

# Artificial Intelligence and High-Energy Physics

Jesse Thaler



Master Your Physics, University of Amsterdam — June 15, 2021

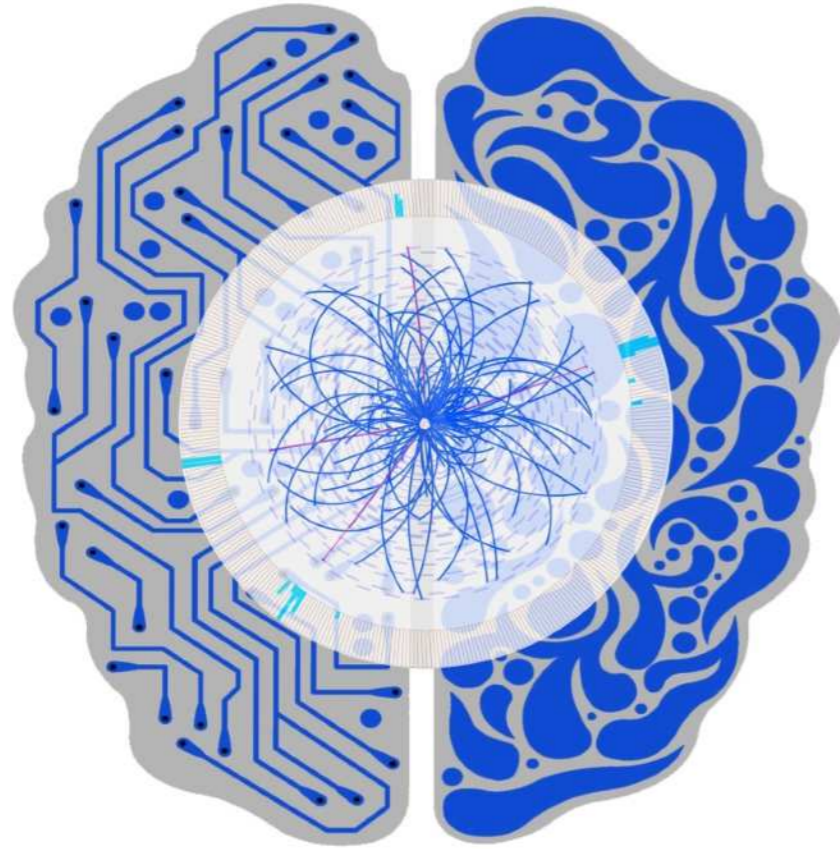
# The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI) *“eye-phi”*

*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]





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

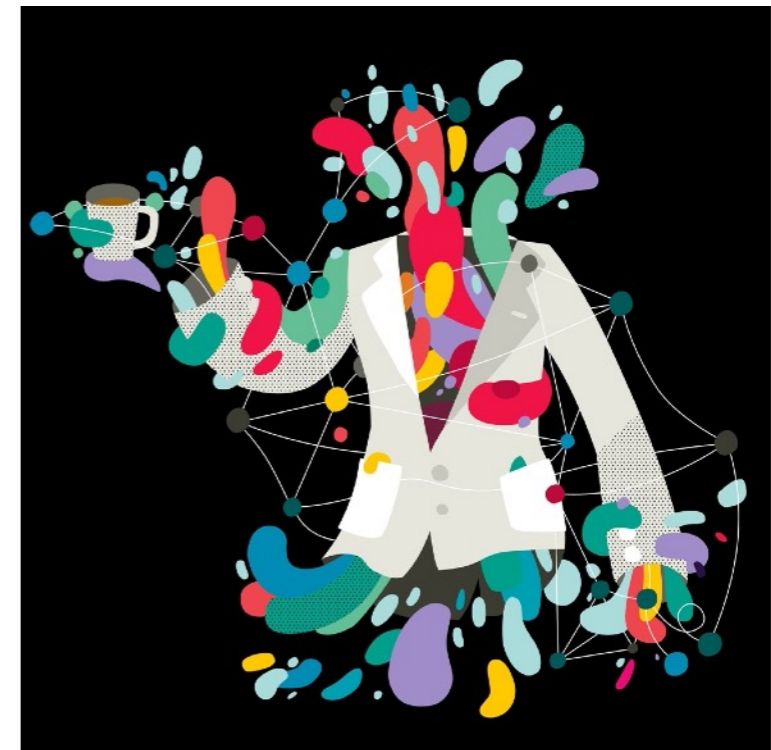
**The New York Times**



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*



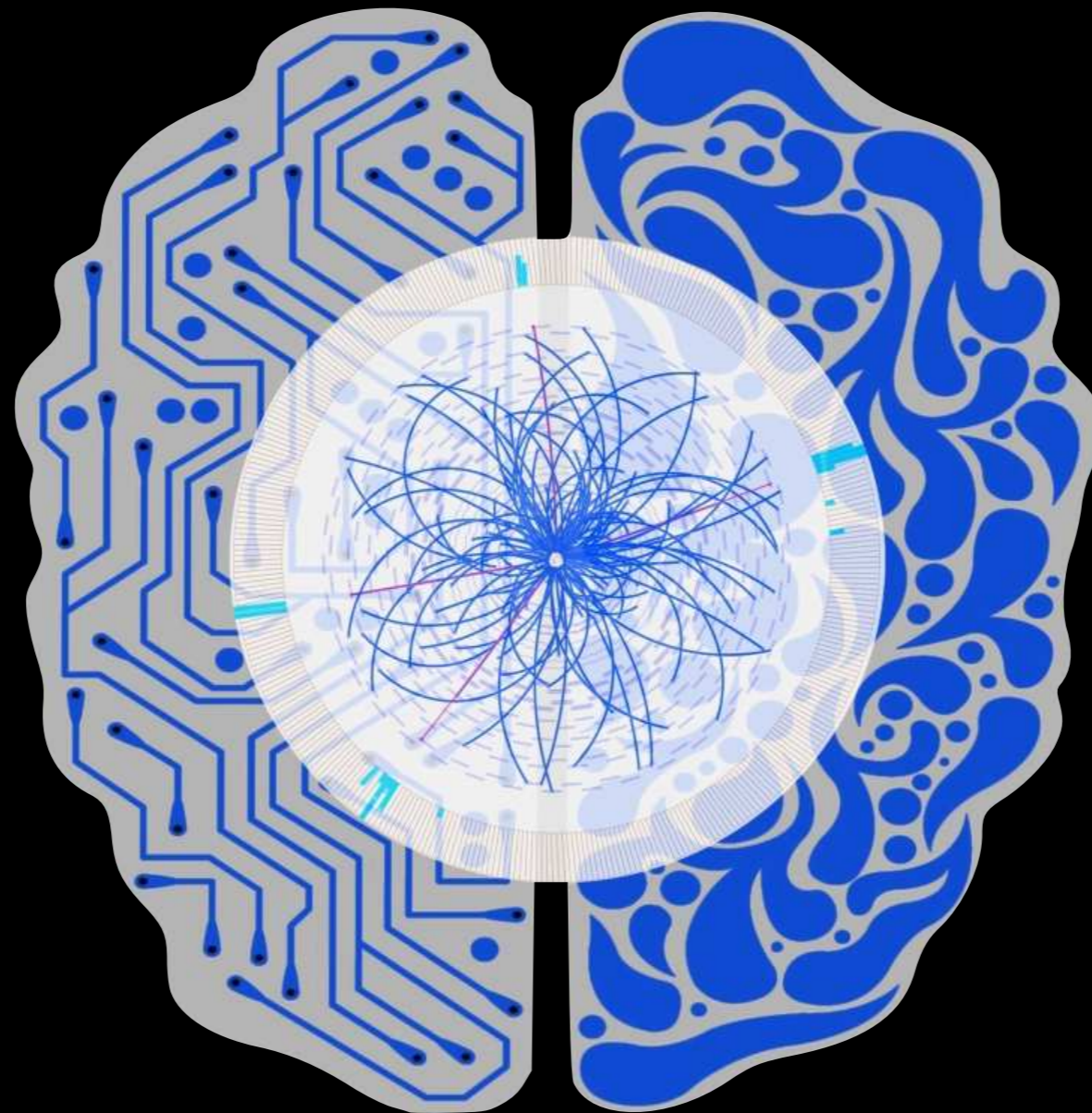
Using randomly initialized neural network (!)

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

[Ulyanov, Vedaldi, Lempitsky, [CVPR 2018](#)]



# The Lens of Machine Learning



*What formalisms are needed to leverage ML for HEP?*

# 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. Cranmer, Pavez, Louppe, [arXiv 2015](#); D’Agnolo, Wulzer, [PRD 2019](#);  
simulation-based inference in Cranmer, Brehmer, Louppe, [PNAS 2020](#);  
relation to f-divergences in Nguyen, Wainwright, Jordan, [AoS 2009](#); Nachman, Thaler, [arXiv 2021](#)]



# 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 focus from solving problems to **specifying problems**

[see e.g. Cranmer, Pavez, Louppe, [arXiv 2015](#); D'Agnolo, Wulzer, [PRD 2019](#);  
simulation-based inference in Cranmer, Brehmer, Louppe, [PNAS 2020](#);  
relation to f-divergences in Nguyen, Wainwright, Jordan, [AoS 2009](#); Nachman, Thaler, [arXiv 2021](#)]

# Machine Learning Requirements

*If you have in hand...*

Well-specified loss  
Reliable training data  
Learnable function

*...then you can leverage ML!*

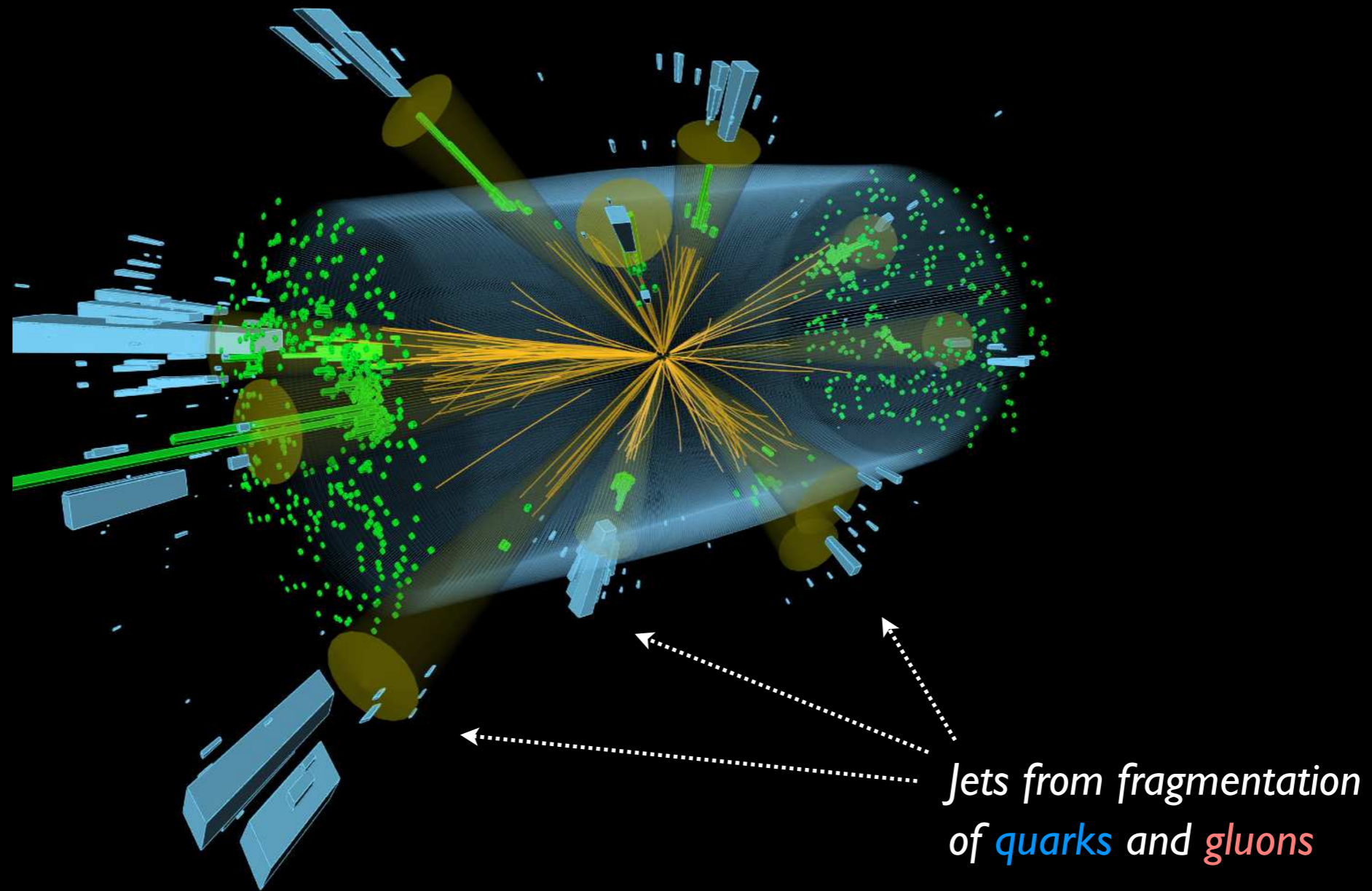
Many HEP tasks can be **phrased in this language**

**Physics input essential** for robust usage of these tools

[see [HEPML-LivingReview](#) for extensive bibliography]



# Machine Learning for High-Energy Physics

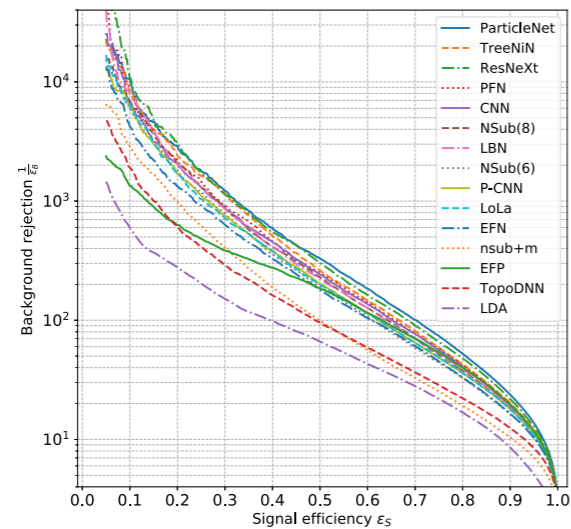


*What tasks are amenable to a machine learned approach?*

# Optimization in Collider Physics

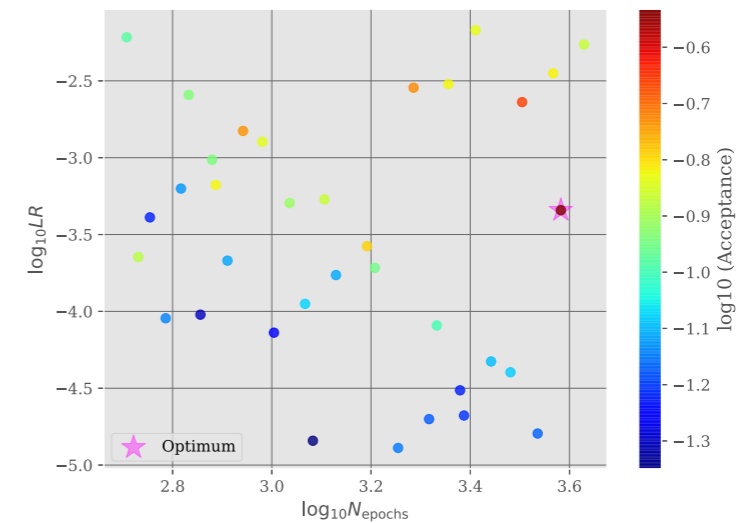
*This slide is far from exhaustive*

## Jet Classification



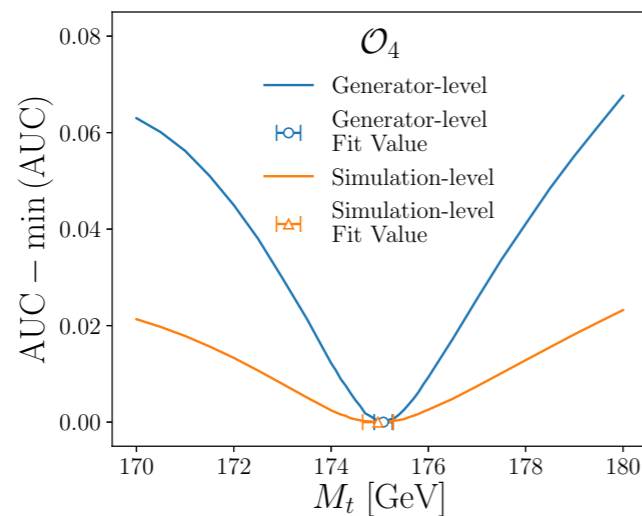
[e.g. Kasieczka, Plehn, et al., [SciPost 2019](#)]

## Phase Space Integration



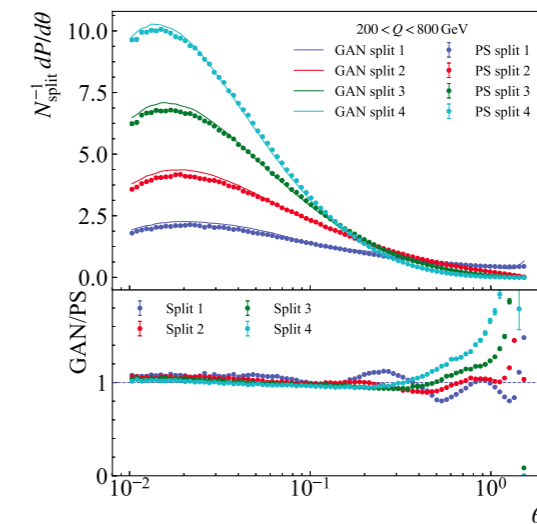
[e.g. Gao, Höche, Isaacson, Krause, Schulz, [PRD 2020](#)]

## Parameter Estimation



[e.g. Andreassen, Hsu, Nachman, Suaysom, Suresh, [PRD 2021](#)]

## Parton Shower Modeling

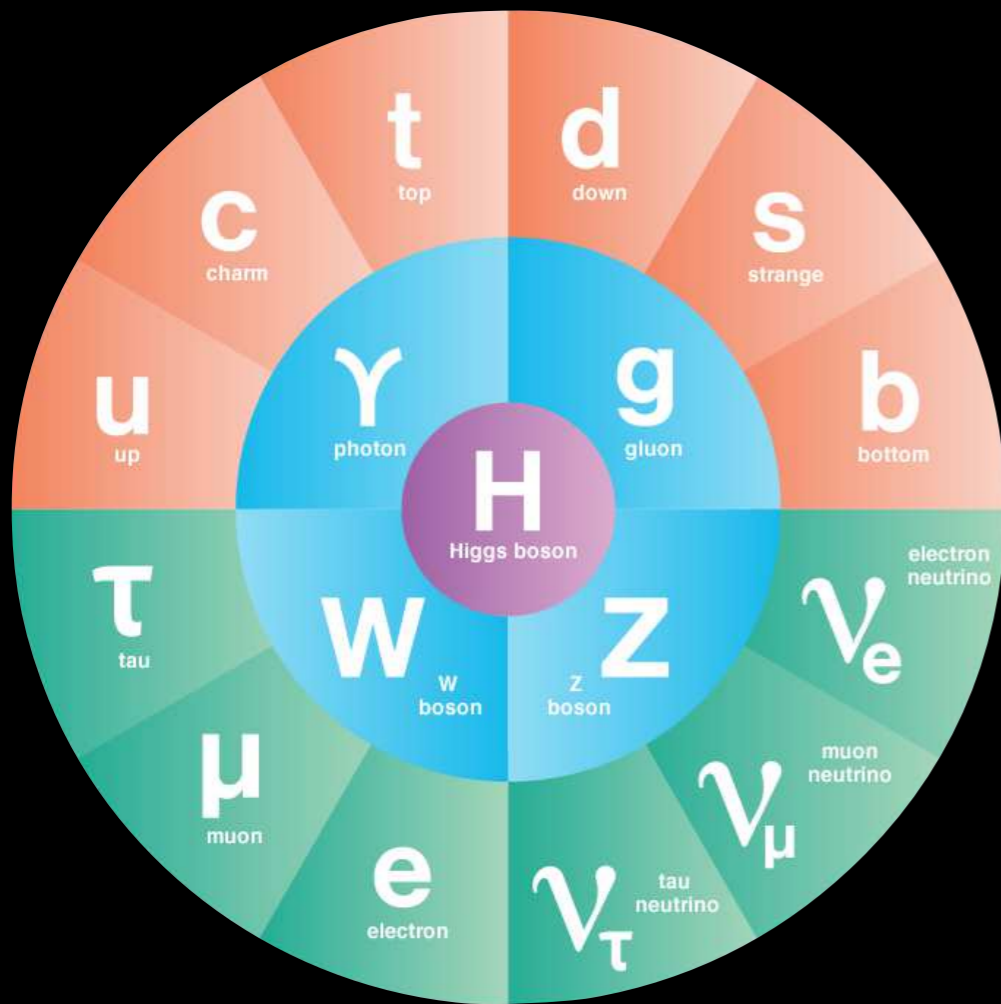


[e.g. Lai, Neill, Płoskoń, Ringer, [arXiv 2020](#)]

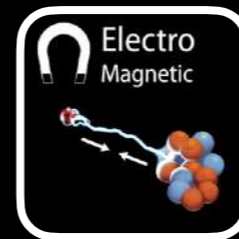
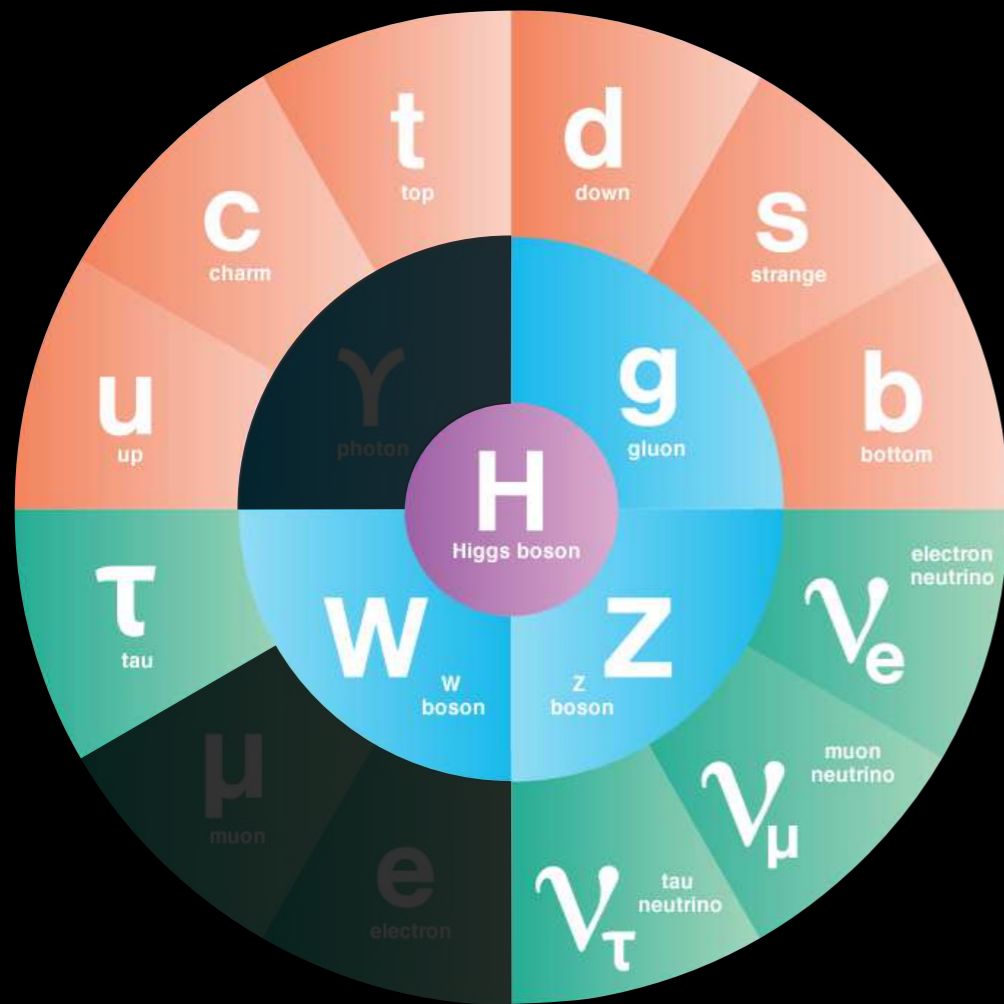
...



# Particle Physics 101



# Particle Physics 101

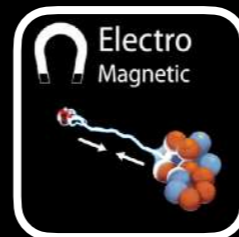
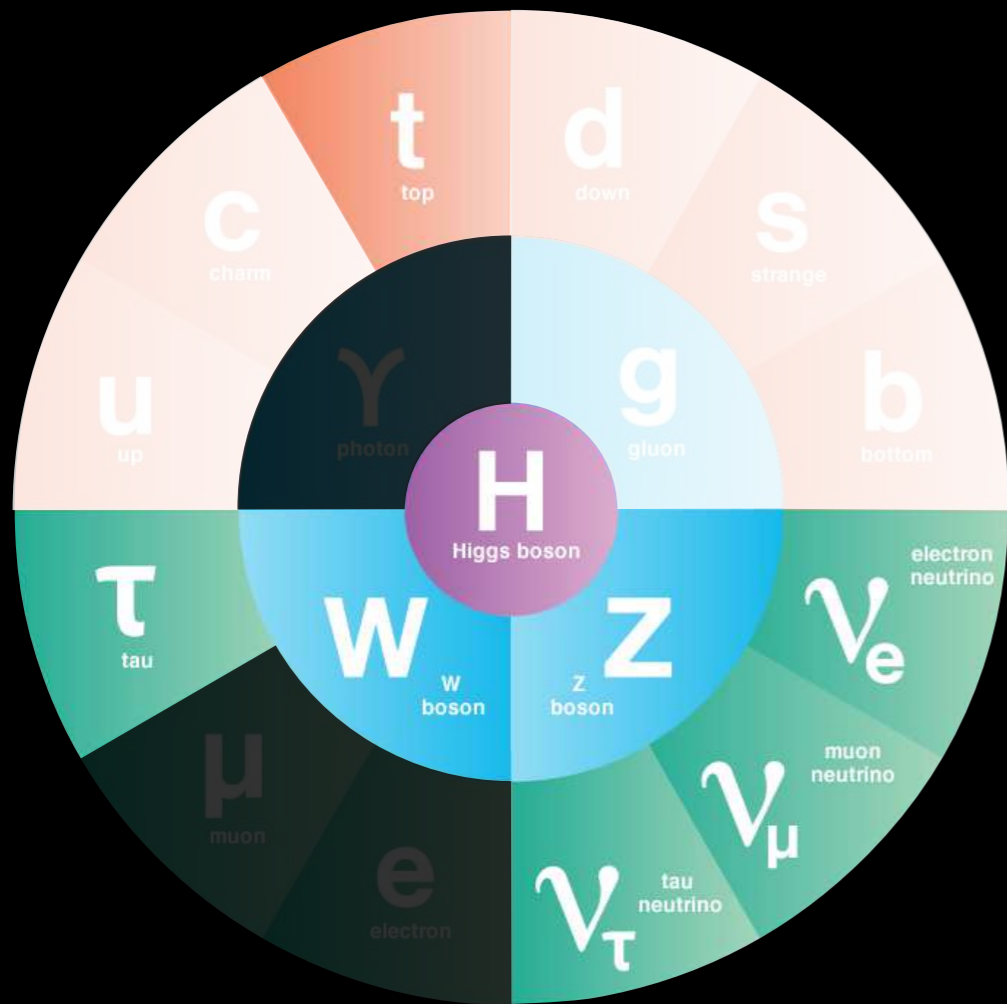


$\gamma$  photon  
 $e^\pm$  electron  
 $\mu^\pm$  muon

elementary

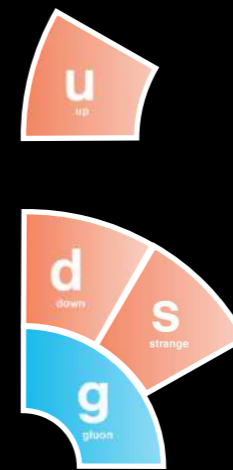
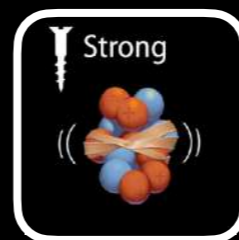


# Particle Physics 101



*QCD Confinement*

Quarks  
&  
Gluons



- $\gamma$  photon
- $e^\pm$  electron
- $\mu^\pm$  muon
- $\pi^\pm$  pion
- $K^\pm$  kaon
- $K_L^0$  K-long
- $p/\bar{p}$  proton
- $n/\bar{n}$  neutron

elementary

composite

T E H M

	●			$\gamma$	photon
●	●			$e^{\pm}$	electron
●	●	●	●	$\mu^{\pm}$	muon
●	●	●		$\pi^{\pm}$	pion
●	●	●		$K^{\pm}$	kaon
	●	●		$K_L^0$	K-long
●	●	●		$p/\bar{p}$	proton
	●	●		$n/\bar{n}$	neutron

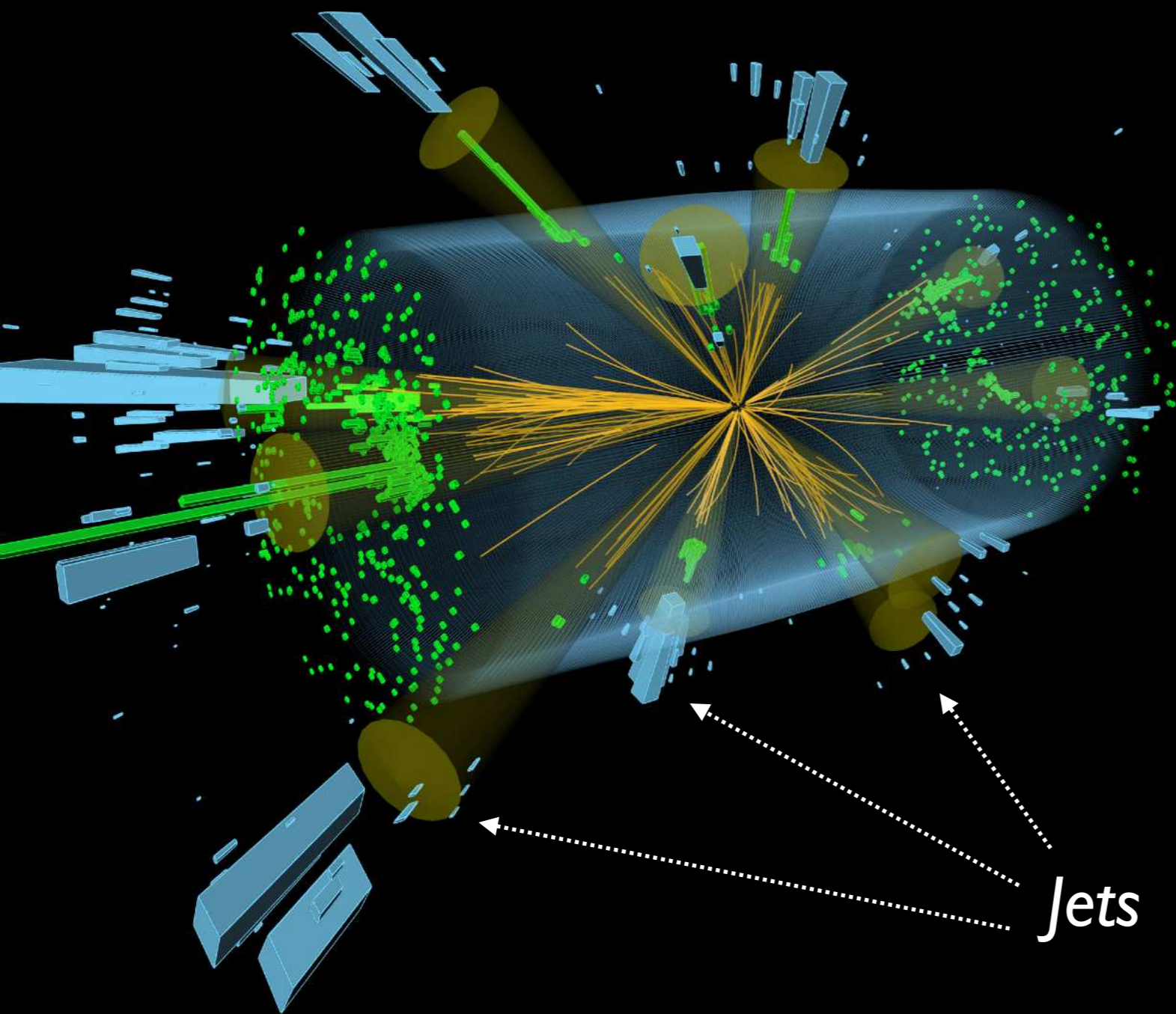
elementary

composite



# Collider Event

Every 25 nanoseconds at the LHC



T E H M

	●	$\gamma$	photon	elementary	
●	●	$e^{\pm}$	electron		
●	●	●	$\mu^{\pm}$		muon
●	●	●	$\pi^{\pm}$		pion
●	●	●	$K^{\pm}$	kaon	composite
	●	●	$K_L^0$	K-long	
●	●	●	$p/\bar{p}$	proton	
	●	●	$n/\bar{n}$	neutron	

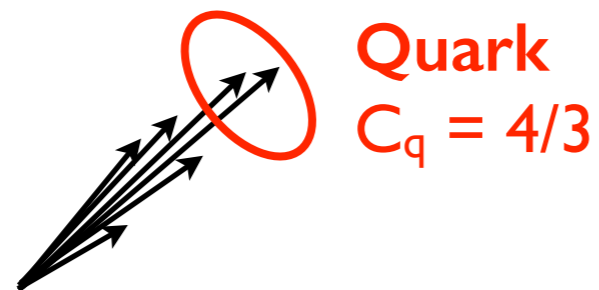
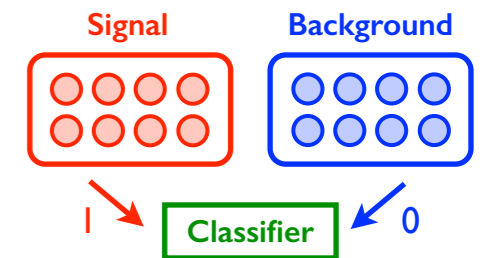
Jets

elementary

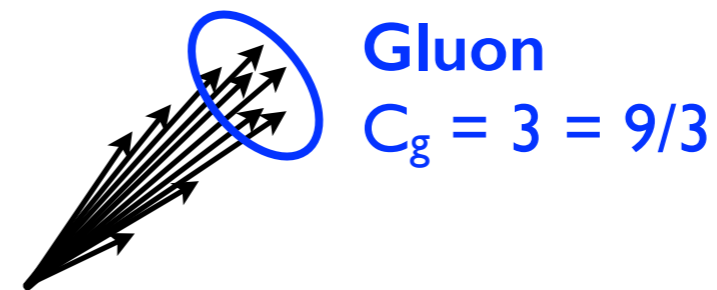
composite

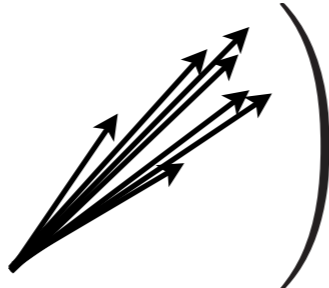
# Quark/Gluon Classification

“Hello, World!” of Jet Physics



vs.



Find  $h$   such that

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

Best you can do:  $h(\mathcal{J}) = \left( 1 + \frac{p(\mathcal{J}|\text{G})}{p(\mathcal{J}|\text{Q})} \right)^{-1}$   
(Neyman-Pearson lemma)

*Likelihood ratio yields optimal binary classifier (and vice versa)*

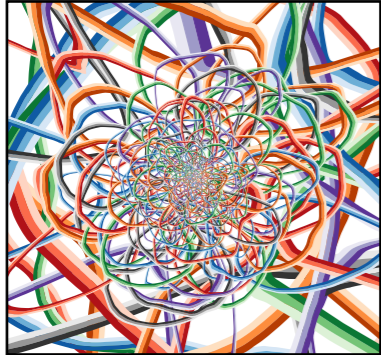
[see e.g. Gras, Höche, Kar, Larkoski, Lönnblad, Plätzer, Siódmok, Skands, Soyez, JDT, JHEP 2017; Komiske, Metodiev, Schwartz, JHEP 2017; Komiske, Metodiev, JDT, JHEP 2018]



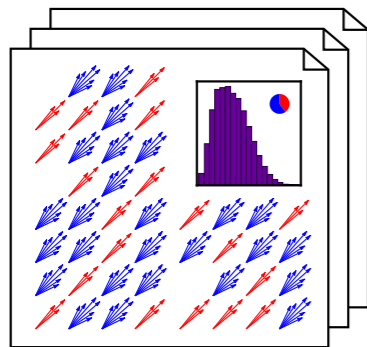
# From Curmudgeon to Evangelist



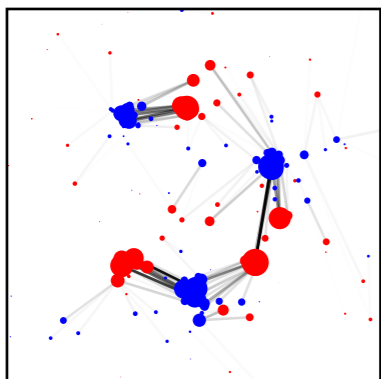
*What have been helpful guides in pursuing ML  $\Leftrightarrow$  HEP?*



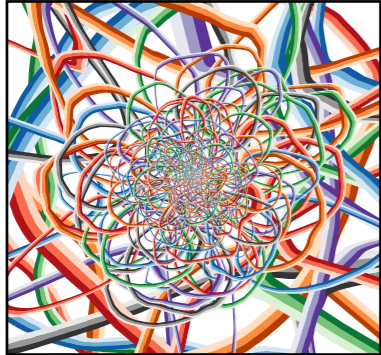
Can *theoretical structures* be encoded directly?



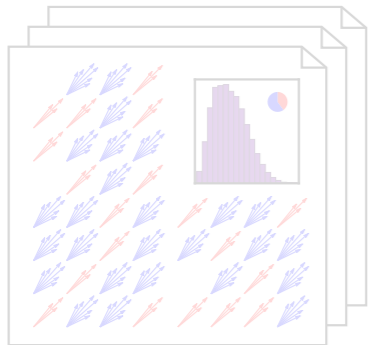
Can strategy be defined on *physical quantities*?



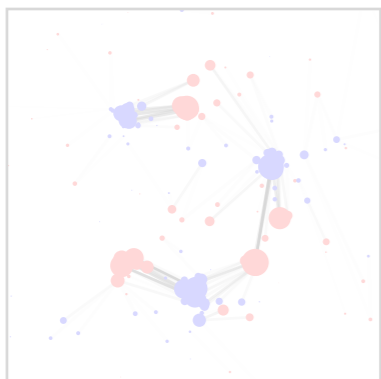
Can we leverage *unsupervised machine learning*?



*Can theoretical structures be encoded directly?*



*Can strategy be defined on physical quantities?*



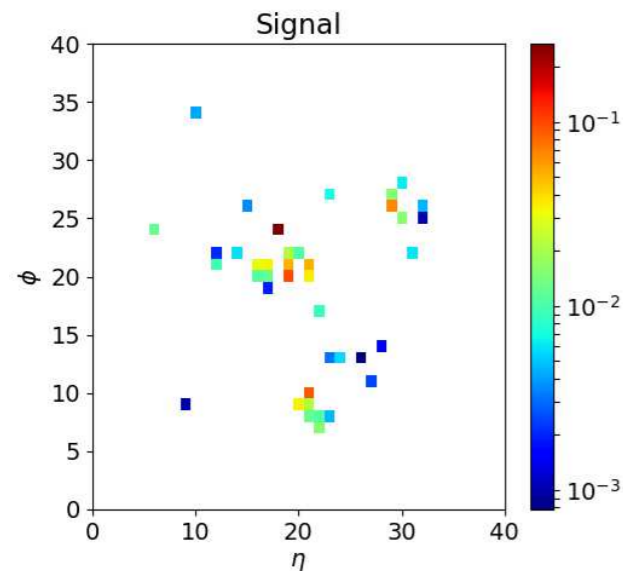
*Can we leverage unsupervised machine learning?*



# Jet Representations

## Pixelized Image

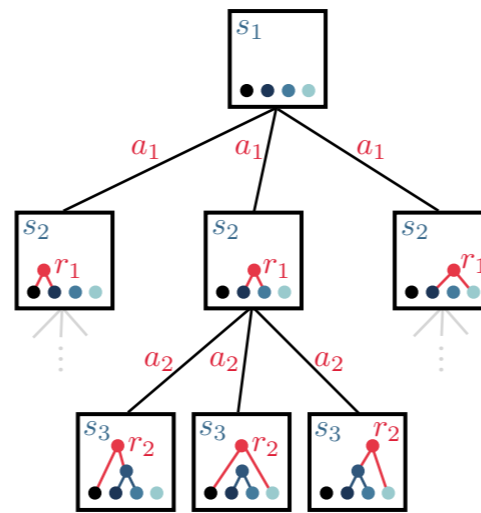
Calorimetry



[review in Kagan, [arXiv 2020](#)]

## Hierarchical Tree

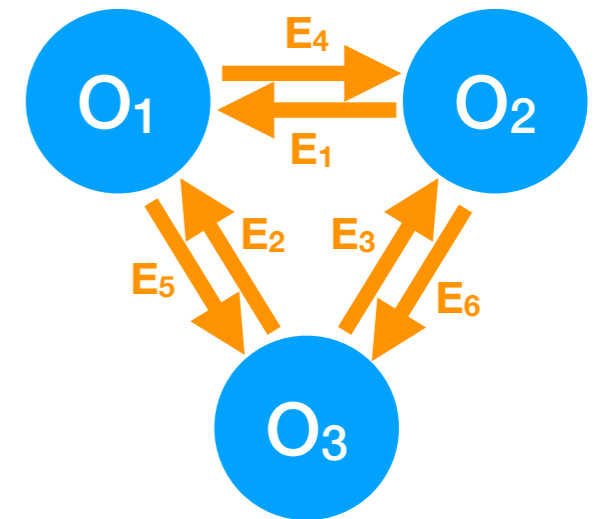
Binary Splittings



[e.g. Brehmer, Macaluso, Pappadopulo, Cranmer, [NeurIPS 2020](#)]

## Graphs

Pairwise Interactions

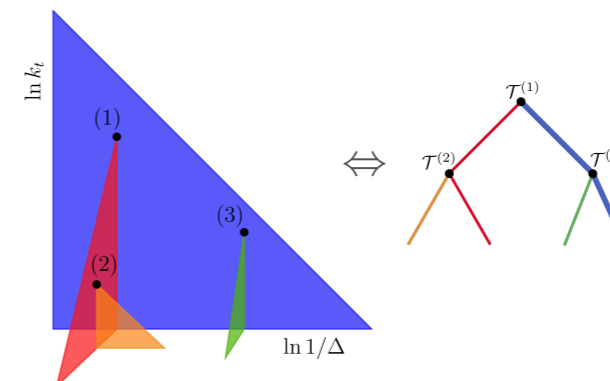


[e.g. Moreno, Cerri, Duarte, Newman, Nguyen, Periwal, Pierini, Serikova, Spiropulu, Vlimant, [EPJC 2020](#)]

Imposes implicit *theoretical prior*; affects choice of *network architecture*

E.g. recent progress with  
*Lund Plane* + *Graph Networks*

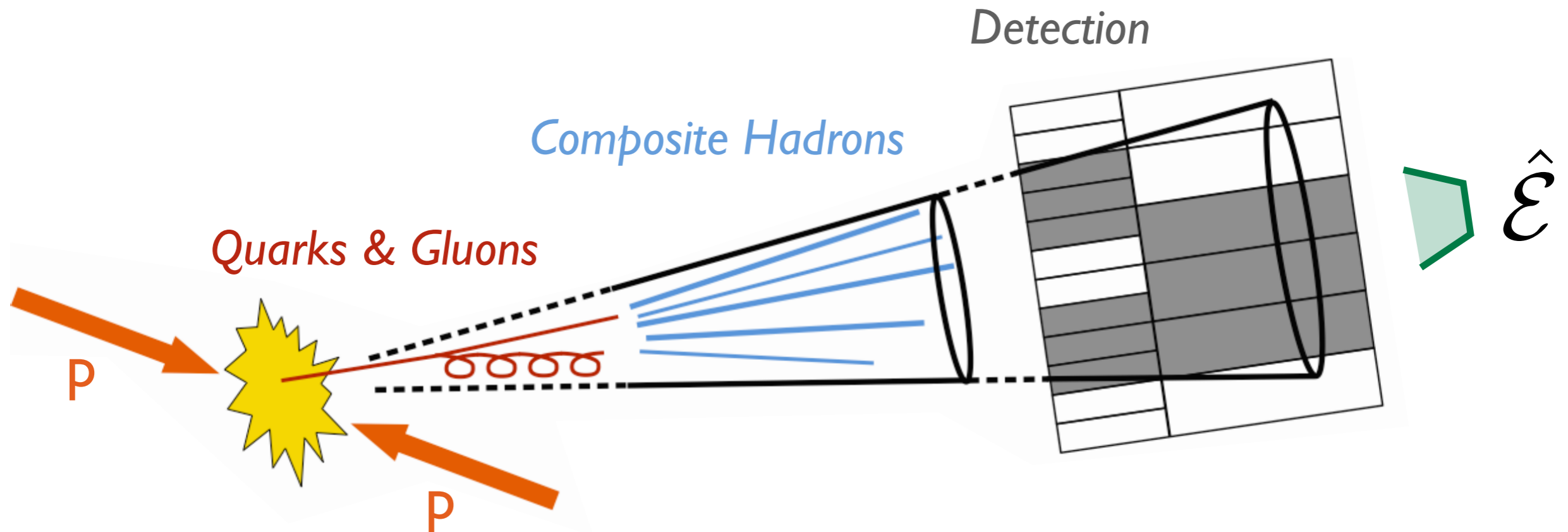
[Dreyer, Qu, [JHEP 2021](#)]



# Energy Flow Representation

Emphasizes *infrared and collinear safety*

Theory



## Energy Flow:

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

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

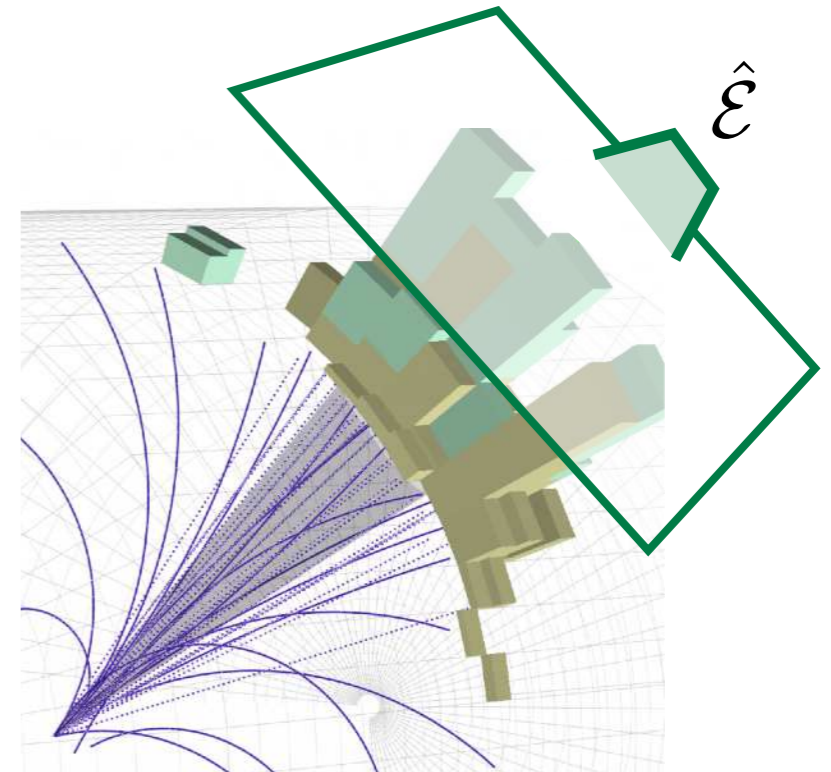
[see e.g. Sveshnikov, Tkachov, [PLB 1996](#); Hofman, Maldacena, [JHEP 2008](#); Mateu, Stewart, [JDT, PRD 2013](#); Belitsky, Hohenegger, Korchemsky, Sokatchev, Zhiboedov, [PRL 2014](#); Chen, Moul, Zhang, Zhu, [PRD 2020](#)]  
[complementary perspective on IRC unsafe information in Chakraborty, Lim, Nojiri, Takeuchi, [JHEP 2020](#)]

# Jets as **Weighted Point Clouds**

- **Energy-Weighted Directions**

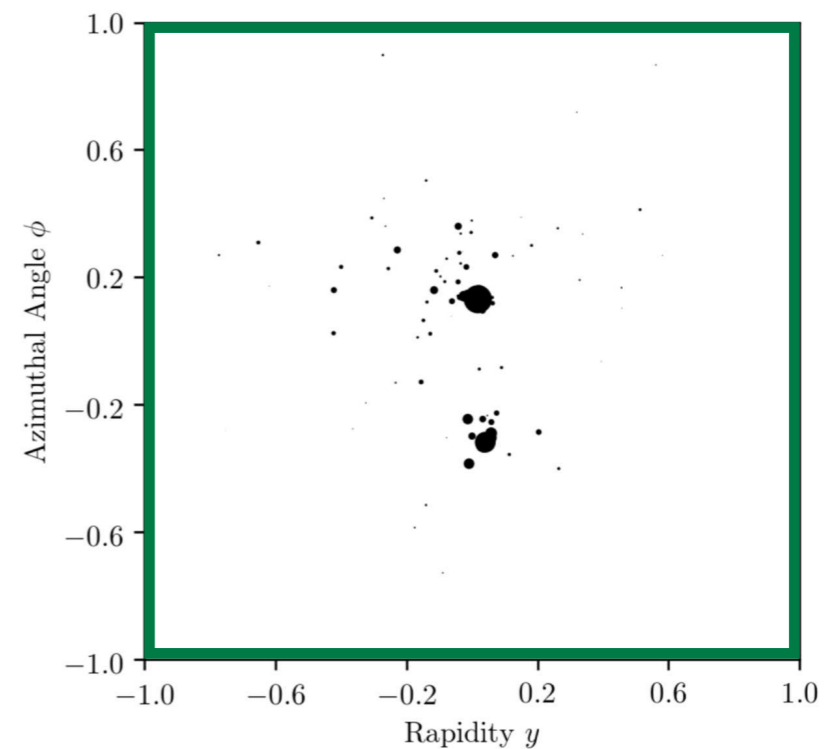
$$\vec{p} = \left\{ \underset{\substack{\uparrow \\ \text{Energy}}}{E}, \underbrace{\hat{n}_x, \hat{n}_y, \hat{n}_z}_{\text{Direction}} \right\}$$

(suppressing “unsafe” charge/flavor information)



- Equivalently: **Energy Density**

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





# 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](https://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, [PRD 2021](#);  
graph-based approach in Moreno, Cerri, Duarte, Newman, Nguyen, Periwal, Pierini, Serikova, Spiropulu, Vlimant, [EPJC 2020](#);  
Lorentz-equivariant approach in Bogatskiy, Anderson, Offermann, Roussi, Miller, Kondor, [arXiv 2020](#);  
histogram pooling in Cranmer, Kreisch, Pisani, Villaescusa-Navarro, Spengel, Ho, [ICLR SimDL 2021](#)]



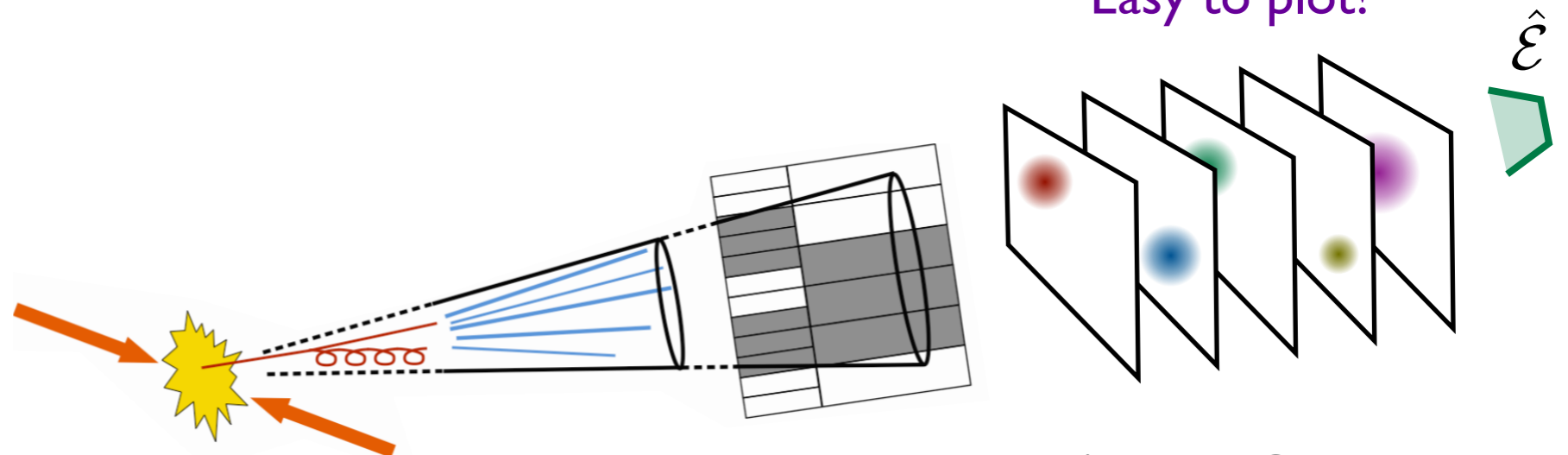
# Energy Flow Networks

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  $\ell$

Easy to plot!



(similar to CNN filter activation)

[Komiske, Metodiev, JDT, [JHEP 2019](#); see also Komiske, Metodiev, JDT, [JHEP 2018](#); code at [energyflow.network](https://energyflow.network); special case of Zaheer, Kottur, Ravanbakhsh, Póczos, Salakhutdinov, Smola, [NIPS 2017](#); other set-based architecture in Qu, Gouskos, [PRD 2020](#); Mikuni, Canelli, [EPJP 2020](#); Dolan, Ore, [PRD 2021](#); graph-based approach in Moreno, Cerri, Duarte, Newman, Nguyen, Periwal, Pierini, Serikova, Spiropulu, Vlimant, [EPJC 2020](#); Lorentz-equivariant approach in Bogatskiy, Anderson, Offermann, Roussi, Miller, Kondor, [arXiv 2020](#); histogram pooling in Cranmer, Kreisch, Pisani, Villaescusa-Navarro, Spergel, Ho, [ICLR SimDL 2021](#)]

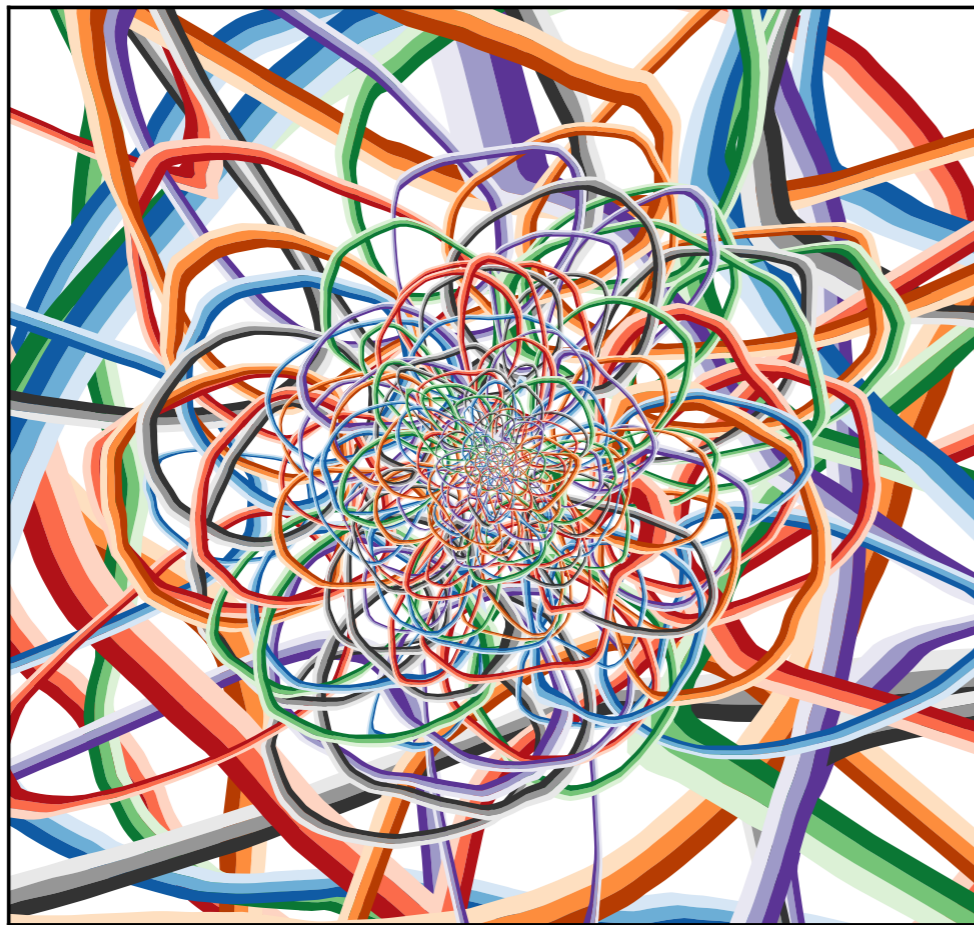


# Energy Flow Networks

Architecture designed around symmetries and *interpretability*

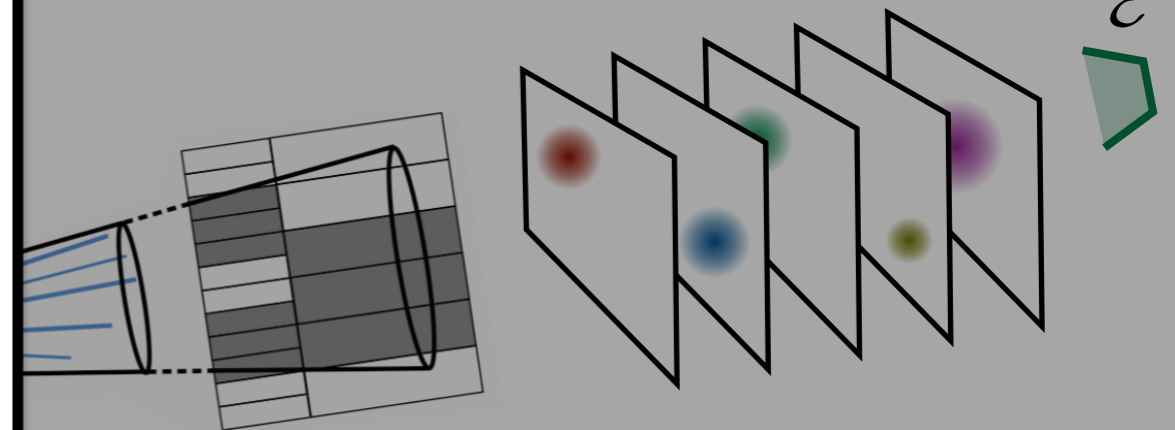
## Psychedelic Network Visualization

Latent Dimension 256



$$V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} E_i \Phi_a(\hat{n}_i)$$

Easy to plot!



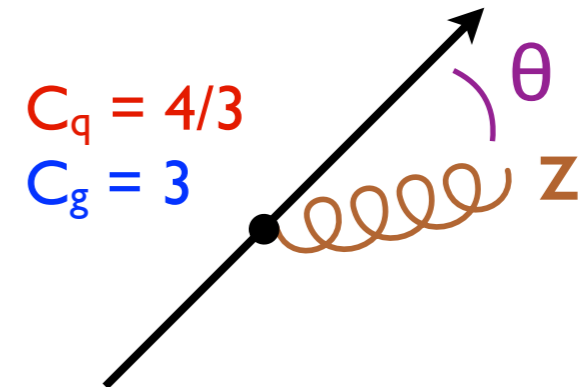
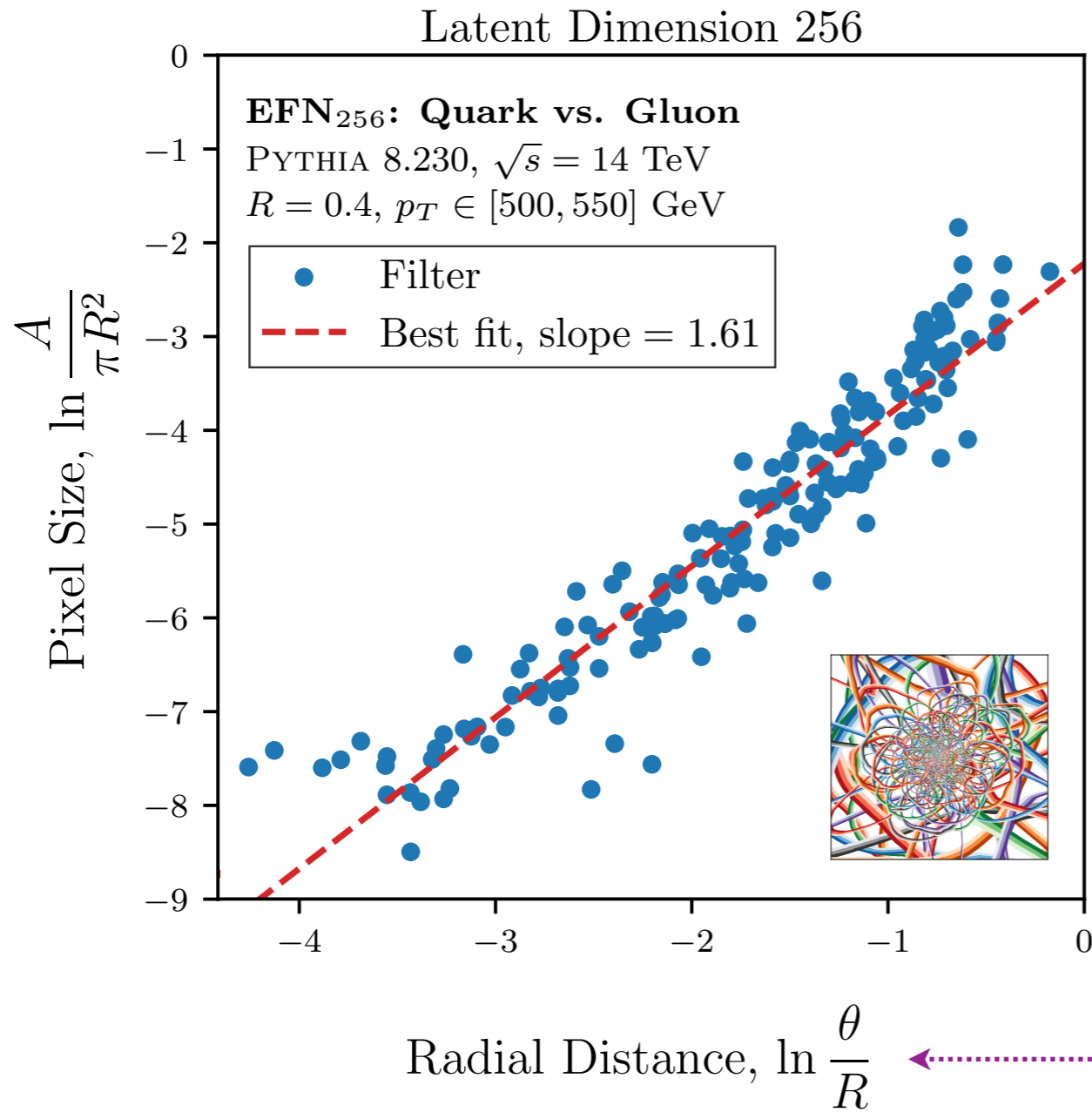
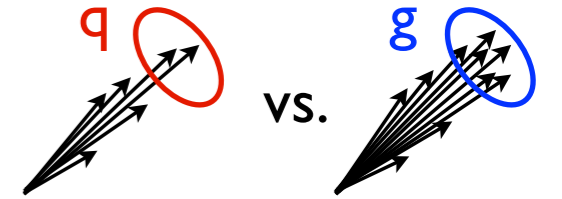
(similar to CNN filter activation)

[Komiske, Metodiev, JDT, [JHEP 2019](#); see also Komiske, Metodiev, JDT, [JHEP 2018](#); code at [energyflow.network](https://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, [PRD 2021](#);  
graph-based approach in Moreno, Cerri, Duarte, Newman, Nguyen, Periwal, Pierini, Serikova, Spiropulu, Vlimant, [EPJC 2020](#);  
Lorentz-equivariant approach in Bogatskiy, Anderson, Offermann, Roussi, Miller, Kondor, [arXiv 2020](#);  
histogram pooling in Cranmer, Kreisch, Pisani, Villaescusa-Navarro, Spergel, Ho, [ICLR SimDL 2021](#)]





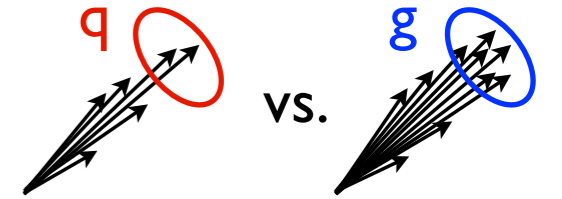
# Machine Learning Collinear QCD



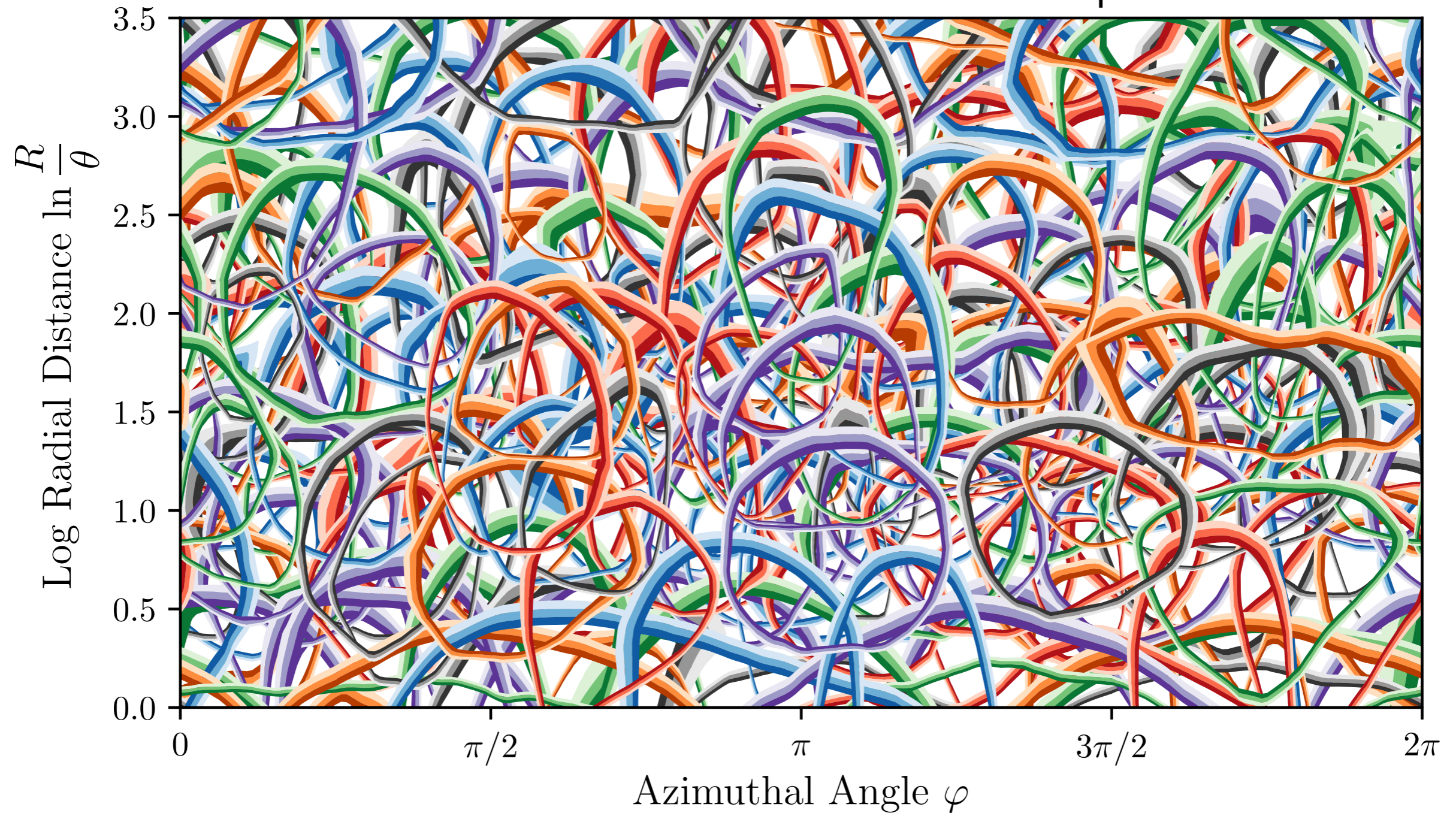
$$dP_{i \rightarrow ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{d\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{dz}{z}}_{\text{Soft}}$$

[Komiske, Metodiev, JDT, JHEP 2019]

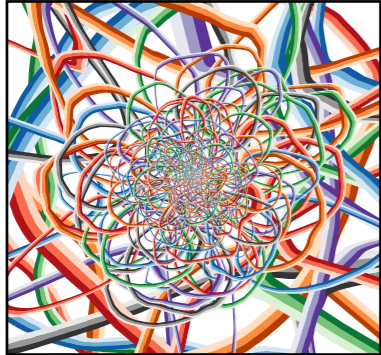
# Ready for the Stedelijk?



Coordinate transformation to the emission plane



[Komiske, Metodiev, JDT, JHEP 2019; see also Dreyer, Salam, Soyez, JHEP 2018]

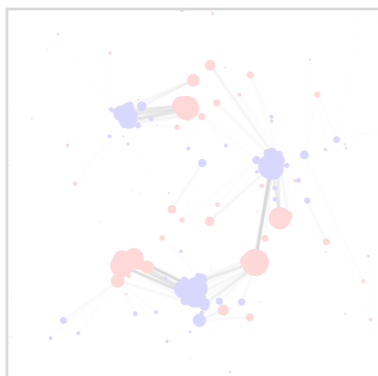


*Can theoretical structures be encoded directly?*

Energy Flow Networks  $\Leftrightarrow$  IRC Safety + Permutations

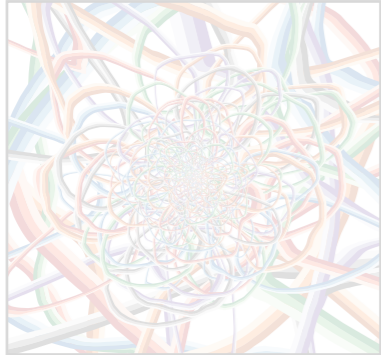


*Can strategy be defined on physical quantities?*



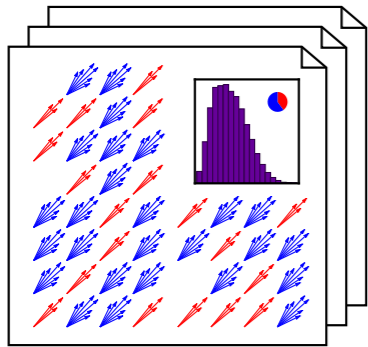
*Can we leverage unsupervised machine learning?*



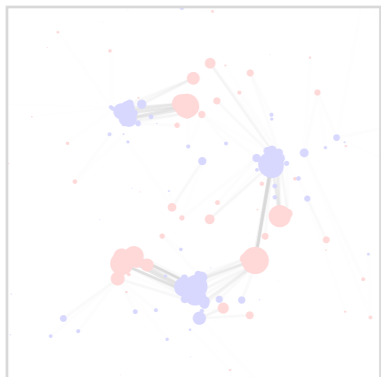


*Can theoretical structures be encoded directly?*

Energy Flow Networks  $\Leftrightarrow$  IRC Safety + Permutations



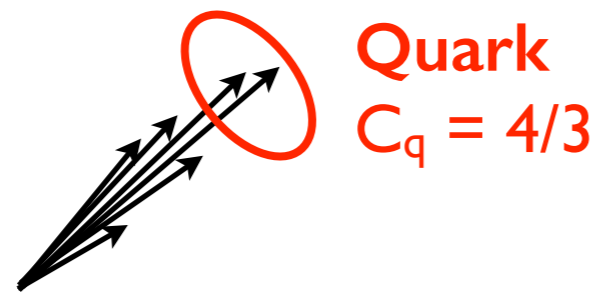
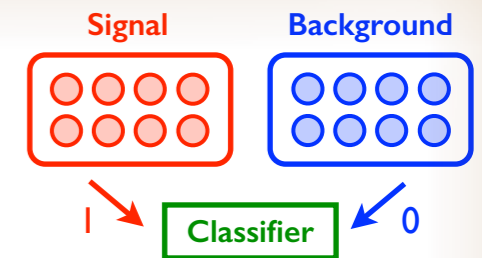
*Can strategy be defined on physical quantities?*



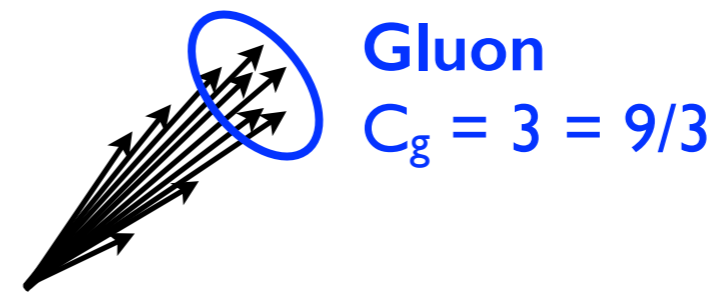
*Can we leverage unsupervised machine learning?*

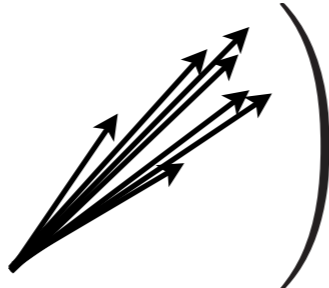
# Quark/Gluon Classification

“Hello, World!” of Jet Physics



vs.



Find  $h$   such that

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

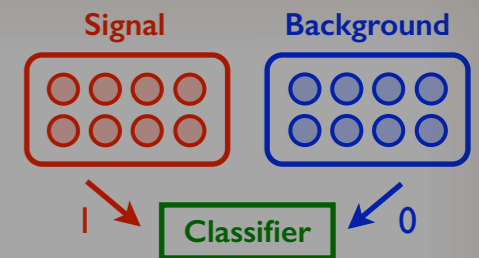
Best you can do:  $h(\mathcal{J}) = \left( 1 + \frac{p(\mathcal{J}|\text{G})}{p(\mathcal{J}|\text{Q})} \right)^{-1}$   
(Neyman-Pearson lemma)

*Likelihood ratio yields optimal binary classifier (and vice versa)*

[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]

# Quark/Gluon Classification

“Hello, World!” of Jet Physics



What do you mean by “quark” and “gluon”?

Jets are clusters of *colorless hadrons!*

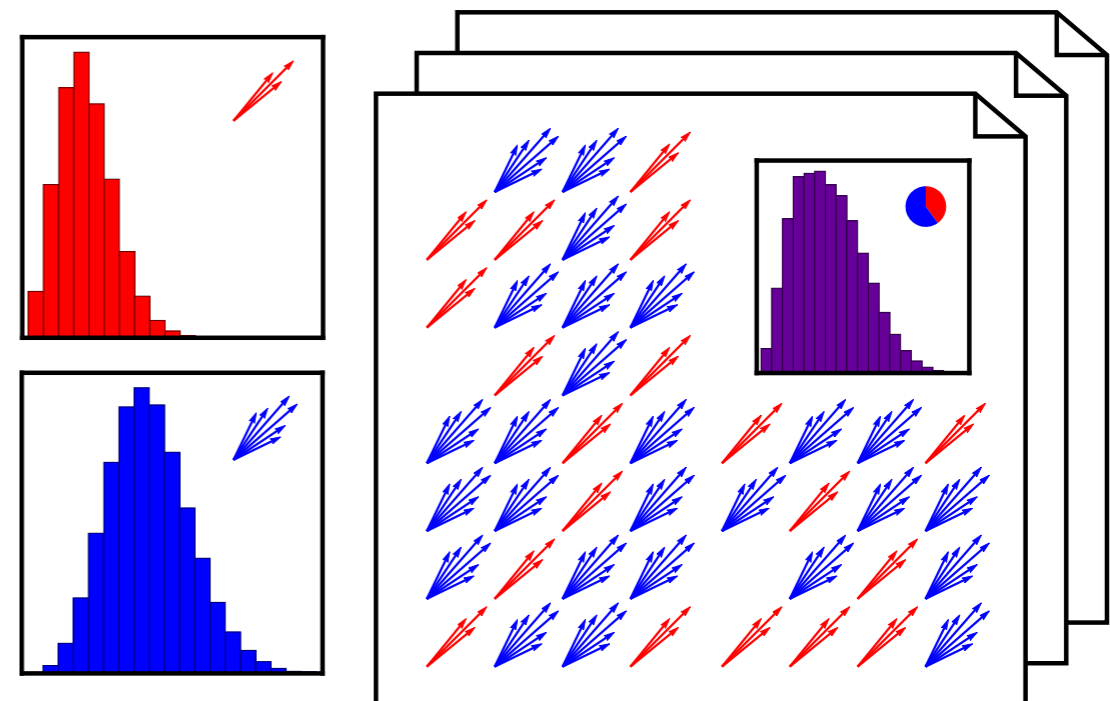
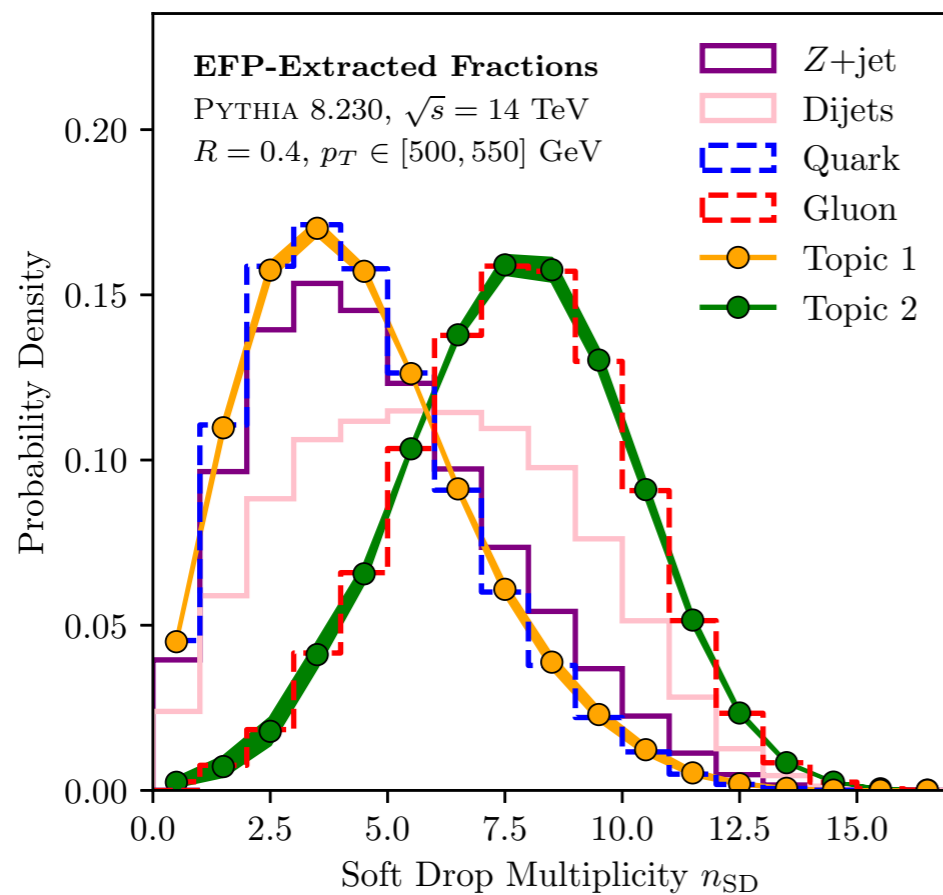
Parton shower “truth” is but a (useful) fiction!

*Likelihood ratio yields optimal binary classifier (and vice versa)*

[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]

# Topic Modeling to Disentangle Jet Categories

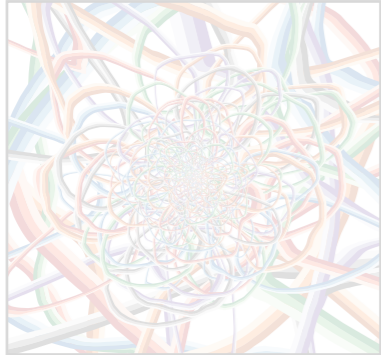
While you can't unambiguously label individual jets, you can extract **quark** and **gluon** distributions from **hadron-level measurements**



Key concept from natural language processing: **“anchor words”**

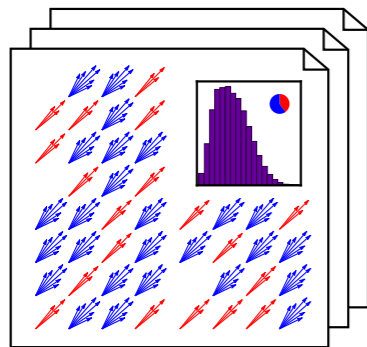
[Komiske, Metodiev, JDT, [JHEP 2018](#); using Metodiev, Nachman, JDT, [JHEP 2017](#); Metodiev, JDT, [PRL 2018](#)]  
see also Blanchard, Flaska, Handy, Pozzi, Scott, [PLMR 2013](#); Katz-Samuels, Blanchard, Scott, [JMLR 2016](#)]





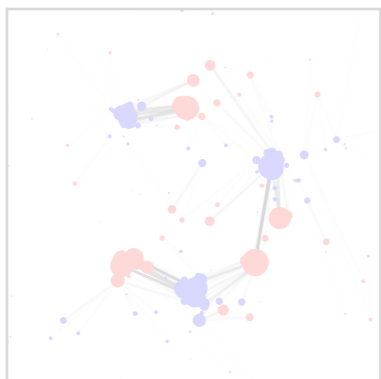
*Can theoretical structures be encoded directly?*

Energy Flow Networks  $\Leftrightarrow$  IRC Safety + Permutations

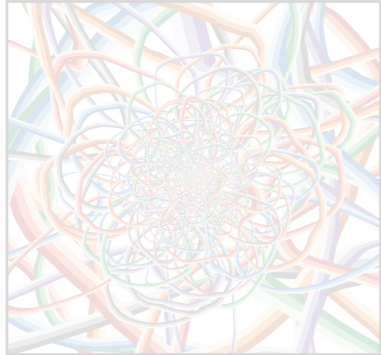


*Can strategy be defined on physical quantities?*

Jet Topics  $\Leftrightarrow$  Hadron-Level Approach to QCD Partons

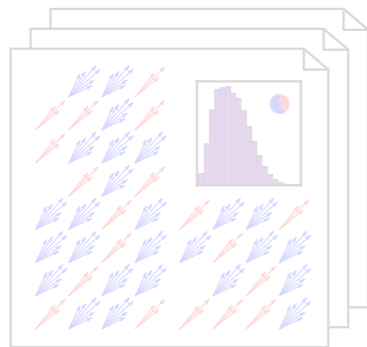


*Can we leverage unsupervised machine learning?*



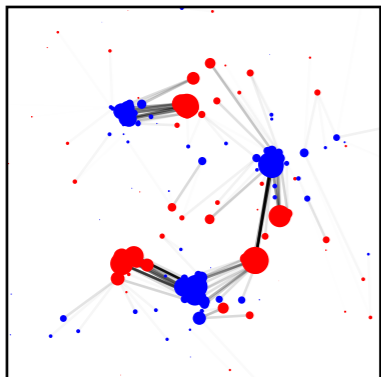
*Can theoretical structures be encoded directly?*

Energy Flow Networks  $\Leftrightarrow$  IRC Safety + Permutations



*Can strategy be defined on physical quantities?*

Jet Topics  $\Leftrightarrow$  Hadron-Level Approach to QCD Partons



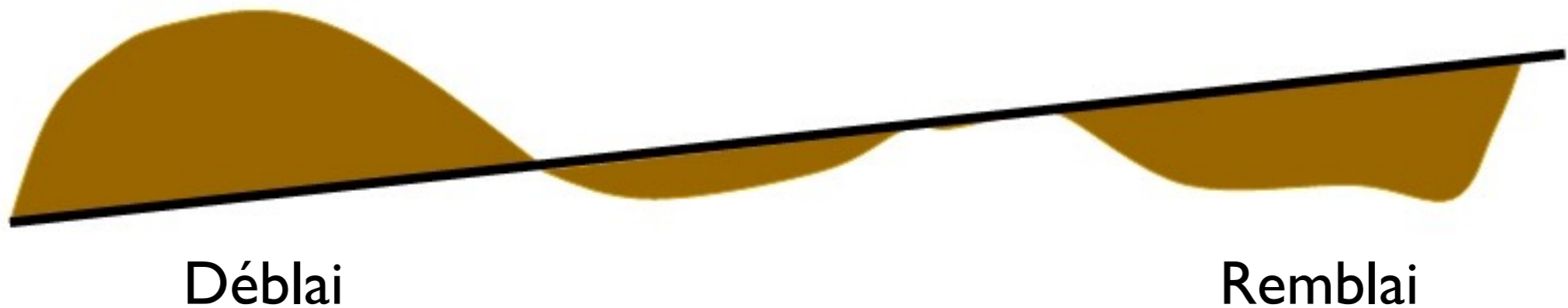
*Can we leverage unsupervised machine learning?*

# 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



Déblai

Remblai

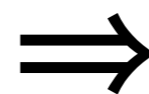
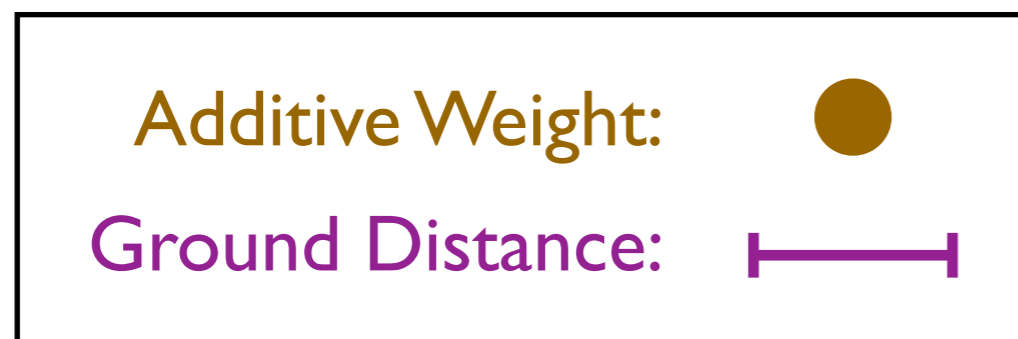
[h/t Niles-Weed, [ML4jets 2020](#); Monge, 1781; Vaserštejn, 1969; [Wikipedia](#)]

# The Earth Mover's Distance

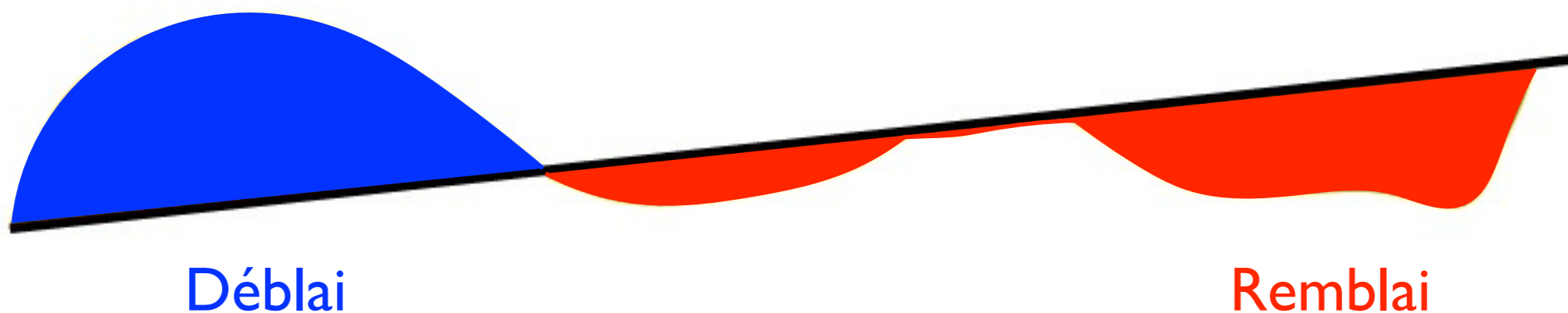
Optimal Transport:

[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](#)]

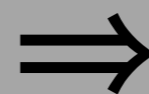
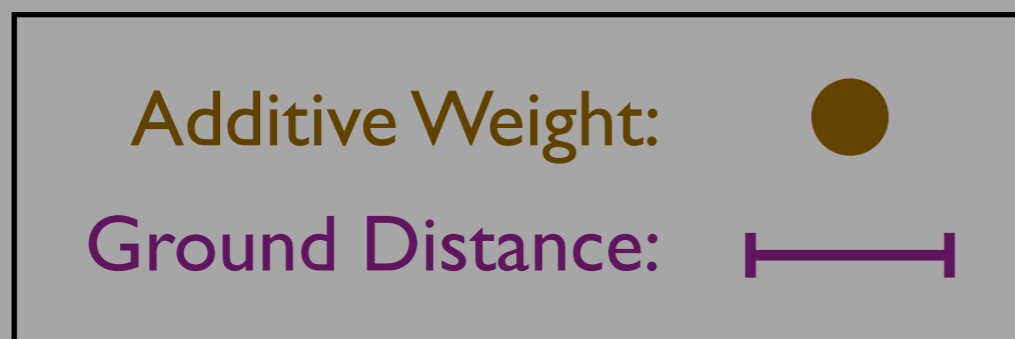


# The Earth Mover's Distance

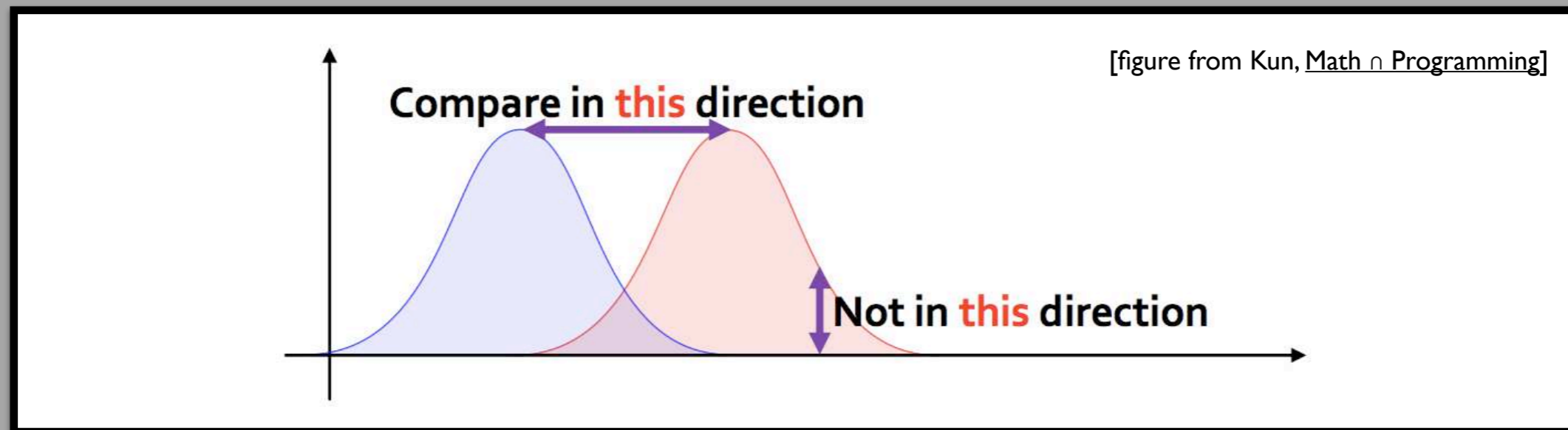
Optimal Transport:

[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**

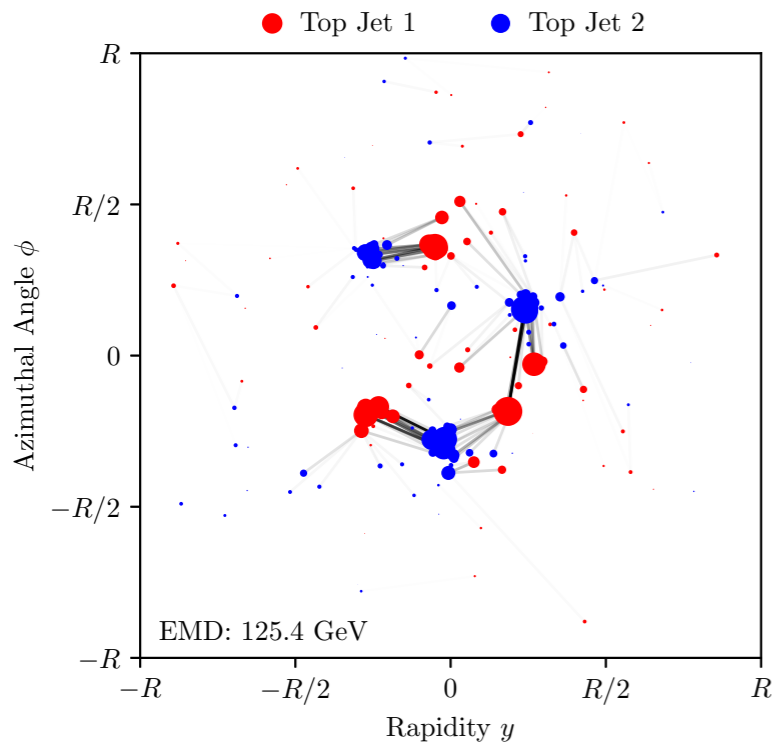
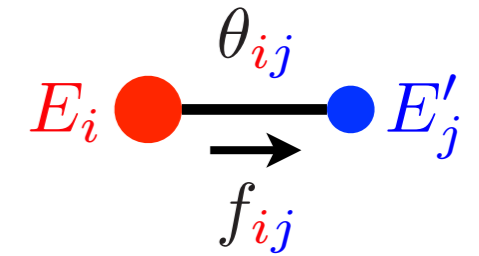


Distance Between  
Distributions



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

# The Energy Mover's Distance



Optimal transport between energy flows...

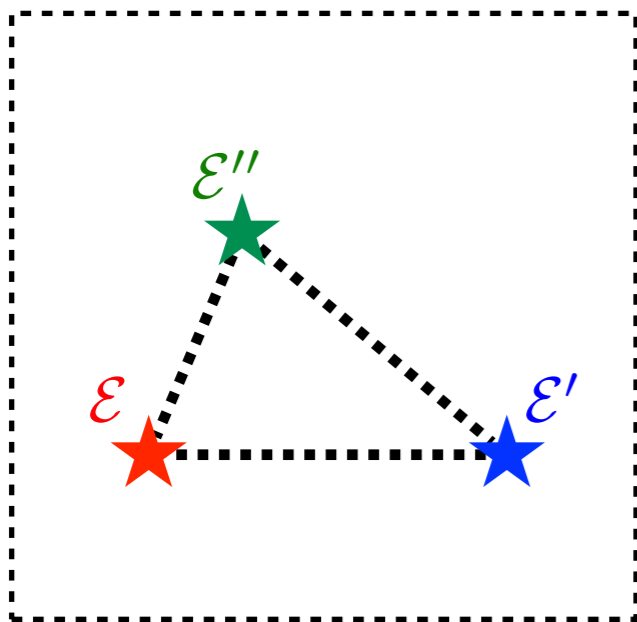
$$\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \underbrace{\sum_i \sum_j f_{ij} \frac{\theta_{ij}}{R}}_{\text{Cost to move energy}} + \underbrace{\left| \sum_i E_i - \sum_j E'_j \right|}_{\text{Cost to create energy}}$$

↑  
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)

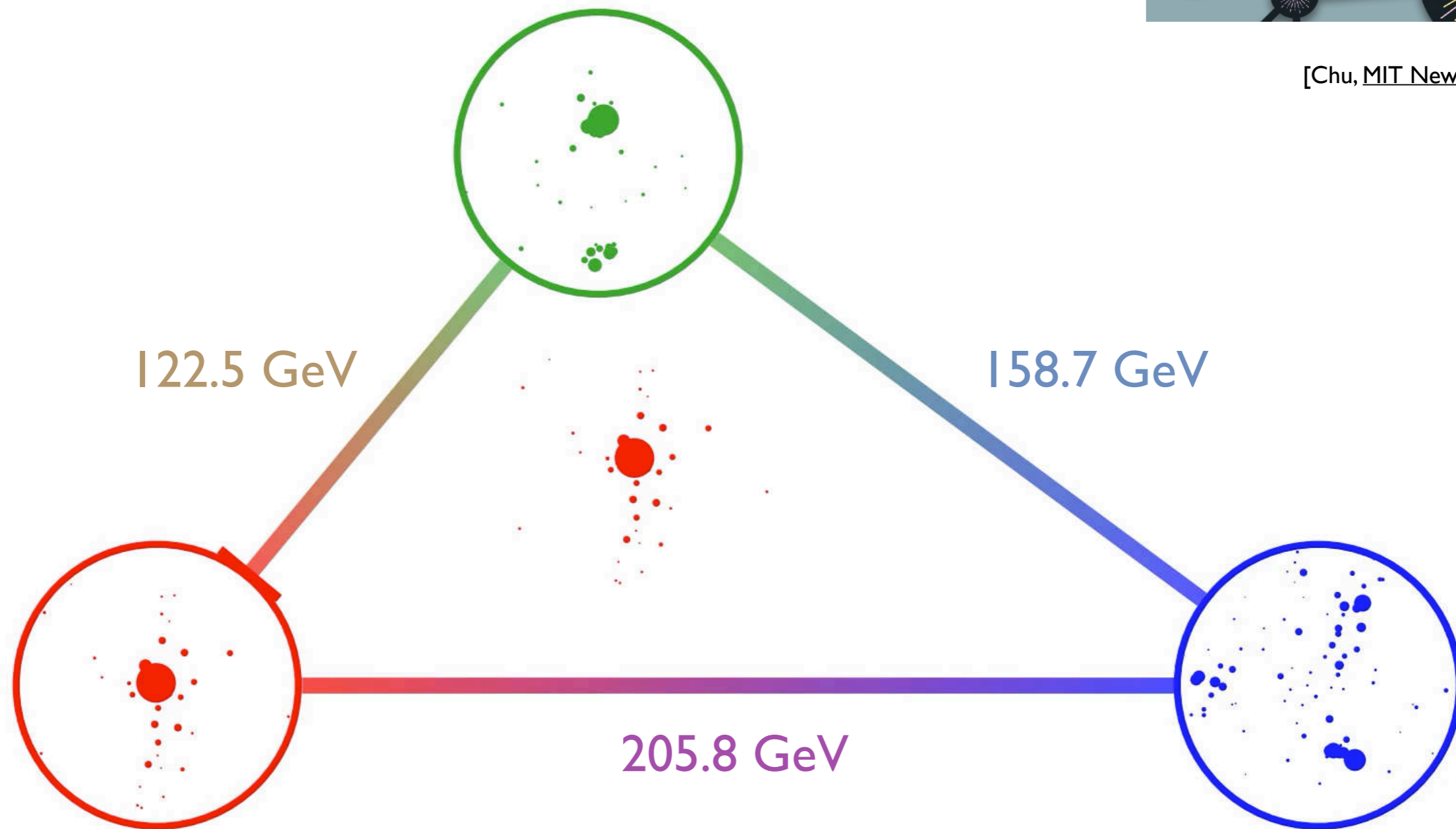


[Komiske, Metodiev, JDT, [PRL 2019](#); see also Pele, Werman, [ECCV 2008](#); Pele, Taskar, [GSI 2013](#)]  
 [see flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, [EPJC 2021](#)]  
 [see computational speed up in Cai, Cheng, Craig, Craig, [PRD 2020](#)]

# Triangulating the Space of Jets



[Chu, [MIT News July 2019](#)]



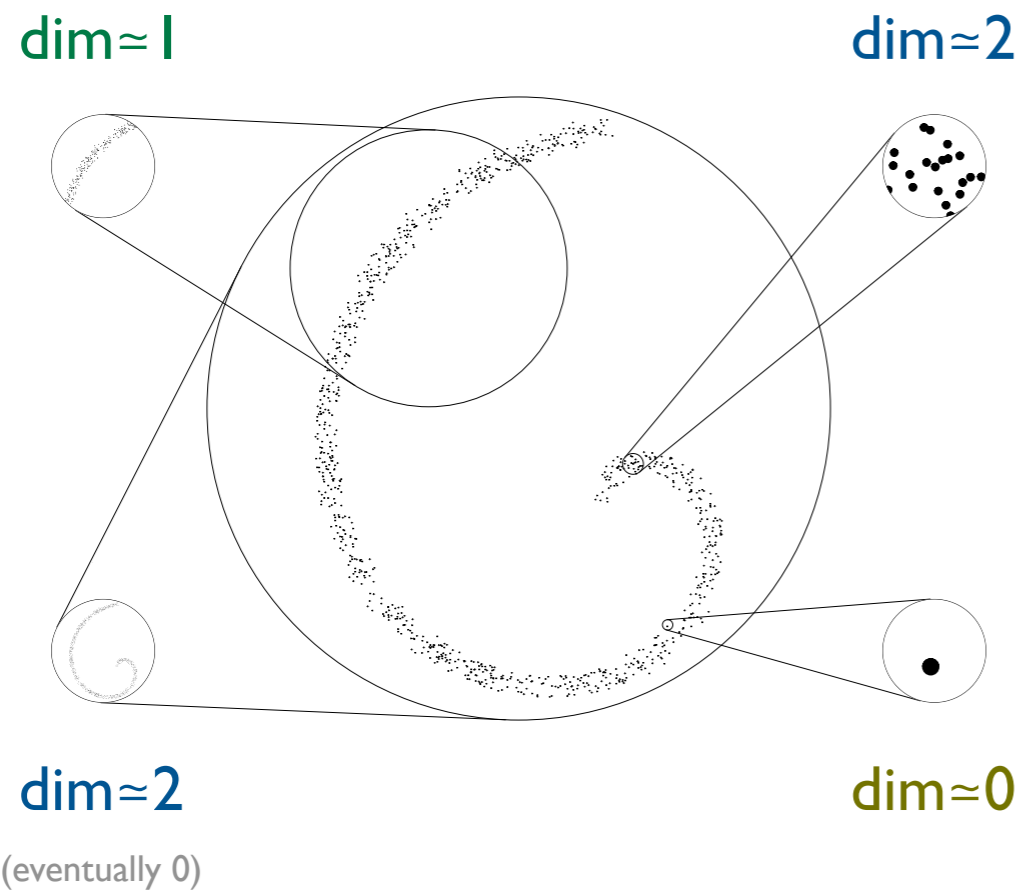
[Komiske, Metodiev, JDT, [PRL 2019](#); code at Komiske, Metodiev, JDT, [energyflow.network](#);  
see alternative graph network approach in Mullin, Pacey, Parker, White, Williams, [JHEP 2021](#)]

# 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]





# Dimensionality of Space of Jets



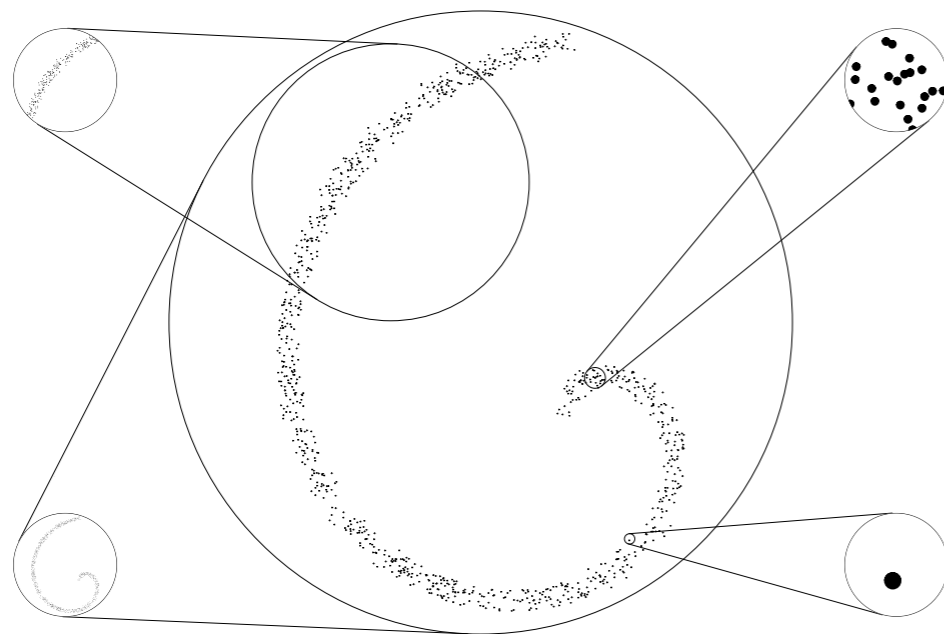
$$N_{\text{neighbors}}(r) \sim r^{\text{dim}}$$

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

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

dim ≈ 1

dim ≈ 2

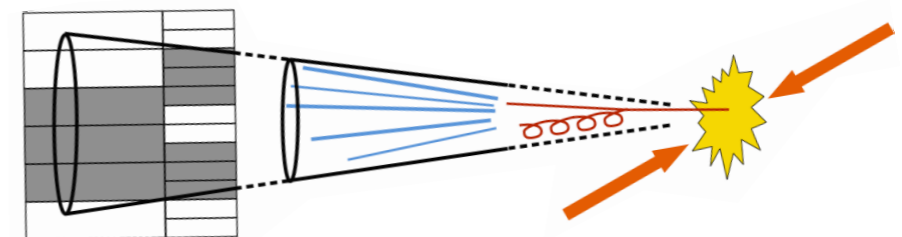
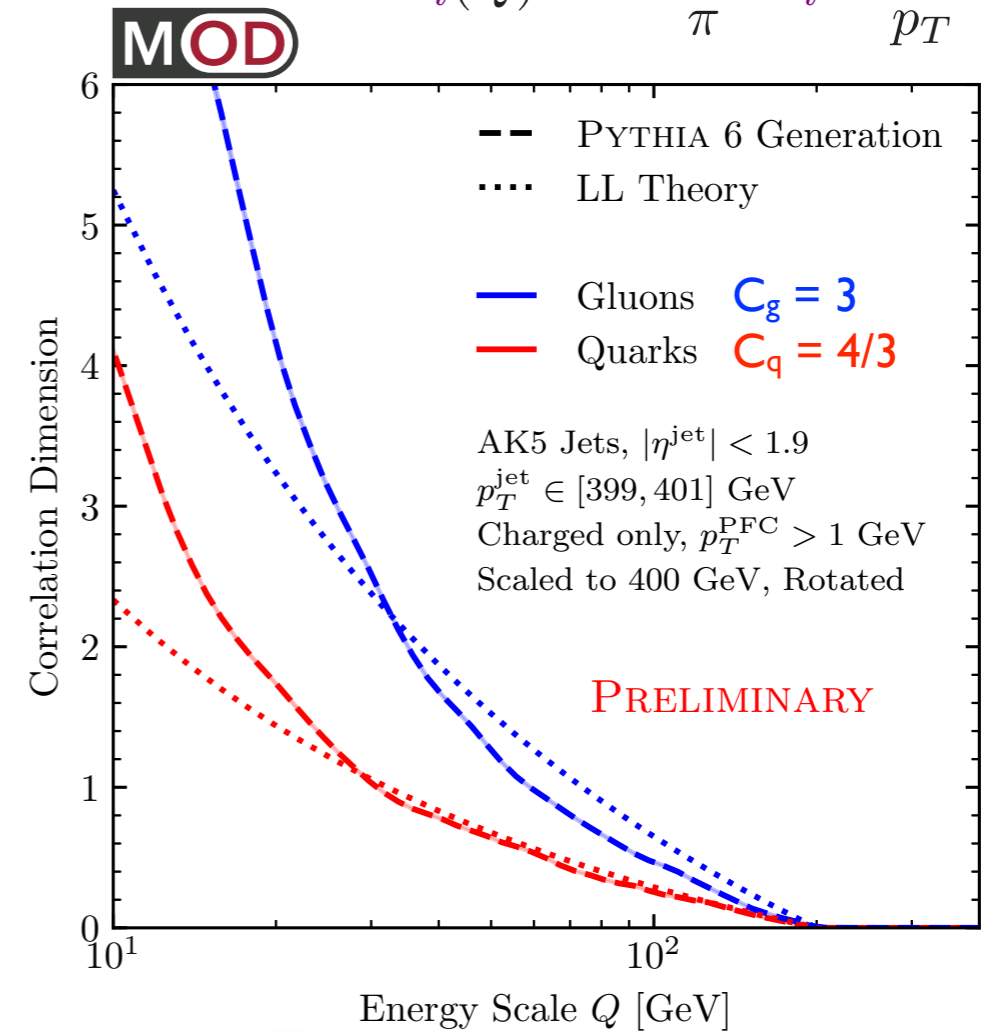


dim ≈ 2

dim ≈ 0

(eventually 0)

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



# Dimensionality of Space of Jets



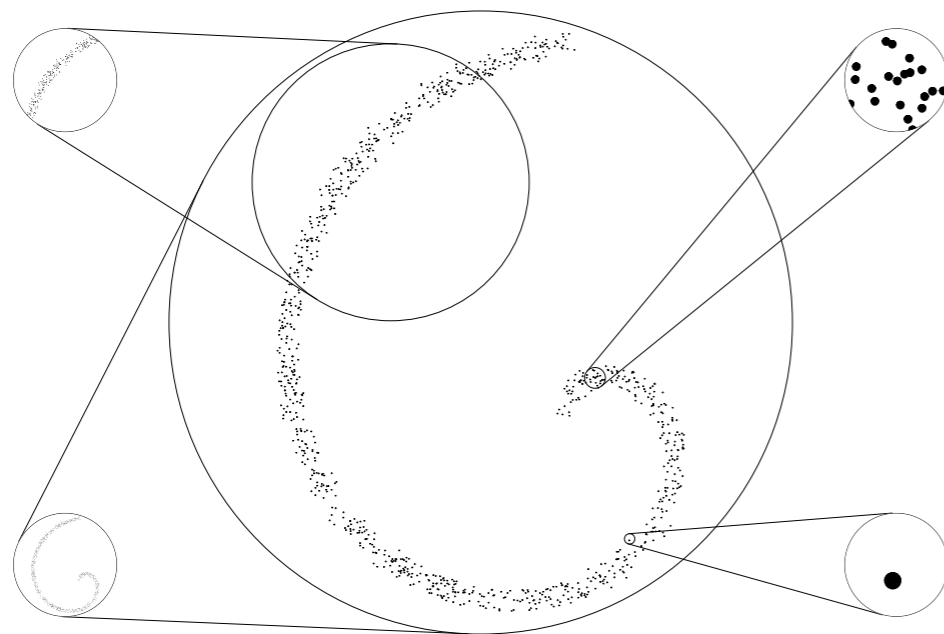
$$N_{\text{neighbors}}(r) \sim r^{\text{dim}}$$

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

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

dim ≈ 1

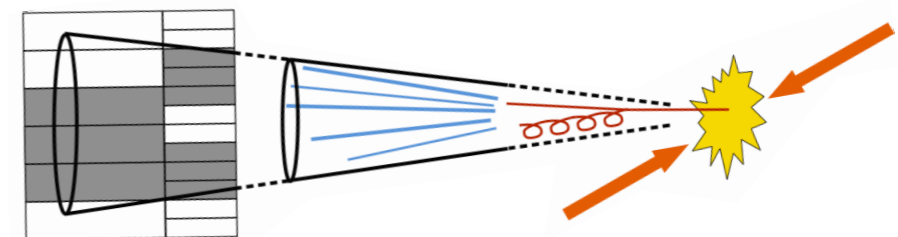
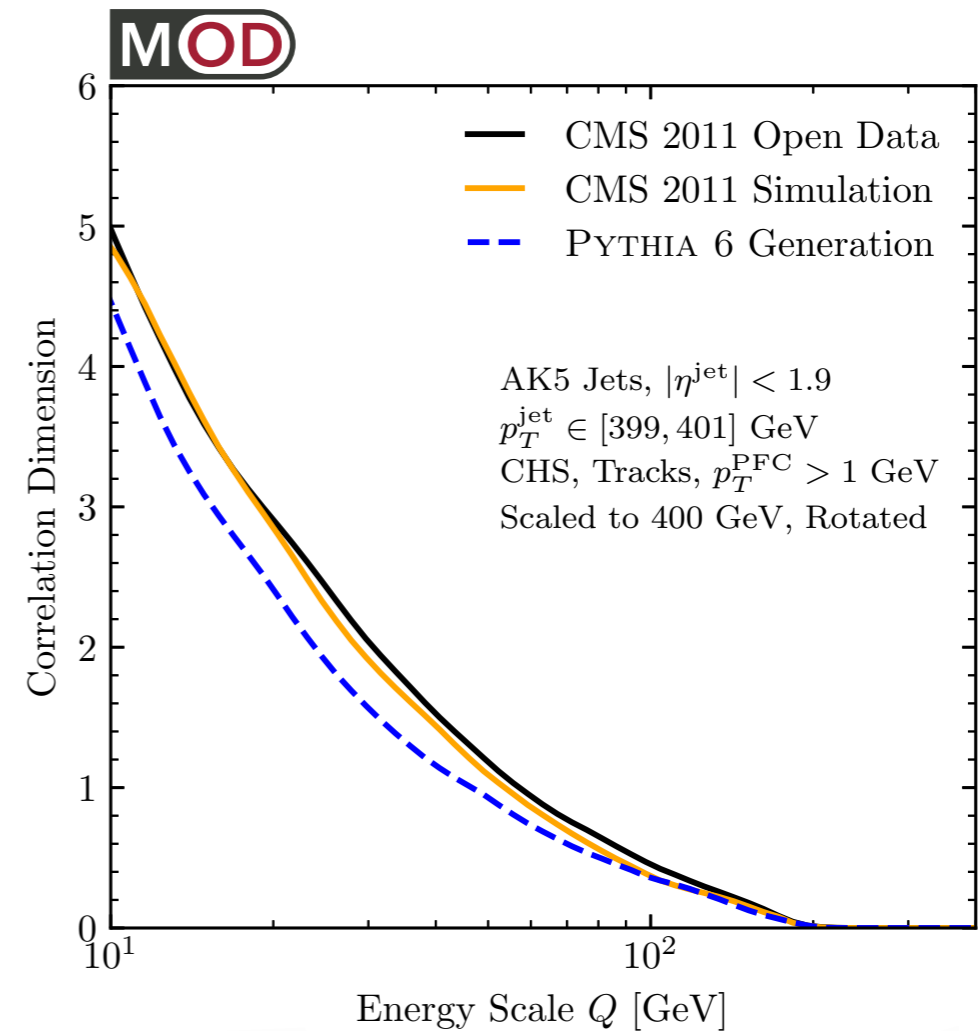
dim ≈ 2



dim ≈ 2

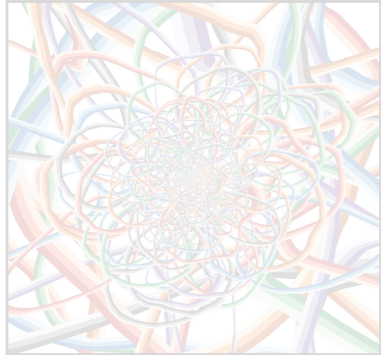
dim ≈ 0

(eventually 0)



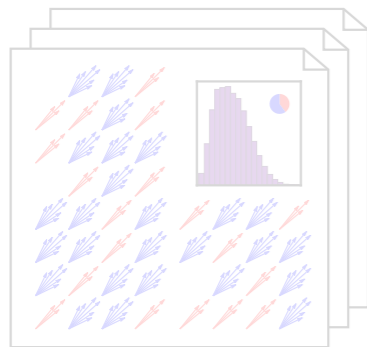
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;  
using CMS Open Data]





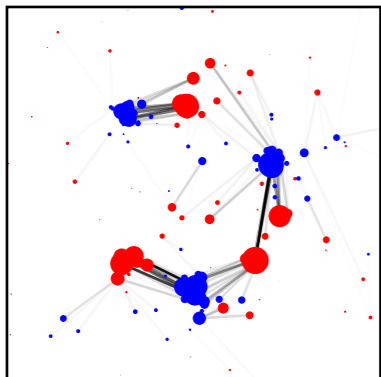
*Can theoretical structures be encoded directly?*

Energy Flow Networks  $\Leftrightarrow$  IRC Safety + Permutations



*Can strategy be defined on physical quantities?*

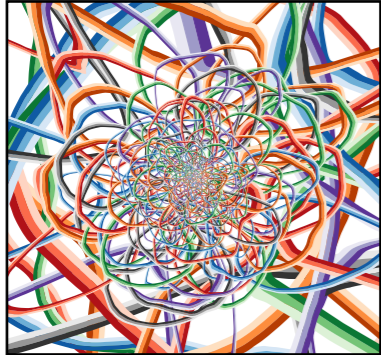
Jet Topics  $\Leftrightarrow$  Hadron-Level Approach to QCD Partons



*Can we leverage **unsupervised machine learning**?*

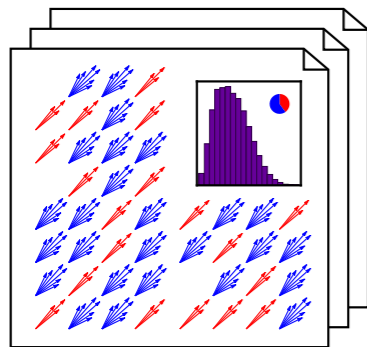
Energy Mover's Distance  $\Leftrightarrow$  **Geometric Strategies** for Collider Physics

# Artificial Intelligence and High-Energy Physics



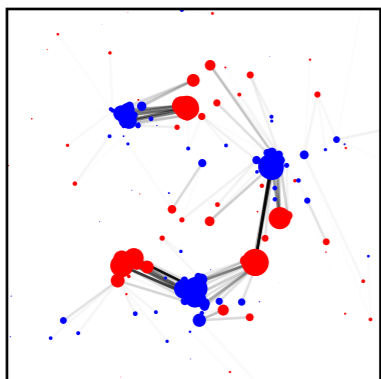
*Can theoretical structures be encoded directly?*

Energy Flow Networks  $\Leftrightarrow$  IRC Safety + Permutations



*Can strategy be defined on physical quantities?*

Jet Topics  $\Leftrightarrow$  Hadron-Level Approach to QCD Partons



*Can we leverage unsupervised machine learning?*

Energy Mover's Distance  $\Leftrightarrow$  Geometric Strategies for Collider Physics

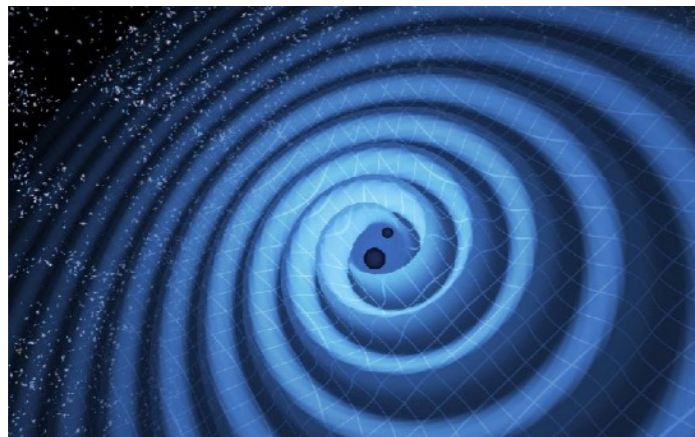
Physics insights essential for developing these tools



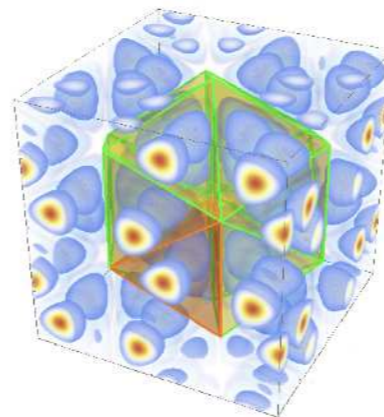
# Artificial Intelligence $\Leftrightarrow$ Fundamental Interactions



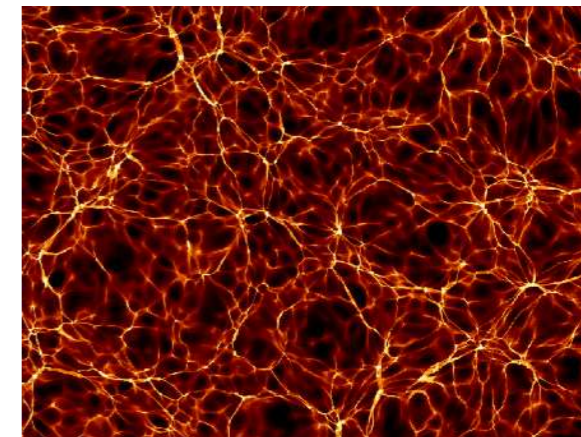
Gravitational Waves



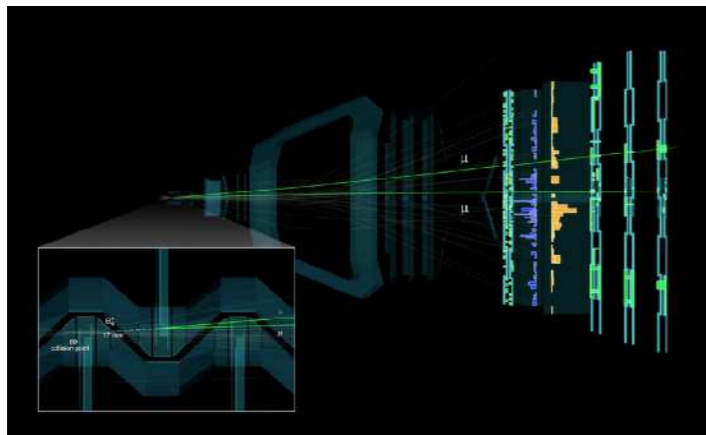
Nuclear Physics



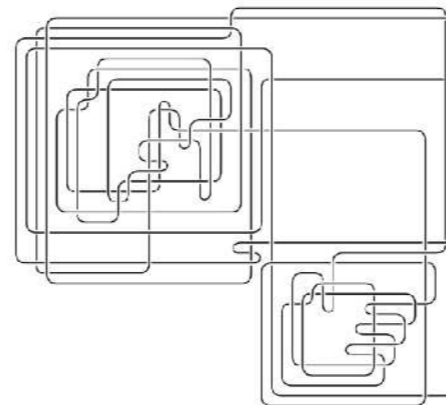
Dark Matter



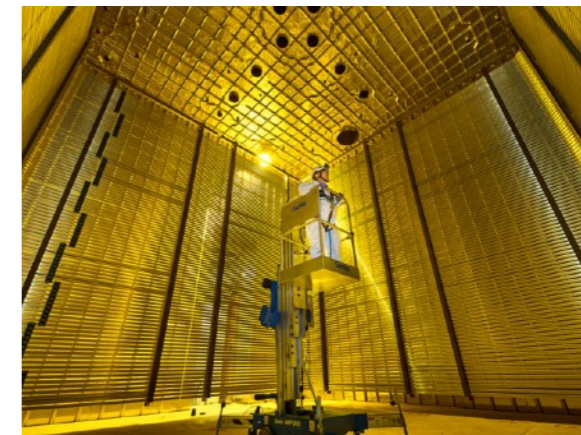
Particle Colliders



Mathematical Physics



Neutrino Detection



...

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

[<http://iaifi.org>]

# Backup Slides

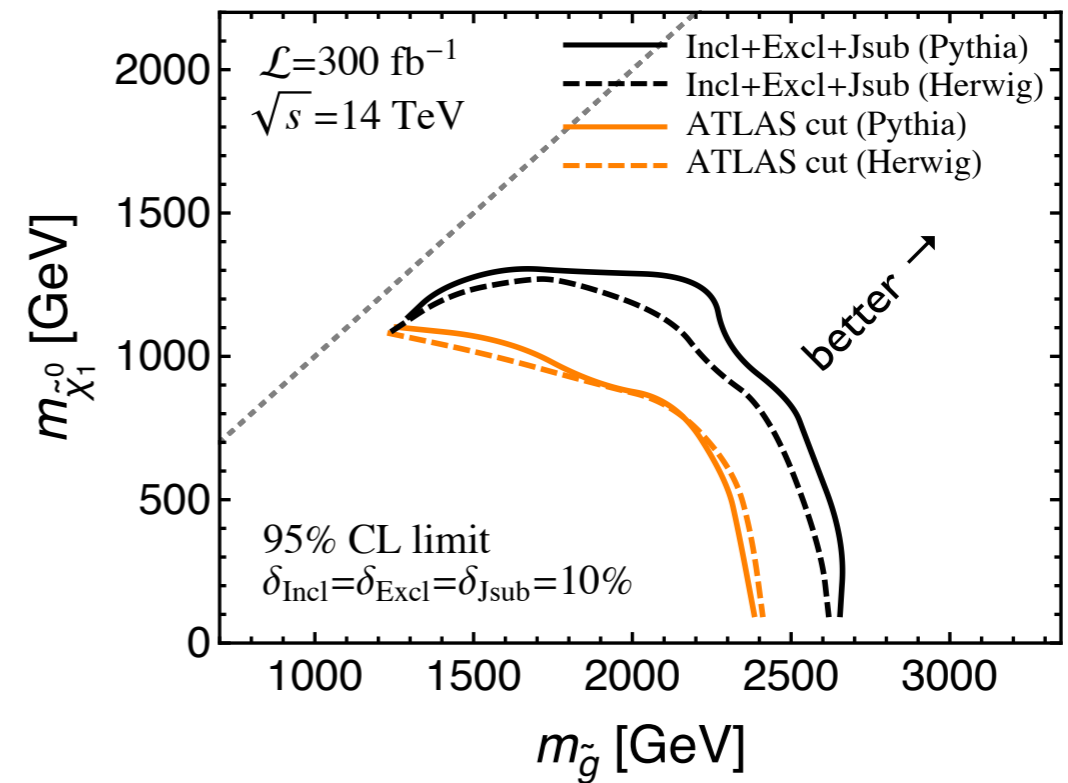
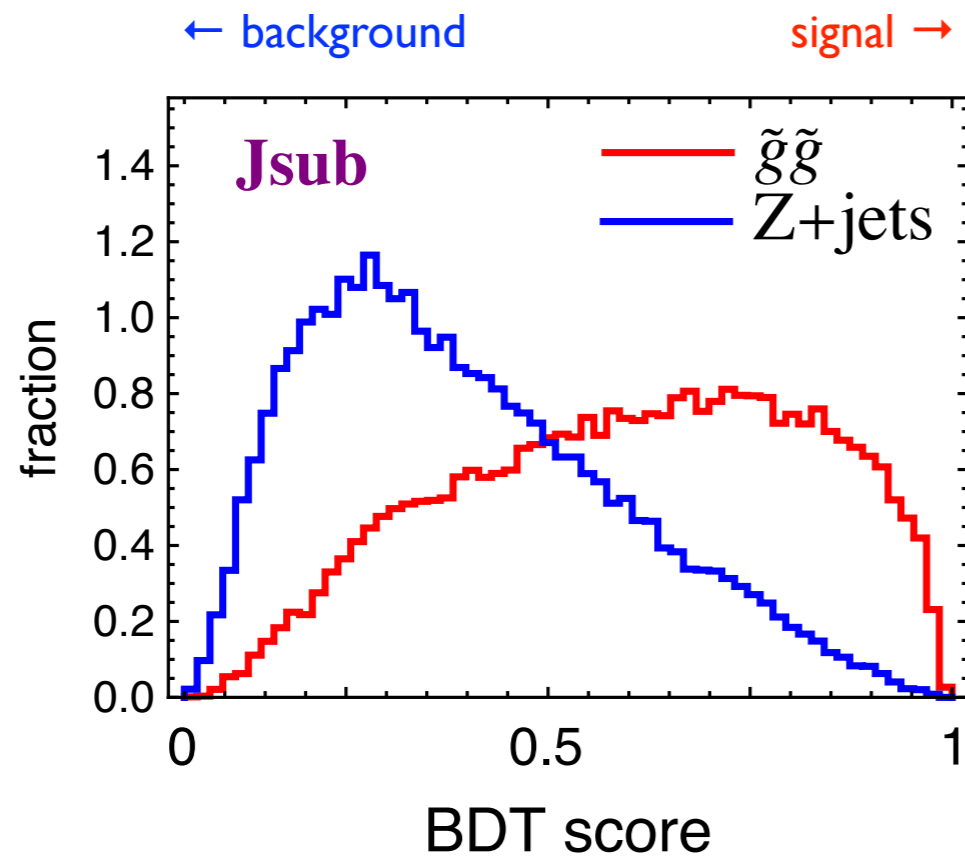
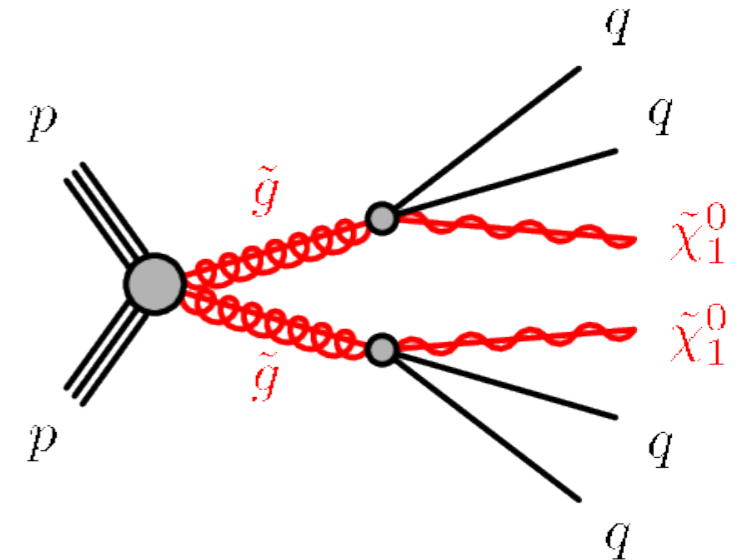
# E.g. Search for Supersymmetry

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

Inputs: Jet mass, width, track multiplicity

Signal: Quark enriched

Background: Gluon enriched



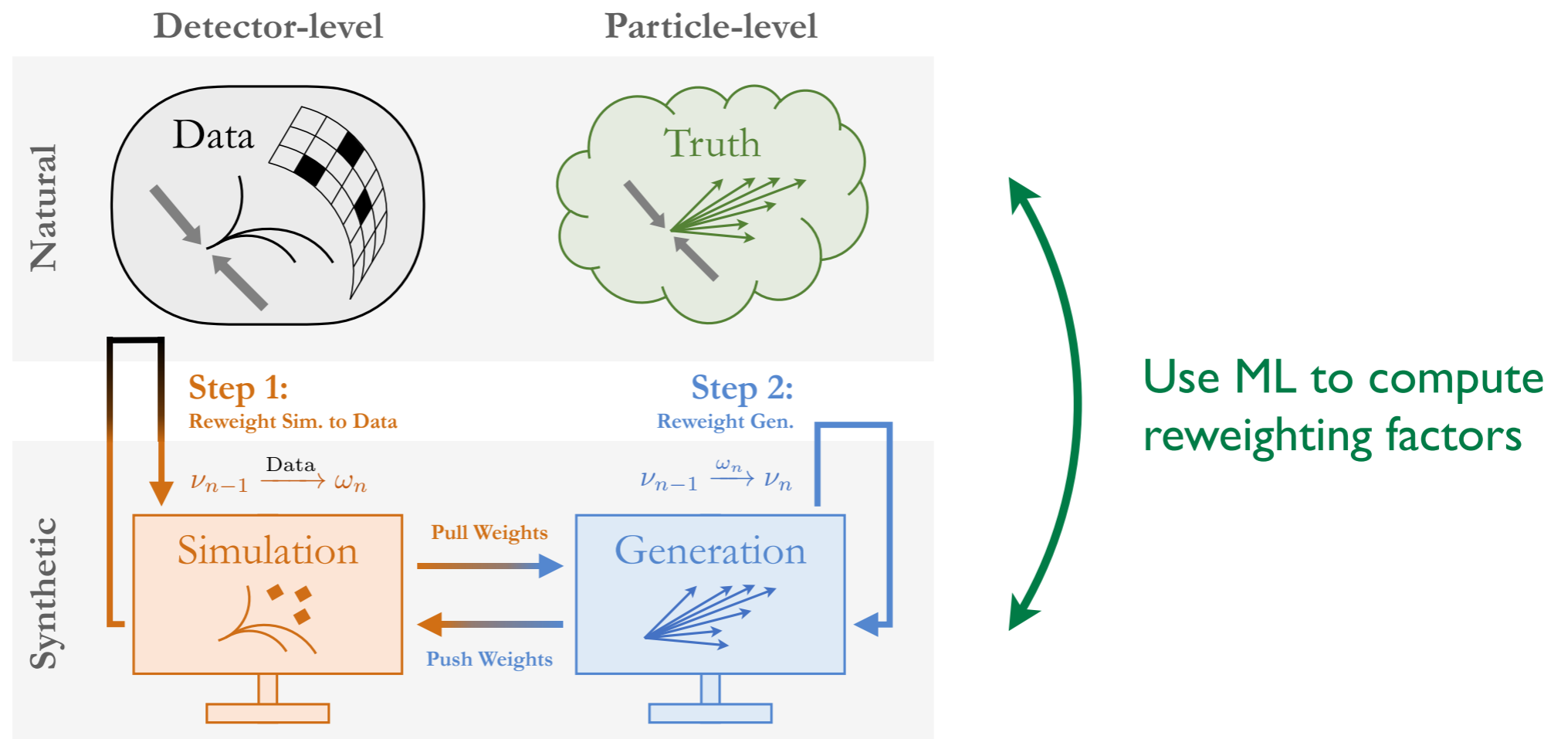
[Bhattacharjee, Mukhopadhyay, Nojiri, Sakakie, Webber, JHEP 2017]

# E.g. Detector Unfolding

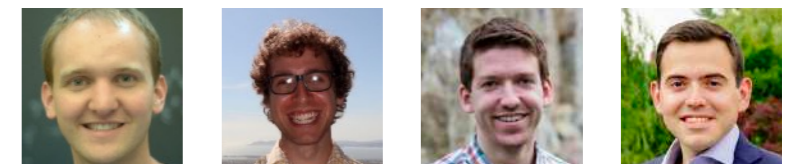
OmniFold



*Multi-dimensional unbinned* detector corrections  
via iterated application of *likelihood ratio trick*



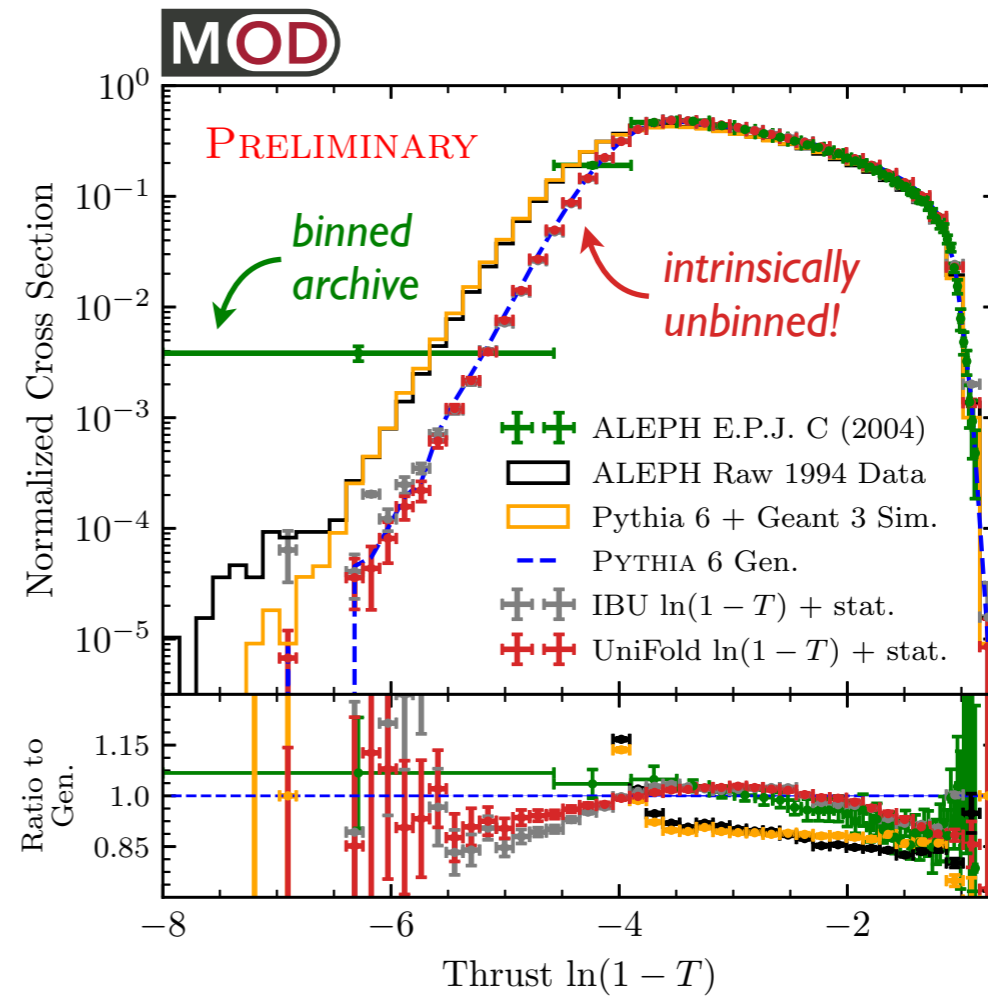
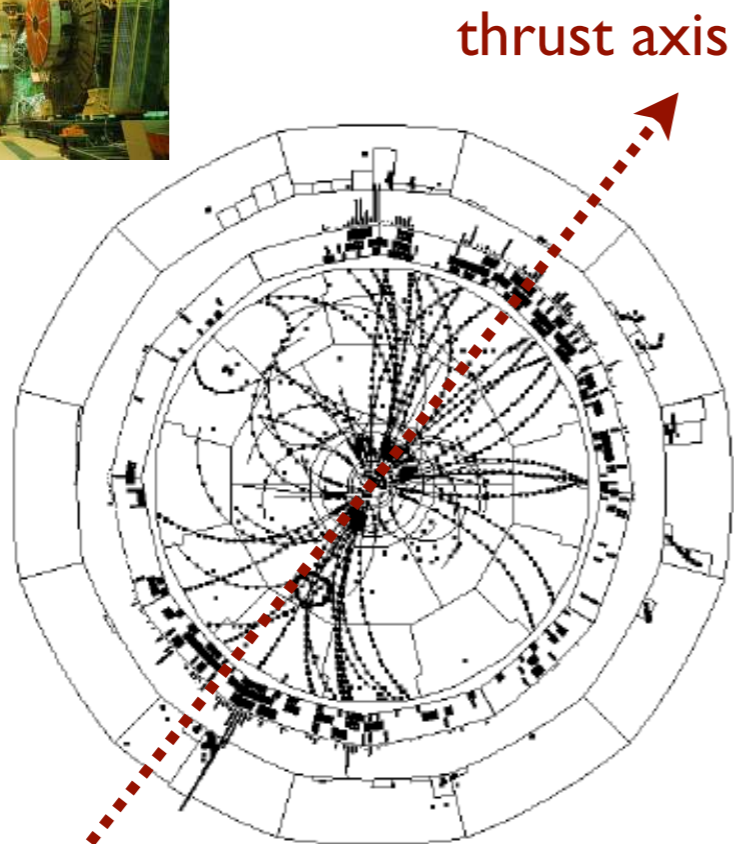
[Andreassen, Komiske, Metodiev, Nachman, JDT, [PRL 2020](#)]





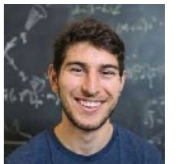
# E.g. Detector Unfolding

## Back to the Future with ALEPH Archival Data

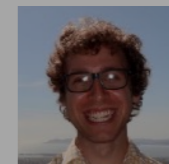


[talk by Badea, ICHEP 2020; cf. ALEPH, EPJ C 2004]

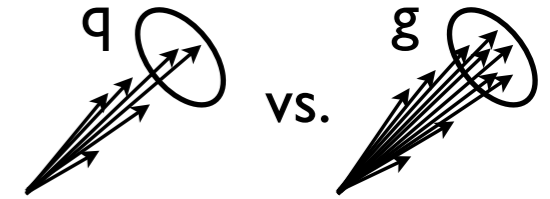
[see also Badea, Baty, Chang, Innocenti, Maggi, McGinn, Peters, Sheng, JDT, Lee, PRL 2019]



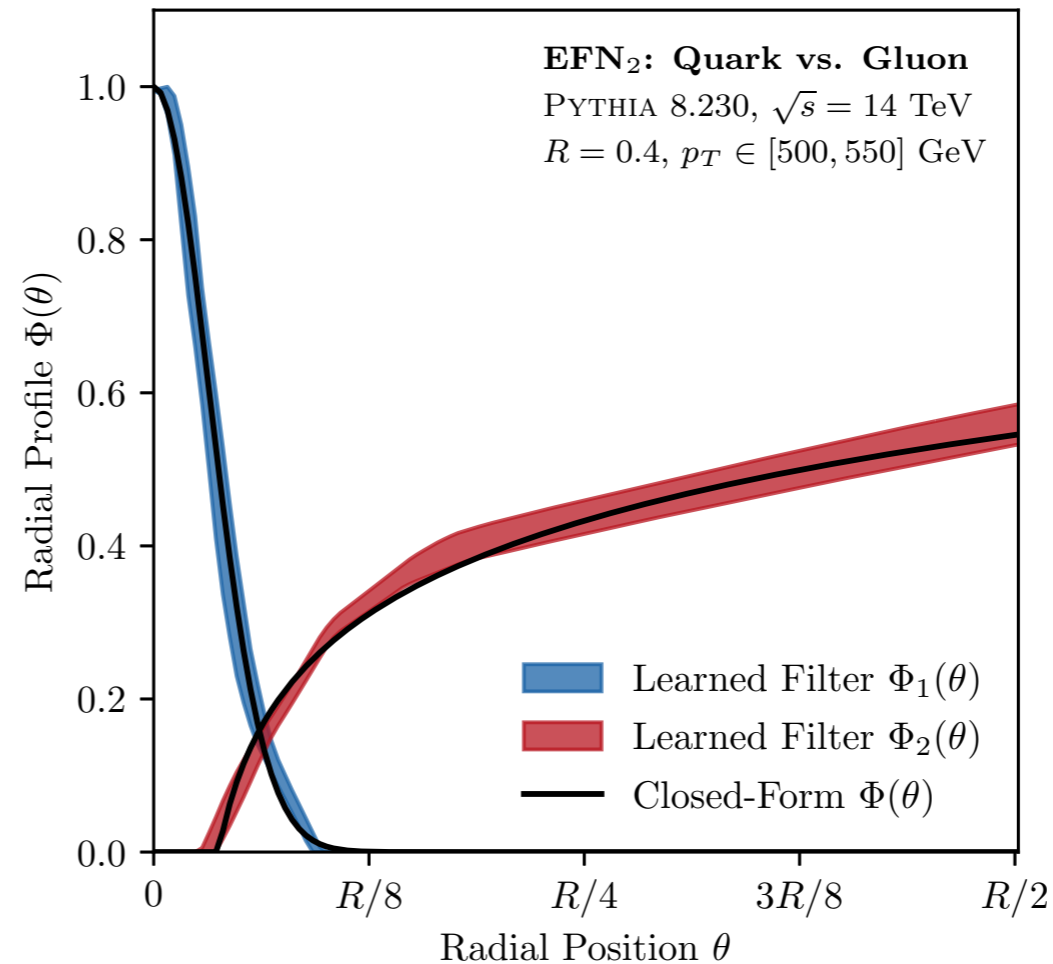
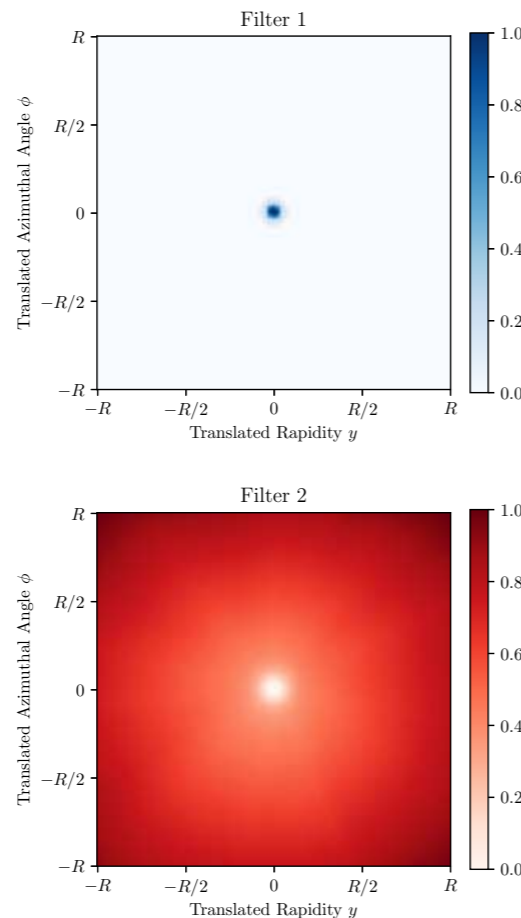
[Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020]



# Learning from the Machine



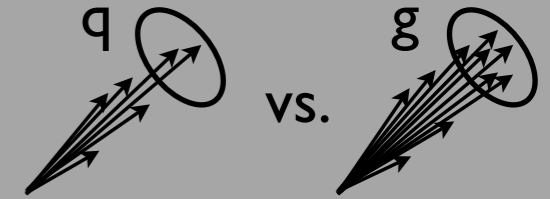
For  $\ell = 2$ , EFN learns radial moments:  $\sum_{i \in \text{jet}} z_i f(\theta_i)$  cf. Angularities:  $f(\theta) = \theta^\beta$



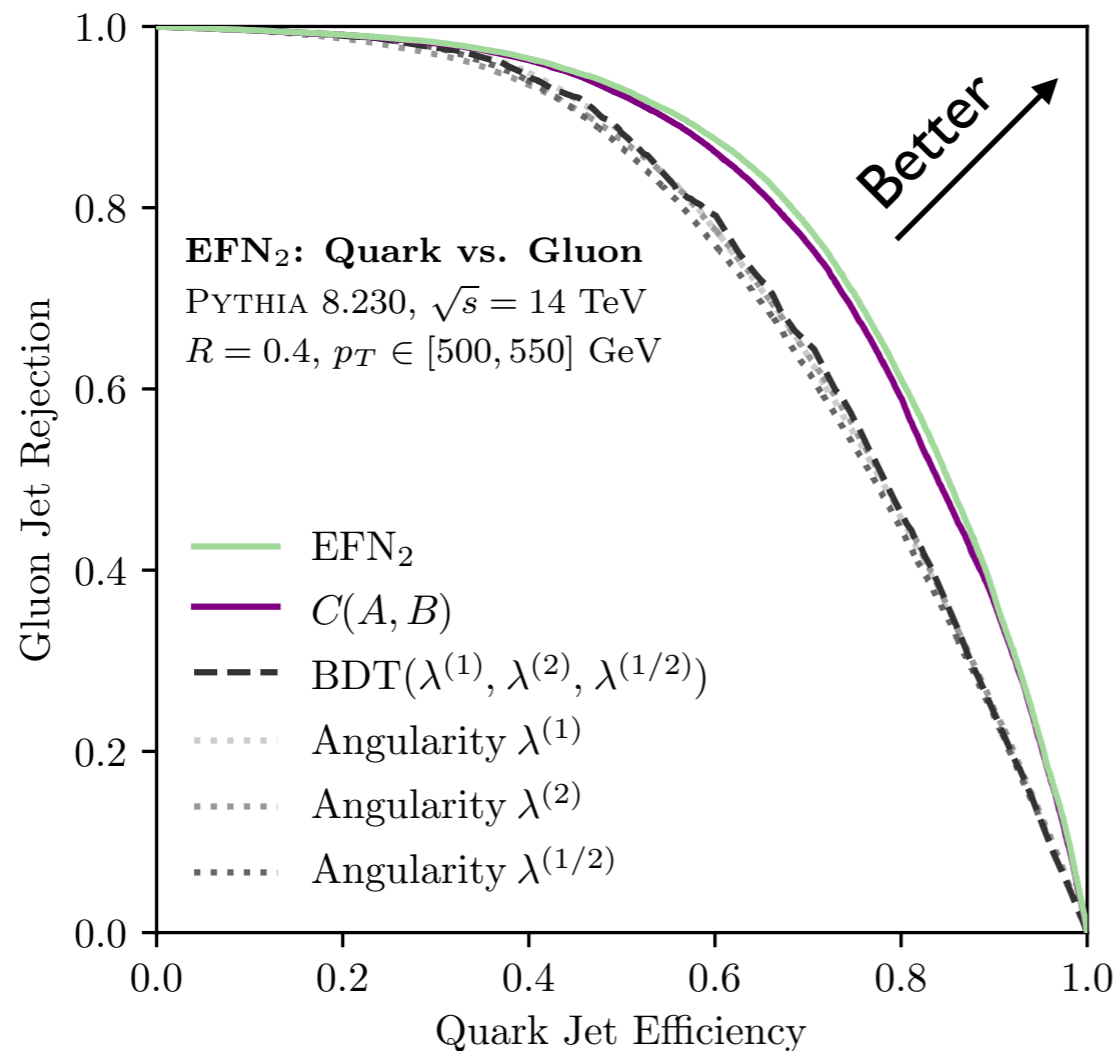
Traditional QCD observables emphasize homogeneous angular scaling  
 But EFN reveals that **likelihood ratio** exhibits **collinear/wide-angle** separation

[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 learns radial moments:  $\sum_{i \in \text{jet}} z_i f(\theta_i)$  cf. Angularities:  $f(\theta) = \theta^\beta$



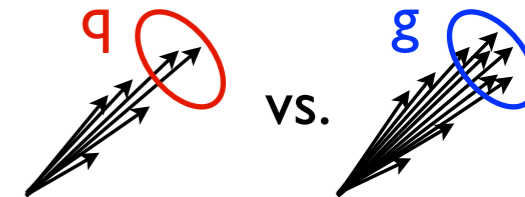
EFN outperformed a domain expert (i.e. me)

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

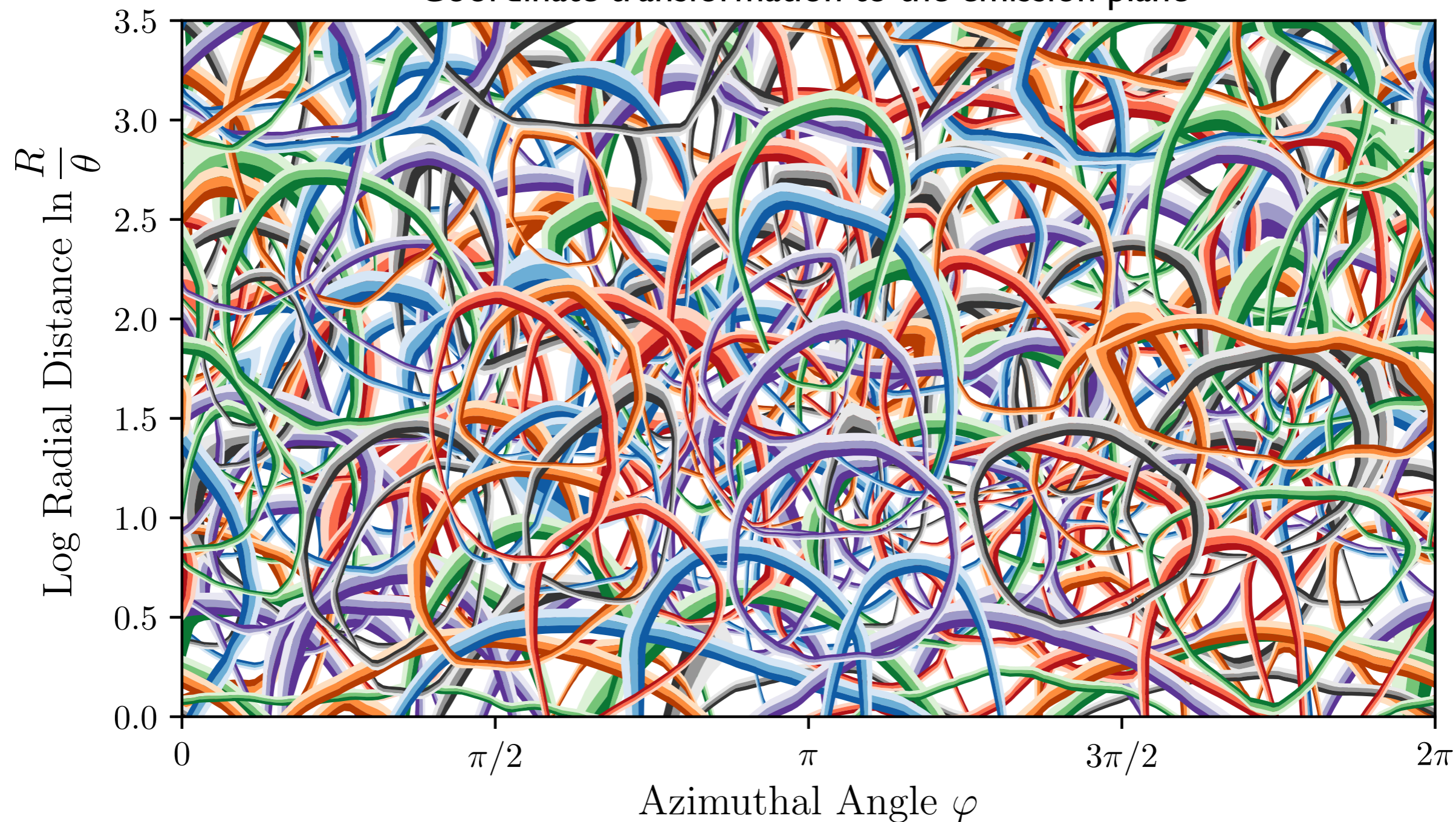
[Komiske, Metodiev, JDT, JHEP 2019;  
 cf. Larkoski, JDT, Waalewijn, JHEP 2014; using Berger, Kucs, Sterman, PRD 2003; Ellis, Vermilion, Walsh, Hornig, Lee, JHEP 2010]



# En Route to the Lund Plane



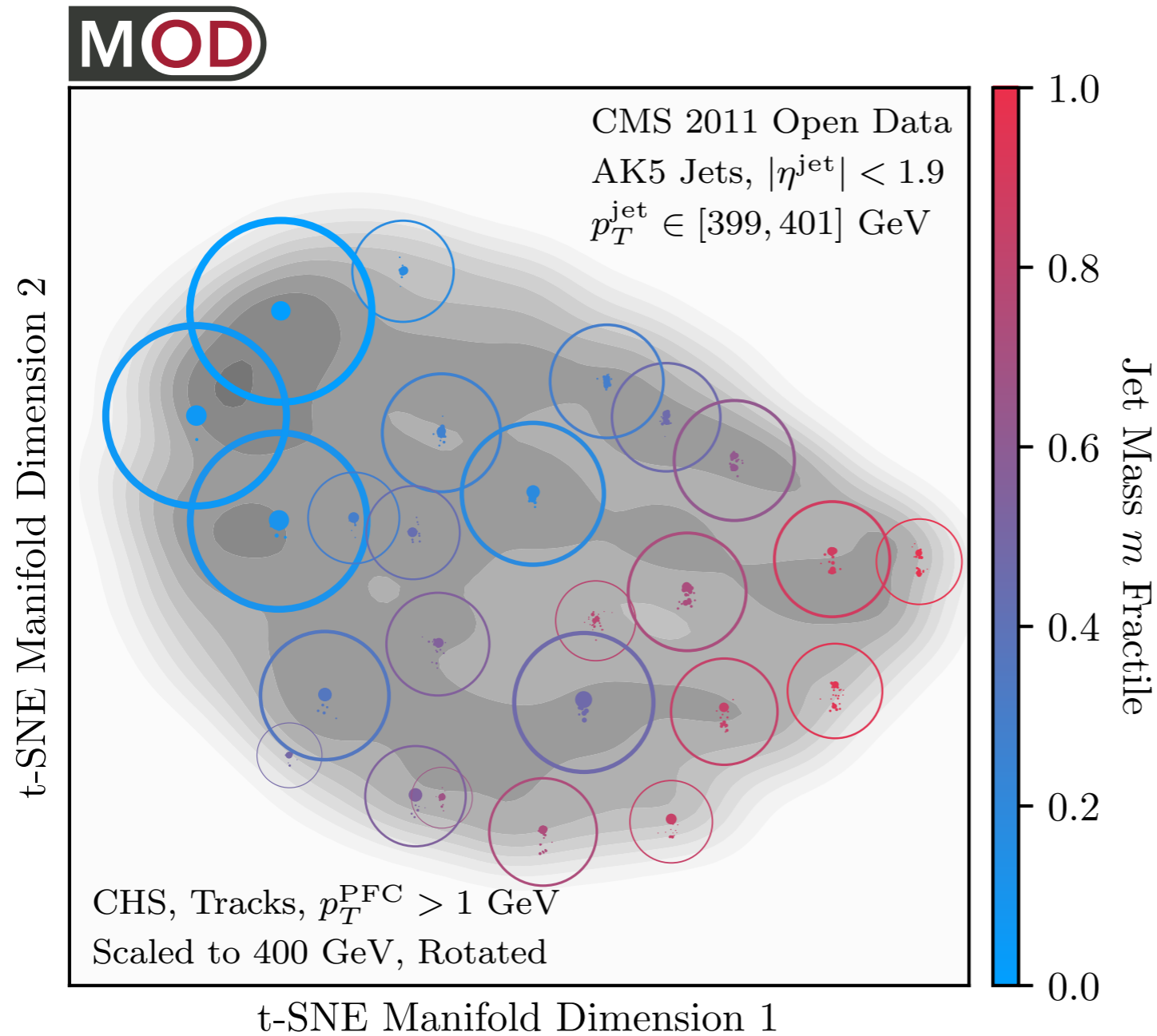
Coordinate transformation to the emission plane



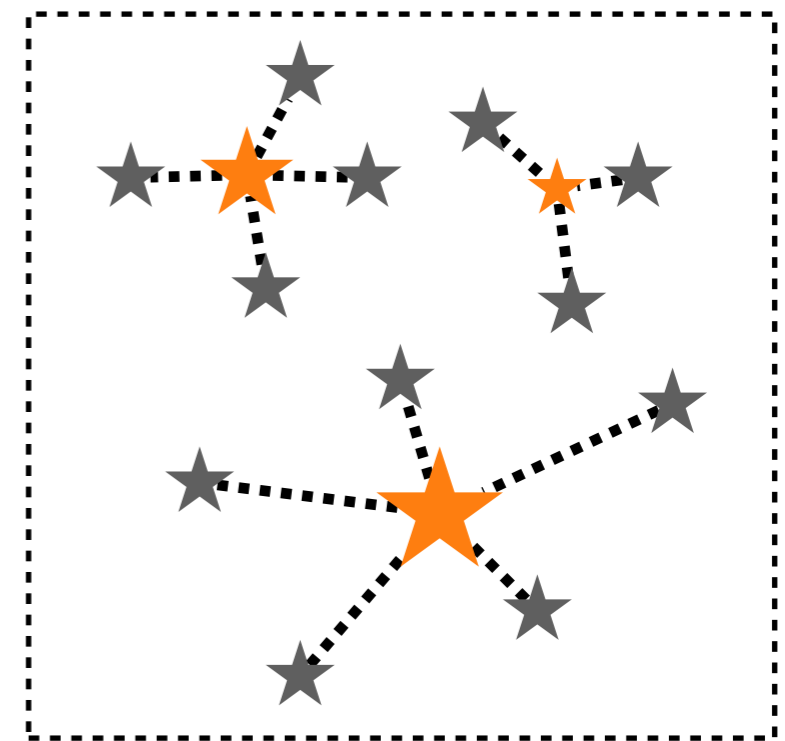
[Komiske, Metodiev, JDT, JHEP 2019; see also Dreyer, Salam, Soyez, JHEP 2018]



# Most Representative Jets



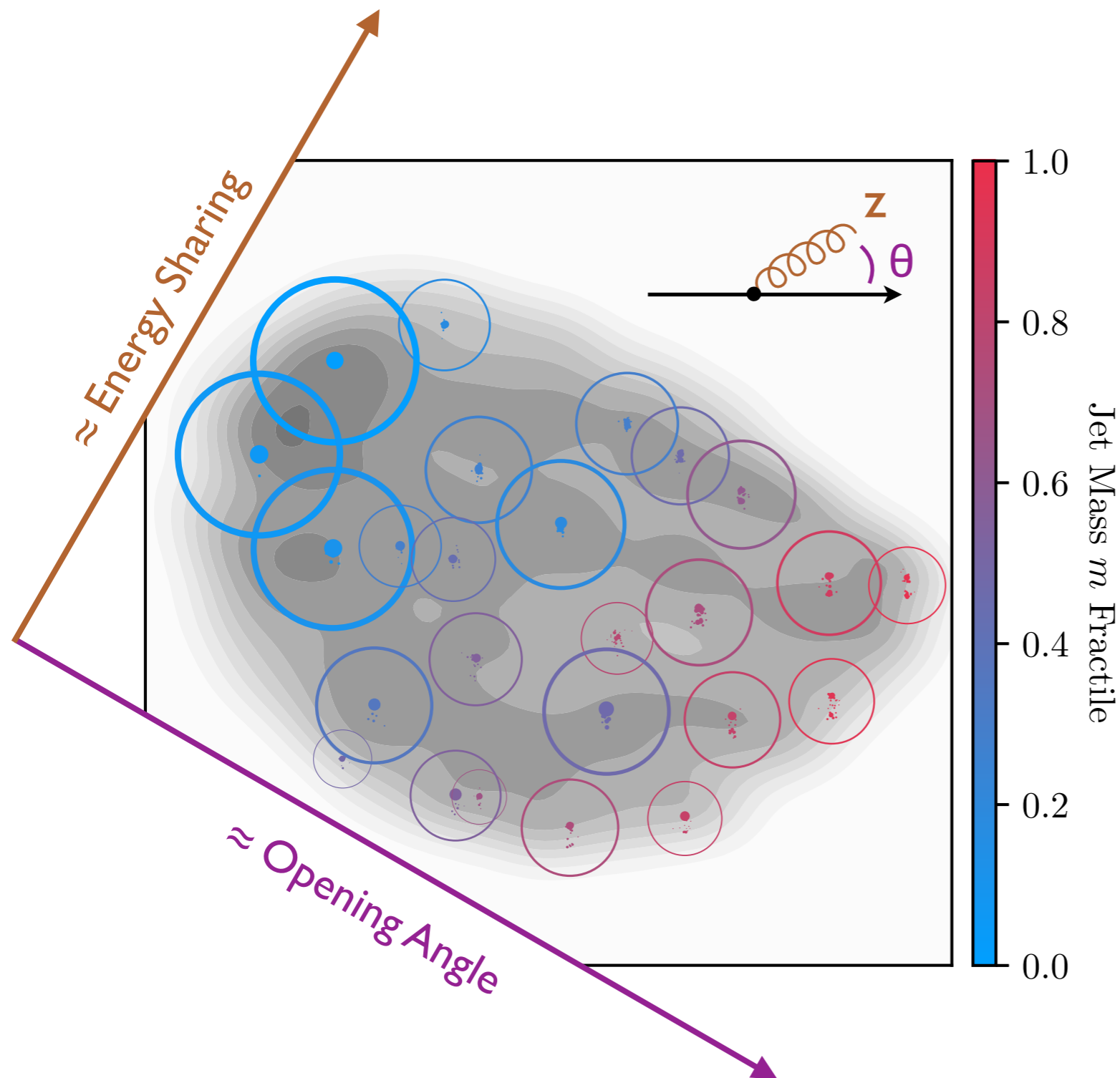
**k-medoids**  
 Arranged via t-SNE



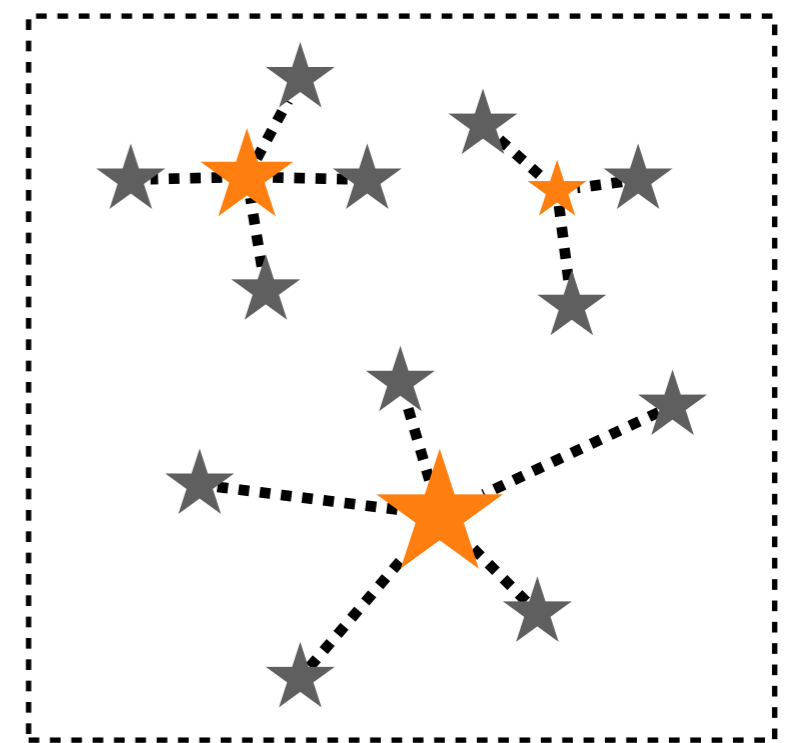
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;  
 using van der Maaten, Hinton, JMLR 2008]



# Most Representative Jets



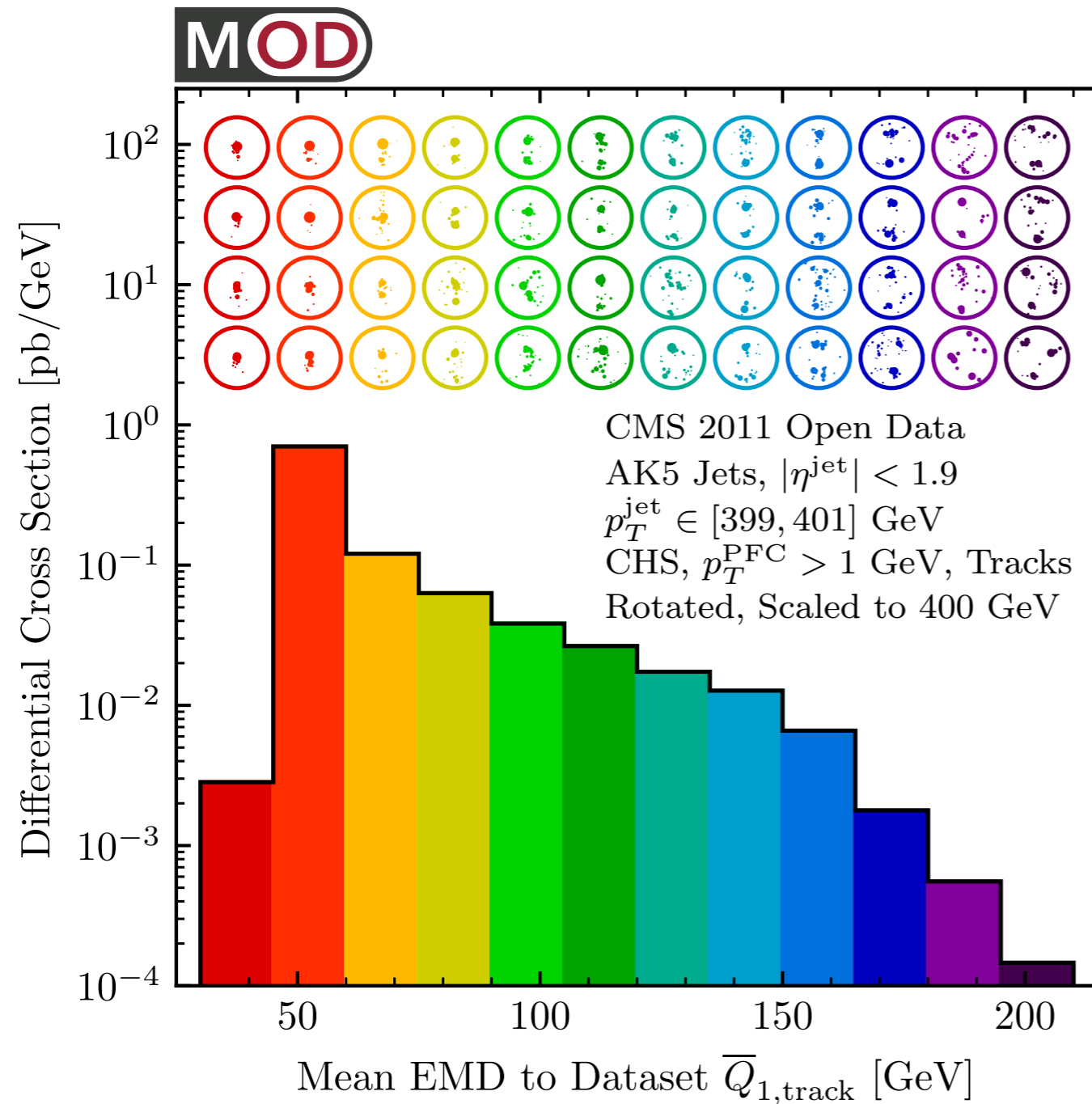
**k-medoids**  
*Arranged via t-SNE*



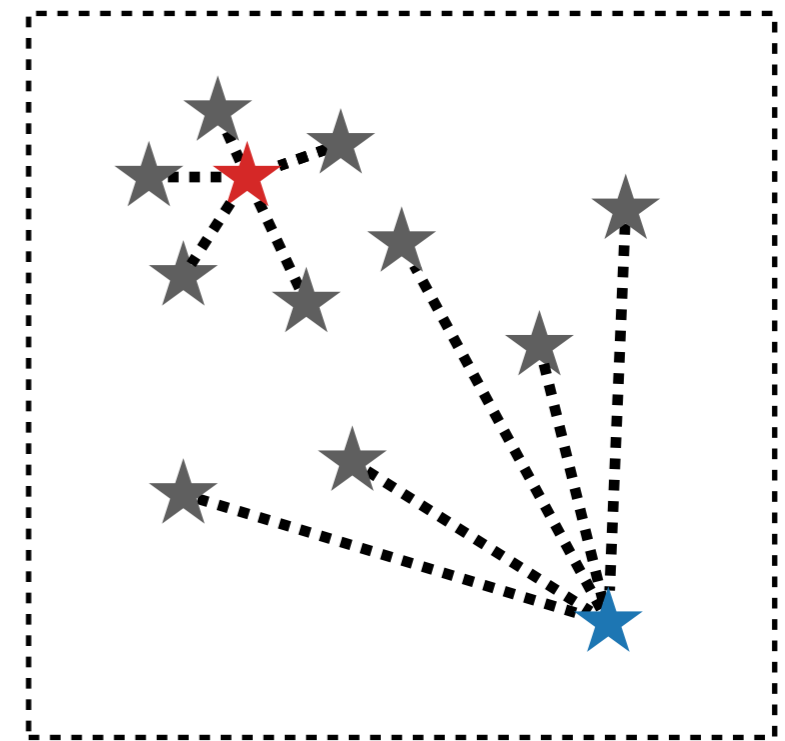
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;  
using van der Maaten, Hinton, JMLR 2008]



# Least Representative Jets



New Physics?  
 Or tails of QCD?



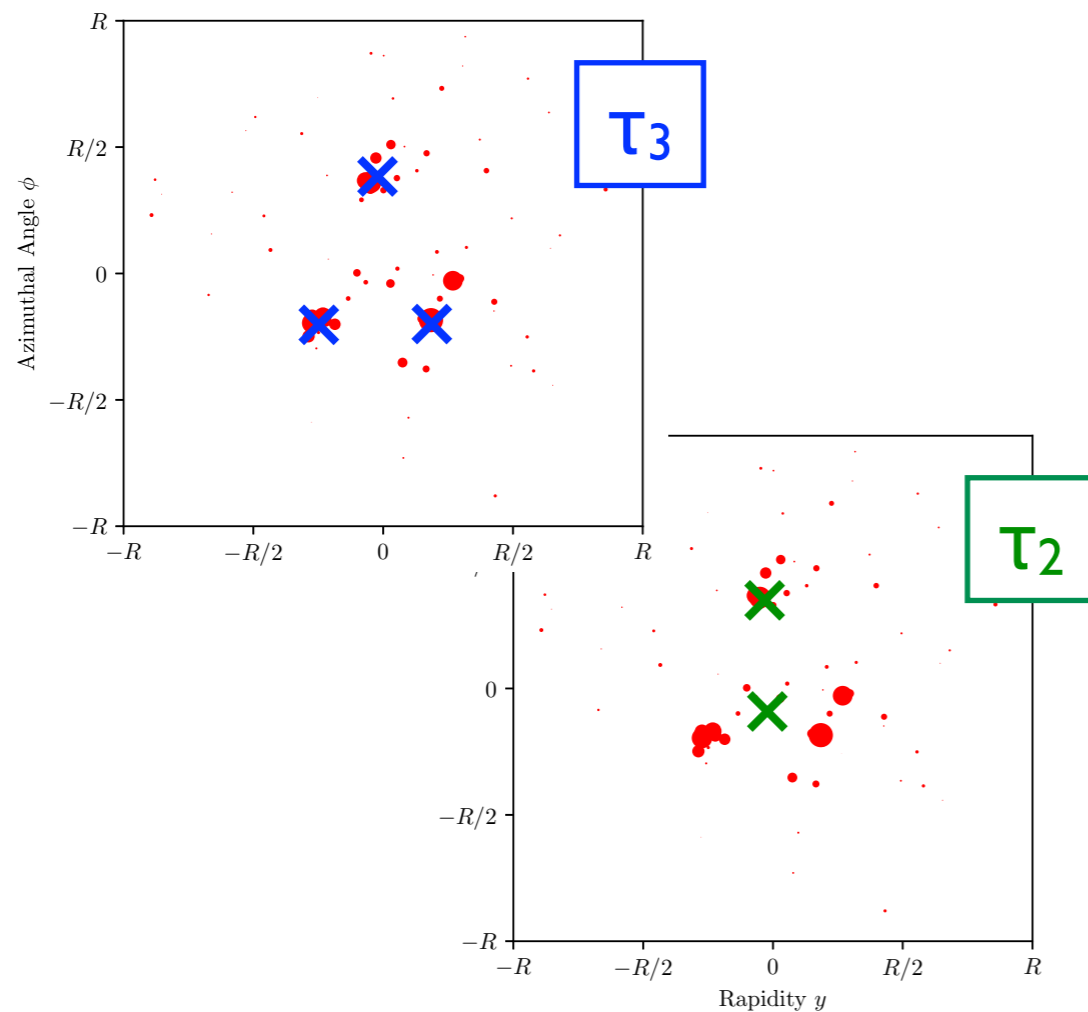
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]



# N-subjettiness

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

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



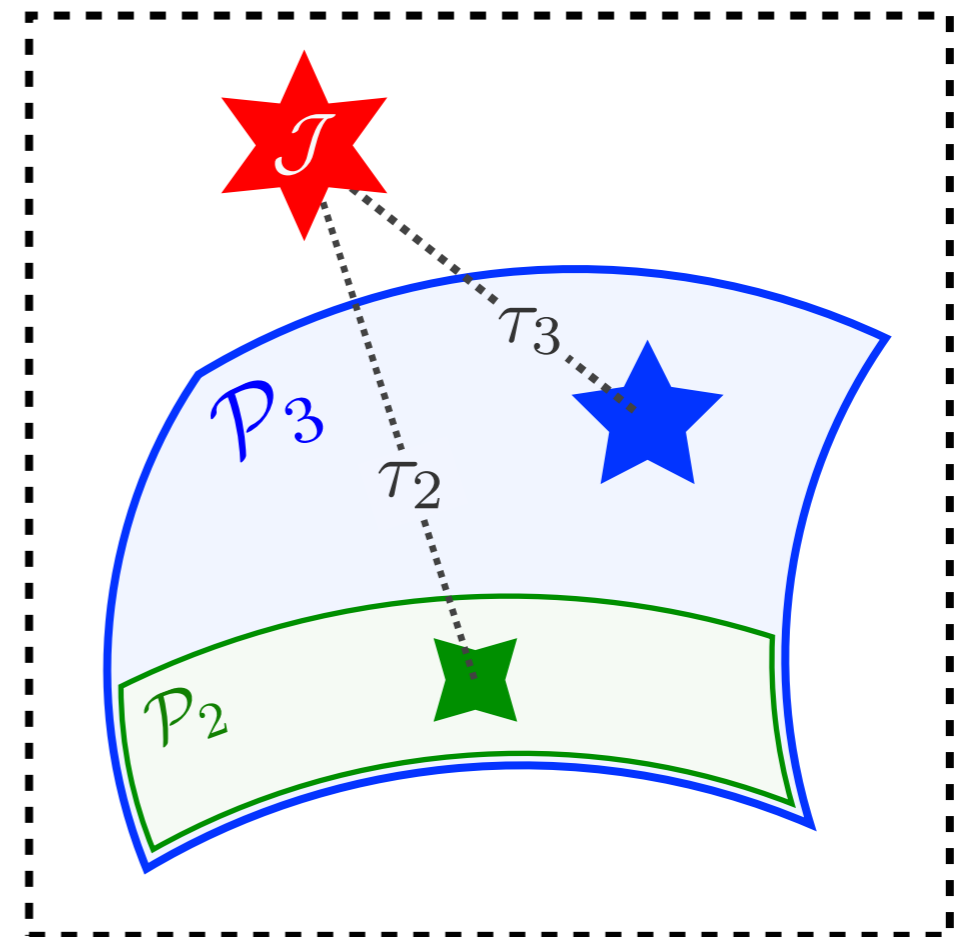
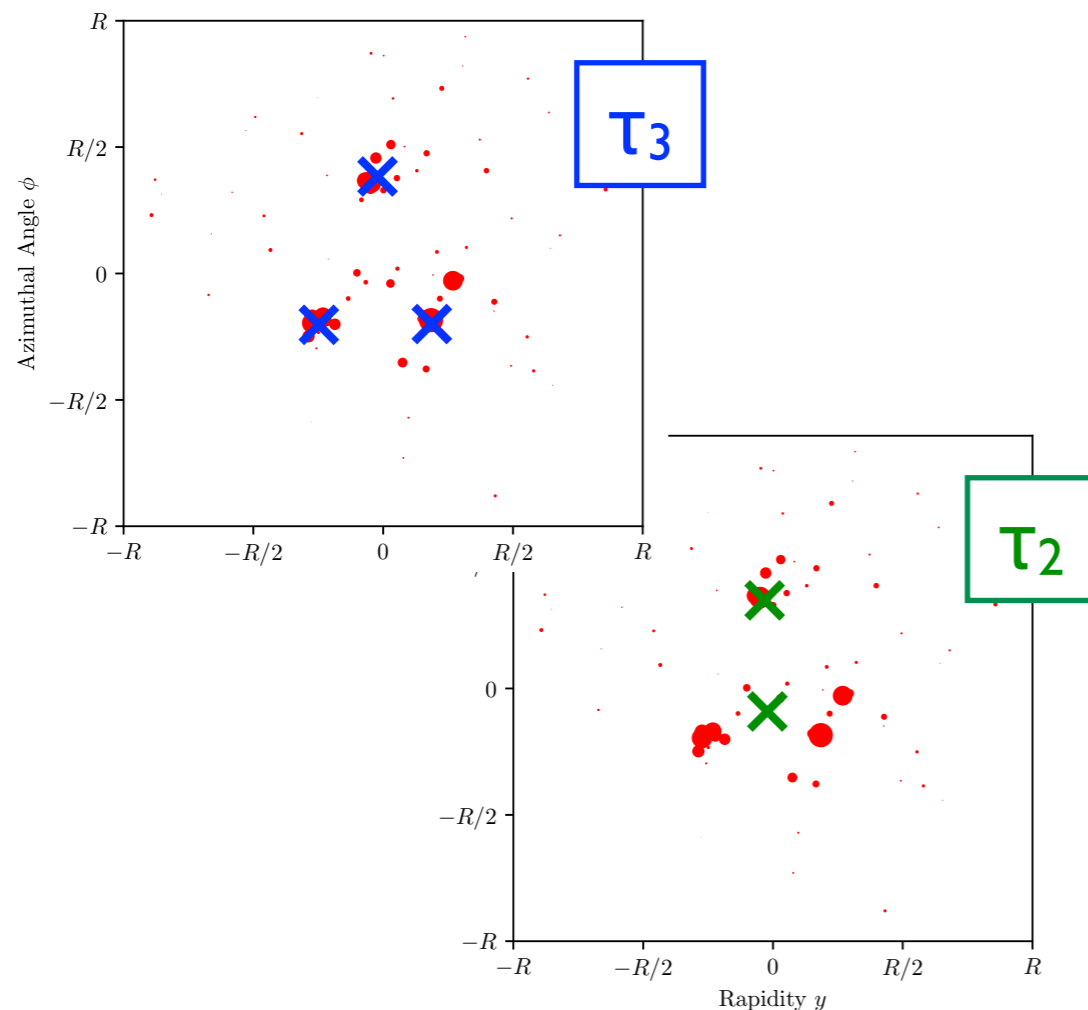
[JDT, Van Tilburg, JHEP 2011, JHEP 2012;  
based on Brandt, Dahmen, ZPC 1979; Stewart, Tackmann, Waalewijn, PRL 2010]



# N-subjettiness = Point to Manifold EMD

...is secretly an optimal transport problem

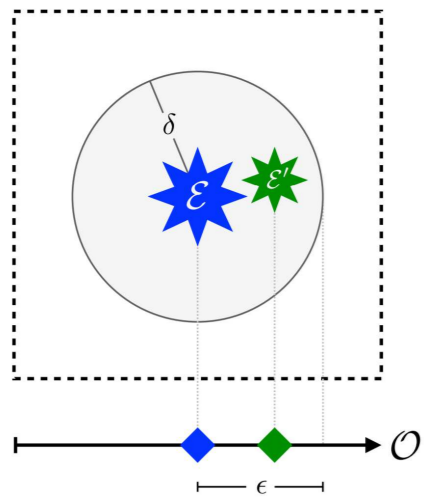
$$\tau_N(\mathcal{J}) = \min_{\mathcal{J}' \in \mathcal{P}_N} \text{EMD}(\mathcal{J}, \mathcal{J}')$$



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

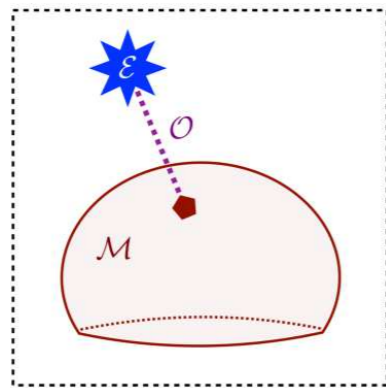
# Six Decades of Collider Physics Translated into a New Geometric Language!

IRC Safety is smoothness in the space of events



Taming infinities

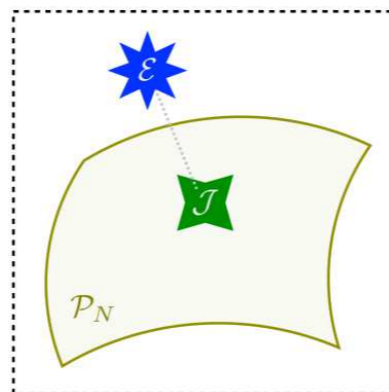
Event shapes are distances from events to manifolds.



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

Event Shapes

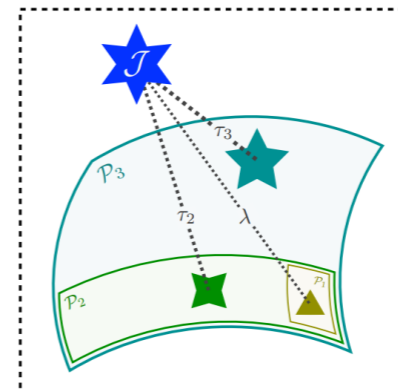
Jets are projections to few-particle manifolds.



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

Jet Algorithms

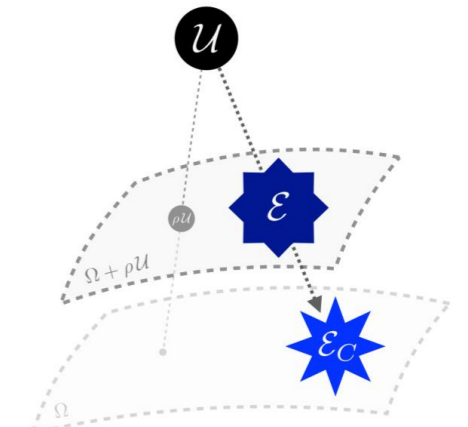
Substructure resolves emissions within the jet.



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

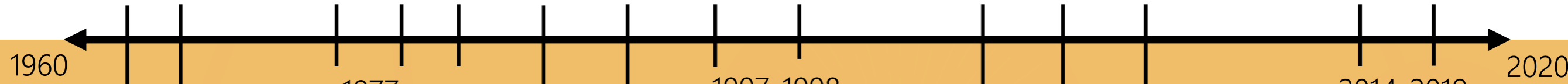
Jet Substructure

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]

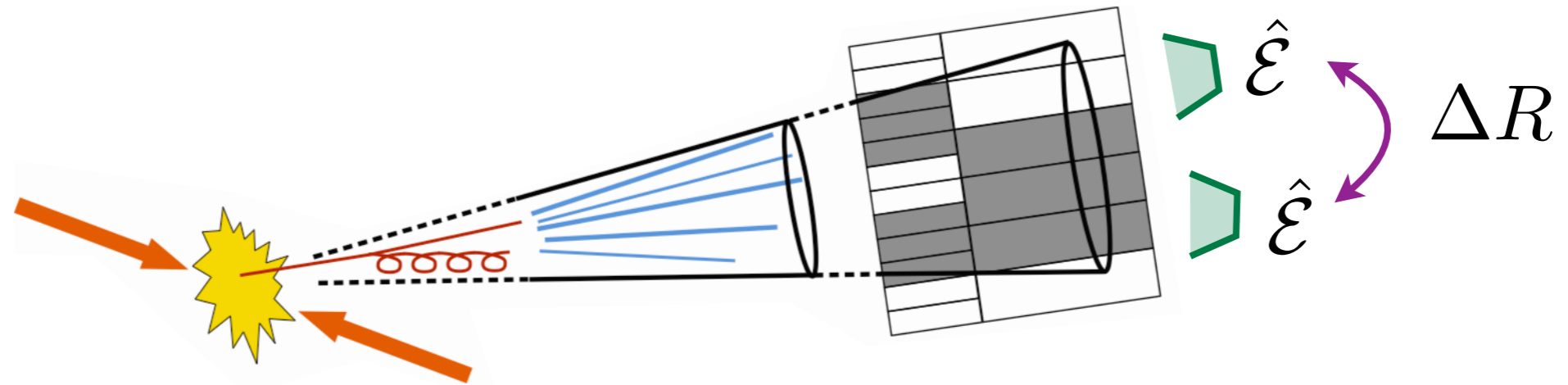
2010-2015  
N-(sub)jettiness, X Cone  
[Stewart, Tackmann, Waalewijn, PRL 2010]  
[Thaler, Van Tilburg, JHEP 2011]  
[Stewart, Tackmann, Thaler, Vermilion, Wilkason, JHEP 2015]

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

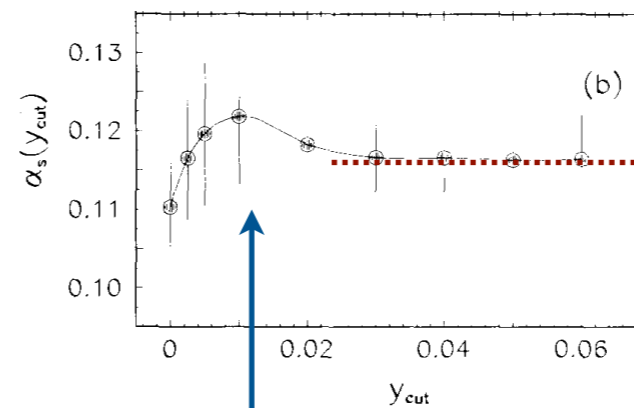
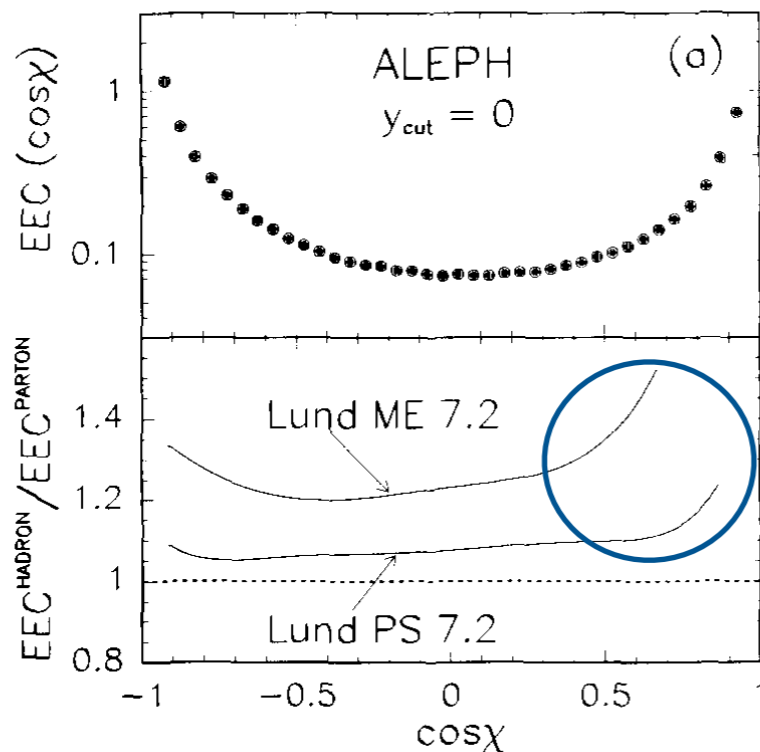
And many more!

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

# Energy-Energy Correlators



A long history in probing collinear dynamics of QCD

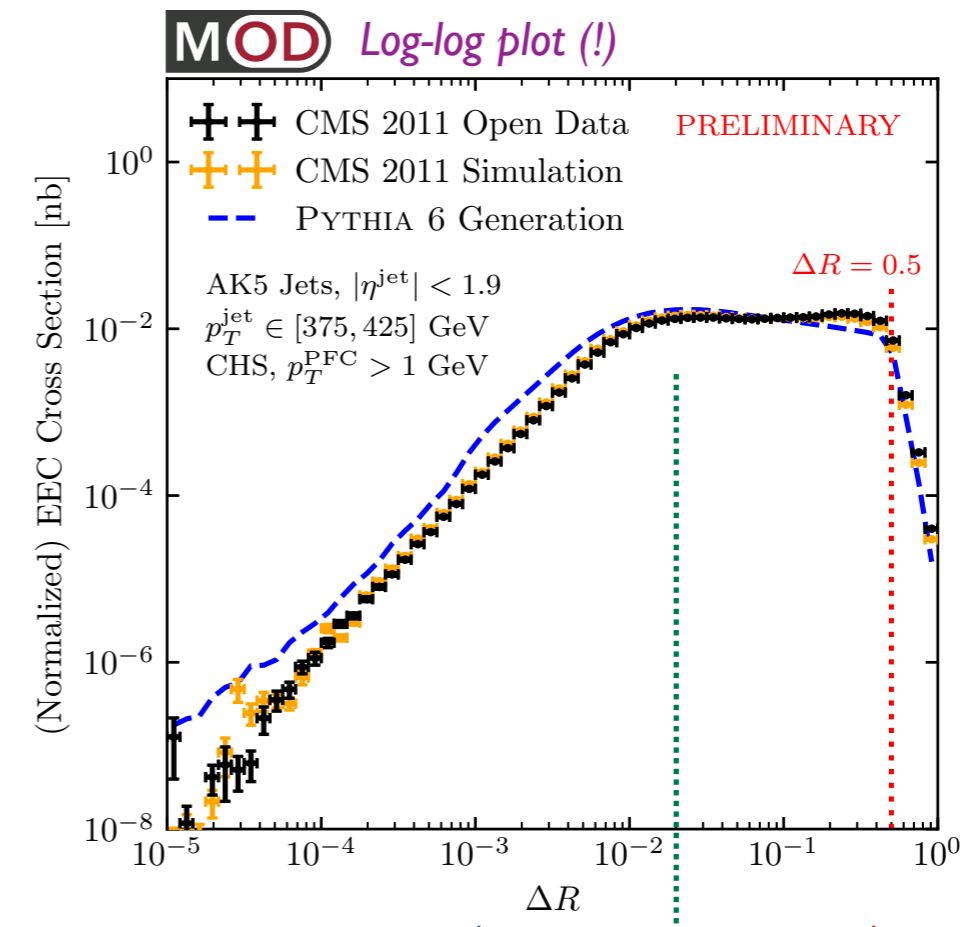
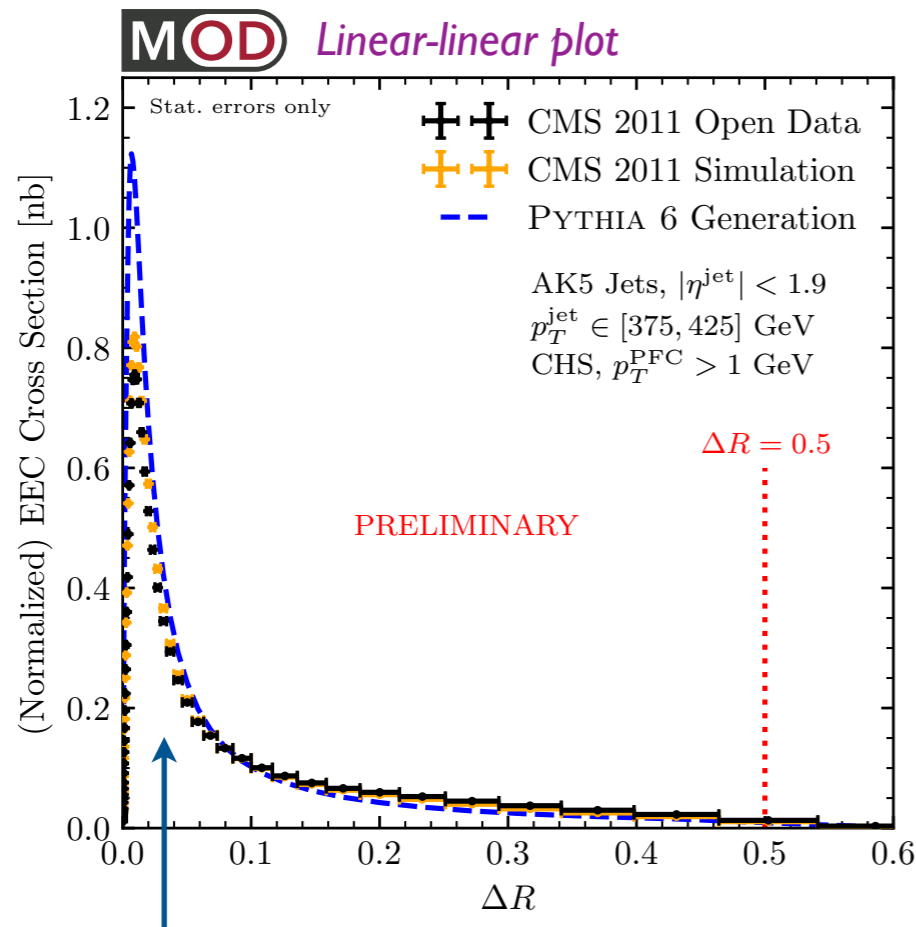


Extracting the strong coupling constant

Theoretical challenges with small angle (collinear) limit

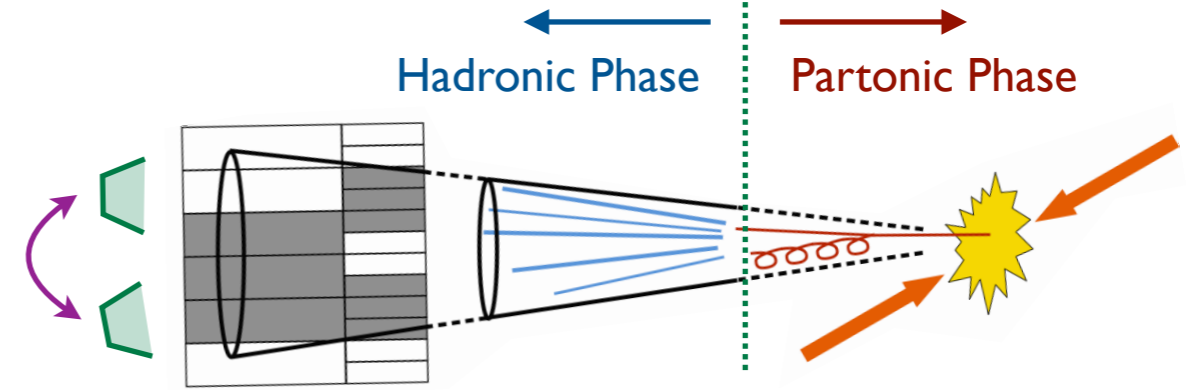
[Basham, Brown, Ellis, Love, *PRL* 1978; ALEPH, *PLB* 1991; see Chen, Mout, Zhang, Zhu, *PRD* 2020]

# 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]

