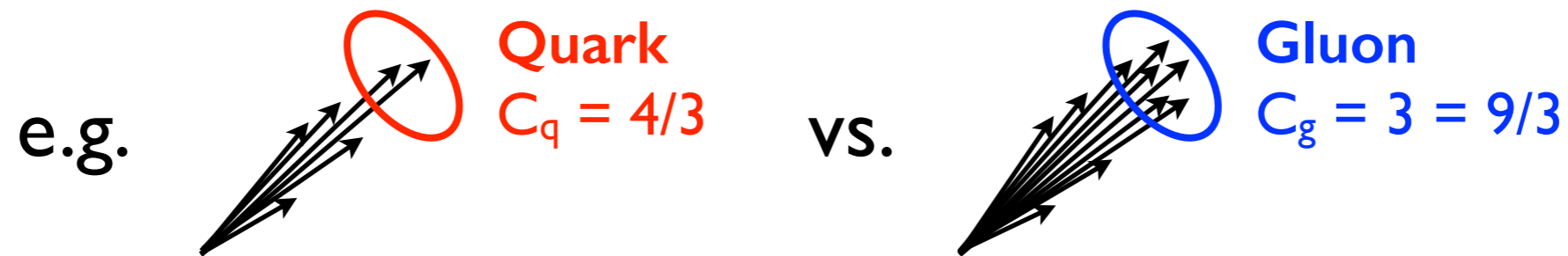
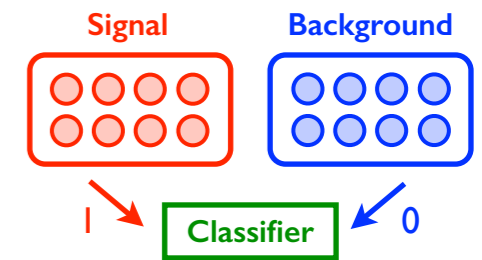


[Komiske, Metodiev, JDT, JHEP 2018;
using Metodiev, Nachman, JDT, JHEP 2017; Metodiev, JDT, PRL 2018; Komiske, Metodiev, JDT, JHEP 2019]



E.g. Quark/Gluon Classification

“Hello, World!” of Jet Physics



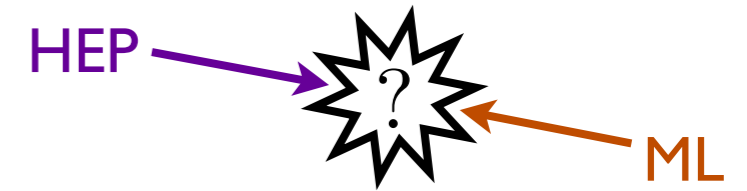
Find $h \left(\text{jet} \right)$ such that

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

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)

[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

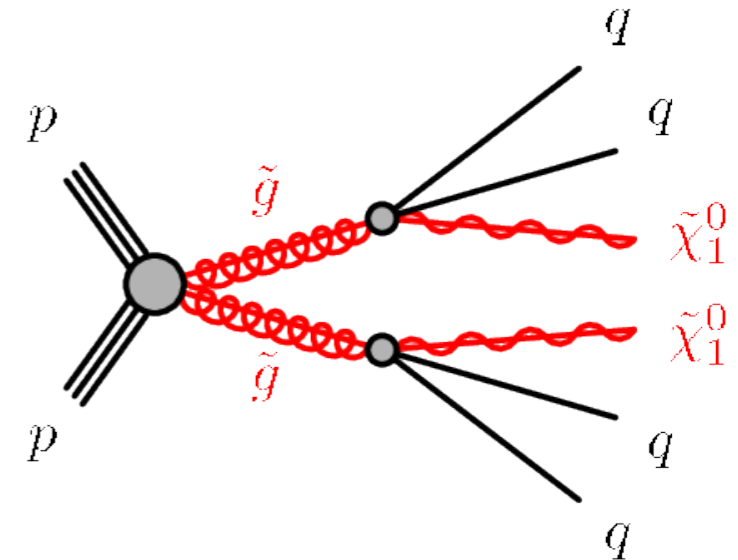


Classifier: Boosted decision tree (for each of 4 jets)

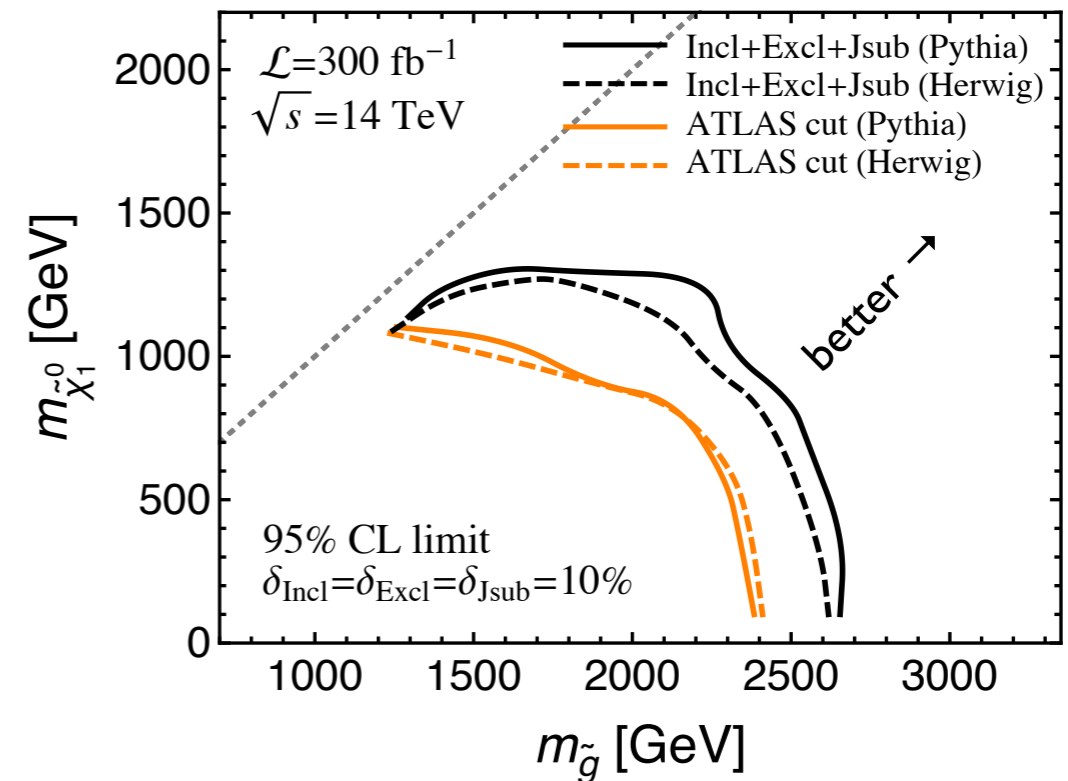
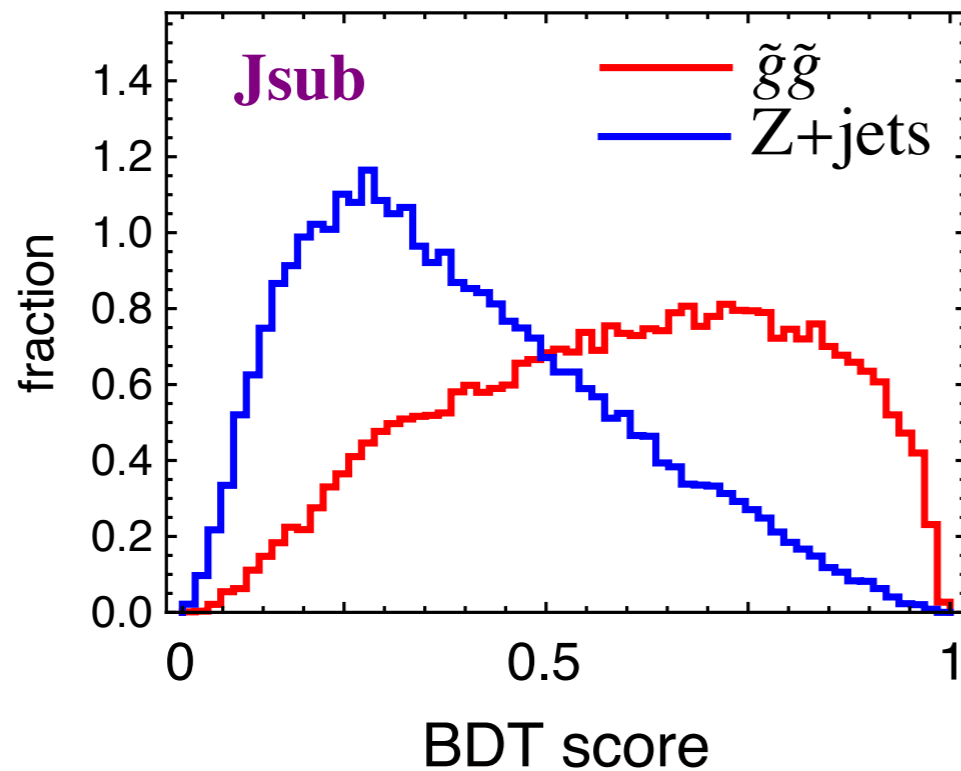
Inputs: Jet mass, width, track multiplicity

Signal: Quark enriched

Background: Gluon enriched

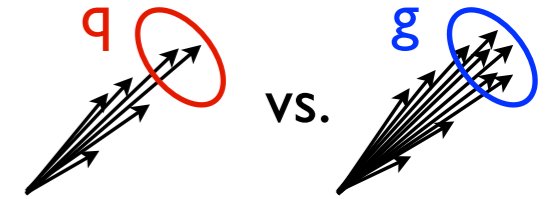


← background signal →



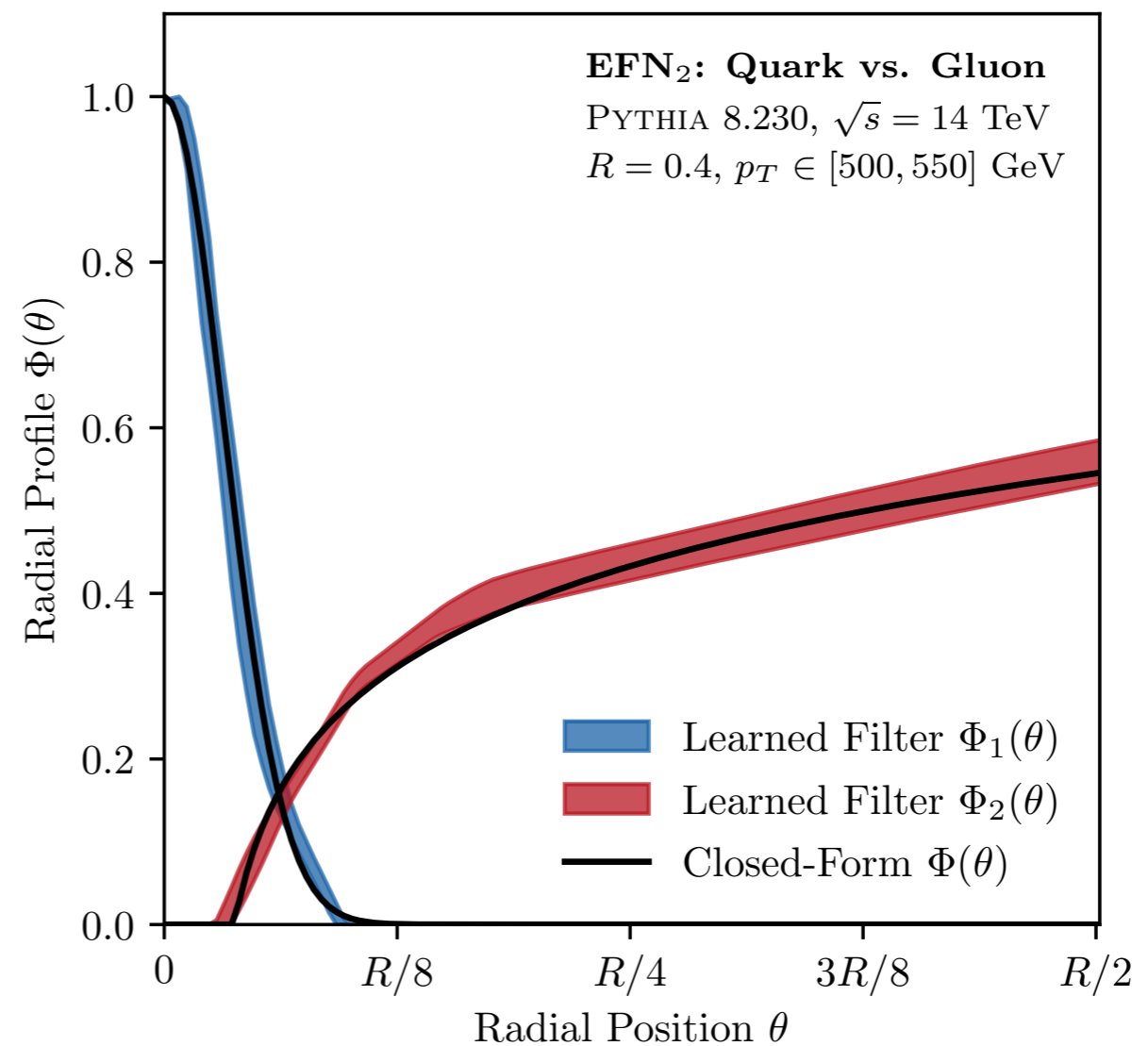
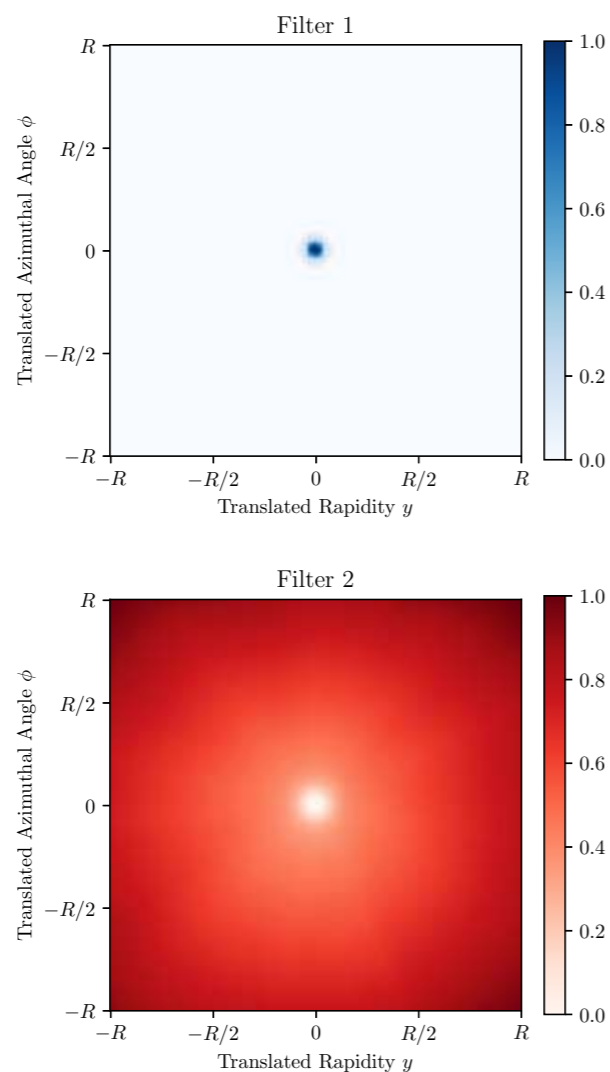
[Bhattacharjee, Mukhopadhyay, Nojiri, Sakakie, Webber, JHEP 2017]

Learning from the Machine



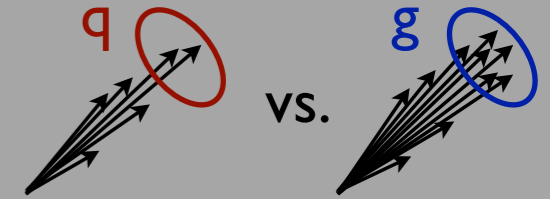
For $\ell = 2$ EFN, radial moments: $\sum_{i \in \text{jet}} z_i f(\theta_i)$

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



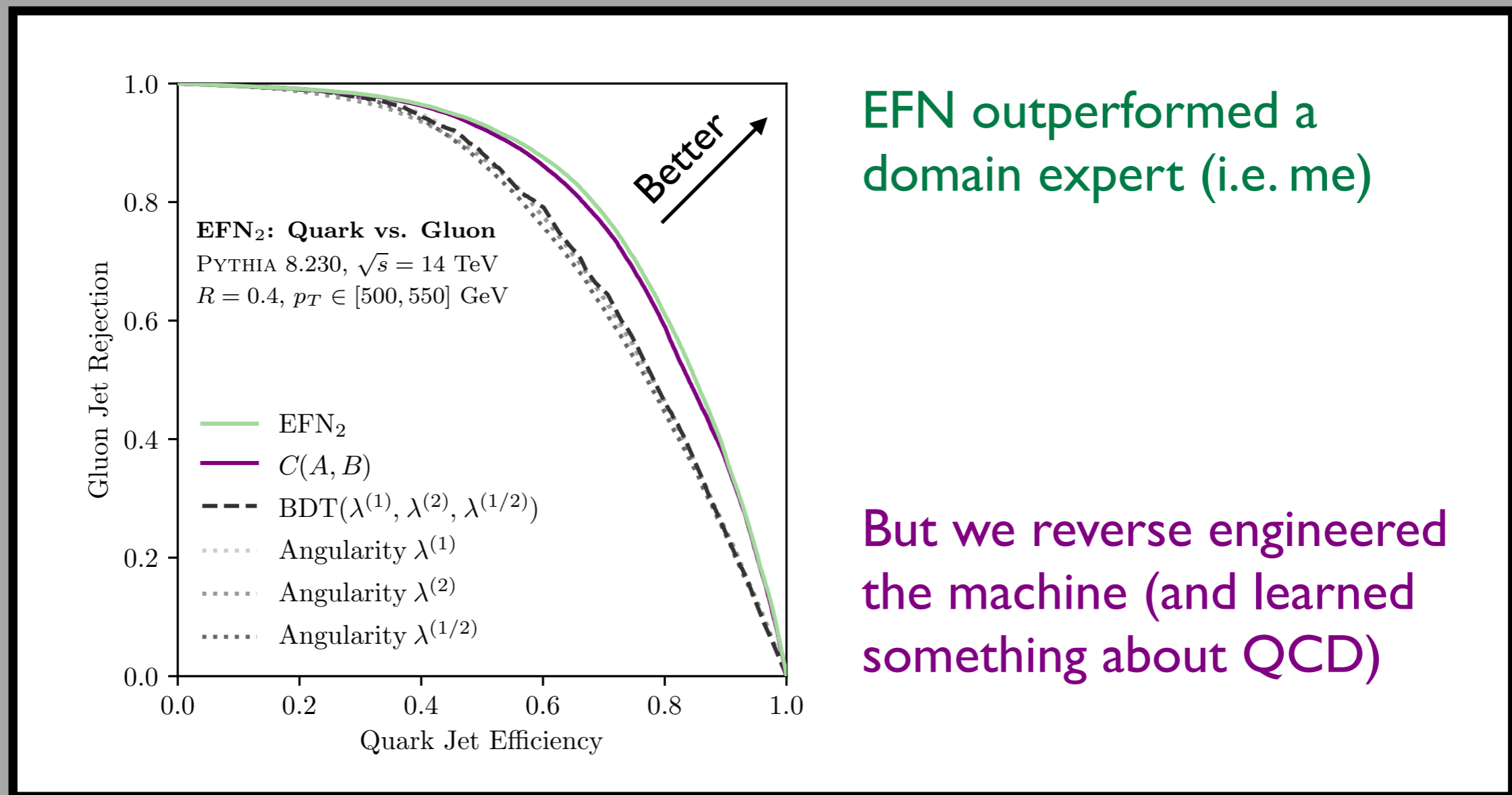
[Komiske, Metodiev, JDT, JHEP 2019;
 cf. Larkoski, JDT, Waalewijn, JHEP 2014; using Berger, Kucs, Sterman, PRD 2003; Ellis, Vermilion, Walsh, Hornig, Lee, JHEP 2010]

Learning from the Machine



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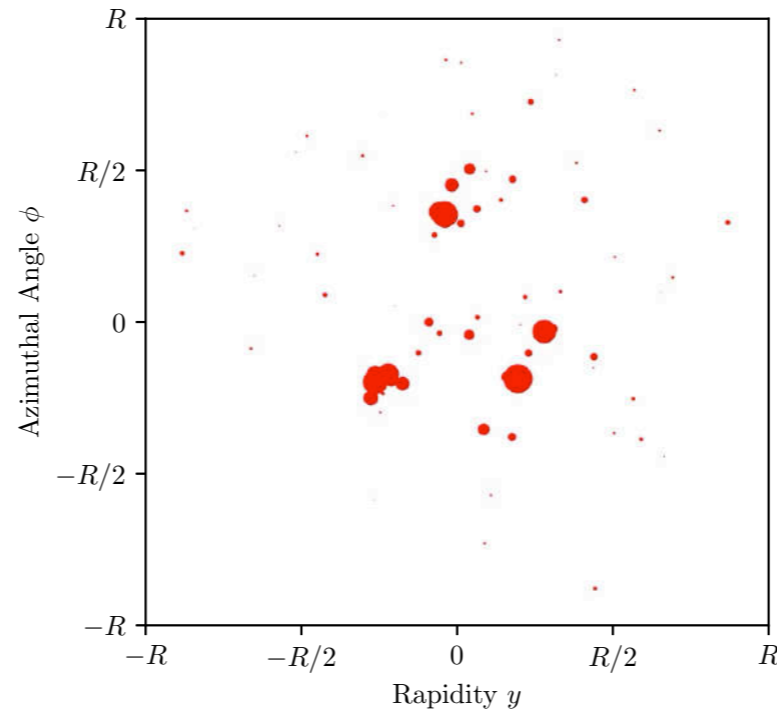
EFN outperformed a domain expert (i.e. me)

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

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

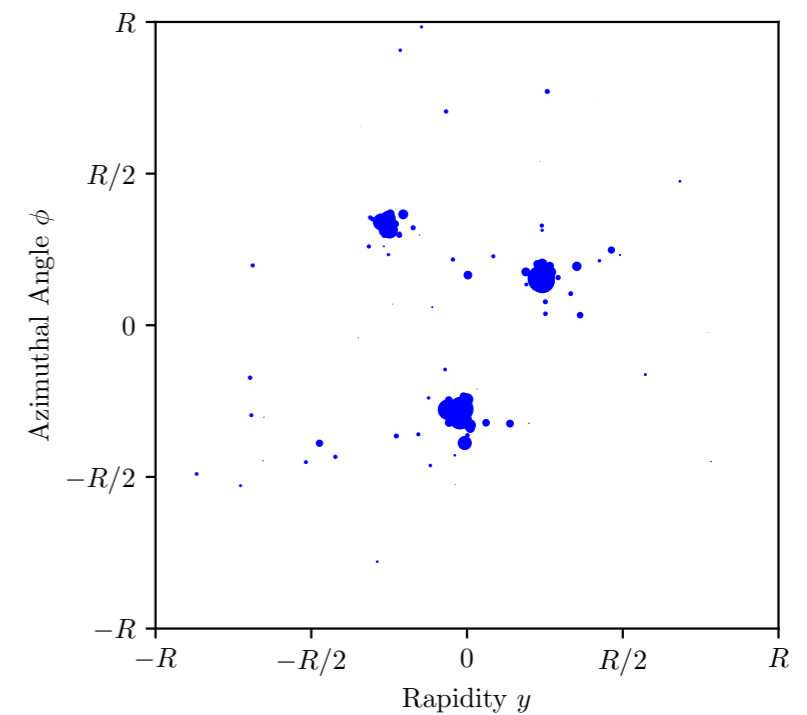
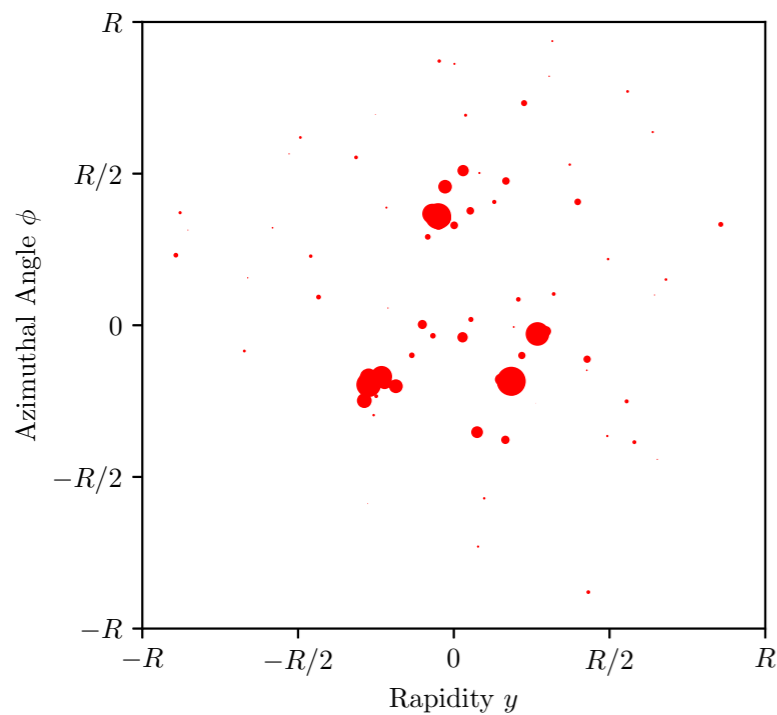
Similarity of Two Energy Flows?

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



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



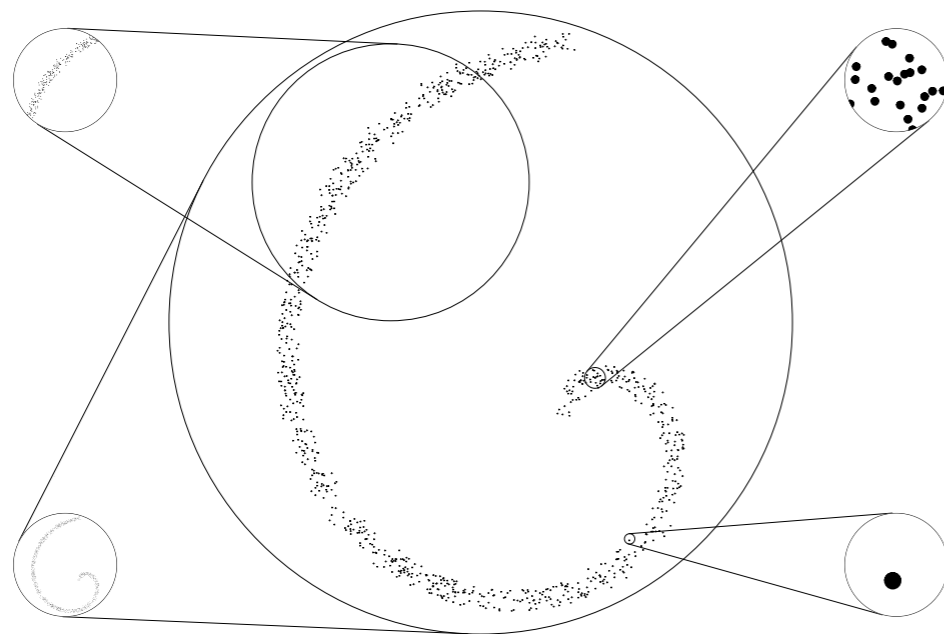
$$N_{\text{neighbors}}(r) \sim r^{\text{dim}}$$

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

[Grassberger, Procaccia, PRL 1983; Kégl, NIPS 2002]

dim ≈ 1

dim ≈ 2

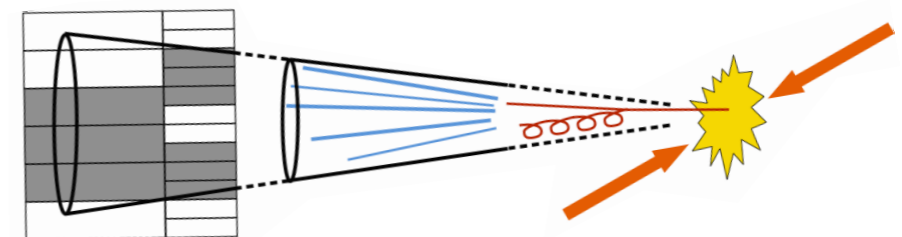
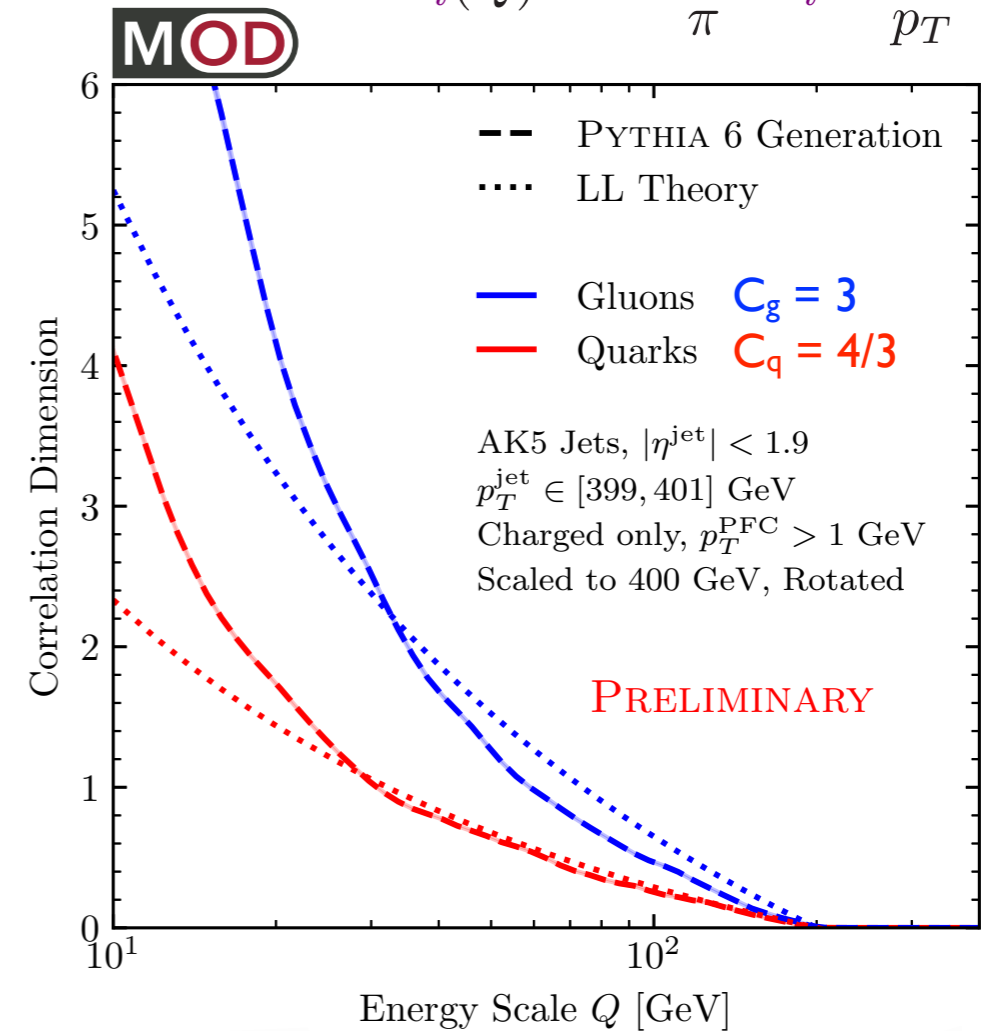


dim ≈ 2

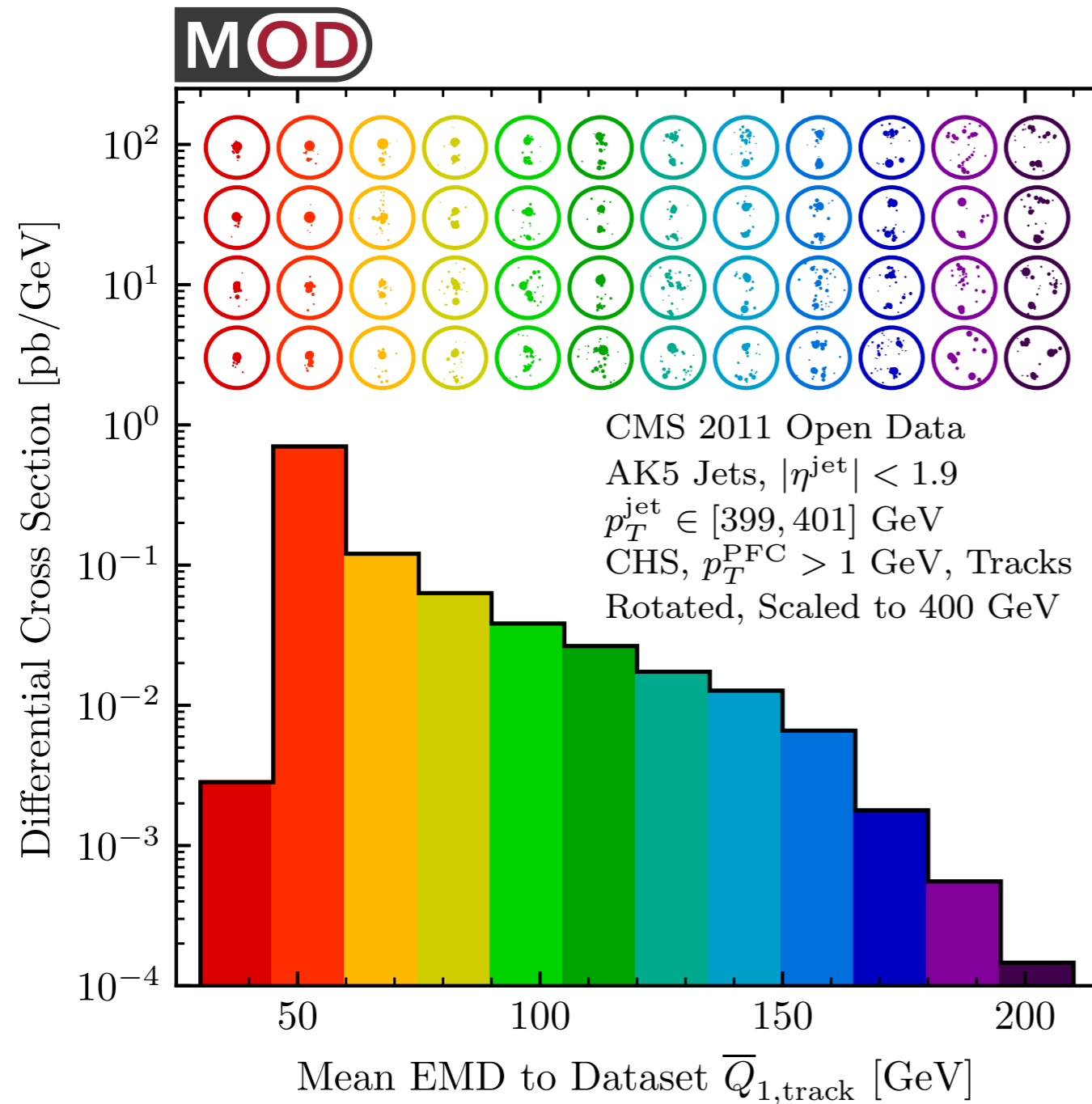
dim ≈ 0

(eventually 0)

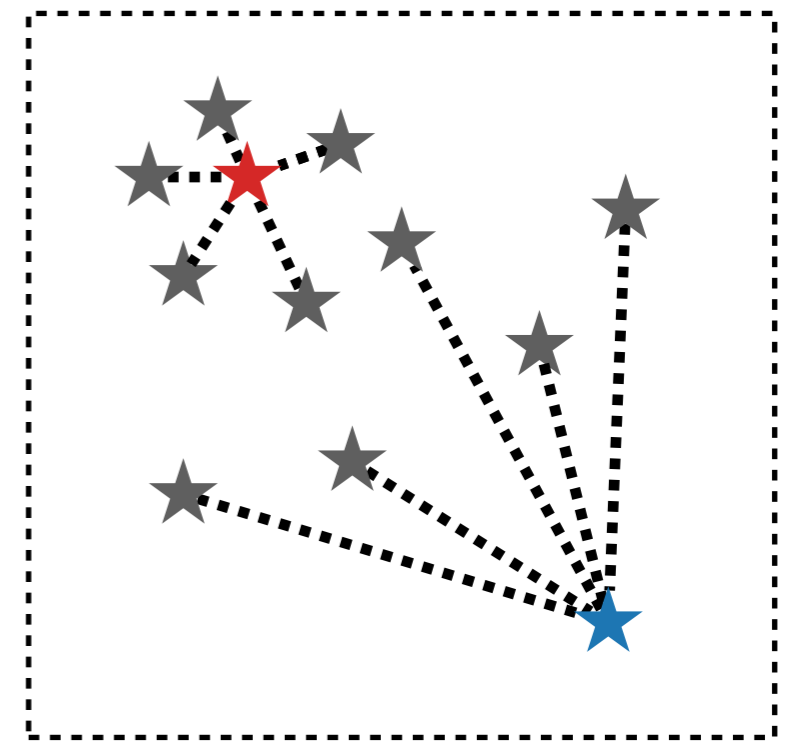
$$\text{dim}_i(Q) \simeq -\frac{8\alpha_s}{\pi} C_i \ln \frac{Q}{p_T}$$



Least Representative Jets



New Physics?
 Or tails of QCD?

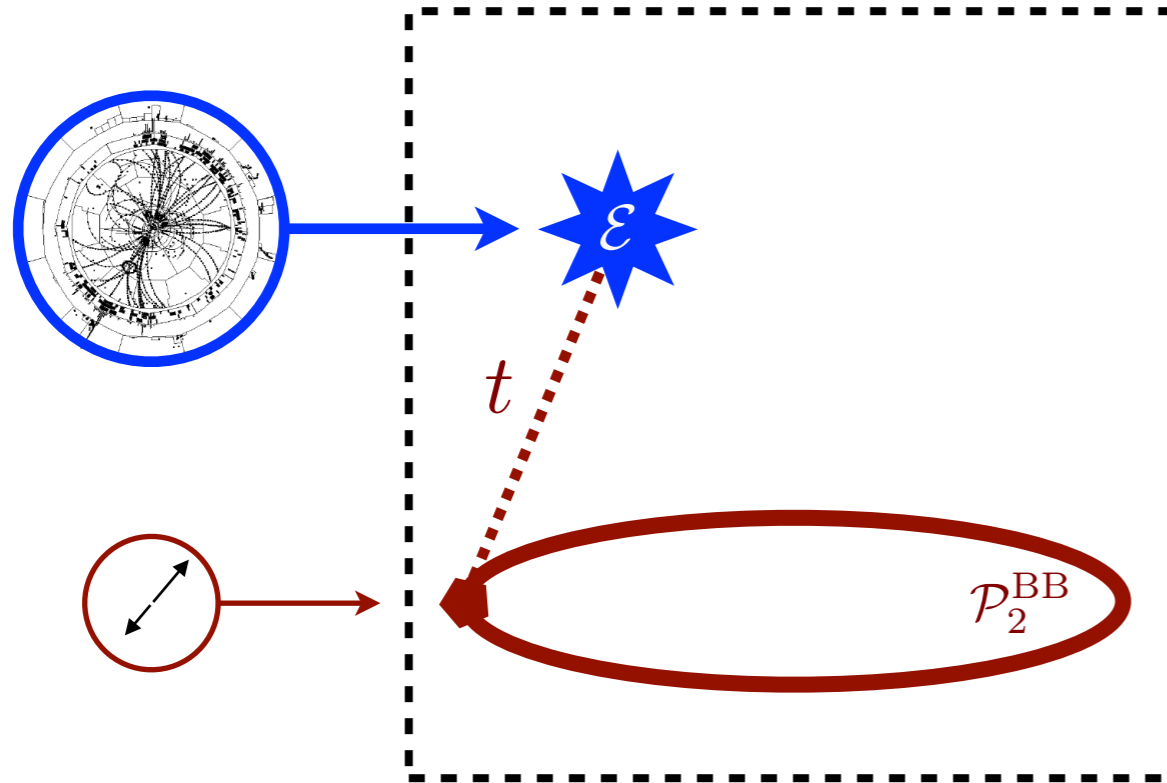


[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]



Back to the Future with Thrust

How dijet-like is an event?

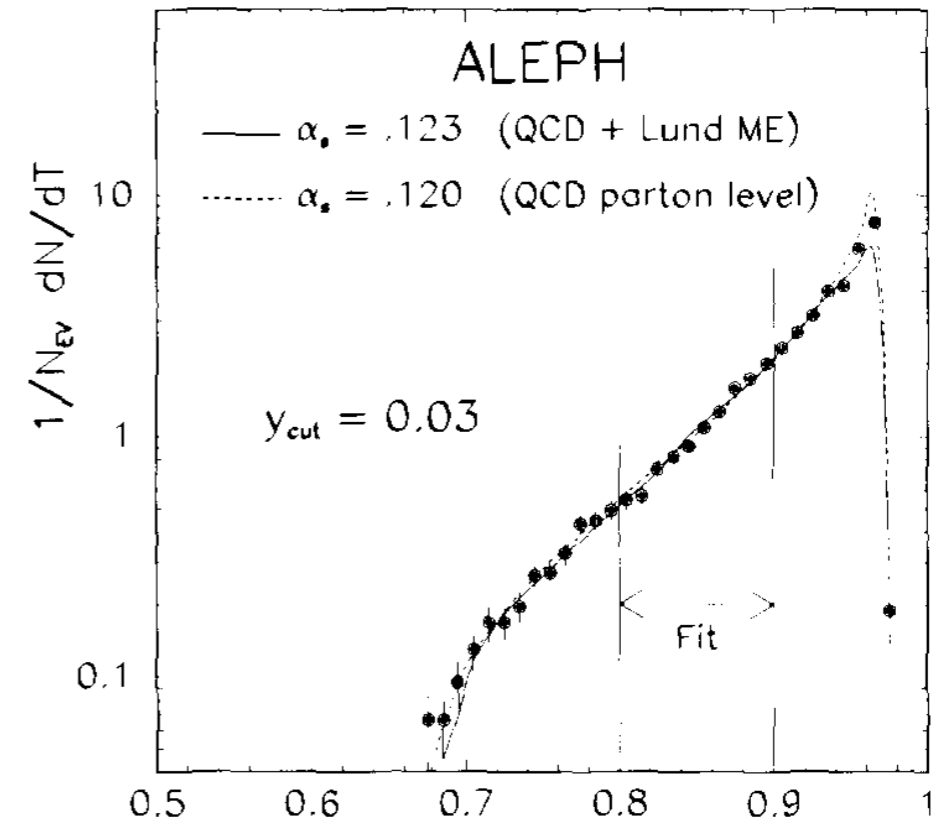


All Back-to-Back Two Particle Configurations

$$\mathcal{P}_2^{\text{BB}} = \left\{ \begin{array}{c} \text{---} \text{---} \text{---} \text{---} \text{---} \end{array} \right\}$$

(using $\beta=2$ EMD variant)

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



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

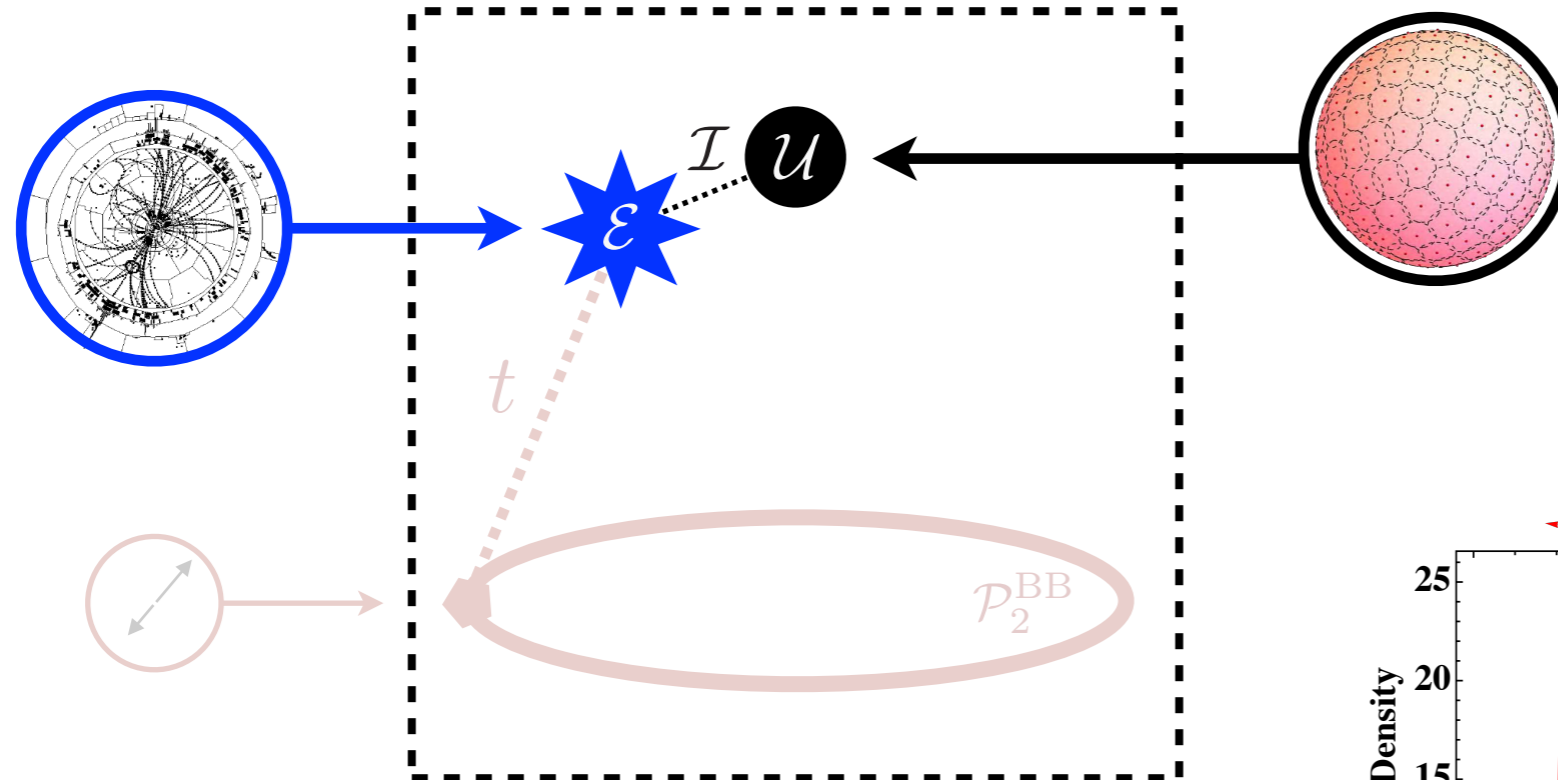
(flipped, linear version of ALEPH thrust plot from before)

[Komiske, Metodiev, JDT, JHEP 2020]

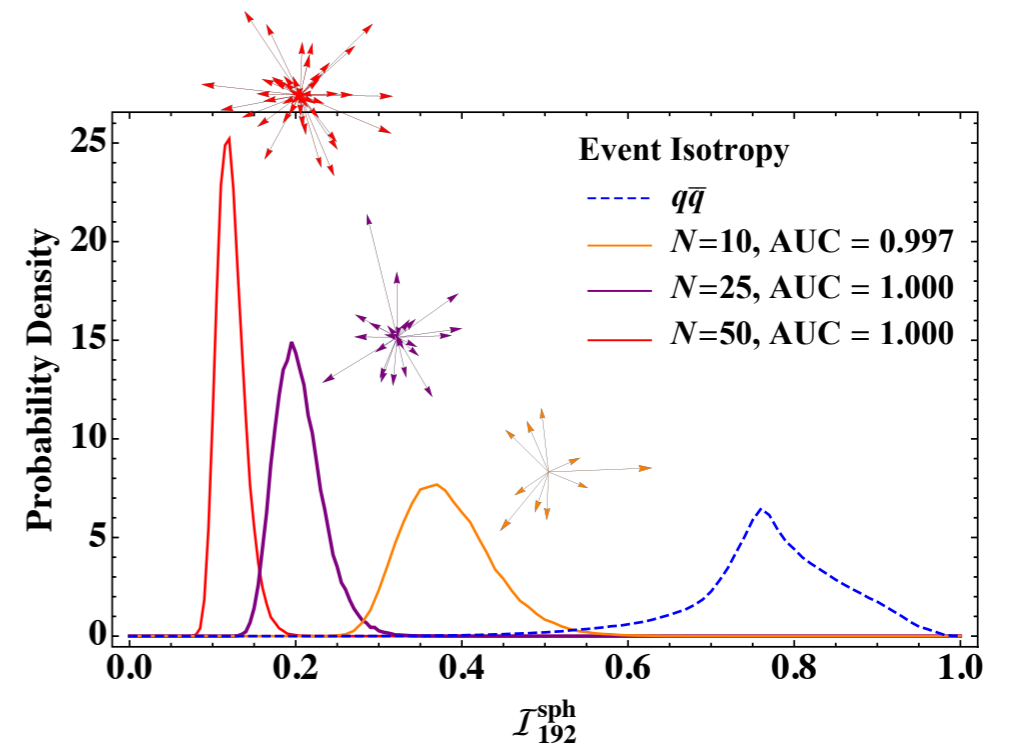
[Brandt, Peyrou, Sosnowski, Wroblewski, PL 1964; Farhi, PRL 1977; ALEPH, PLB 1991]

Event Isotropy from Collider Geometry

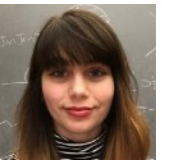
How uniform is an event?



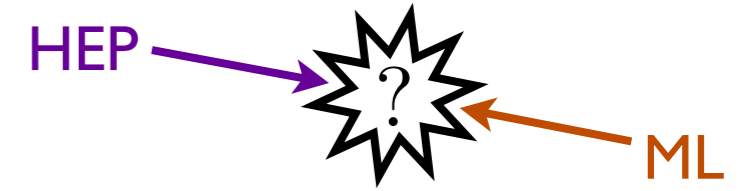
$$\mathcal{I}(\mathcal{E}) = \text{EMD}(\mathcal{E}, \mathcal{U})$$



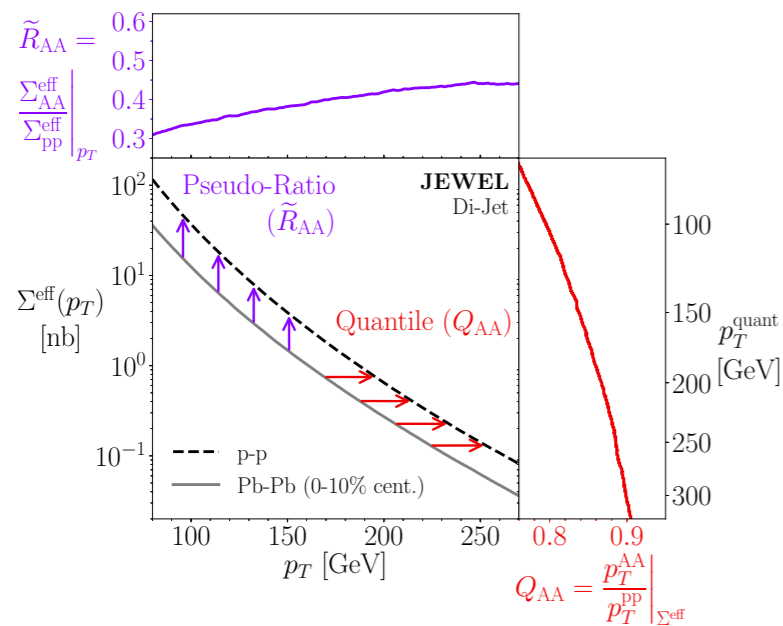
[Cesarotti, JDT, JHEP 2020;
see also Cesarotti, Reece, Strassler, arXiv 2020]



More Collisions

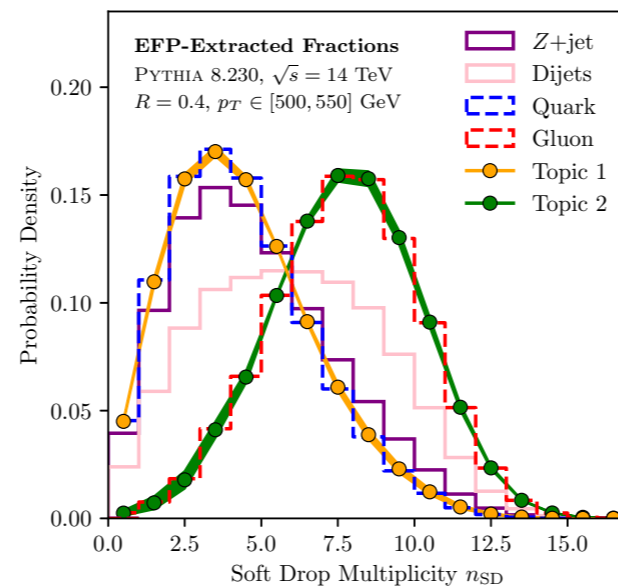


Jet Quenching via Optimal Transport



[Brewer, Milhano, JDT, PRL 2019]

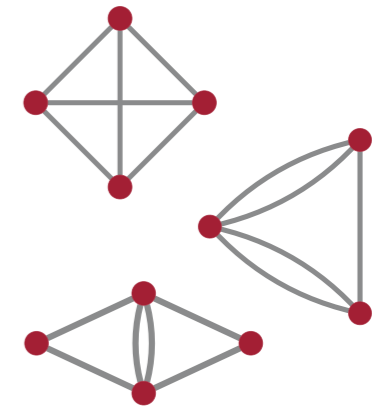
Quark/Gluon Definitions via Blind Source Separation



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

Kinematic Decomposition via Graph Theory

Edges d	Leafless Multigraphs	
	Connected	All
1	0	0
2	1	1
3	2	2
4	4	5
5	9	11
6	26	34
7	68	87
8	217	279
9	718	897
10	2553	3129
11	9574	11458
12	38005	44576
13	157306	181071
14	679682	770237
15	3047699	3407332
16	14150278	15641159



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