

Machine Learning

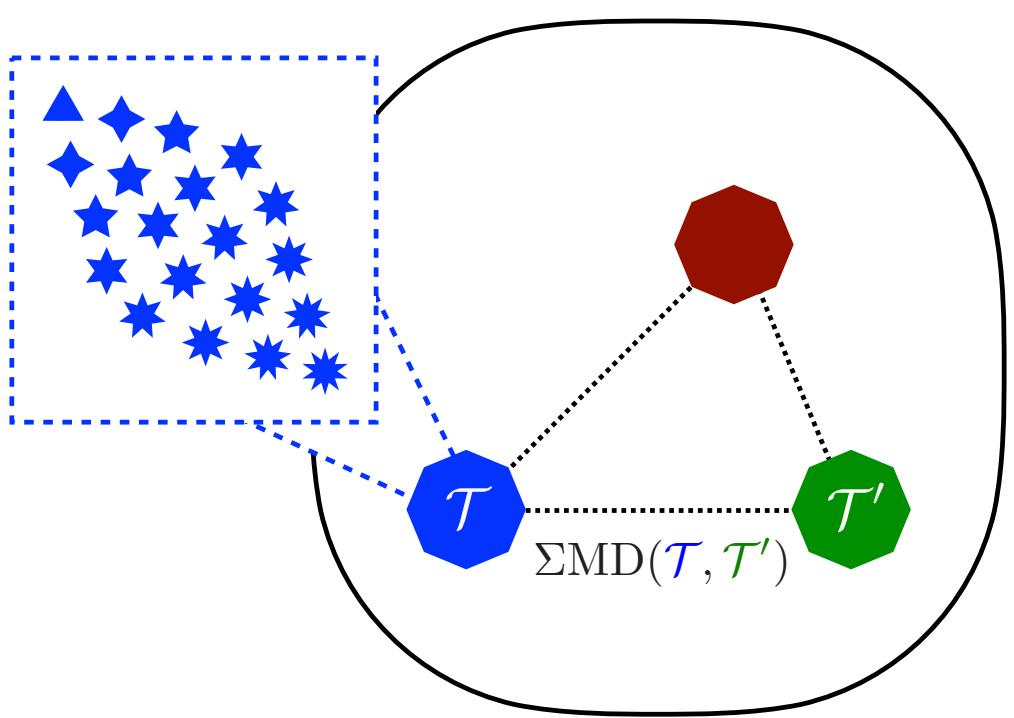
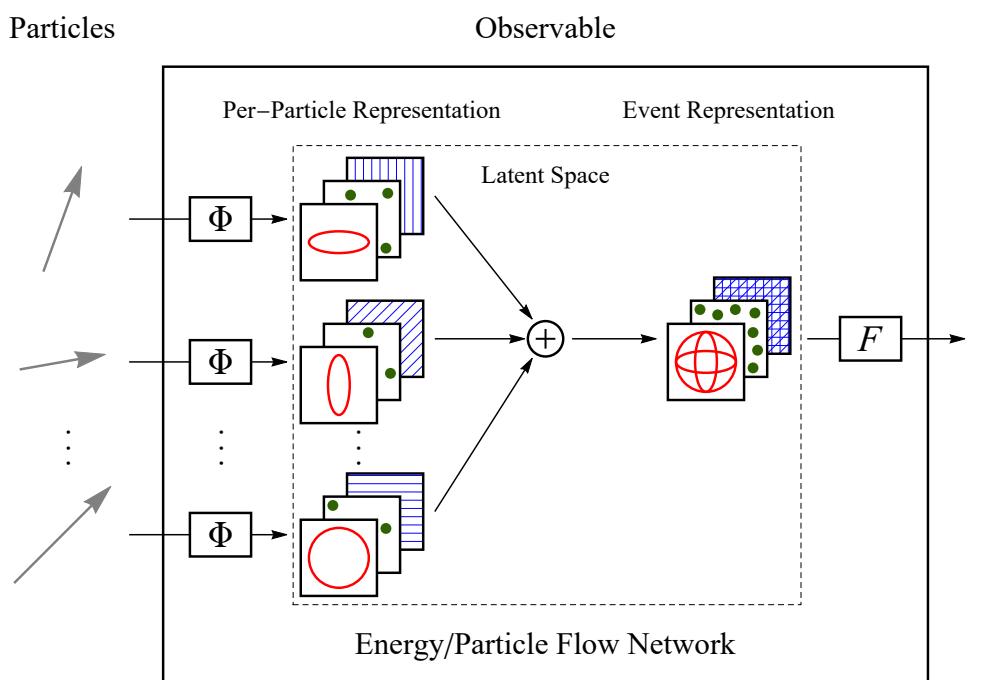
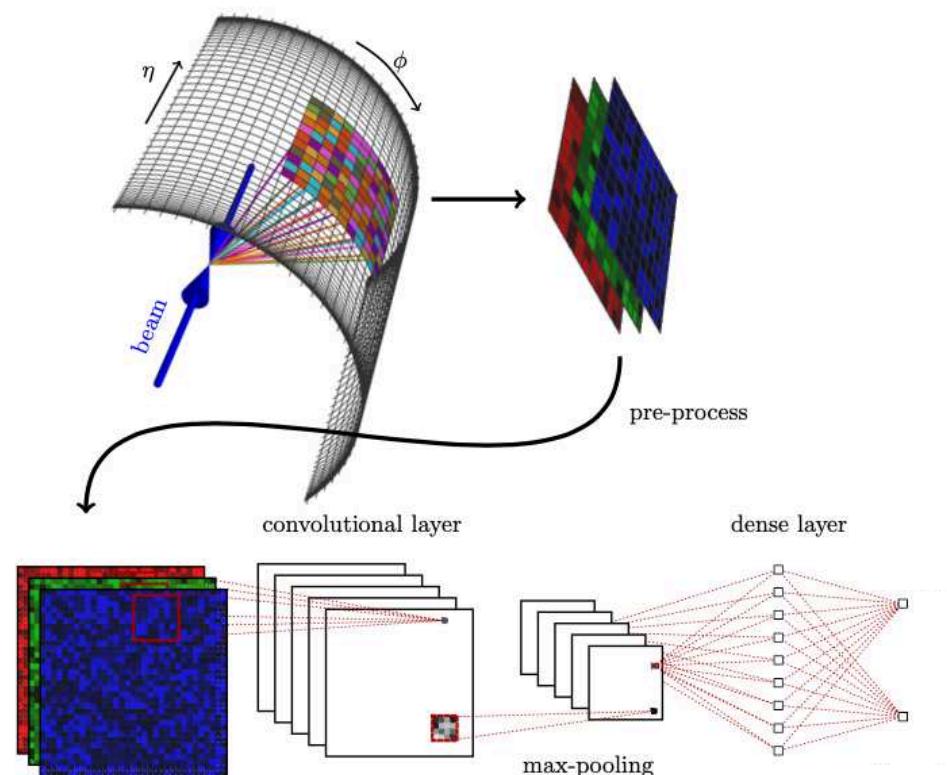
An Essential Toolkit for Particle Physics

Patrick T. Komiske III

Massachusetts Institute of Technology
Center for Theoretical Physics

Snowmass Computational Frontier Workshop – ML Subgroup

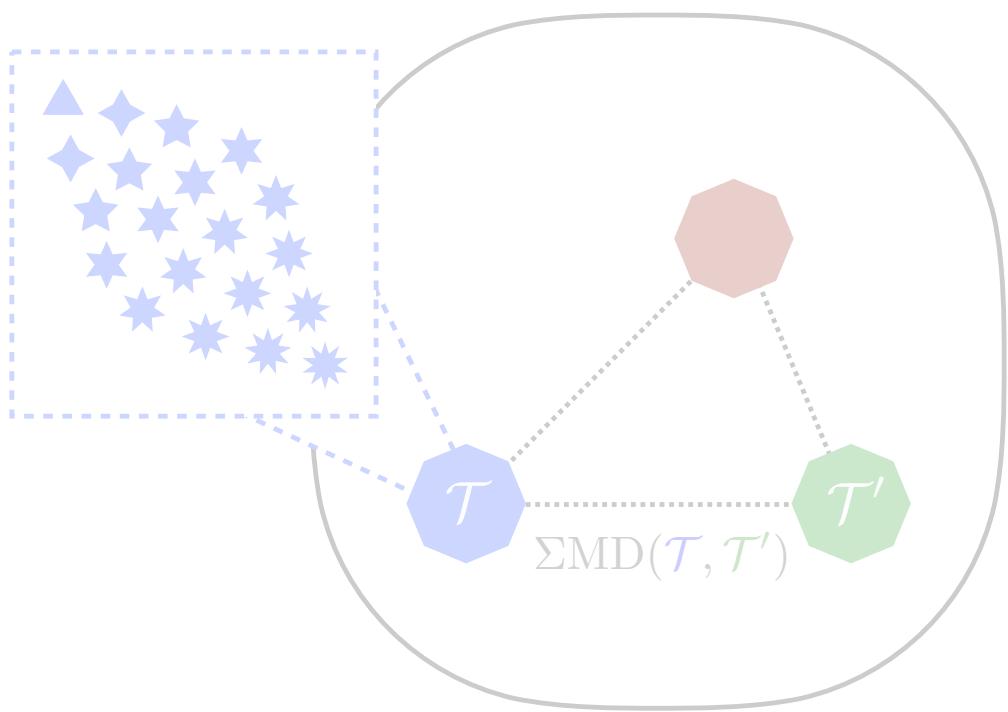
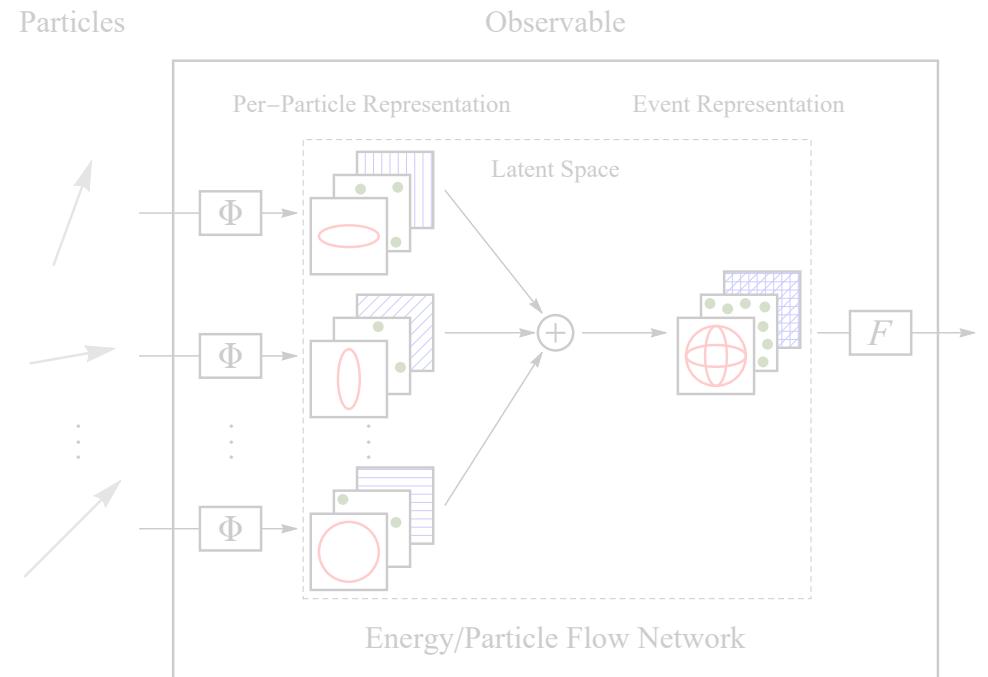
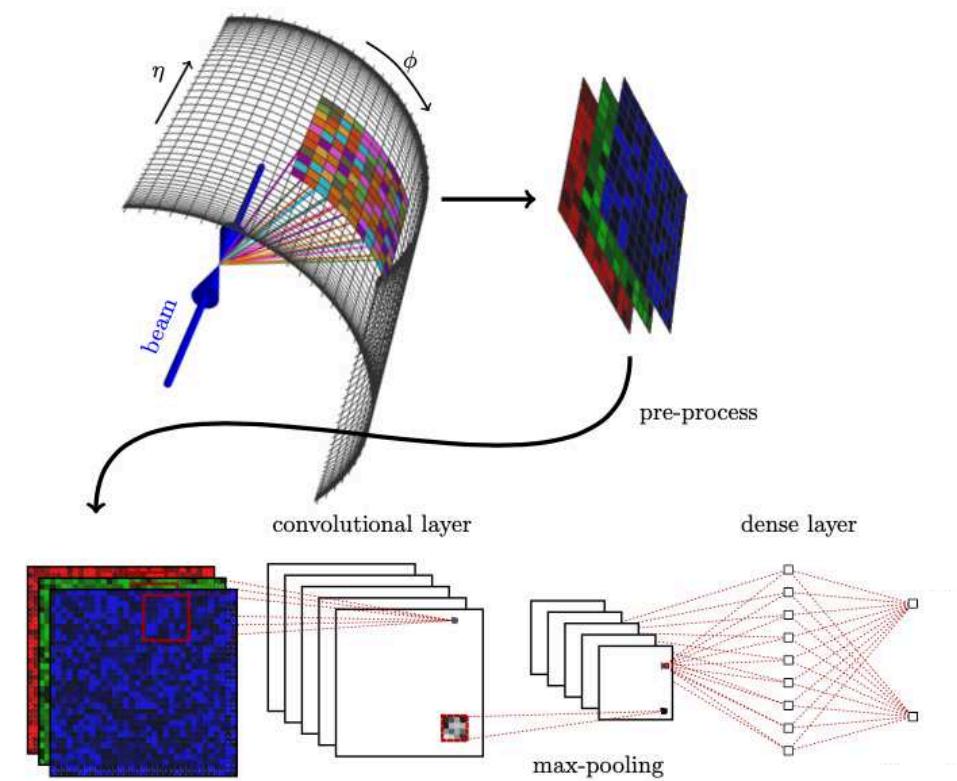
August 10, 2020



Ubiquity of ML in HEP

Lightning Review

Future Directions

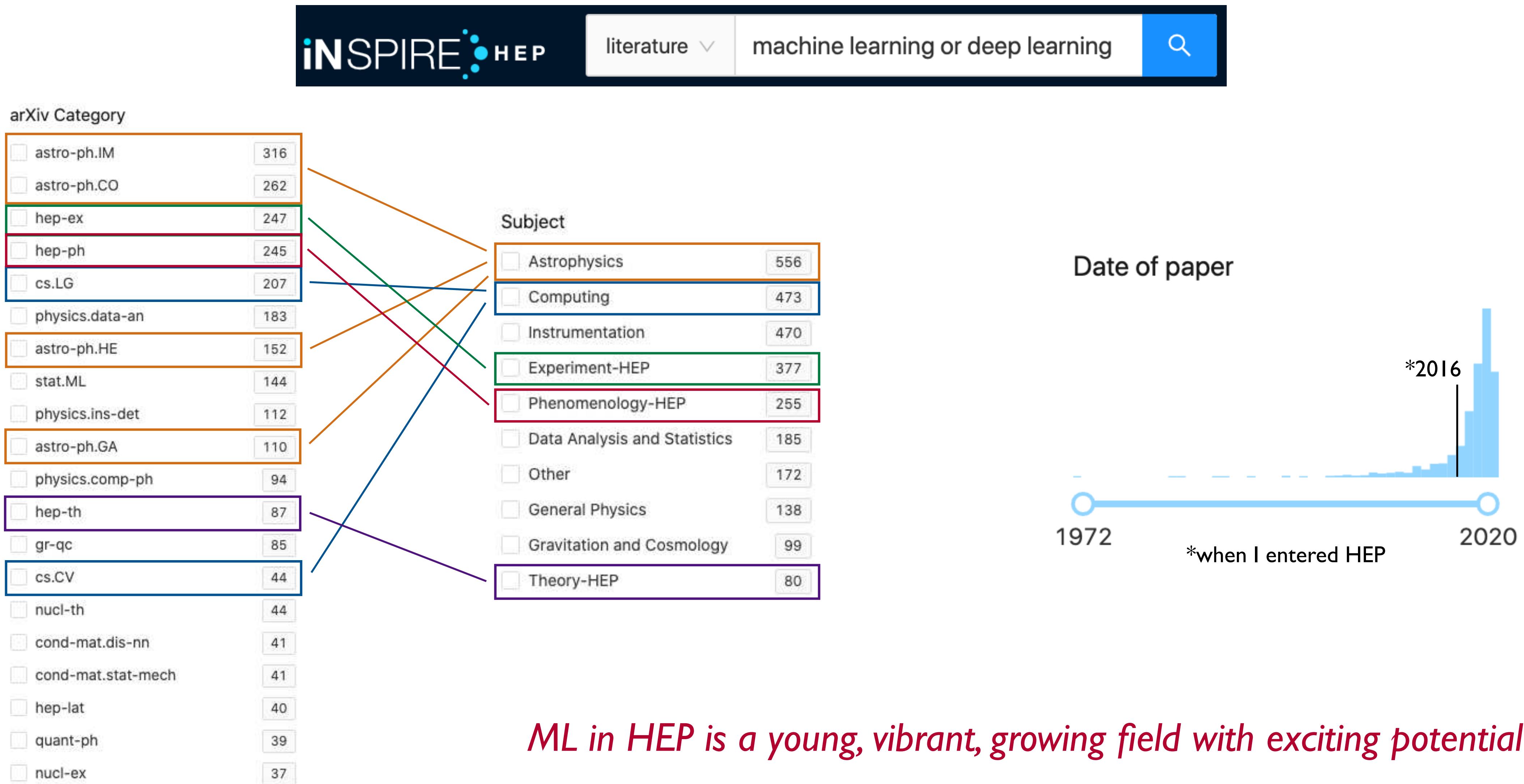


Ubiquity of ML in HEP

Lightning Review

Future Directions

Machine Learning Permeates High-Energy Physics



Machine Learning Fundamentals

The Power of ML

Comes at a cost

► *Interpolation in high-dimensional spaces*

Combats the curse of dimensionality

Loses analytic understandability/tractability

► *Automatic feature extraction*

Ensures relevant features are not missed

Cannot easily convey what features are used

► *Asymptotically optimizes performance*

Provides useful/practical statistical power

Training is difficult with few global guarantees

Responsible ML Considerations

► *Available data*

Data source, number of samples, labels, reliability

► *Learning paradigm*

Fully/weakly/un-supervised, classification/regression/generation

► *Inputs and outputs*

Size/shape, symmetries, dimensionality

► *Model architecture*

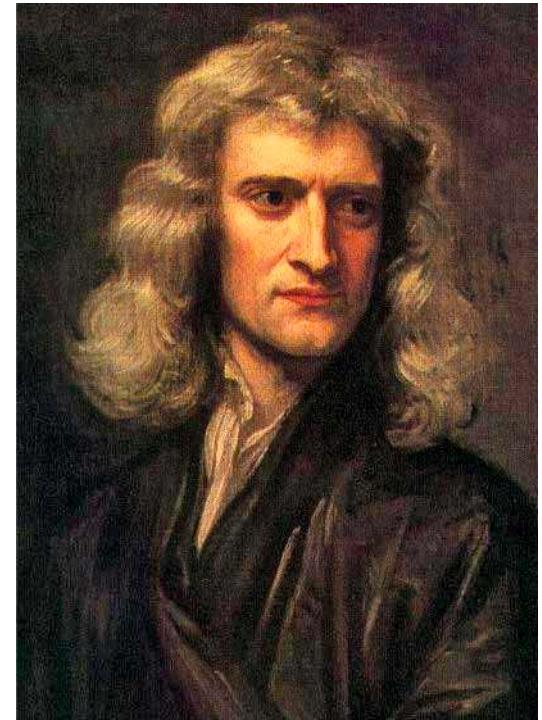
Expressibility, loss function, hyperparameters, validation/testing

► *Deployment strategy*

Model implementation, training/evaluation speed, uncertainties

My Perspective on ML in HEP

Machine learning is here to stay in high-energy physics

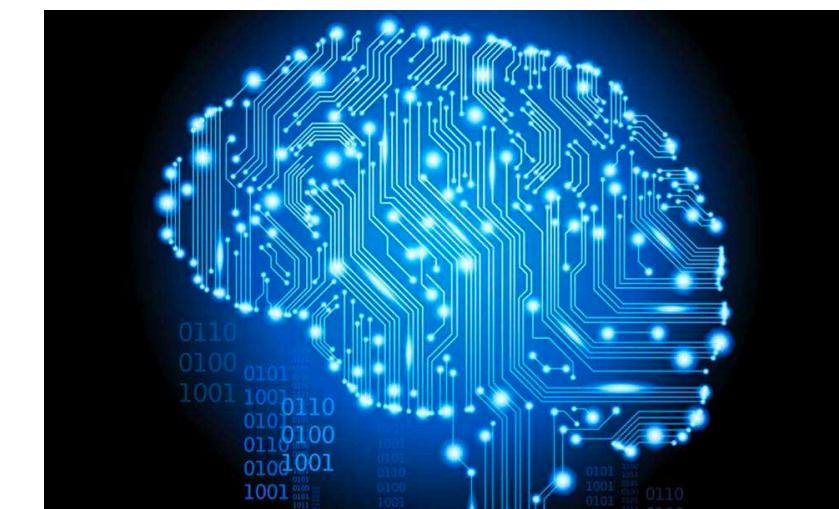


Calculus

- ▶ Fundamental to quantitative study of functions
- ▶ Taught to all undergraduate physics students
- ▶ Essential for understanding modern physics

Machine Learning

- ▶ Fundamental to statistical data analysis
- ▶ Increasingly taught in undergrad science programs
- ▶ Increasingly essential for modern physics/science



Machine learning straddles theory/experiment/computation divide

Close coordination between theory and experiment is essential
in the current era of uncertainty in particle physics

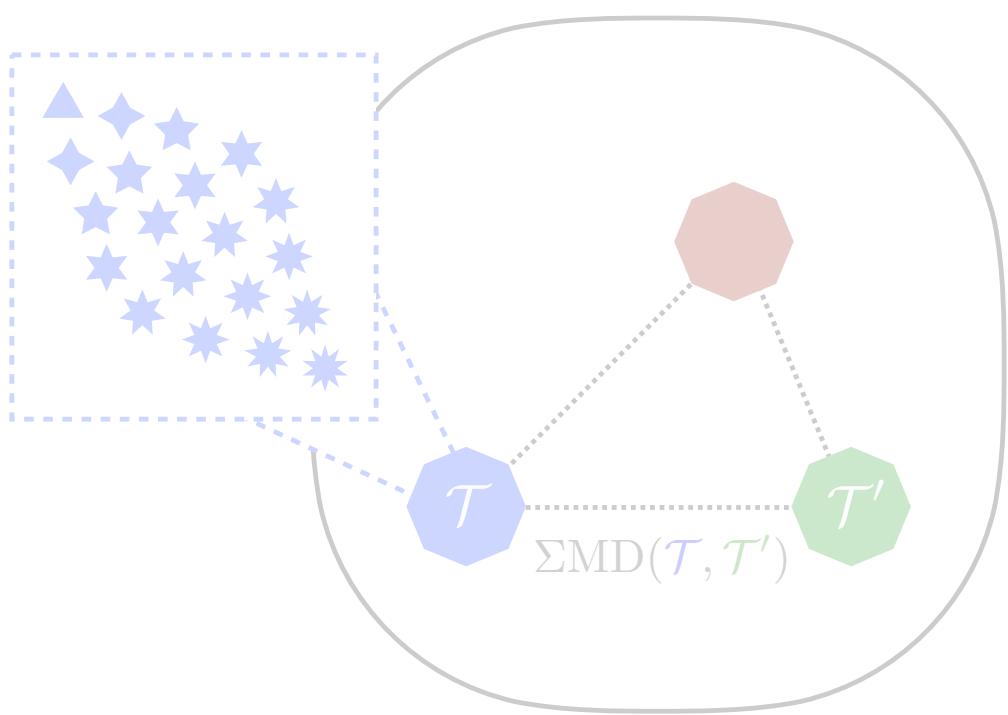
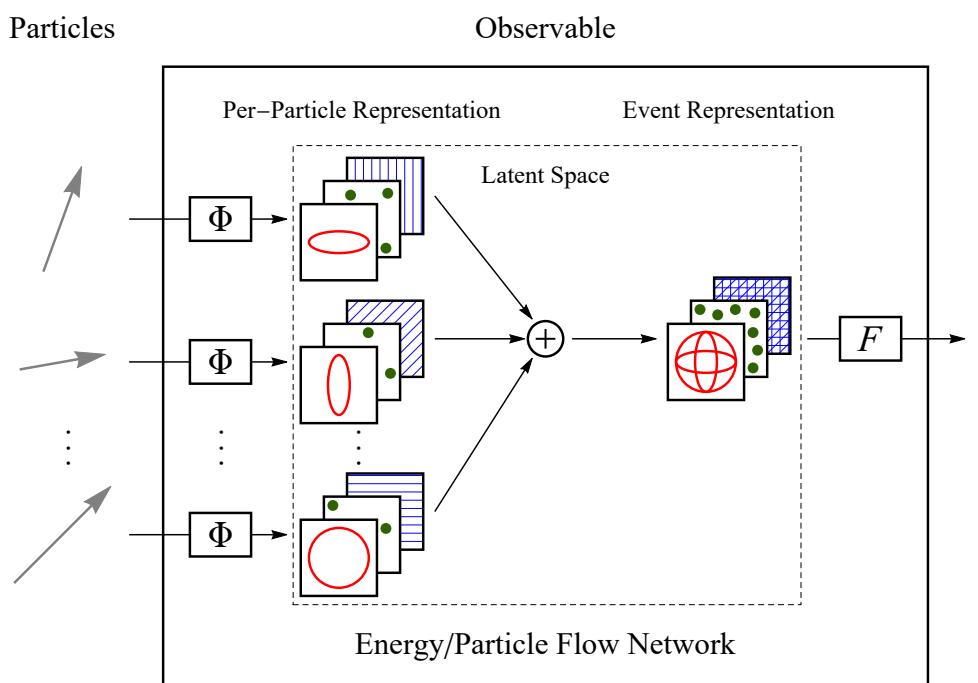
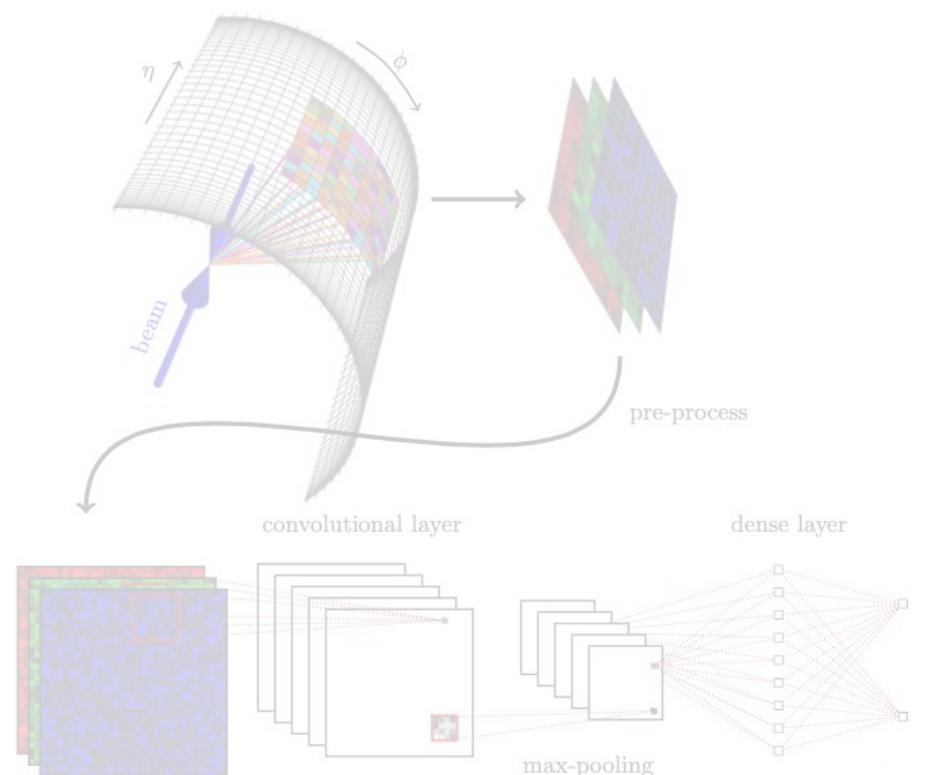
▶ Where has ML already had an impact in high-energy physics?

Key Questions During the Snowmass Process

▶ What is the role of ML in particle physics (and vice-versa) in the future?

[Part II](#) of this talk

[Part III](#) of this talk



Ubiquity of ML in HEP

Lightning Review

Disclaimers

- ▶ Examples biased towards collider physics
- ▶ References are not exhaustive

Future Directions

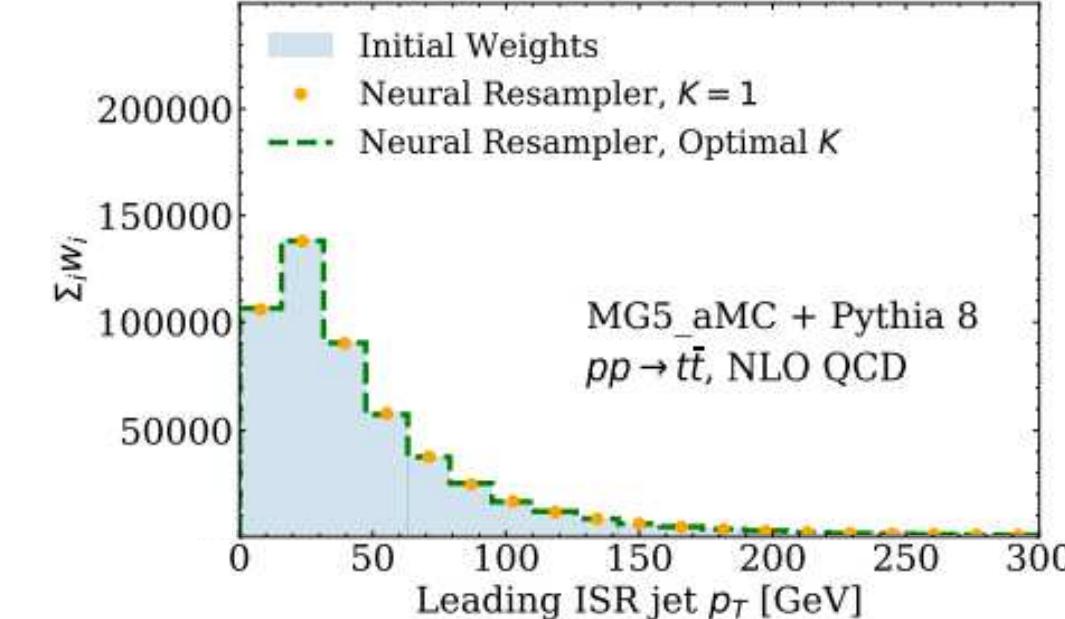
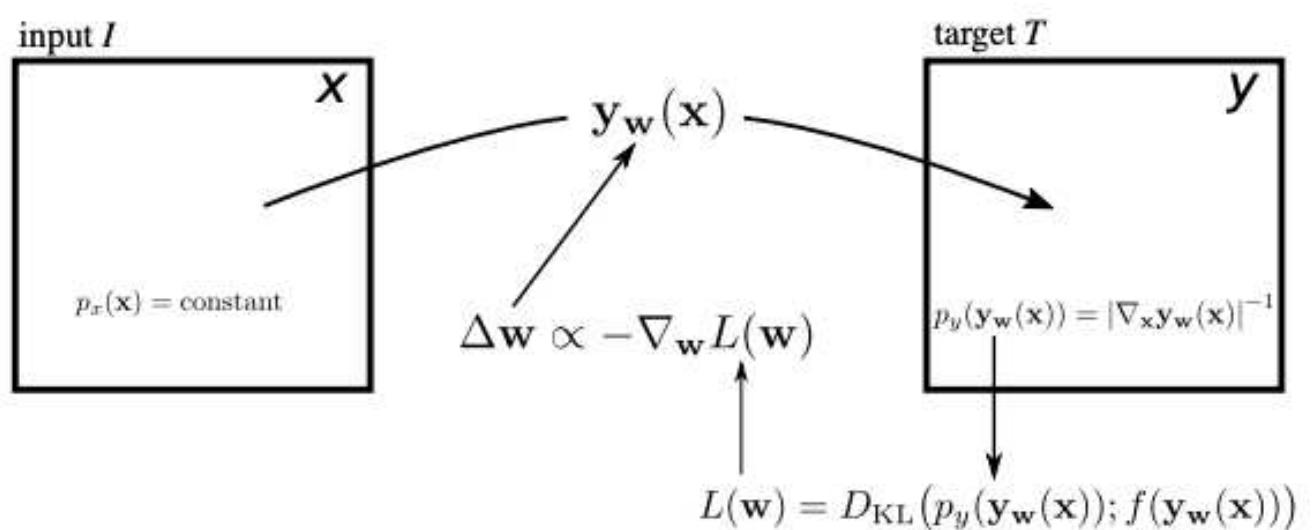
“Uncontroversial” Applications of Machine Learning in HEP

ML can provide a uniformly improved, drop-in replacement for some mathematical tasks

Efficient Monte Carlo Integration

[Bendavid, [1707.00028](#); Klimek, Perelstein, [1810.111509](#)]

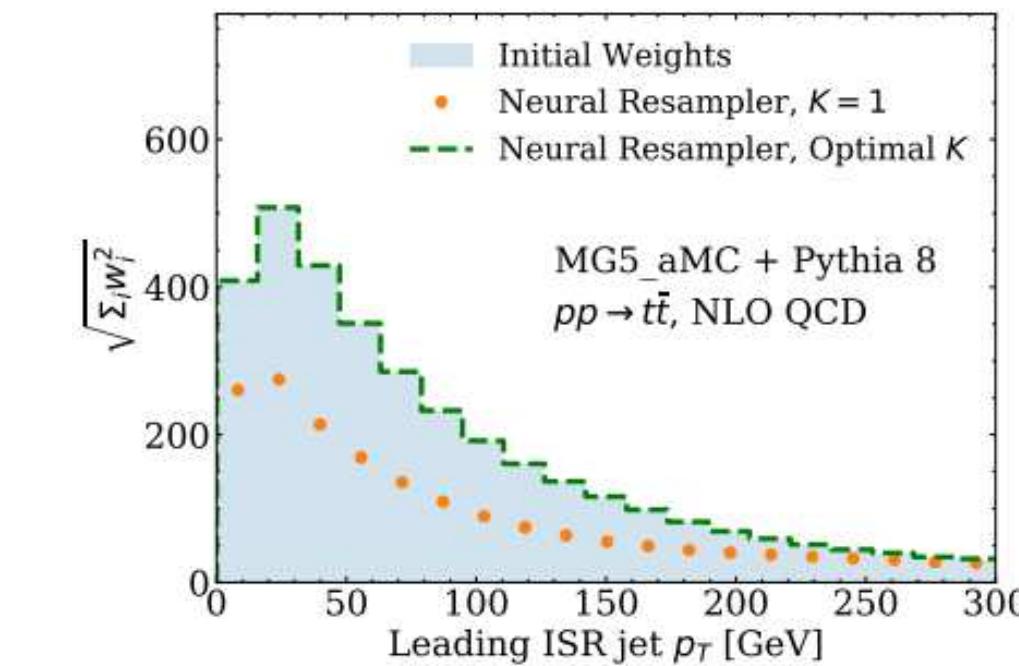
“A continuum implementation of the VEGAS algorithm”



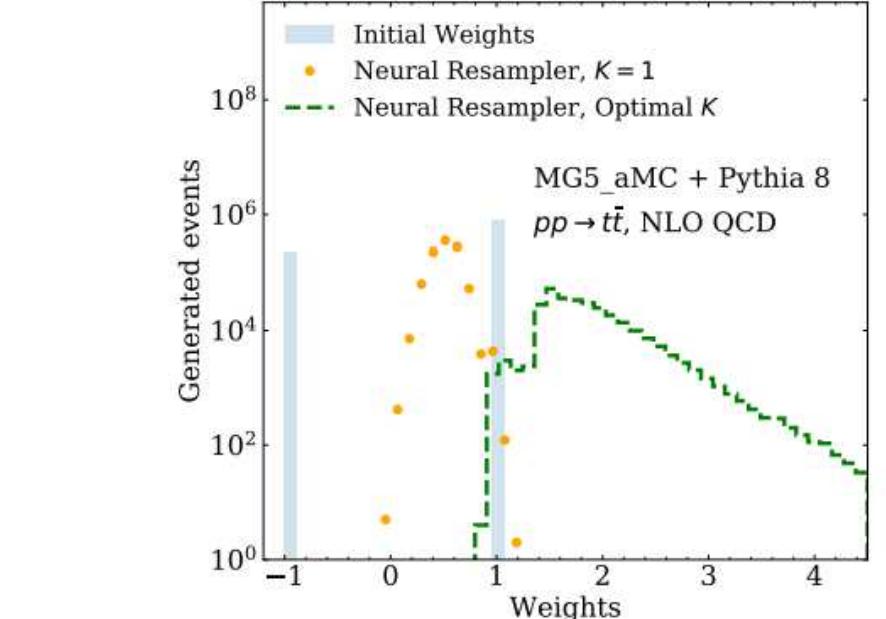
Central value preserved ...

Algorithm	# of Func. Evals	$\sigma_w / < w >$	σ_I / I
VEGAS	300,000	2.820	$\pm 2.0 \times 10^{-3}$
Foam	3,855,289	0.319	$\pm 2.3 \times 10^{-4}$
Generative BDT	300,000	0.082	$\pm 5.8 \times 10^{-5}$
Generative BDT (staged)	300,000	0.077	$\pm 5.4 \times 10^{-5}$
Generative DNN	294,912	0.083	$\pm 5.9 \times 10^{-5}$
Generative DNN (staged)	294,912	0.030	$\pm 2.1 \times 10^{-5}$

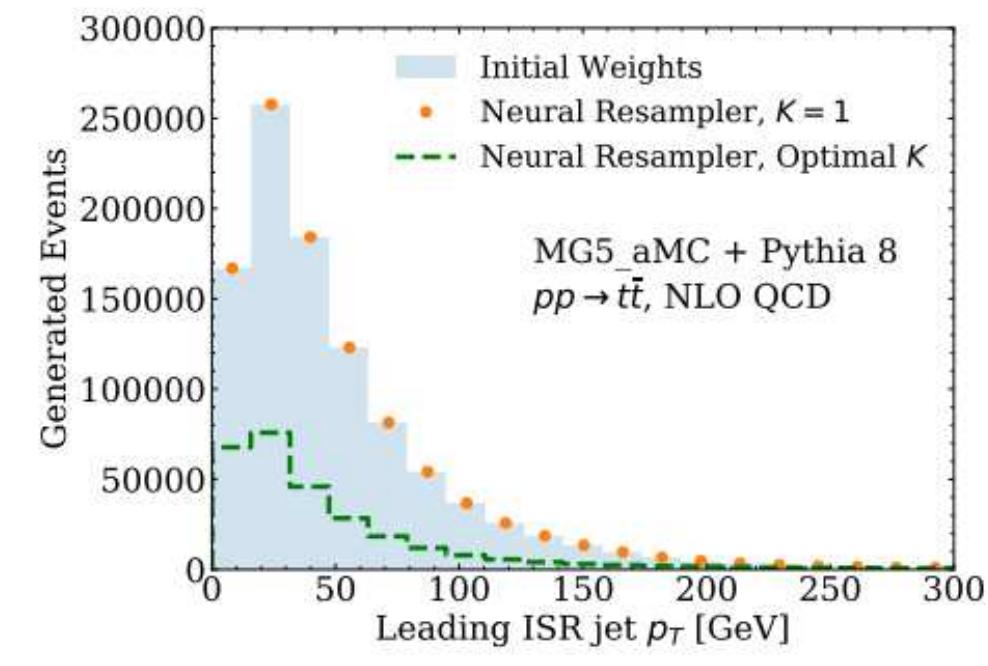
DNN has 10-100x smaller error with the same or fewer samples!



while preserving uncertainty ...



using only positive weights ...



and requiring fewer events!

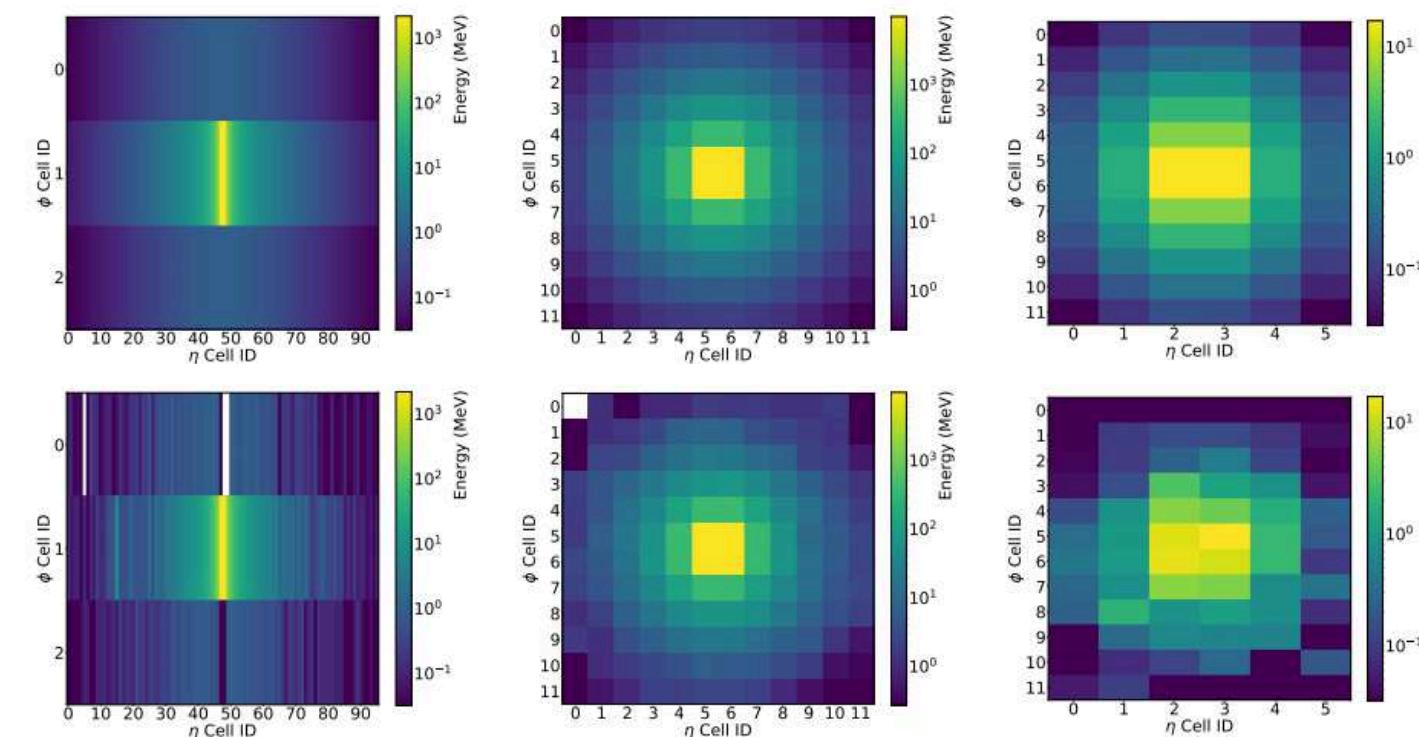
Improvement to Computational Speed/Efficiency with ML

Fast Electromagnetic Calorimeter Simulation

[Paganini, de Oliveira, Nachman, [1705.02355](#) [1712.10321](#); Erdmann, Glombitza, Quast, [1807.01954](#)]

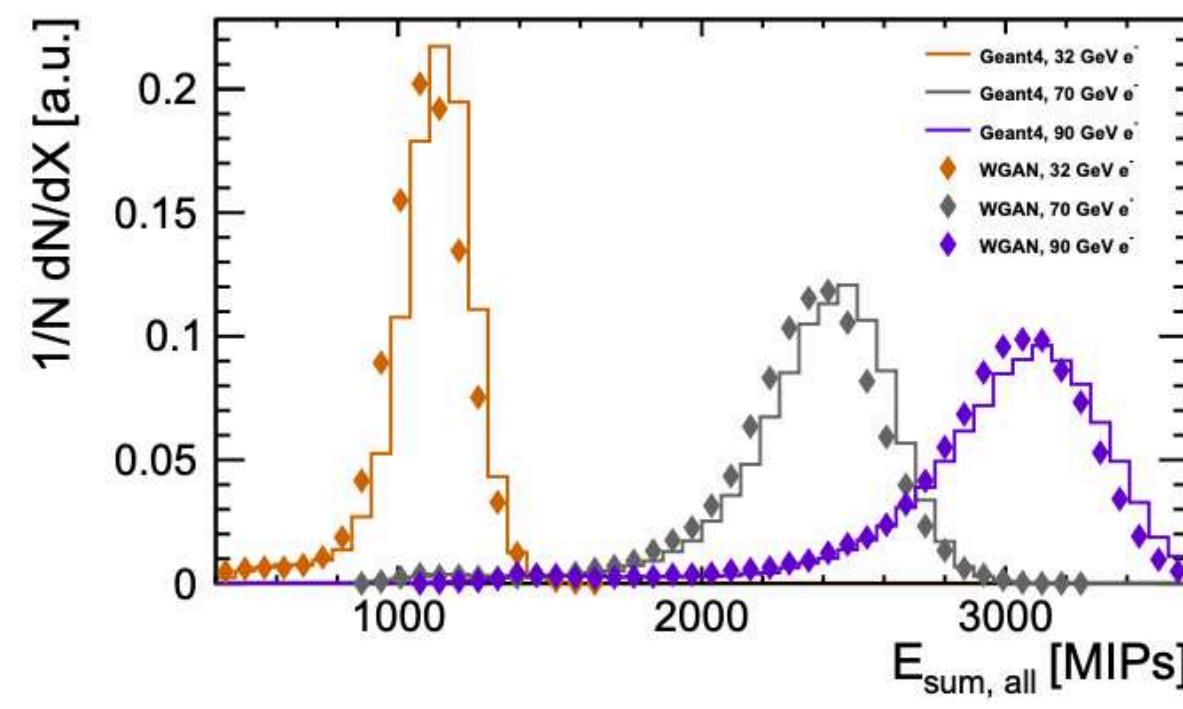
Generative models can be $O(10^2\text{-}10^5) \times$ quicker than full detector-simulation

Geant4



GAN

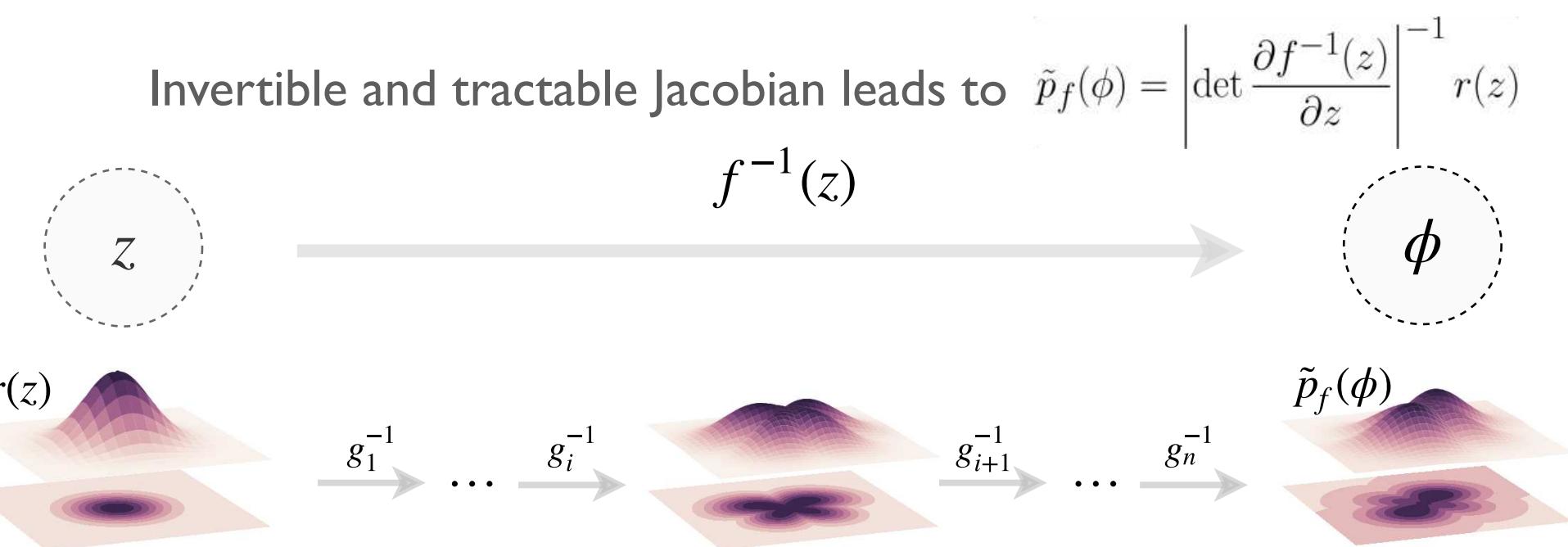
Wasserstein GANs have stabler training and good agreement



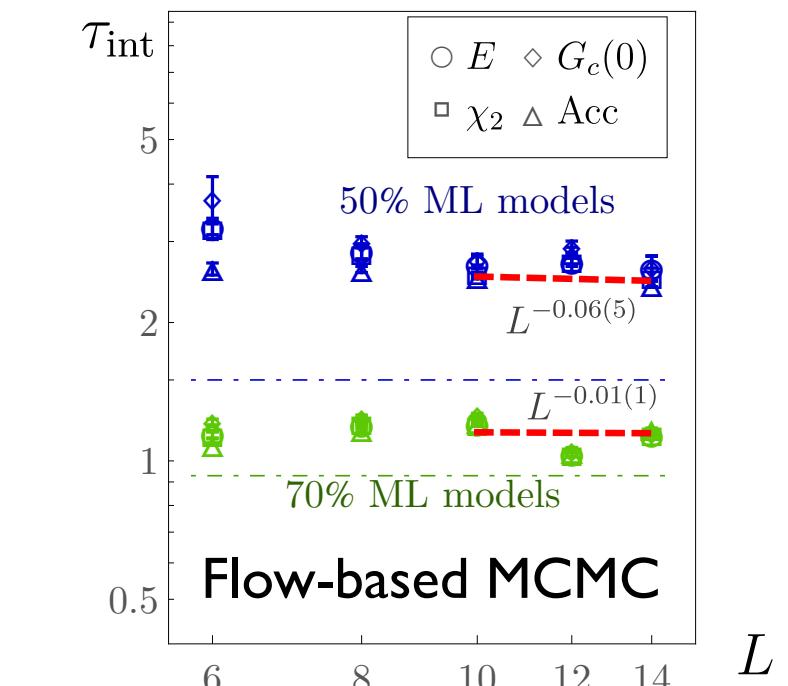
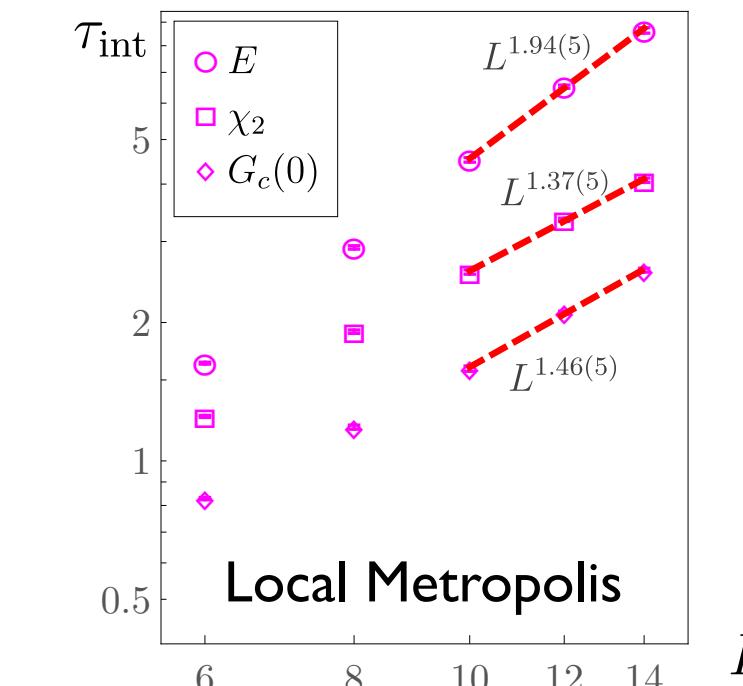
Improved MCMC for Lattice Field Theory

[Albergo, Kanwar, Shanahan, [1904.12072](#); Talk by G. Kanwar]

Normalizing flows can be used to sample from complicated distributions



Power law growth of autocorrelation time avoided with ML

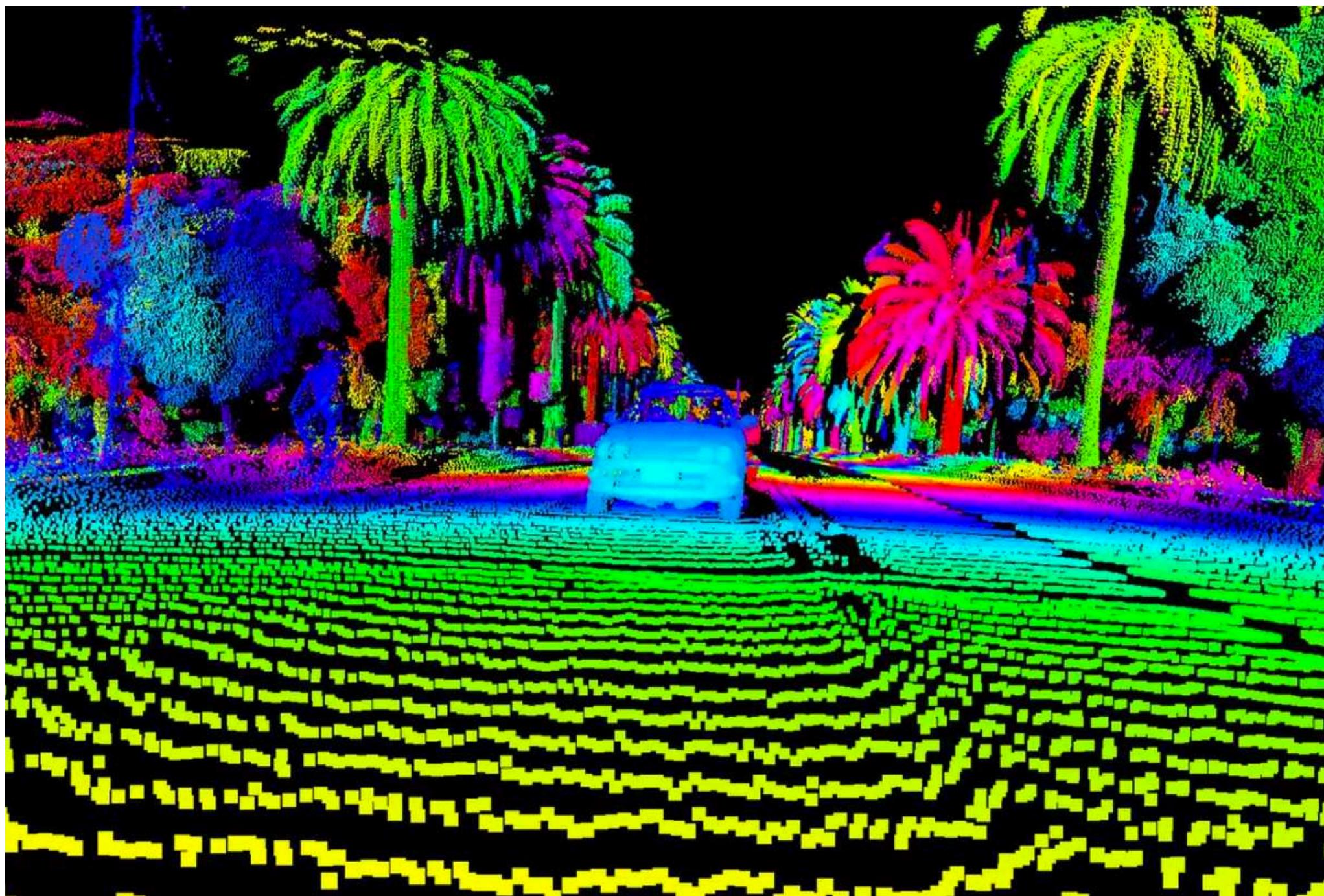


Neural Network Architectures for Particle Physics

Maximally appropriate ML architectures respect symmetries of the underlying data

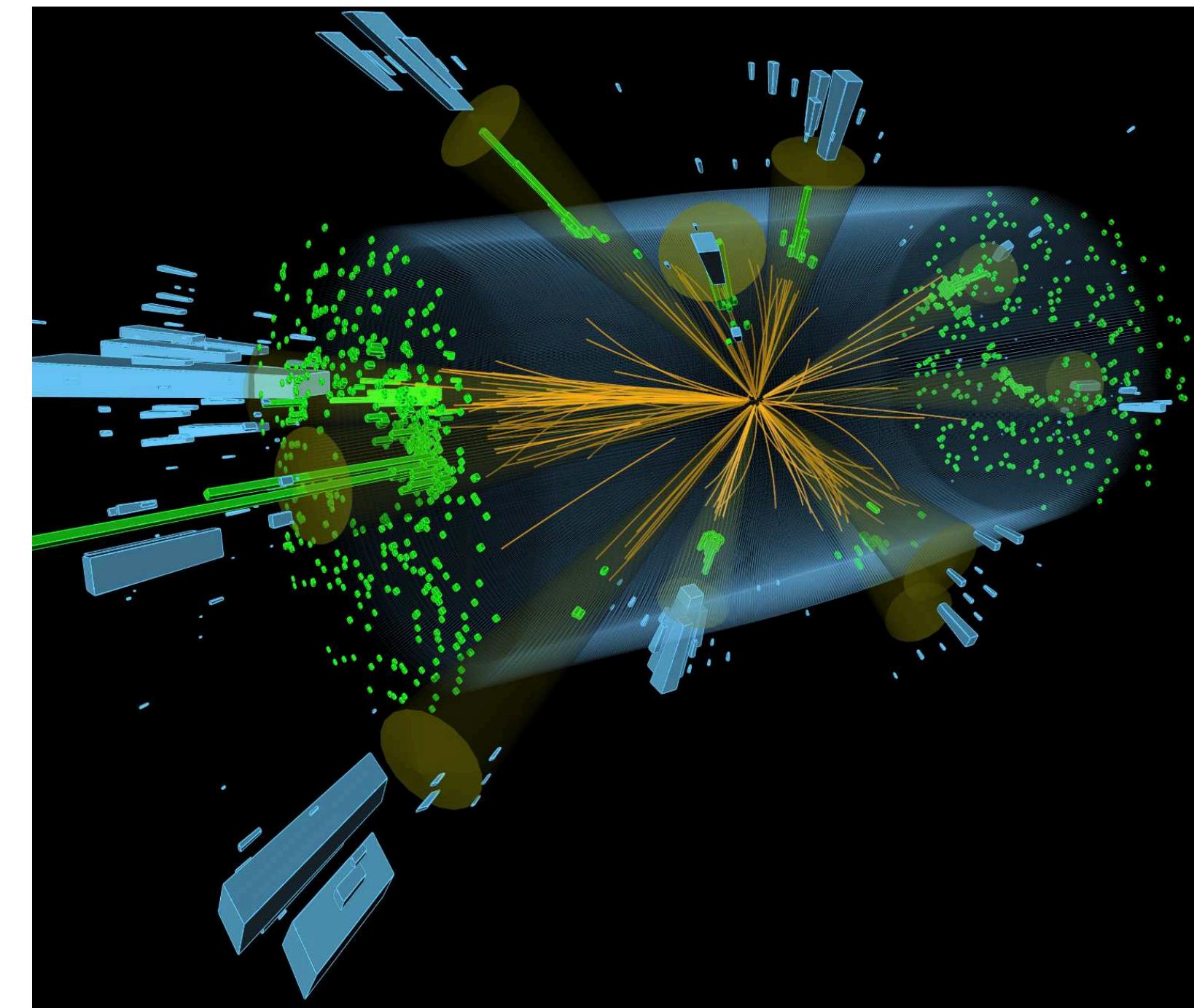
Particle physics events are naturally point clouds (alternatively, images e.g. calorimeters)

Point cloud: "A set of data points in space" –Wikipedia



LIDAR data from self-driving car sensor

An **unordered, variable length** collection of particles

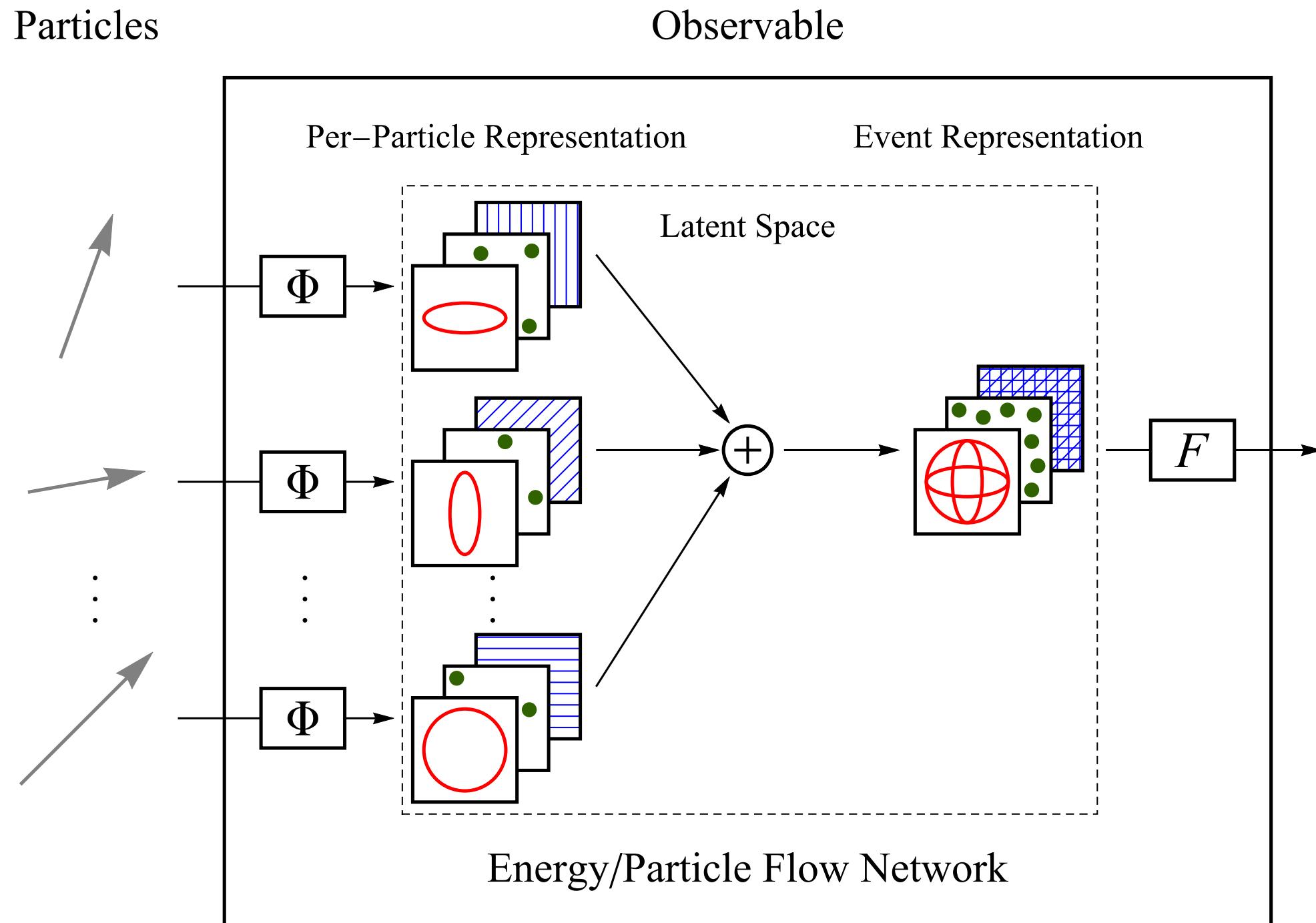


Due to quantum-mechanical indistinguishability

Due to probabilistic nature of event formation

Deep Sets for Particle Jets

[Zaheer, Kottur, Ravanbakhsh, Póczos, Salakhutdinov, Smola, [I703.06114](#);
 PTK, Metodiev, Thaler, [I810.05165](#);
[EnergyFlow Python Package](#)]



Particle Flow Network (PFN)

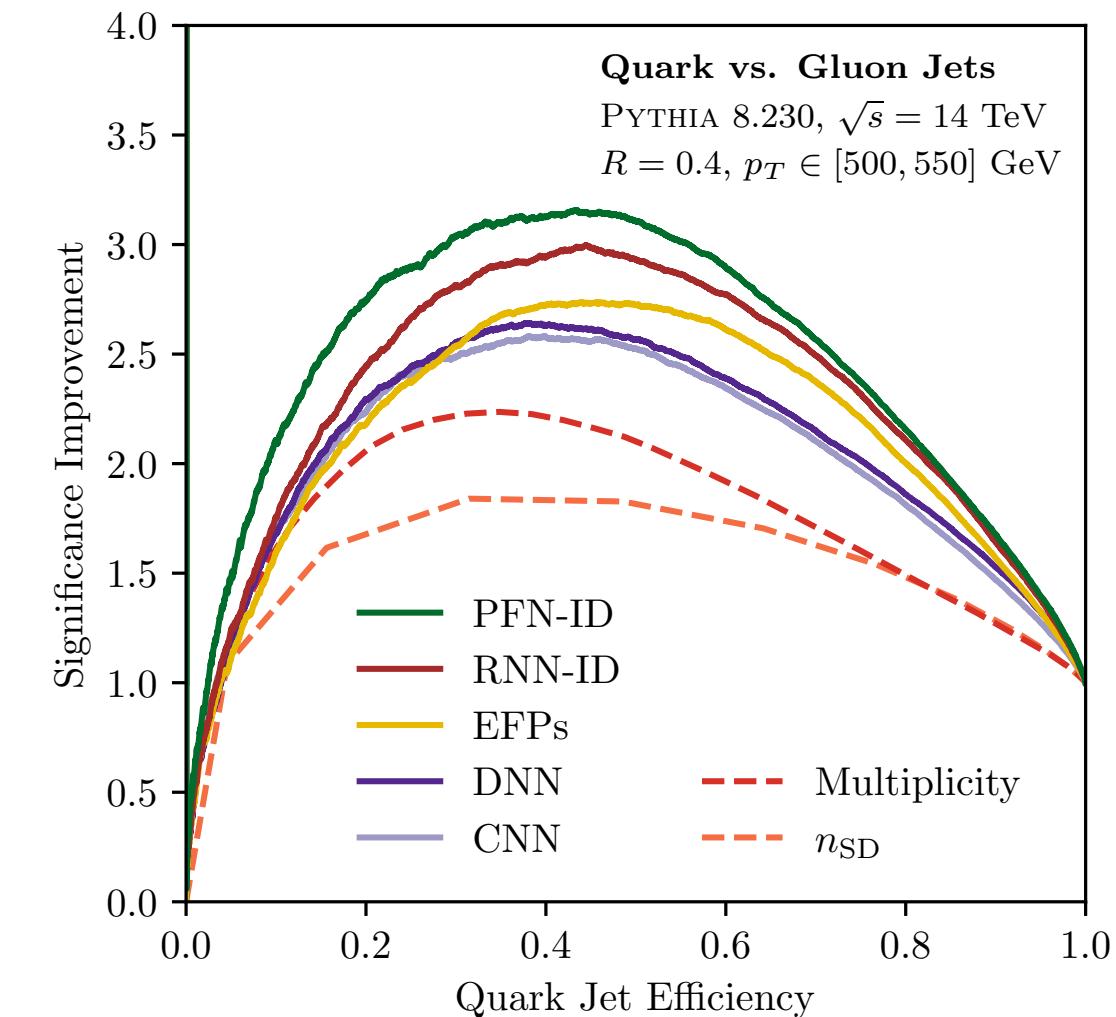
$$\text{PFN}(\{p_1^\mu, \dots, p_M^\mu\}) = F \left(\sum_{i=1}^M \Phi(p_i^\mu) \right)$$

Fully general latent space

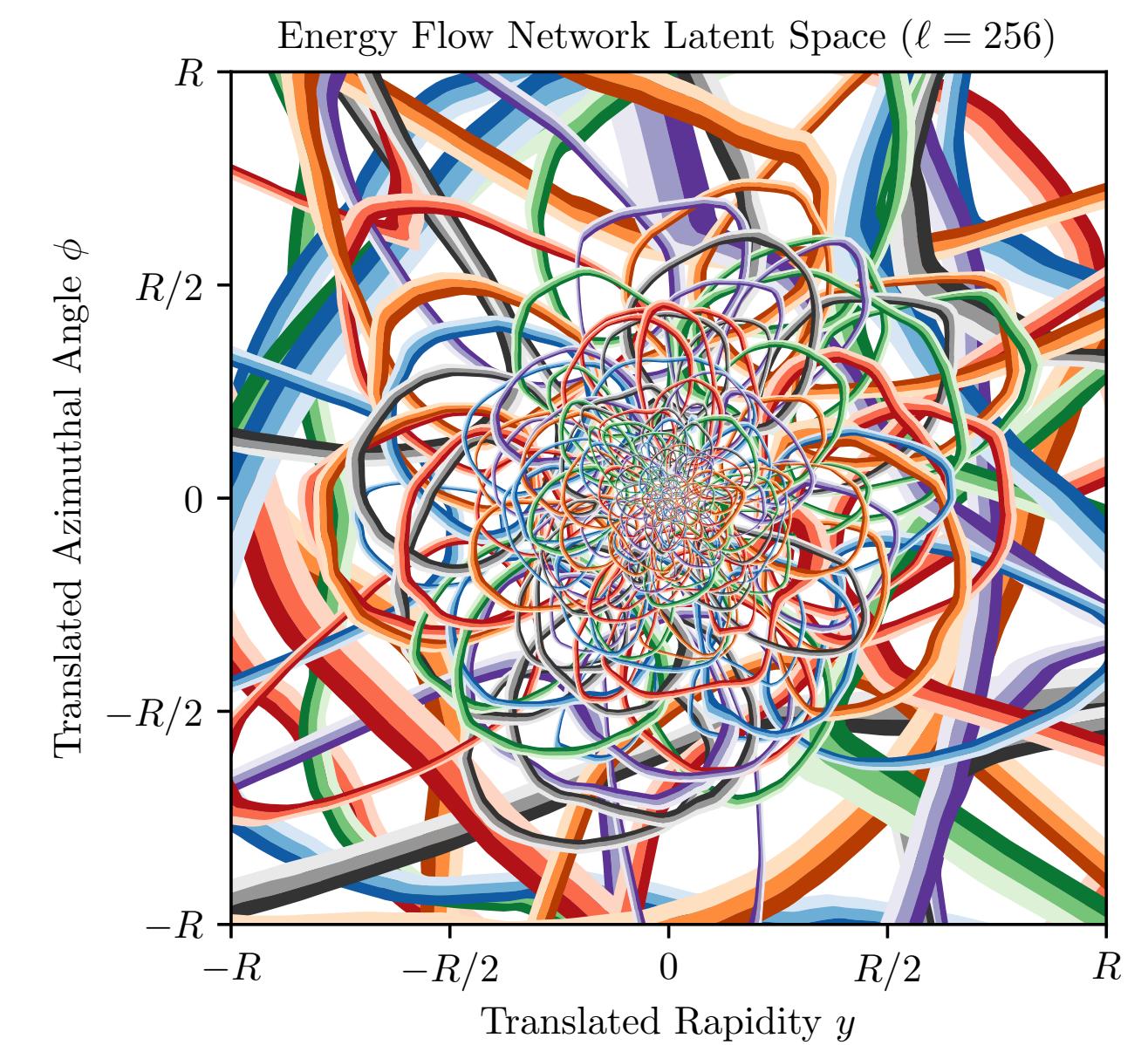
Energy Flow Network (EFN)

$$\text{EFN}(\{p_1^\mu, \dots, p_M^\mu\}) = F \left(\sum_{i=1}^M \textcolor{brown}{z}_i \Phi(\hat{p}_i) \right)$$

IRC-safe latent space



Improved performance (and training)
 compared to RNN and CNN



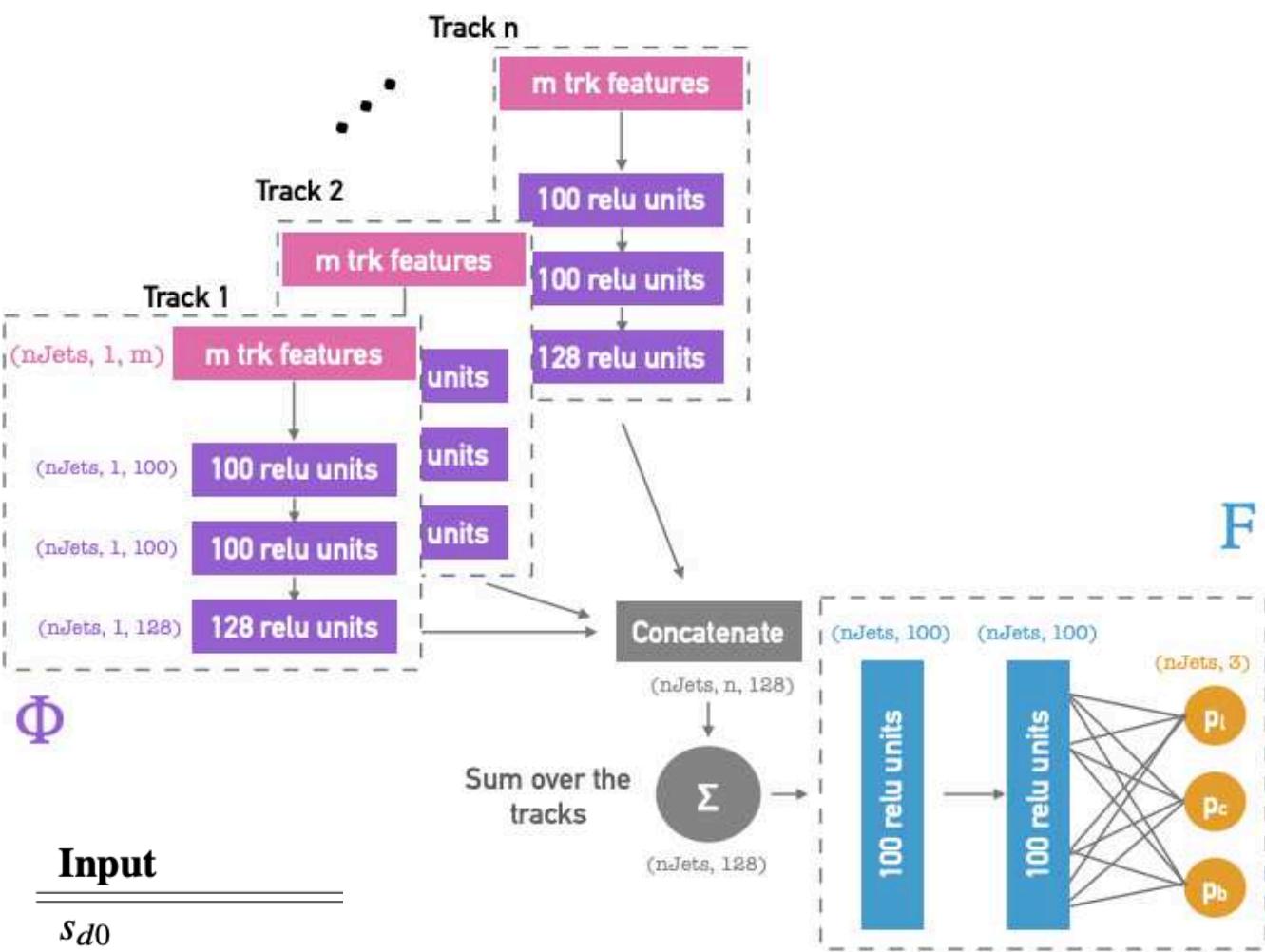
Latent space visualization reveals
 what the network has learned

Dynamic pixel sizing related to
 collinear singularity of QCD!

Other Physics-Inspired Architectures

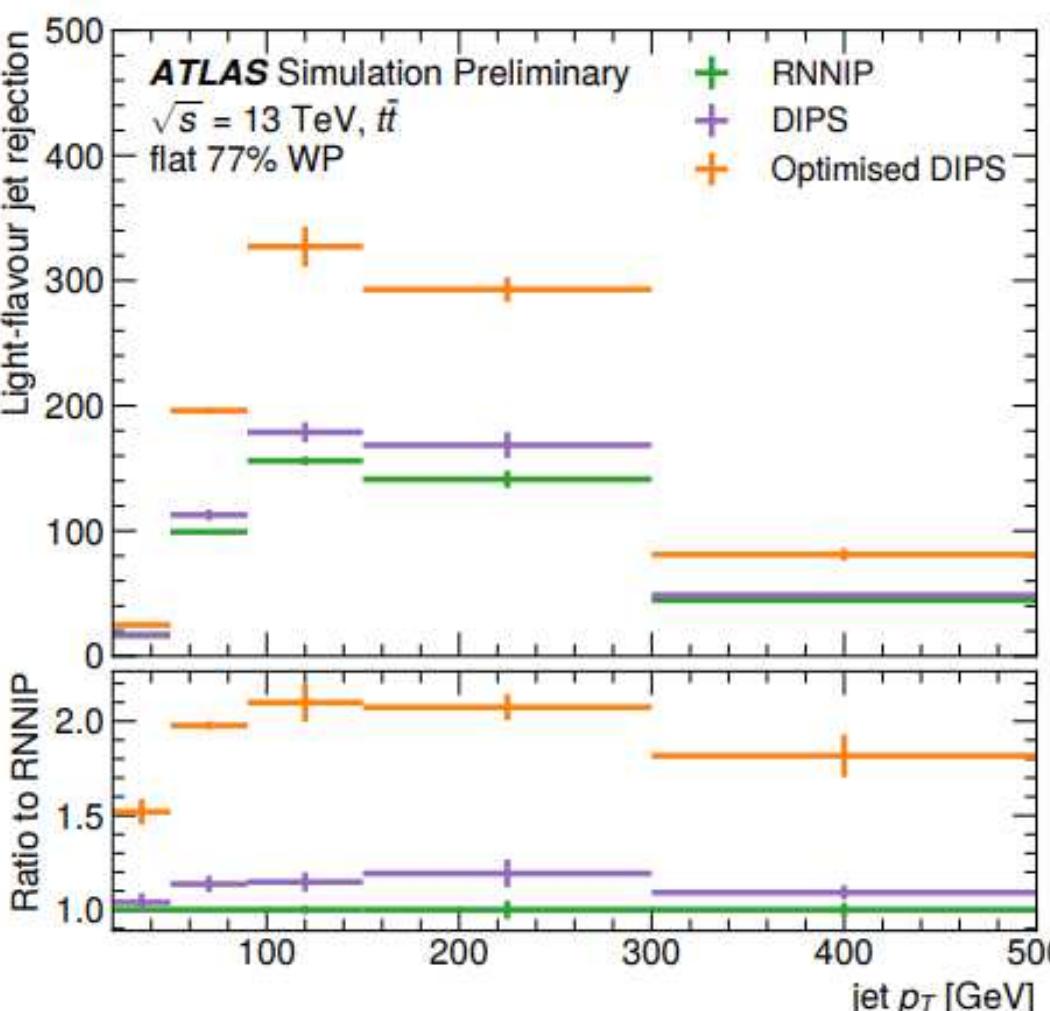
Deep Impact Parameter Sets

[ATL-PHYS-PUB-2020-014]



Input

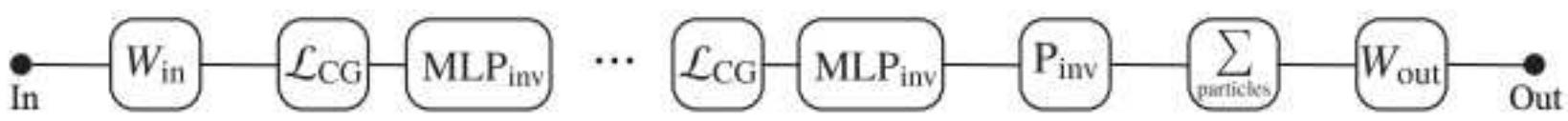
- s_{d0}
- s_{z0}
- $\log p_T^{\text{frac}}$
- $\log \Delta R$
- IBL hits
- PIX1 hits
- shared IBL hits
- split IBL hits
- nPixHits
- shared pixel hits
- split pixel hits
- nSCTHits
- shared SCT hits



Achieves 2x better flavor tagging than an RNN
“Optimised” includes additional features per track

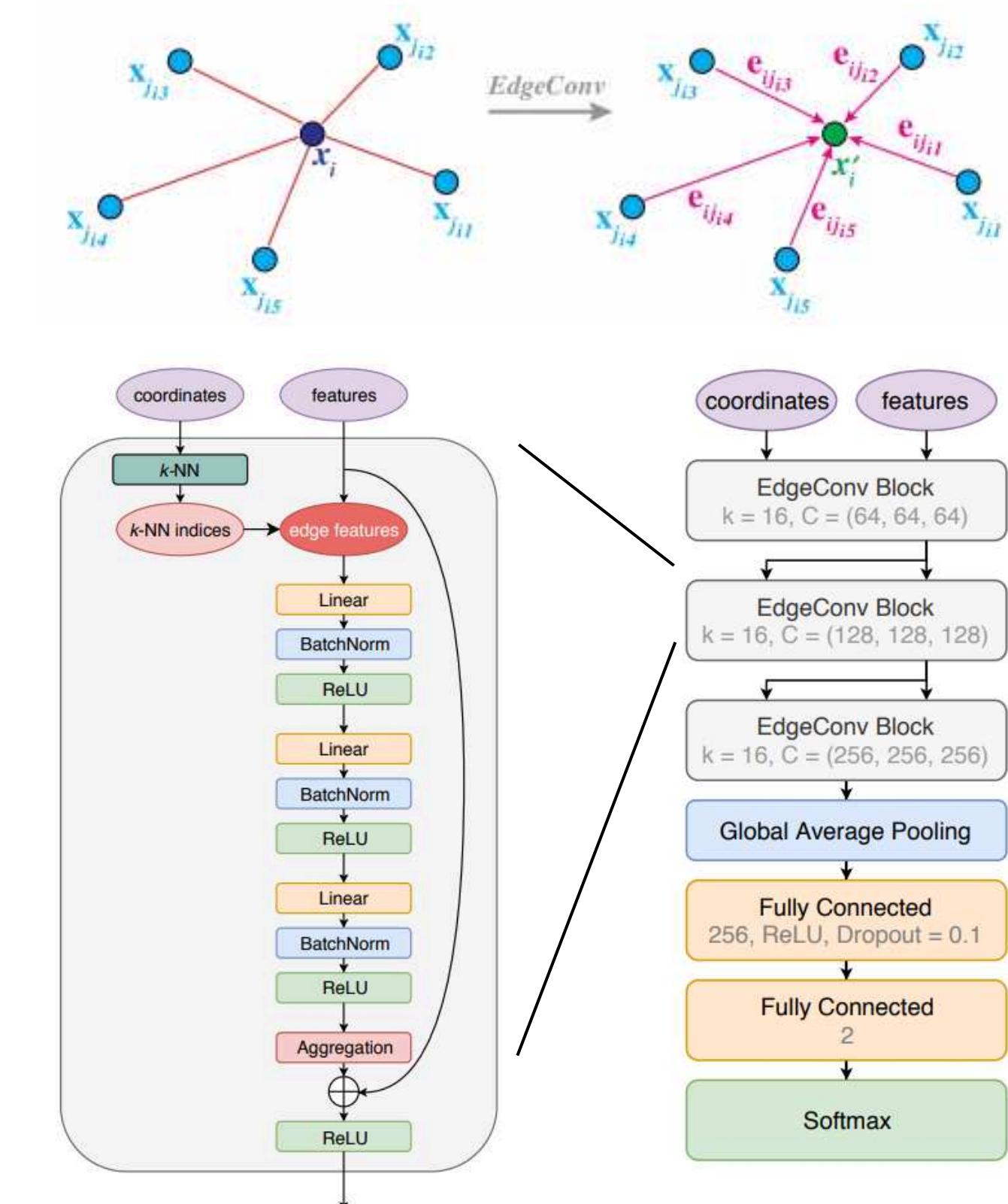
Lorentz Group Equivariant NN

[Bogatskiy, Anderson, Offermann, Roussi, Miller, Kondor, 2006.04780]



Dynamic Graph CNNs (e.g. Particle Net)

[Wang, Sun, Liu, Sarma, Bronstein, Solomon, 1801.07829; Qu, Gouskos, 1902.08570]



Preserves permutation symmetry while prioritizing relationships between inputs

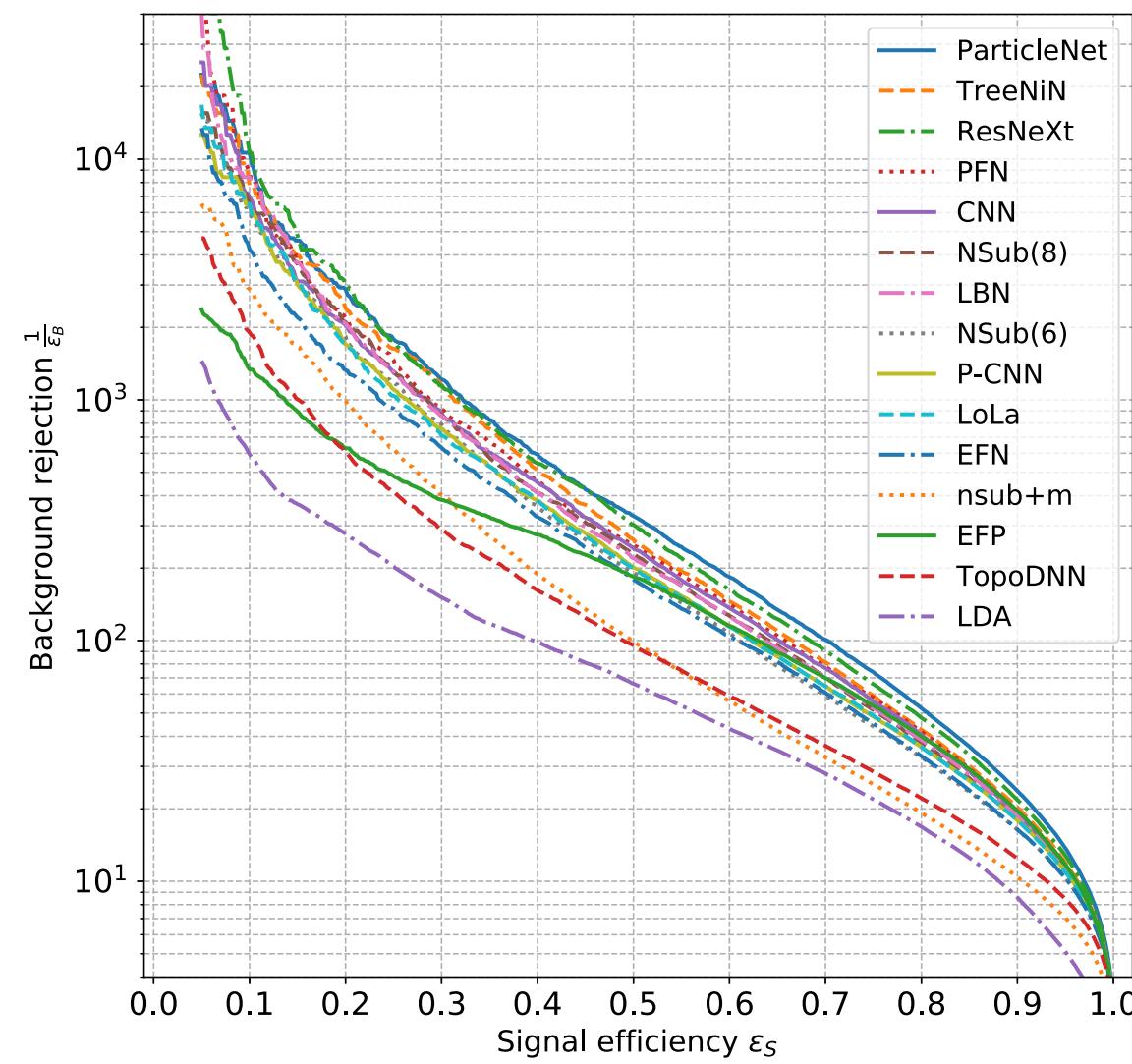
Improved Performance on Classic HEP Tasks with ML

ML optimizes performance

(Jet) Classification

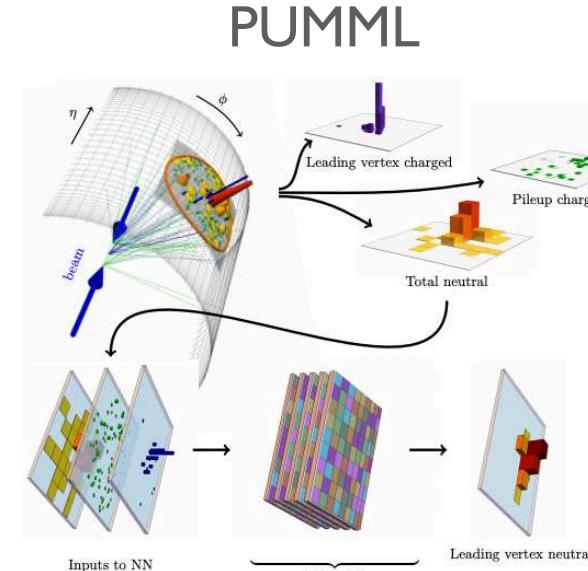
[Kasieczka, Plehn, et al., [1902.09914](#); many many other references...]

Community top-tagging comparison



Regression (e.g. to remove pileup)

[PTK, Metodiev, Nachman, Schwartz, [1707.08600](#); ATL-PHYS-PUB-2019-028; see also Arjona Martínez, Cerri, Spiropulu, Vlimant, Pierini [1810.07988](#)]



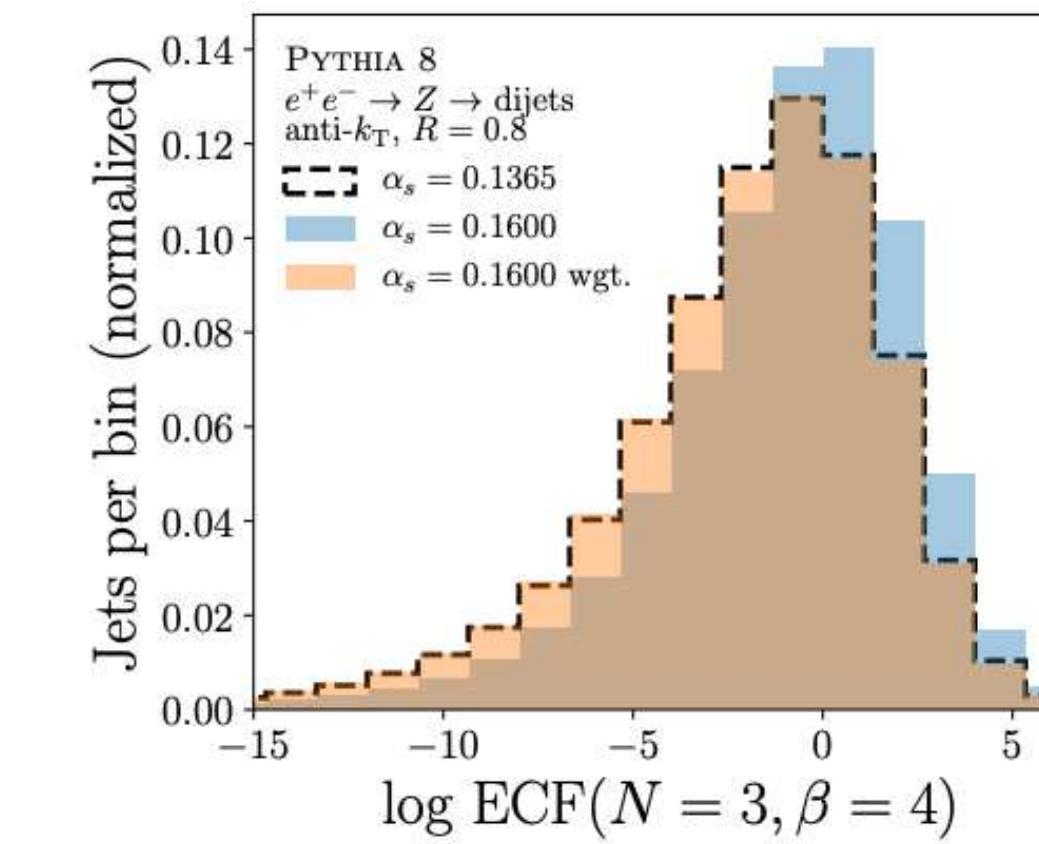
ML can enable an unbinned version of a binned method

(Full) Phase-Space Reweighting

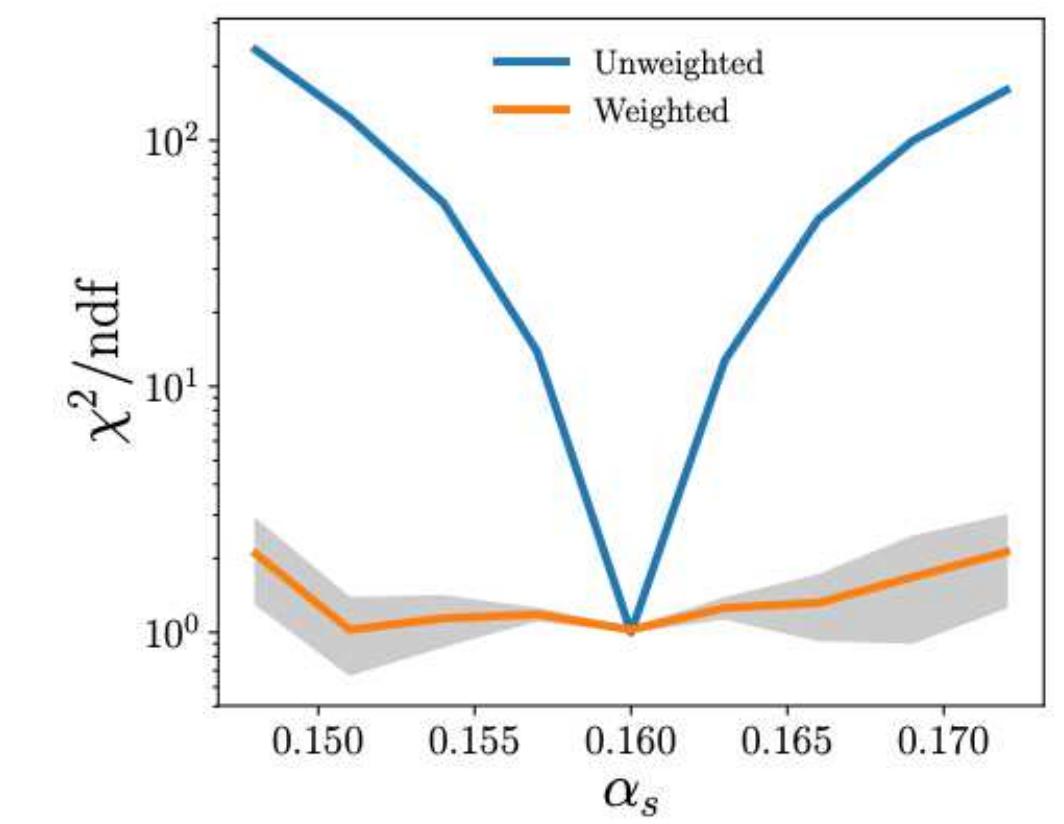
[Cranmer, Pavez, Louppe, [1506.02169](#); Andreassen, Nachman, [1907.08209](#)]

Likelihood-free inference via classification and Neyman-Pearson

DCTR uses a single high-dimensional reweighting...



to match ECF distributions ...



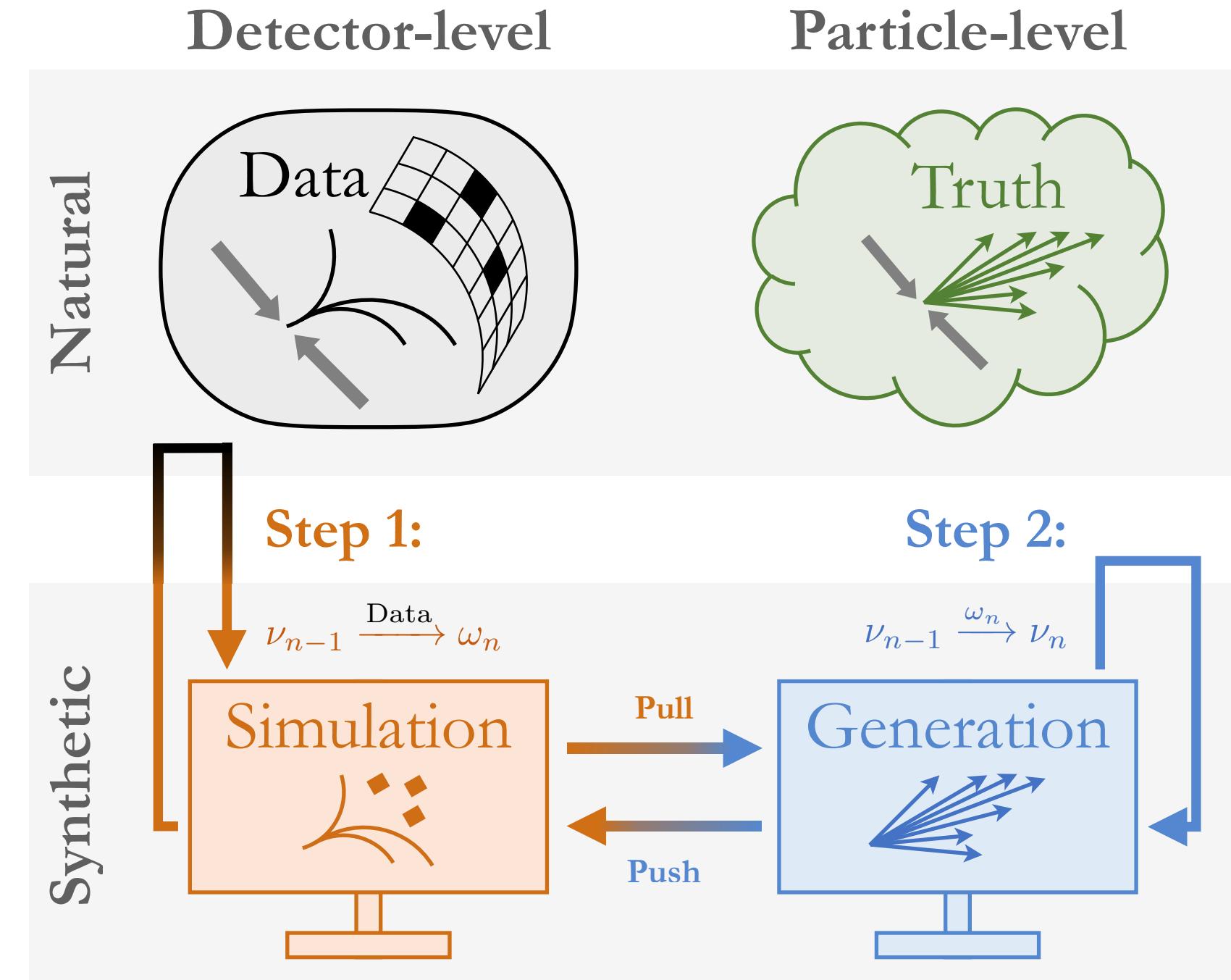
and multiplicity distributions!

High-dimensional reweighting is useful for many tasks ...

OmniFold – Unbinned, Full Phase-Space Unfolding



OmniFold weights particle-level *Gen* to be consistent with *Data* once passed through the detector



Step 1 – Reweights Sim_{n-1} to data, pulls weights back to particle-level Gen_{n-1}

Step 2 – Reweights Gen_{n-1} to (step 1)-weighted gen_{n-1} , pushes weights to detector-level Sim_n

[Andreassen, PTK, Metodiev, Nachman, Thaler, [1911.09107](#);
PTK talk at ML4Jets 2020]

OmniFold – i.e. continuous IBU

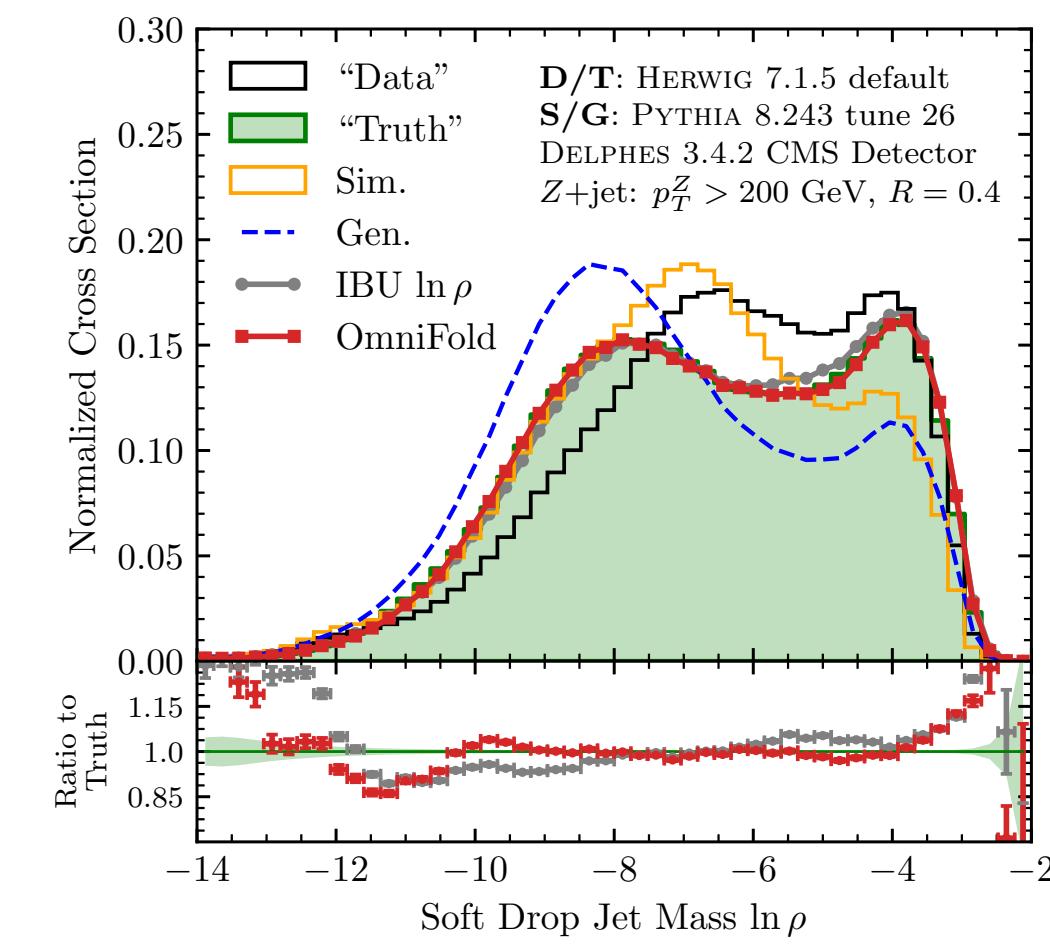
$$\text{Step 1} - \omega_n(m) = \nu_{n-1}^{\text{push}} \times L[(1, \text{Data}), (\nu_{n-1}^{\text{push}}, \text{Sim})](m)$$

$$\text{Step 2} - \nu_n(t) = \nu_{n-1}(t) \times L[(\omega_n^{\text{pull}}, \text{Gen}), (\nu_{n-1}, \text{Gen})](t)$$

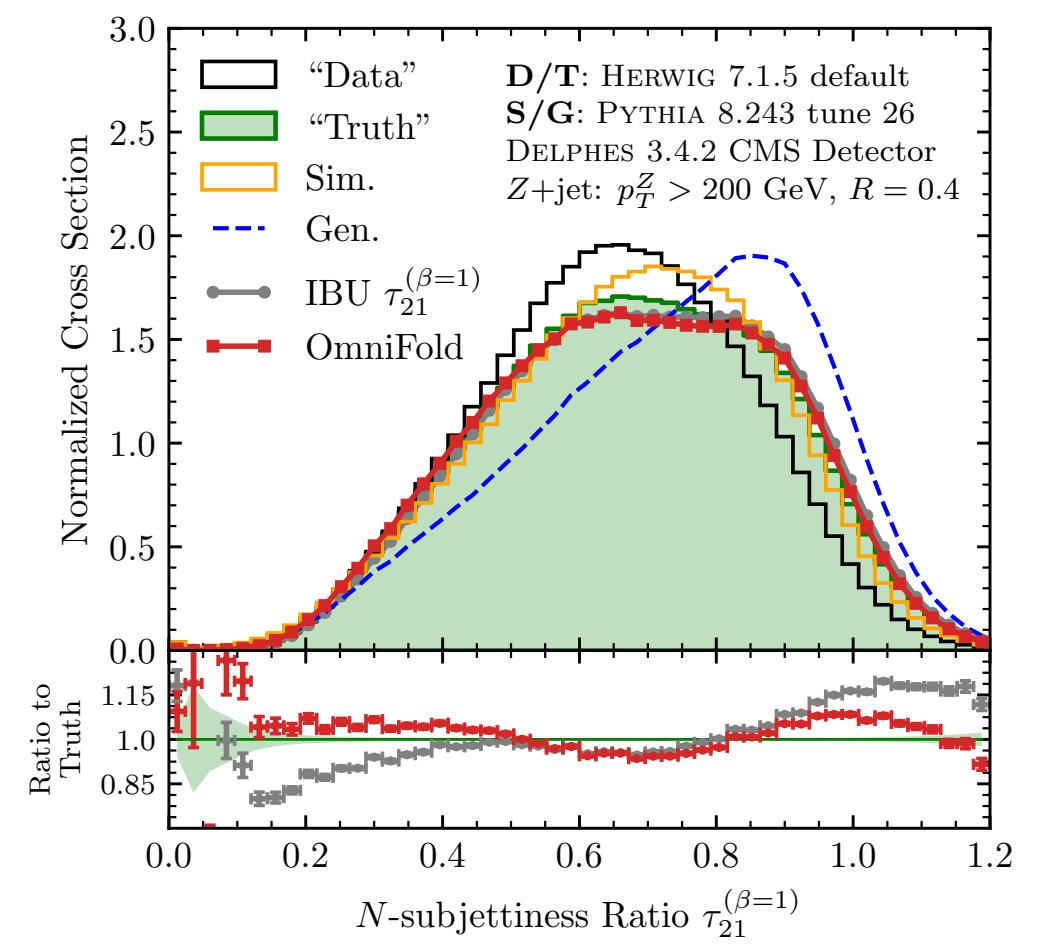
Unfold any* observable $p_{\text{Gen}(t)}$ using universal weights $\nu_n(t)$

$$p_{\text{unfolded}}^{(n)}(t) = \nu_n(t) \times p_{\text{Gen}}(t)$$

*Observables should be chosen responsibly



IRC safe



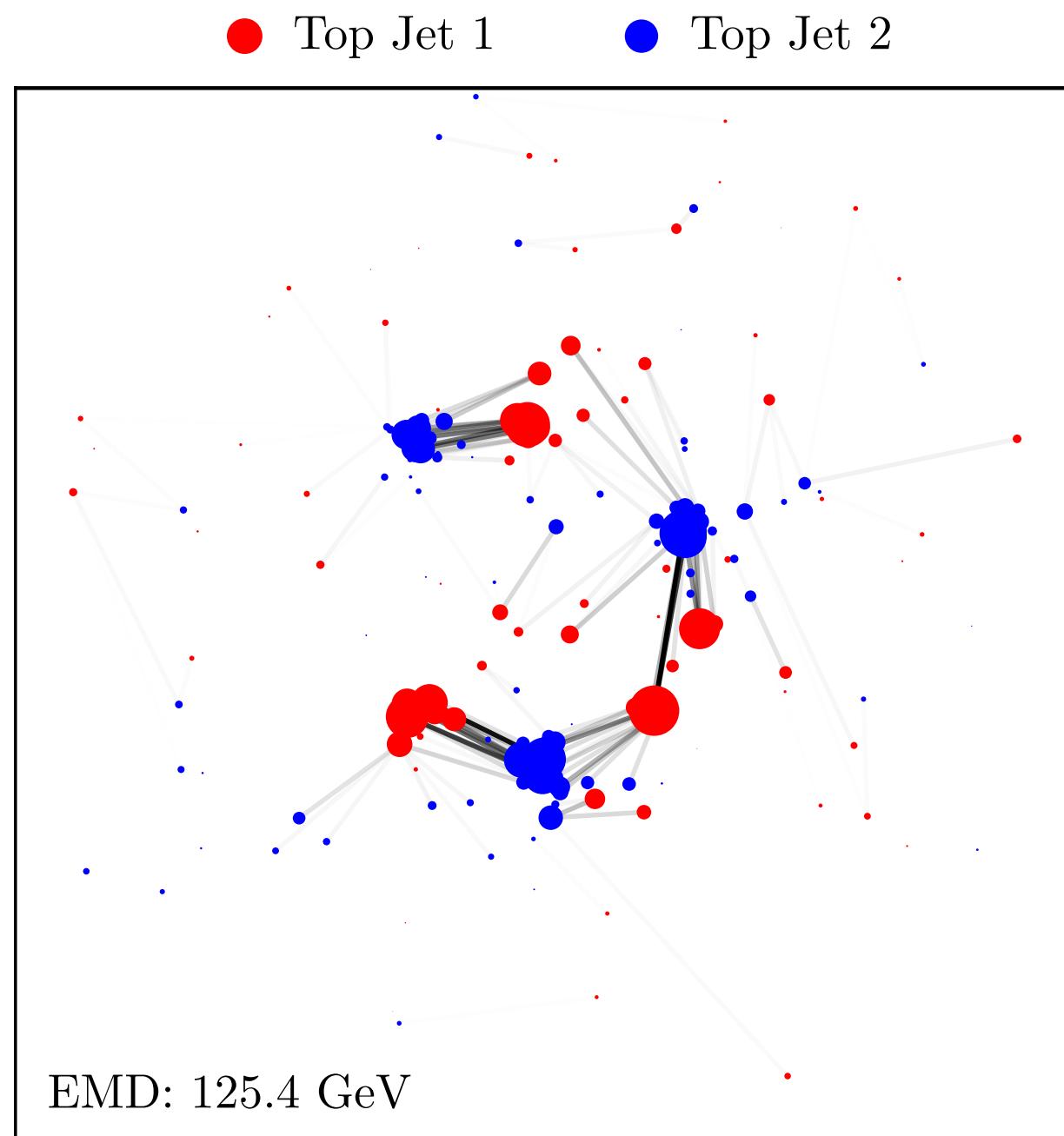
Sudakov safe

Non-Parametric ML – The Energy Mover's Distance (EMD)

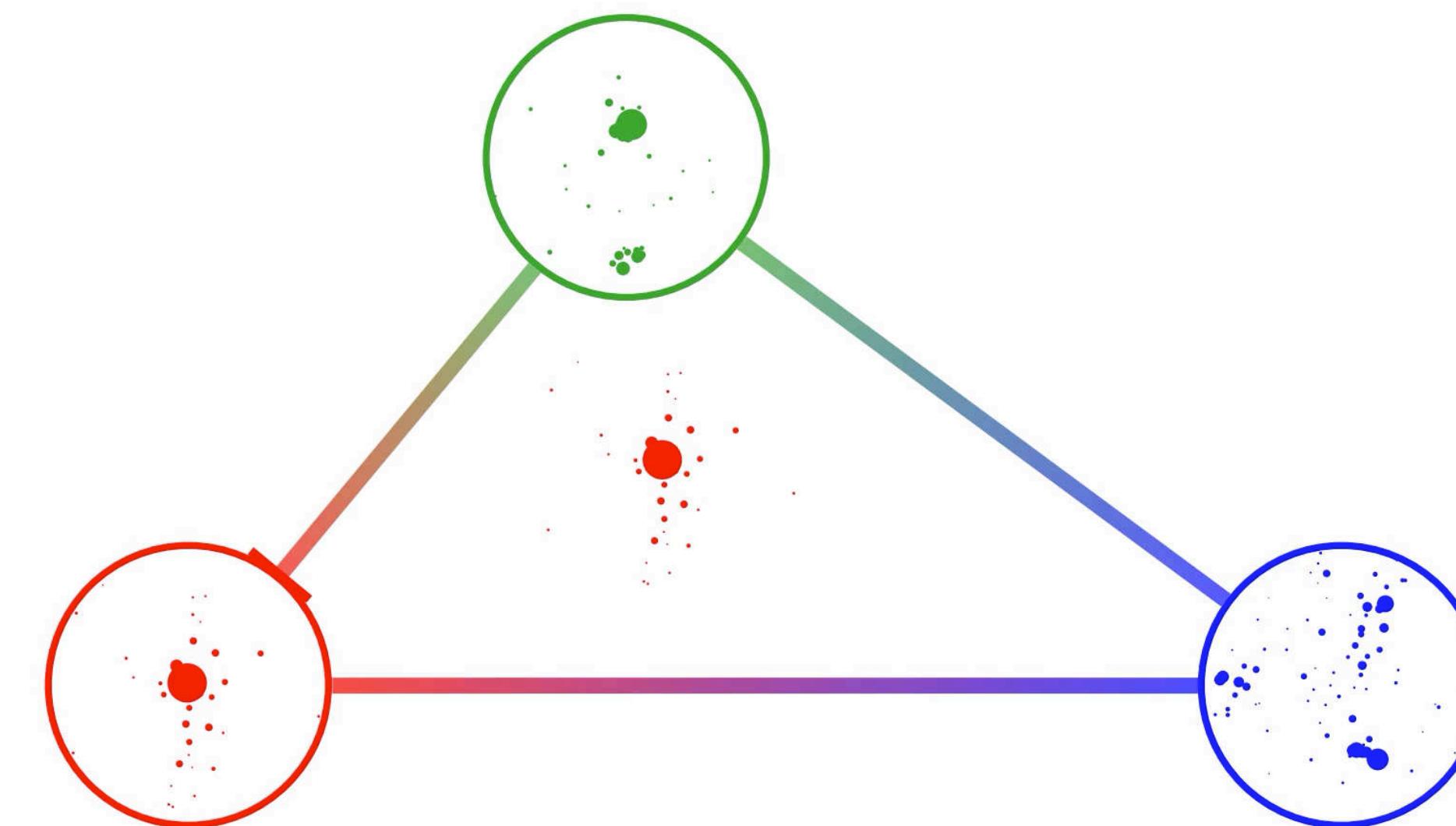
[PTK, Metodiev, Thaler, [PRL 2019](#);

applied on CMS Open Data: PTK, Mastandrea, Metodiev, Naik, Thaler, [1908.08542](#)]

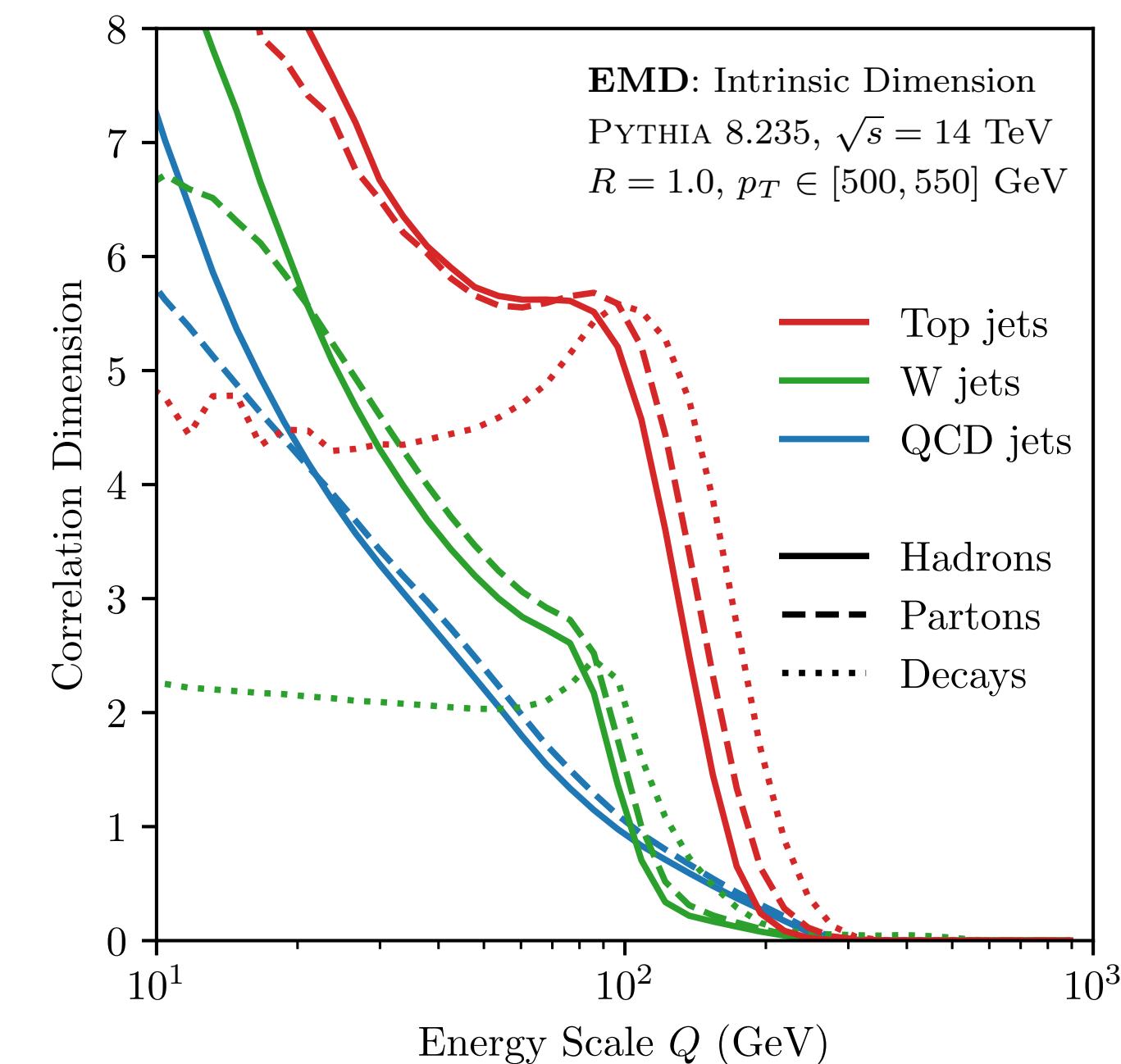
EMD between energy flows defines a metric on the space of events



EMD is the work required to rearrange one event into another



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



Intrinsic dimensionality of dataset highlights physics at all scales

Handling Uncertainties

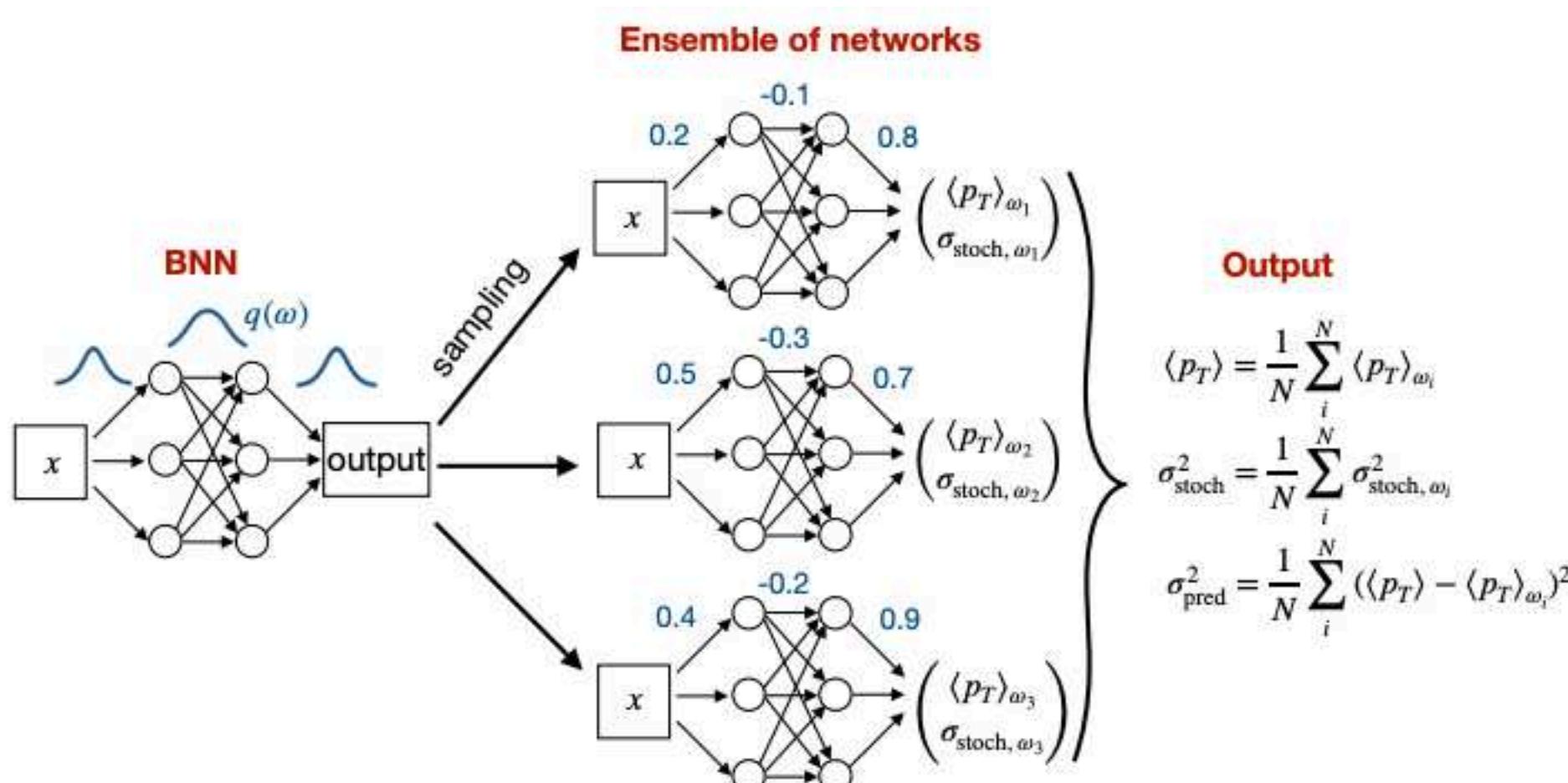
ML can assist in handling uncertainties (but can also create its own difficulties)

Adversarial training to reduce dependence on uncertain regions

[Englert, Galler, Harris, Spannowsky, [1807.08763](#)]

Bayesian neural networks can estimate some uncertainties

[Bollweg, Haußmann, Kasieczka, Luchmann, Plehn, Thompson, [1904.10004](#);
Kasieczka, Luchmann, Otterpohl, Plehn, [2003.11099](#)]



Sources of uncertainty in a statistical analysis

Precision / Optimality: $\text{NN}(x) \neq \frac{p_{\text{true}}(x|S+B)}{p_{\text{true}}(x|B)}$

$p_{\text{train}}(x) \neq p_{\text{true}}(x)$

inaccurate training data

$\text{NN}(x)|_{p_{\text{true}}=p_{\text{train}}} \neq \frac{p_{\text{true}}(x|S+B)}{p_{\text{true}}(x|B)}$

model/optimization flexibility

Statistical uncertainty

limited prediction statistics

Accuracy / Bias: $p_{\text{prediction}}(\text{NN}) \neq p_{\text{true}}(\text{NN})$

[Nachman, [1909.03081](#)]

Parametrized models could enable efficient profiling to handle systematic uncertainties

[similar to Baldi, Cranmer, Faubert, Sadowski, Whiteson, [1601.07913](#)]

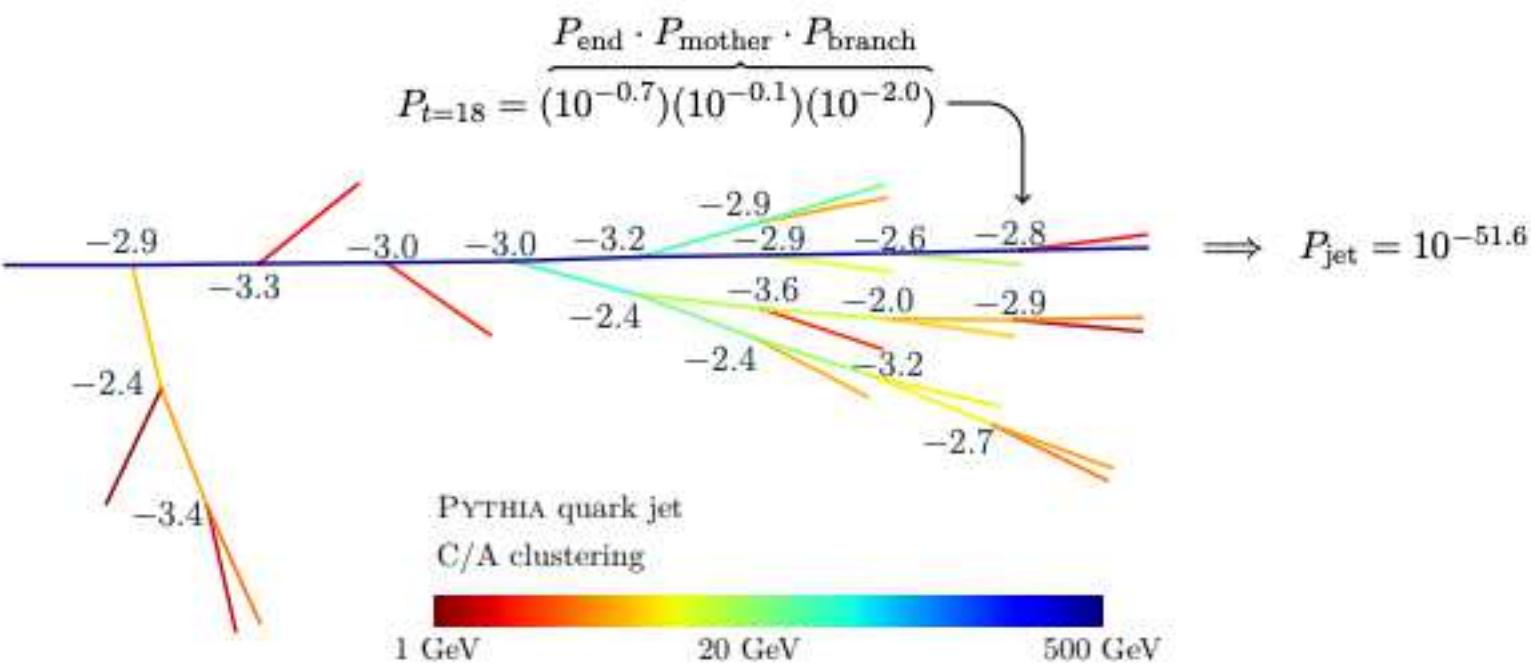
... And So Much More HEP-Specific ML

Weakly Supervised Learning e.g. LLP, CWoLa

[Dery, Nachman, Rubbo, Schwartzman, [1702.00414](#);
Metodiev, Nachman, Thaler, [1708.02949](#);
Cohen, Freytsis, Ostdiek, [1706.09451](#);
PTK, Metodiev, Nachman, Schwartz, [1801.10158](#)]

Unsupervised Learning e.g. JUNIPR

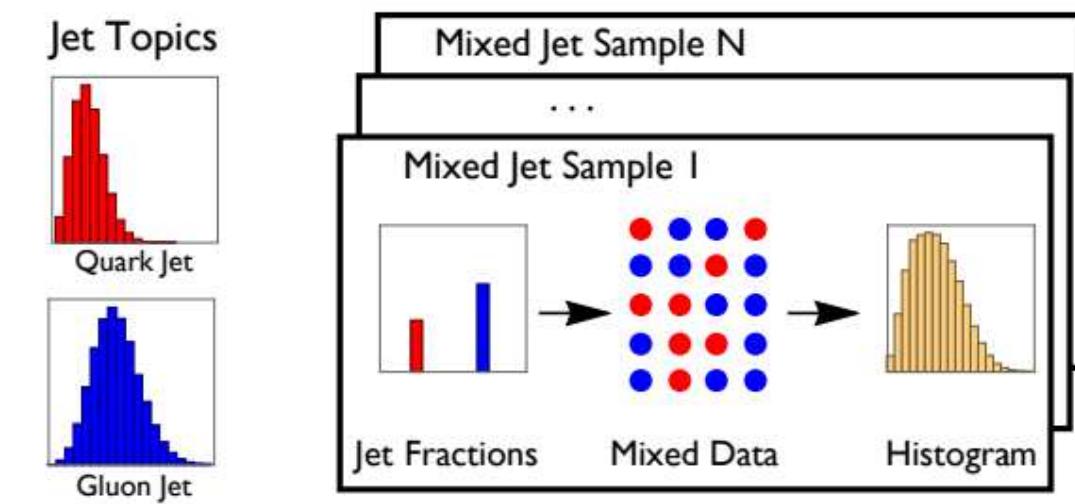
[Andreassen, Feige, Frye, Schwartz, [1804.09720](#), [1906.10137](#)]



Probabilistic formation of a Pythia jet

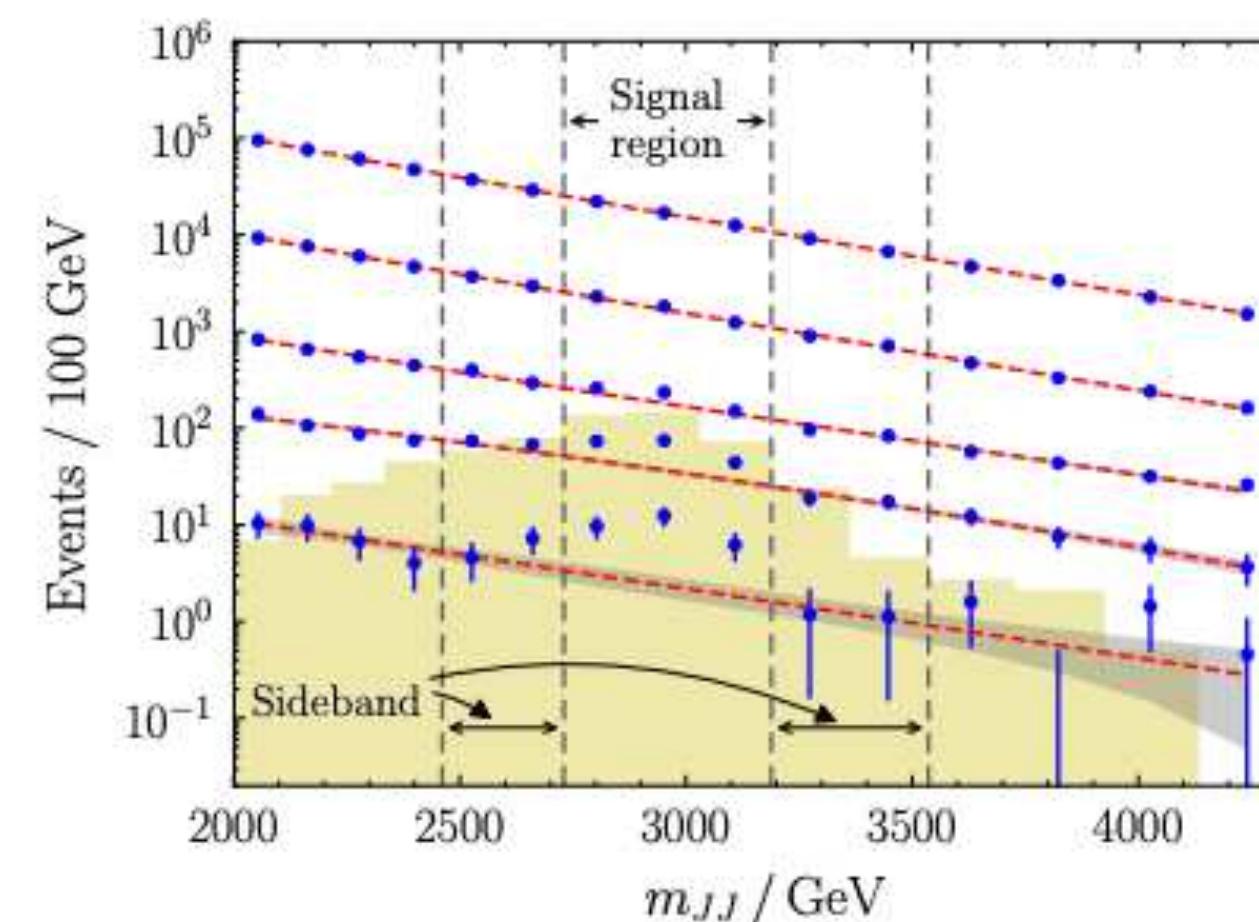
Topic Modeling e.g. Jet Topics

[Metodiev, Thaler, [1802.00008](#);
PTK, Metodiev, Thaler, [1809.01140](#)]



Anomaly Detection *tons of recent work*

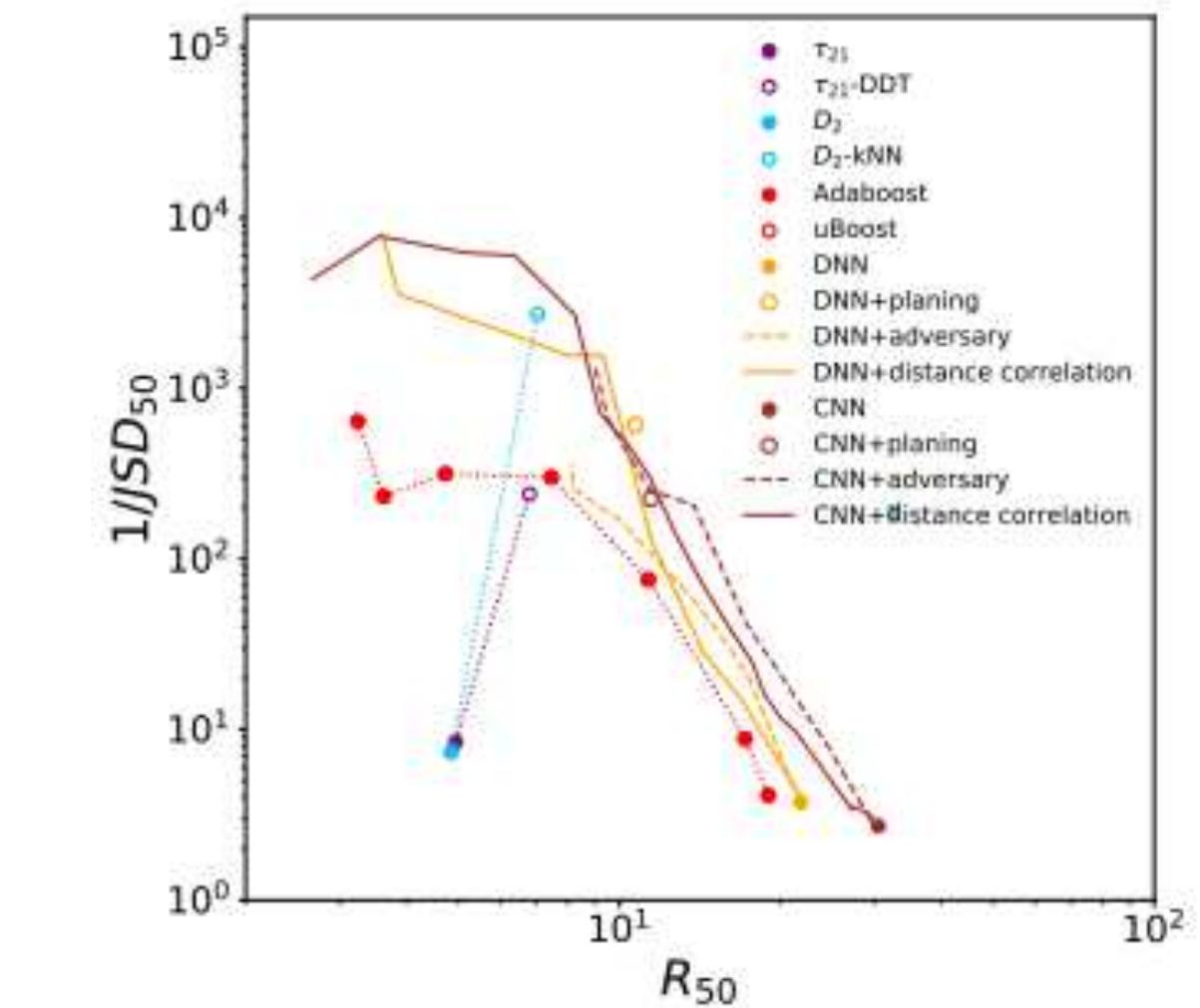
[Collins, Howe, Nachman, [1805.02664](#);
Farina, Nakai, Shih, [1808.08992](#);
Heimel, Kasieczka, Plehn, Thompson, [1808.08979](#);
Cerri, Nguyen, Pierini, Spiropulu, Vlimant, [1811.10276](#);
Blance, Spannowsky, Waite, [1905.10384](#);
See LHC Olympics 2020 anomaly detection workshop]



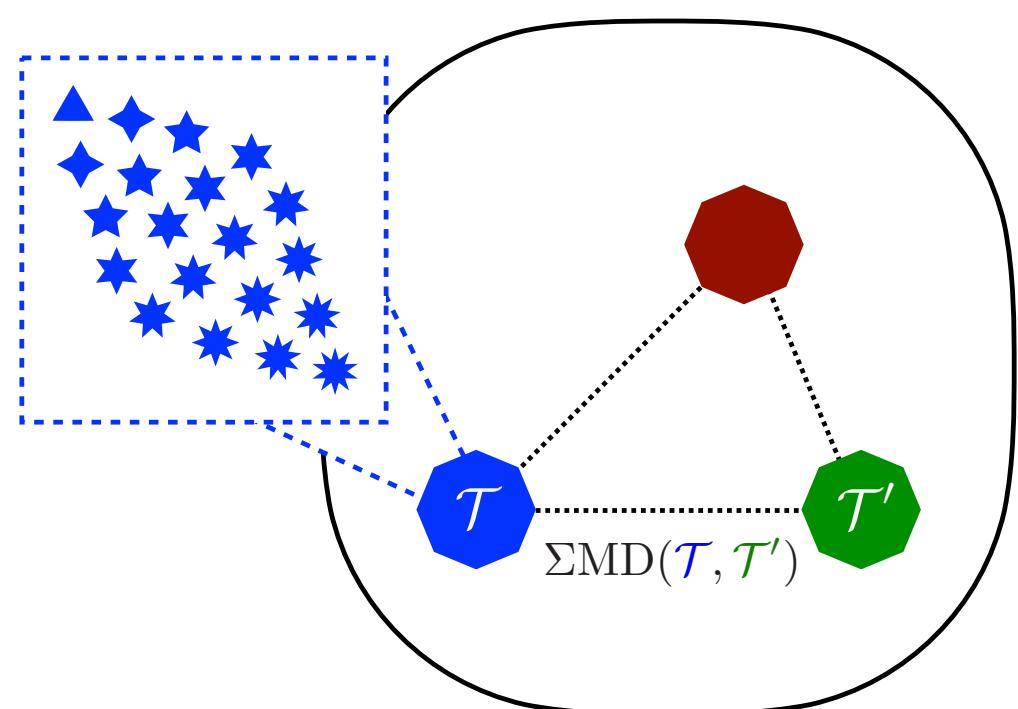
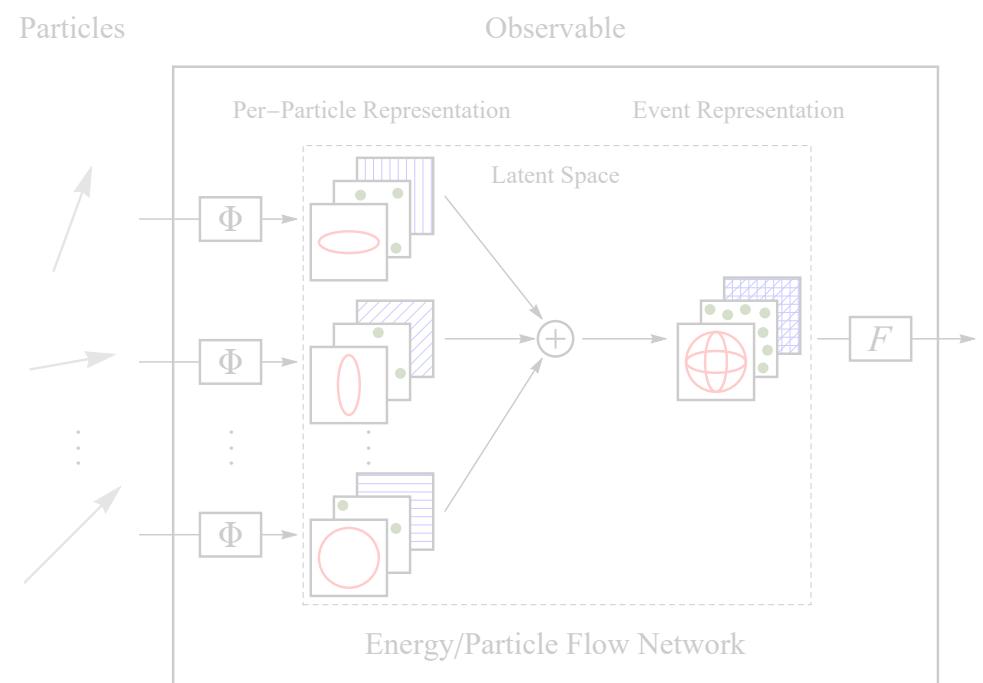
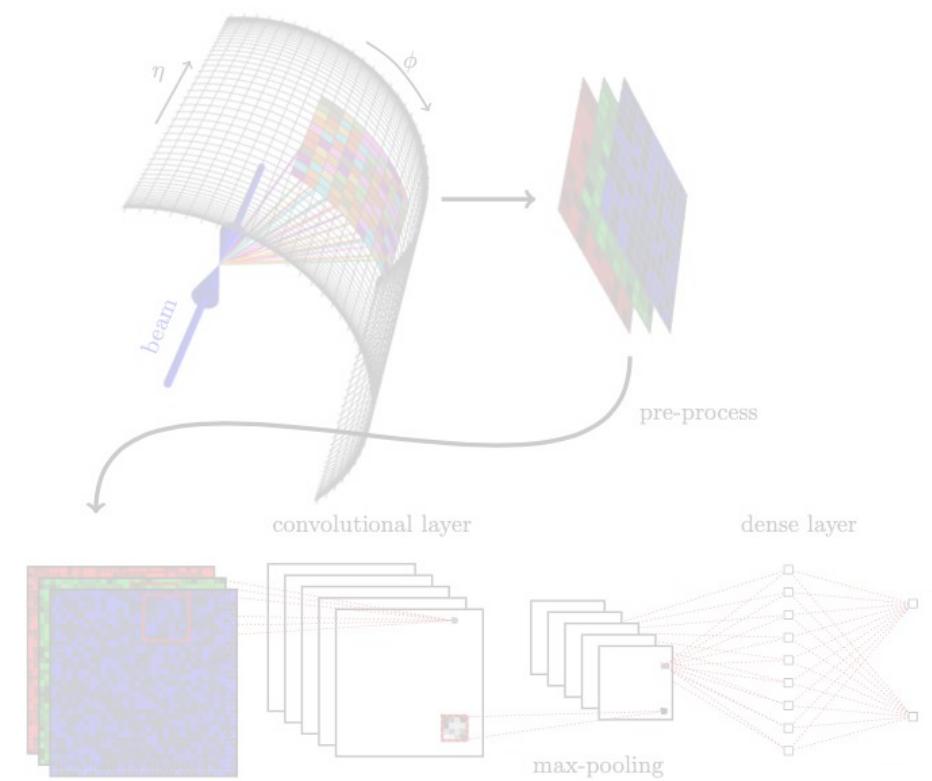
CWoLa hunting to enhance a resonance search

Decorrelation Methods e.g. DDT, Planing, DisCo

[Dolen, Harris, Marzani, Rappoccio, Tran, [1603.00027](#);
Chang, Cohen, Ostdiek, [1709.10106](#);
Kasieczka, Shih, [2001.05310](#);
Kasieczka, Nachman, Schwartz, Shih, [2007.14400](#)]



Decorrelating ML taggers from a key observable



Ubiquity of ML in HEP

Lightning Review

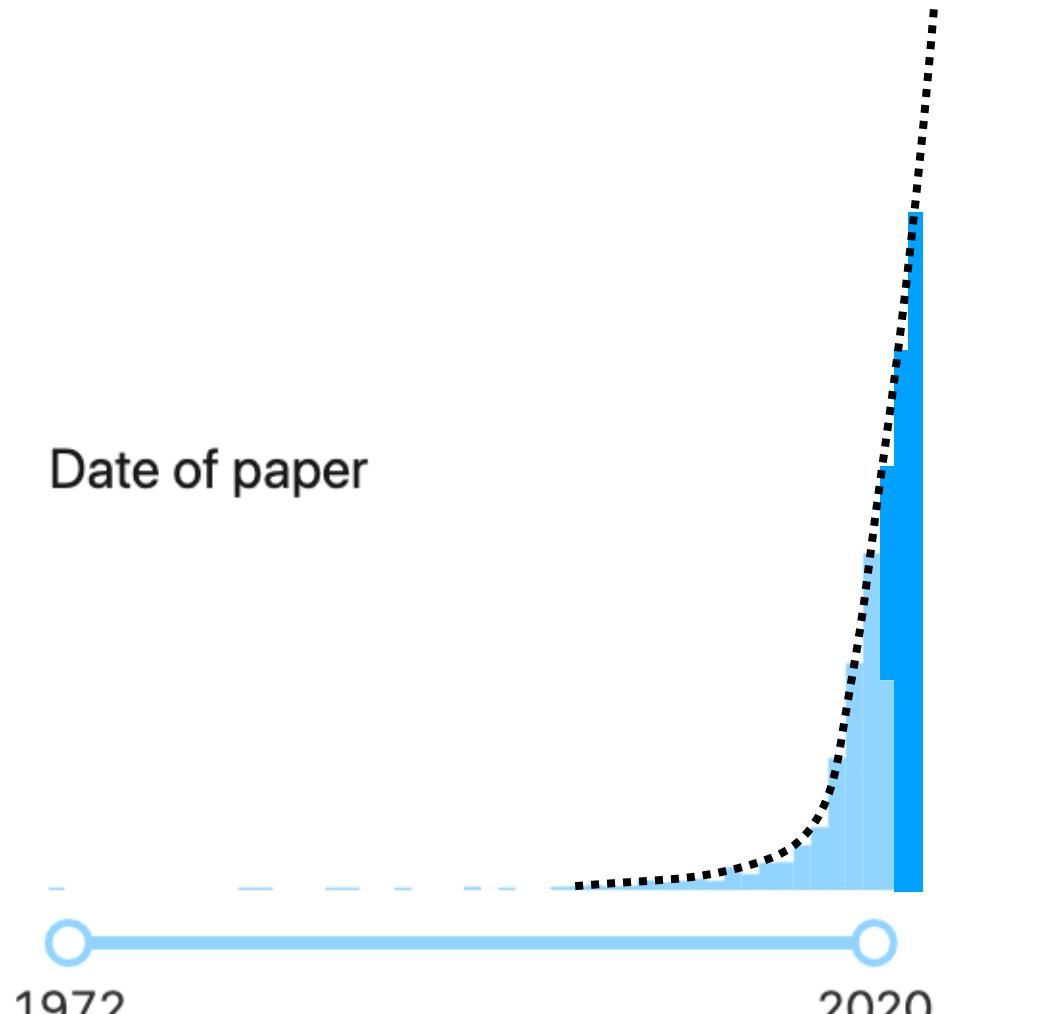
Future Directions

Thoughts on the Future

► *Machine learning will be essential in maximizing HEP potential*

We should capitalize on the opportunity to optimize

ML is both a computational tool and a useful formalism/language



► *Diversity of applications is impressive and will become more so*

Rapidly advancing beyond “hammer and nail” approach for ML in HEP

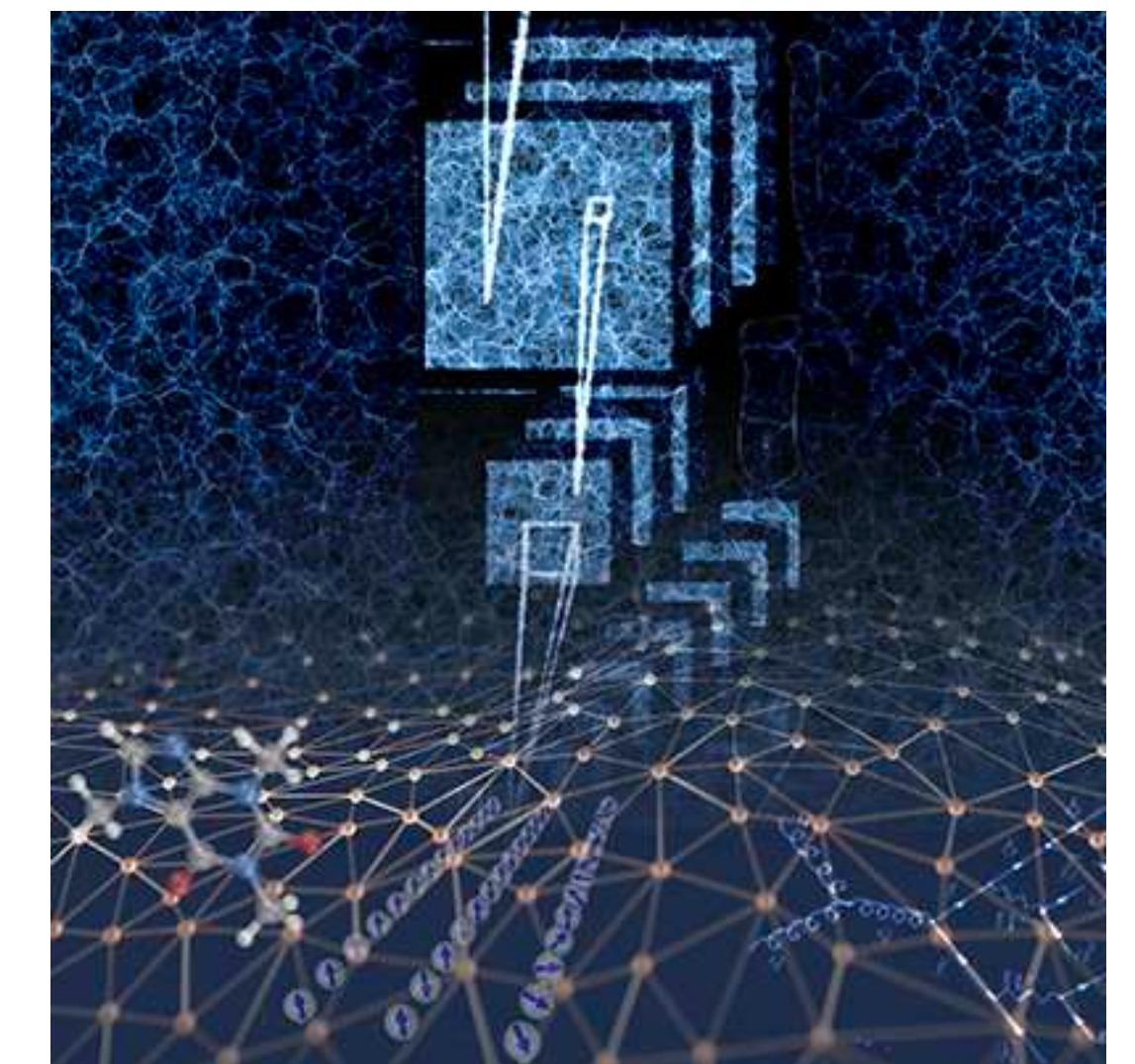
New observables, architectures, paradigms have been developed

HEPML-LivingReview has a thorough
and organized list of papers

► *Collaboration across traditional lines will enable success*

Learn from and contribute to the highly-vibrant ML community

ML in HEP needs insight from theory and experiment



► *ML strongly overlaps with other computational frontier areas*

Software workflows, reproducible analyses, public datasets are critical

[Reviews of Modern Physics Cover December 2019
from Machine learning and the physical sciences]

Thank You!

EnergyFlow Python Package

pip3 install energyflow

Keras/Tensorflow implementations of Energy/Particle Flow Networks
Interfaces with reprocessed [CMS 2011A Jet Primary Dataset](#) hosted on [Zenodo](#)
Detailed [examples](#), [demos](#), and [documentation](#)

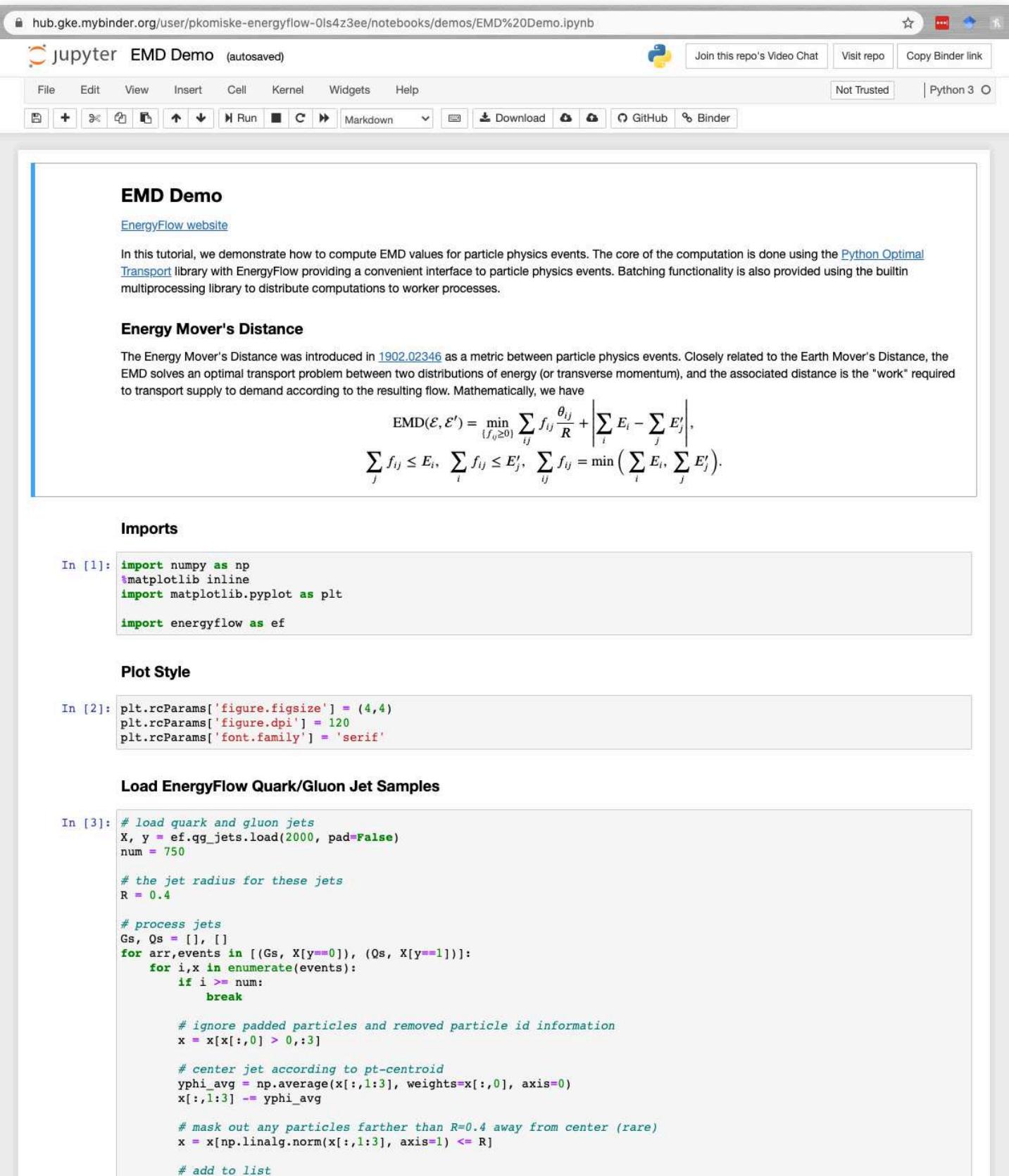
 **Welcome to EnergyFlow**

EnergyFlow is a Python package containing a suite of particle physics tools:

- **Energy Flow Polynomials:** EFPs are a collection of jet substructure observables which form a complete linear basis of IRC-safe observables. EnergyFlow provides tools to compute EFPs on events for several energy and angular measures as well as custom measures.
- **Energy Flow Networks:** EFNs are infrared- and collinear-safe models designed for learning from collider events as unordered, variable-length sets of particles. EnergyFlow contains customizable Keras implementations of EFNs. Available from version [0.10.0](#) onward.
- **Particle Flow Networks:** PFNs are general models designed for learning from collider events as unordered, variable-length sets of particles, based on the [Deep Sets](#) framework. EnergyFlow contains customizable Keras implementations of PFNs. Available from version [0.10.0](#) onward.
- **Energy Mover's Distance:** The EMD is a common metric between probability distributions that has been adapted for use as a metric between collider events. EnergyFlow contains code to facilitate the computation of the EMD between events based on an underlying implementation provided by the [Python Optimal Transport \(POT\)](#) library. Available from version [0.11.0](#) onward.
- **Energy Flow Moments:** EFM moments built out of particle energies and momenta that can be evaluated in linear time in the number of particles. They provide a highly efficient means of implementing $\beta = 2$ EFPs and are also very useful for reasoning about linear redundancies that appear between EFPs. Available from version [1.0.0](#) onward.

The EnergyFlow package also provides easy access to particle physics datasets and useful supplementary features:

- **CMS Open Data in MOD HDF5 Format:** Reprocessed datasets from the CMS Open Data,



In this tutorial, we demonstrate how to compute EMD values for particle physics events. The core of the computation is done using the [Python Optimal Transport](#) library with EnergyFlow providing a convenient interface to particle physics events. Batching functionality is also provided using the builtin multiprocessing library to distribute computations to worker processes.

Energy Mover's Distance

The Energy Mover's Distance was introduced in [1902.02346](#) as a metric between particle physics events. Closely related to the Earth Mover's Distance, the EMD solves an optimal transport problem between two distributions of energy (or transverse momentum), and the associated distance is the "work" required to transport supply to demand according to the resulting flow. Mathematically, we have

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

Imports

```
In [1]: import numpy as np
%matplotlib inline
import matplotlib.pyplot as plt
import energyflow as ef
```

Plot Style

```
In [2]: plt.rcParams['figure.figsize'] = (4,4)
plt.rcParams['figure.dpi'] = 120
plt.rcParams['font.family'] = 'serif'
```

Load EnergyFlow Quark/Gluon Jet Samples

```
In [3]: # load quark and gluon jets
x, y = ef.qg_jets.load(2000, pad=False)
num = 750

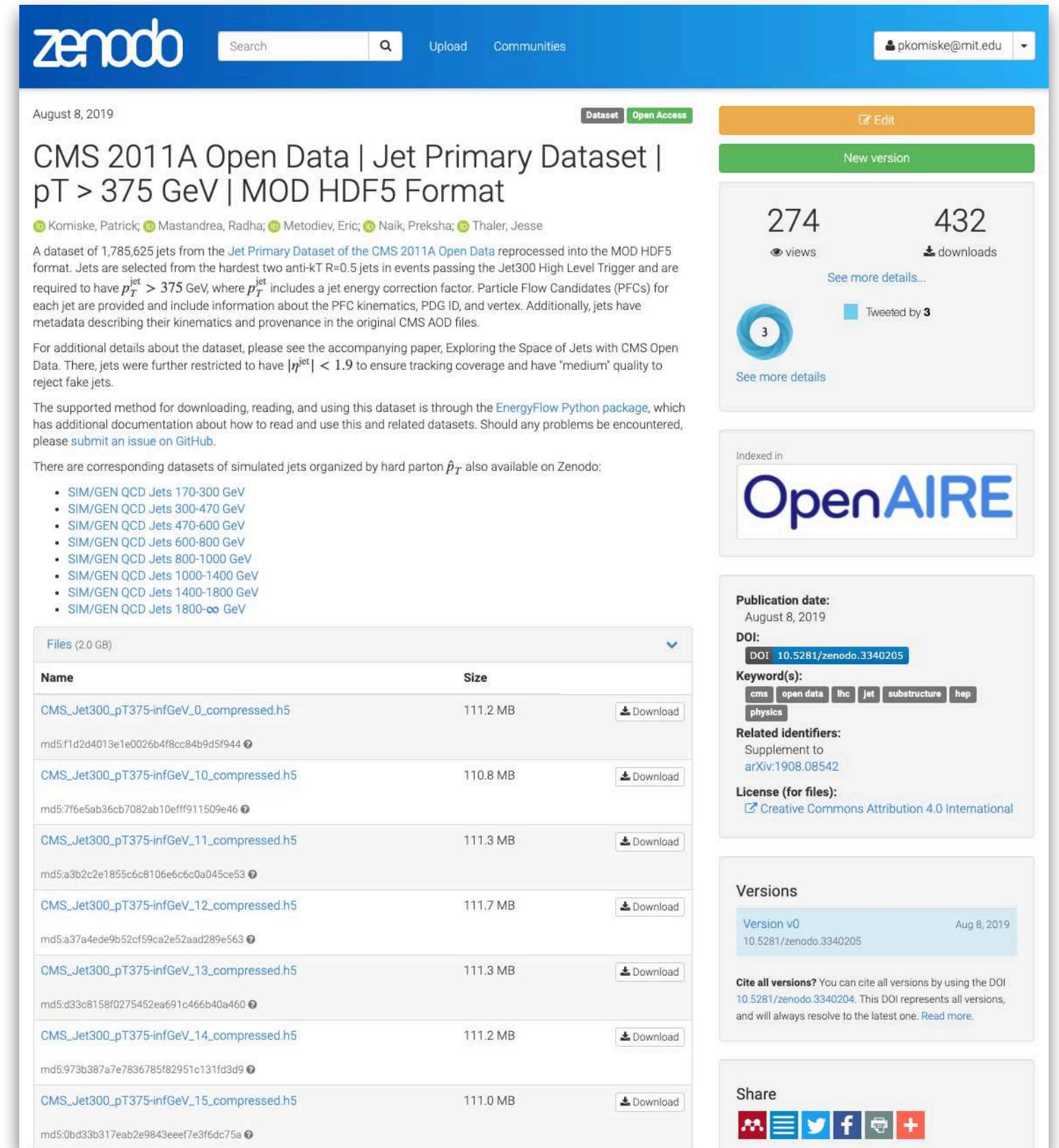
# the jet radius for these jets
R = 0.4

# process jets
Gs, Qs = [], []
for arr,events in [(Gs, X[y==0]), (Qs, X[y==1])]:
    for i,x in enumerate(events):
        if i >= num:
            break
        # ignore padded particles and removed particle id information
        x = x[x[:,0] > 0,:]

        # center jet according to pt-centroid
        yphi_avg = np.average(x[:,1:3], weights=x[:,0], axis=0)
        x[:,1:3] -= yphi_avg

        # mask out any particles farther than R=0.4 away from center (rare)
        x = x[np.linalg.norm(x[:,1:3], axis=1) <= R]

    # add to list
    Gs.append(Gs)
    Qs.append(Qs)
```



August 8, 2019

CMS 2011A Open Data | Jet Primary Dataset | pT > 375 GeV | MOD HDF5 Format

Komiske, Patrick; Mastandrea, Radha; Metodiev, Eric; Naik, Preksha; Thaler, Jesse

A dataset of 1,785 jets from the Jet Primary Dataset of the CMS 2011A Open Data reprocessed into the MOD HDF5 format. Jets are selected from the hardest two anti- $R=0.5$ jets in events passing the Jet300 High Level Trigger and are required to have $p_T^{\text{jet}} > 375$ GeV, where p_T^{jet} includes a jet energy correction factor. Particle Flow Candidates (PFCs) for each jet are provided and include information about the PFC kinematics, PDG ID, and vertex. Additionally, jets have metadata describing their kinematics and provenance in the original CMS AOD files.

For additional details about the dataset, please see the accompanying paper, Exploring the Space of Jets with CMS Open Data. There, jets were further restricted to have $|\eta^{\text{jet}}| < 1.9$ to ensure tracking coverage and have "medium" quality to reject fake jets.

The supported method for downloading, reading, and using this dataset is through the EnergyFlow Python package, which has additional documentation about how to read and use this and related datasets. Should any problems be encountered, please submit an issue on GitHub.

There are corresponding datasets of simulated jets organized by hard parton \hat{p}_T also available on Zenodo:

- SIM/GEN QCD Jets 170-300 GeV
- SIM/GEN QCD Jets 300-470 GeV
- SIM/GEN QCD Jets 470-600 GeV
- SIM/GEN QCD Jets 600-800 GeV
- SIM/GEN QCD Jets 800-1000 GeV
- SIM/GEN QCD Jets 1000-1400 GeV
- SIM/GEN QCD Jets 1400-1800 GeV
- SIM/GEN QCD Jets 1800-∞ GeV

Files (2.0 GB)

Name	Size
CMS_Jet300_pT375-infGeV_0_compressed.h5	111.2 MB
md5:fd2d4013e1e0026b4f8cc84b9d5f94	
CMS_Jet300_pT375-infGeV_10_compressed.h5	110.8 MB
md5:7f6e5ab36cb7082ab10eff911509e46	
CMS_Jet300_pT375-infGeV_11_compressed.h5	111.3 MB
md5:a3b2c2e1855dc8106e6c6c0a045ce53	
CMS_Jet300_pT375-infGeV_12_compressed.h5	111.7 MB
md5:a37a4ede9b52cf59ca2e52a2ad289e563	
CMS_Jet300_pT375-infGeV_13_compressed.h5	111.3 MB
md5:d3c815bf0275452ea691c466b40a460	
CMS_Jet300_pT375-infGeV_14_compressed.h5	111.2 MB
md5:973b387a7e7836785f82951c131fd3d9	
CMS_Jet300_pT375-infGeV_15_compressed.h5	111.0 MB
md5:0bd33b917eab2e9843eeef7e3f6dc75a	

Publication date: August 8, 2019

DOI: [10.5281/zenodo.3340205](#)

Keyword(s): cms, open data, lhc, jet, substructure, hep, physics

Related identifiers: Supplement to arXiv:1908.08542

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Versions

Version v0 Aug 8, 2019

[10.5281/zenodo.3340205](#)

Cite all versions? You can cite all versions by using the DOI 10.5281/zenodo.3340204. This DOI represents all versions, and will always resolve to the latest one. [Read more](#).

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Iterated Bayesian Unfolding (IBU)

Histogram-based unfolding method for a small number of observables

Choose observable(s) and binning at **detector-level** and **particle-level**

measured distribution: $m_i = \Pr(\text{measure } i)$ true distribution: $t_j^{(0)} = \Pr(\text{truth is } j)$

Calculate *response matrix* R_{ij} from **generated**/**simulated** pairs of events

$R_{ij} = \Pr(\text{measure } i \mid \text{truth is } j)$ R is in general non-square and non-invertible

Calculate new particle-level distribution using Bayes' theorem

$$t_j^{(n)} = \sum_i \Pr(\text{truth}_{n-1} \text{ is } j \mid \text{measure } i) \times \Pr(\text{measure } i) = \sum_i \frac{R_{ij} t_j^{(n-1)}}{\sum_k R_{ik} t_k^{(n-1)}} \times m_i$$

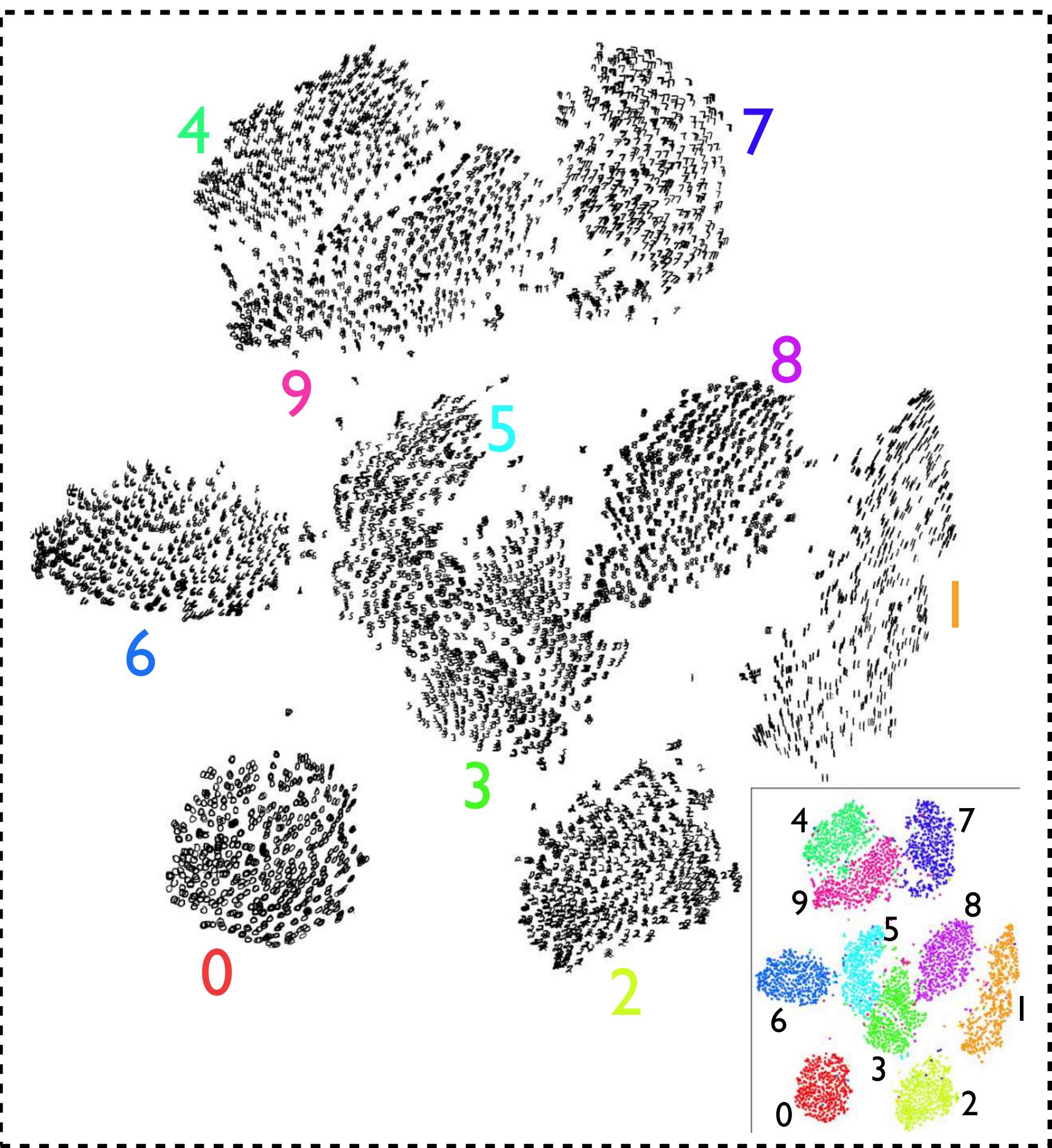
Iterate procedure to remove dependence on prior

[Richardson, 1972; Lucy, 1974; D'Agostini, 1995]

Visualizing Geometry in the Space of Events

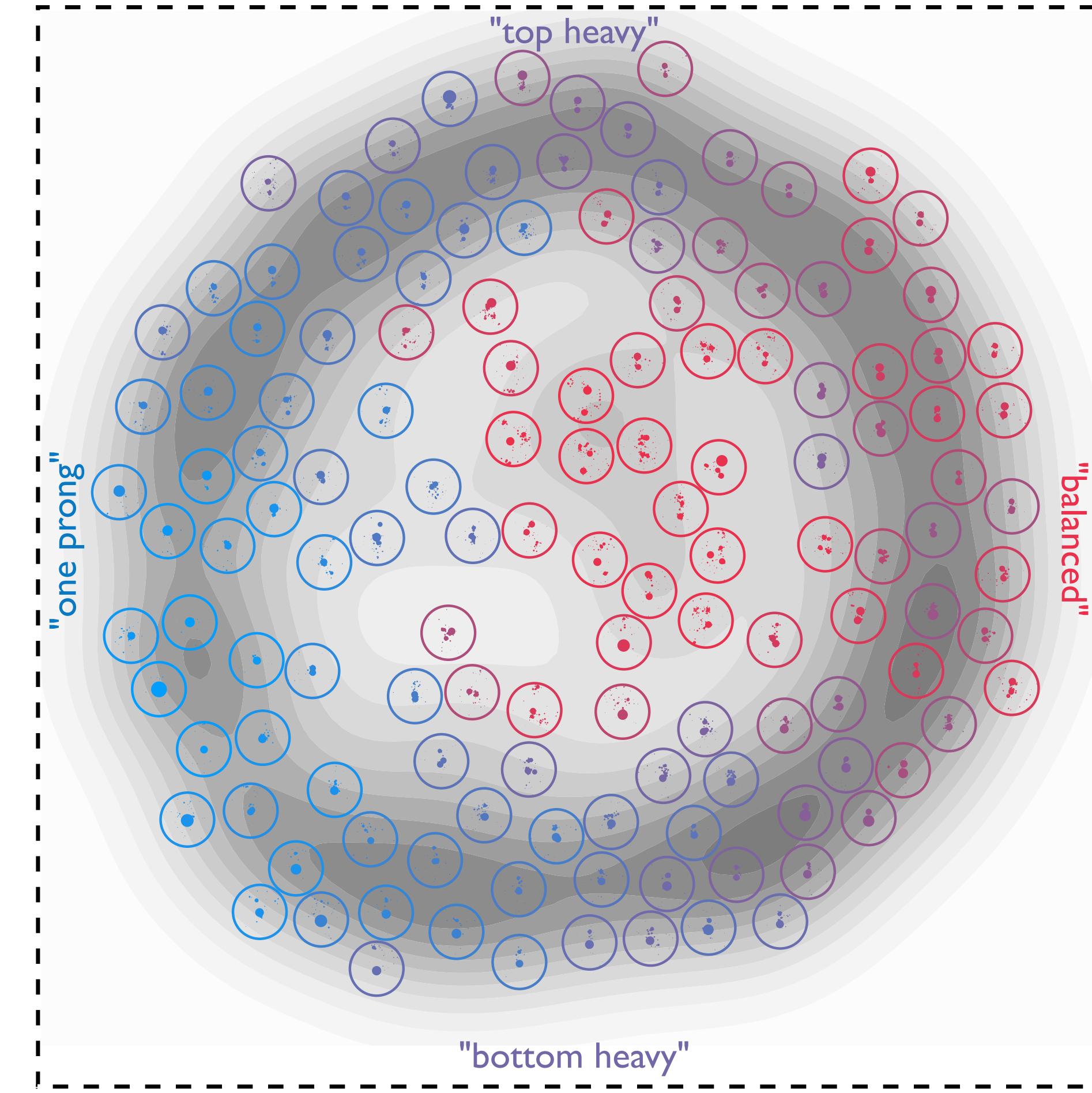
[PTK, Metodiev, Thaler, PRL 2019]

t-Distributed Stochastic Neighbor Embedding (t-SNE)
MNIST handwritten digits

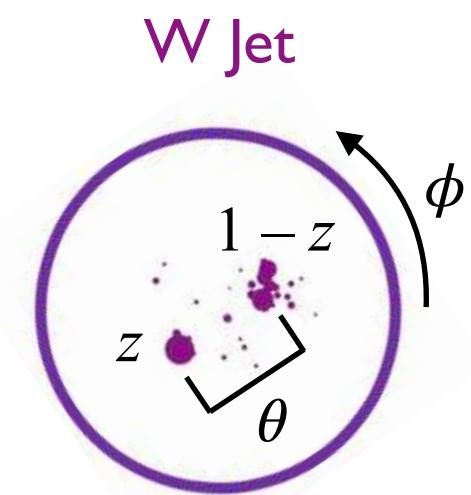


[L. van der Maaten, G. Hinton, JMLR 2008]

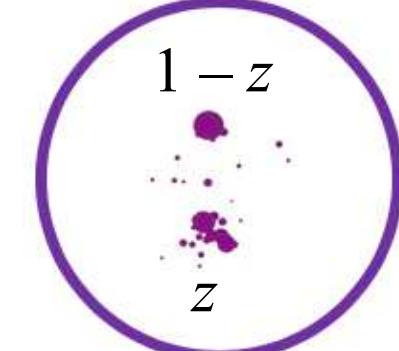
Geometric space of W jets



Gray contours represent the density of jets
Each circle is a particular W jet

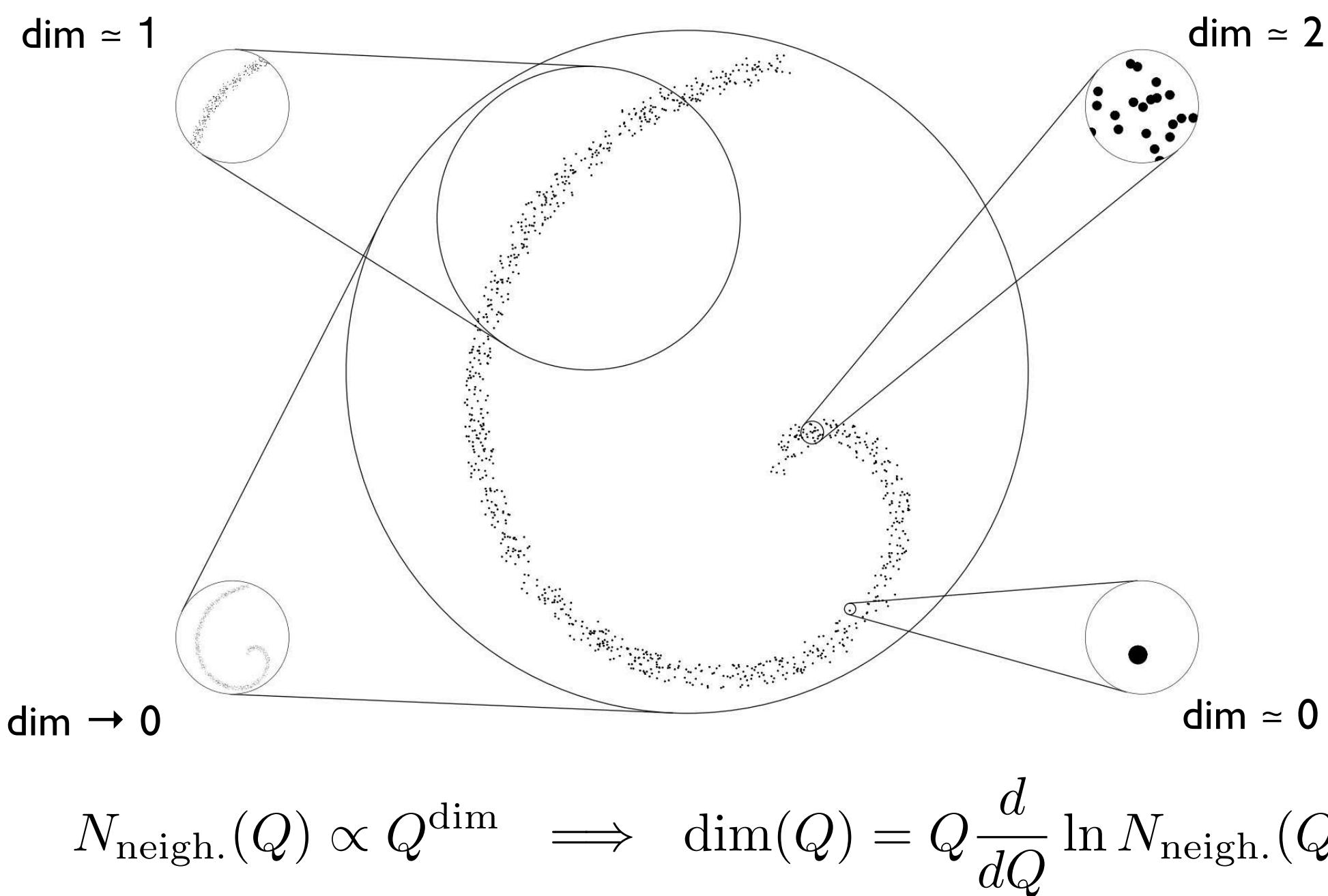


Constraints: W Mass and
 $\phi = 0$ preprocessing



Quantifying Event-Space Manifolds

Correlation dimension: how does the # of elements within a ball of size Q change?



Correlation dimension lessons:

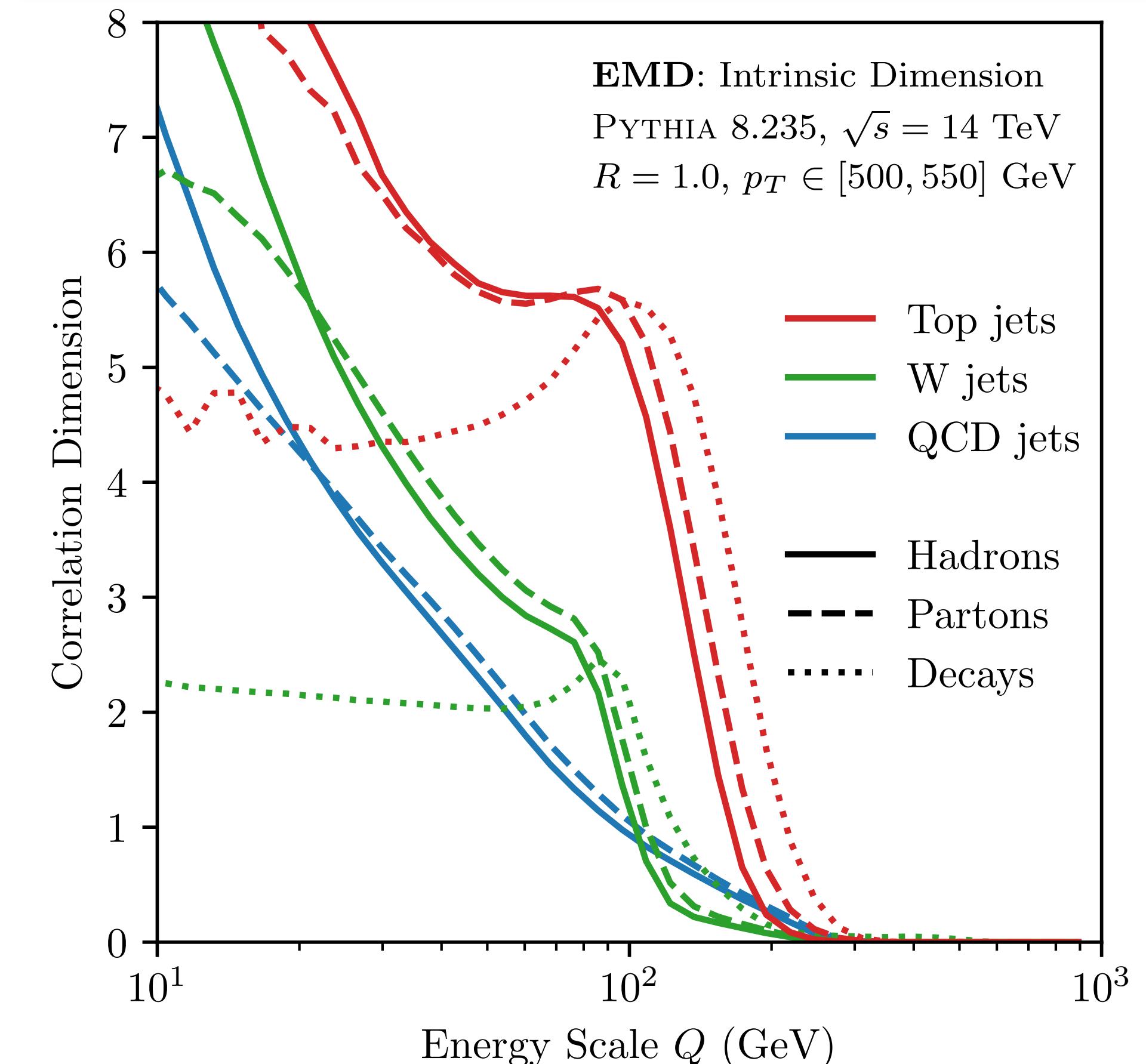
Decays are "constant" dim. at low Q

Complexity hierarchy: QCD < W < Top

Fragmentation increases dim. at smaller scales

Hadronization important around 20-30 GeV

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

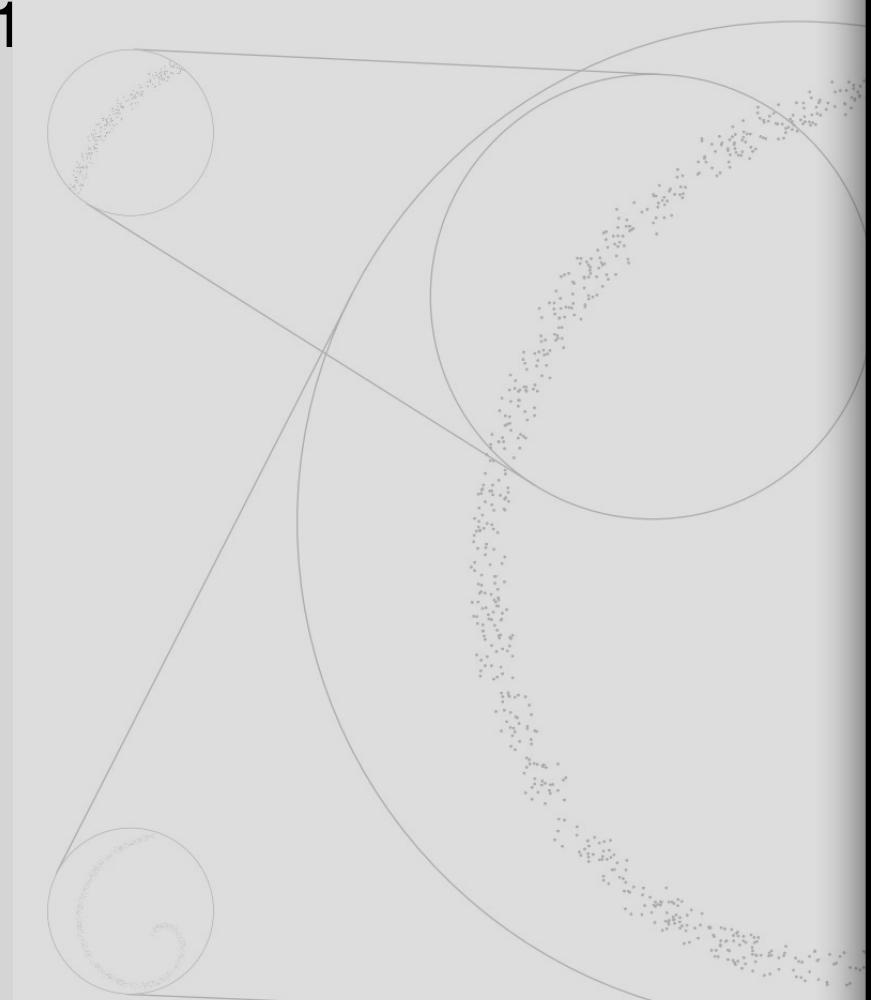


[Grassberger, Procaccia, [PRL 1983](#); PTK, Metodiev, Thaler, [PRL 2019](#)]

Quantifying Event-Space Manifolds

Correlation dimension
elements within a ball

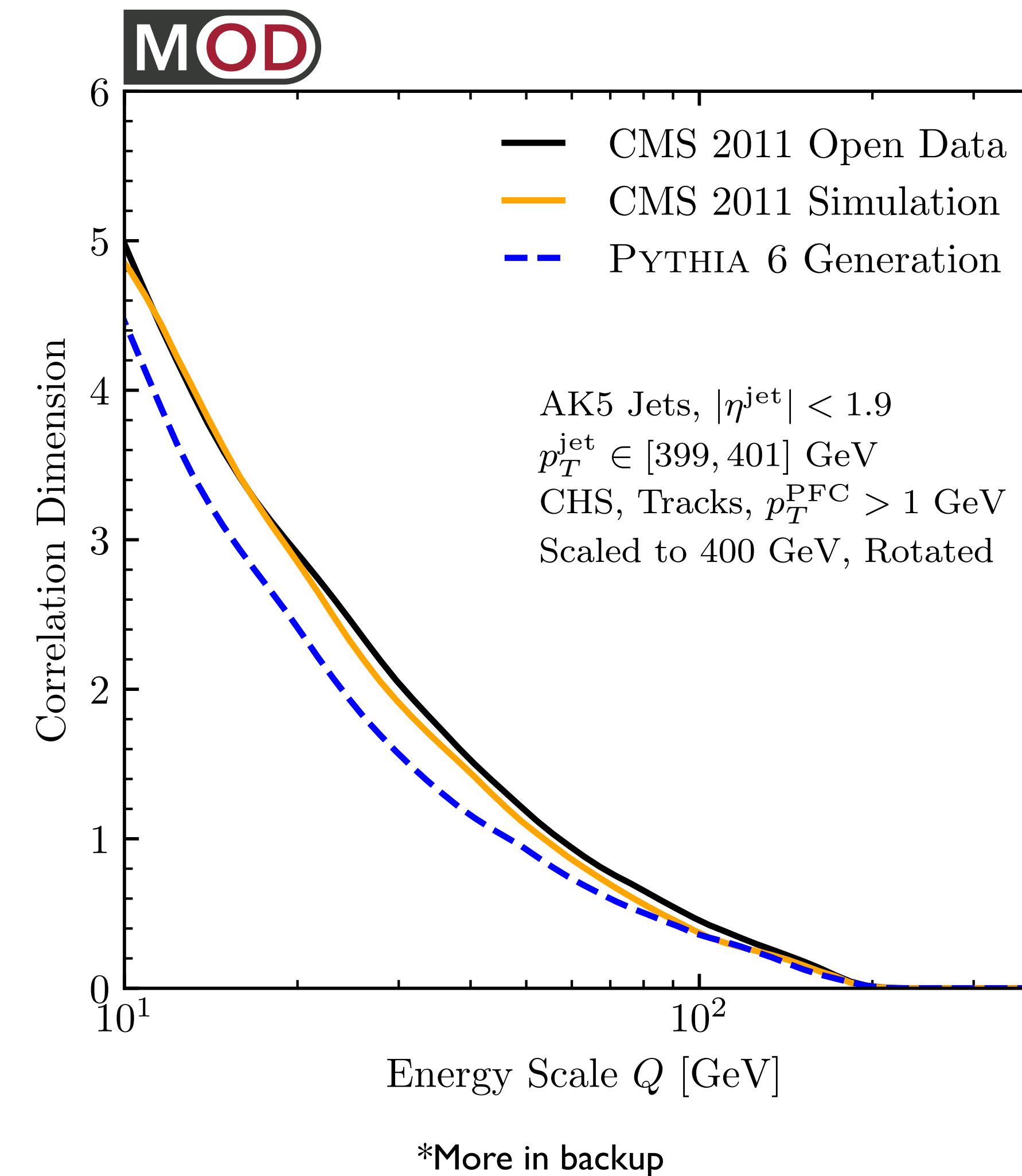
$\text{dim} \approx 1$



$$N_{\text{neigh.}}(Q) \propto Q^{\text{dim}} \implies \text{dim} \approx 1$$

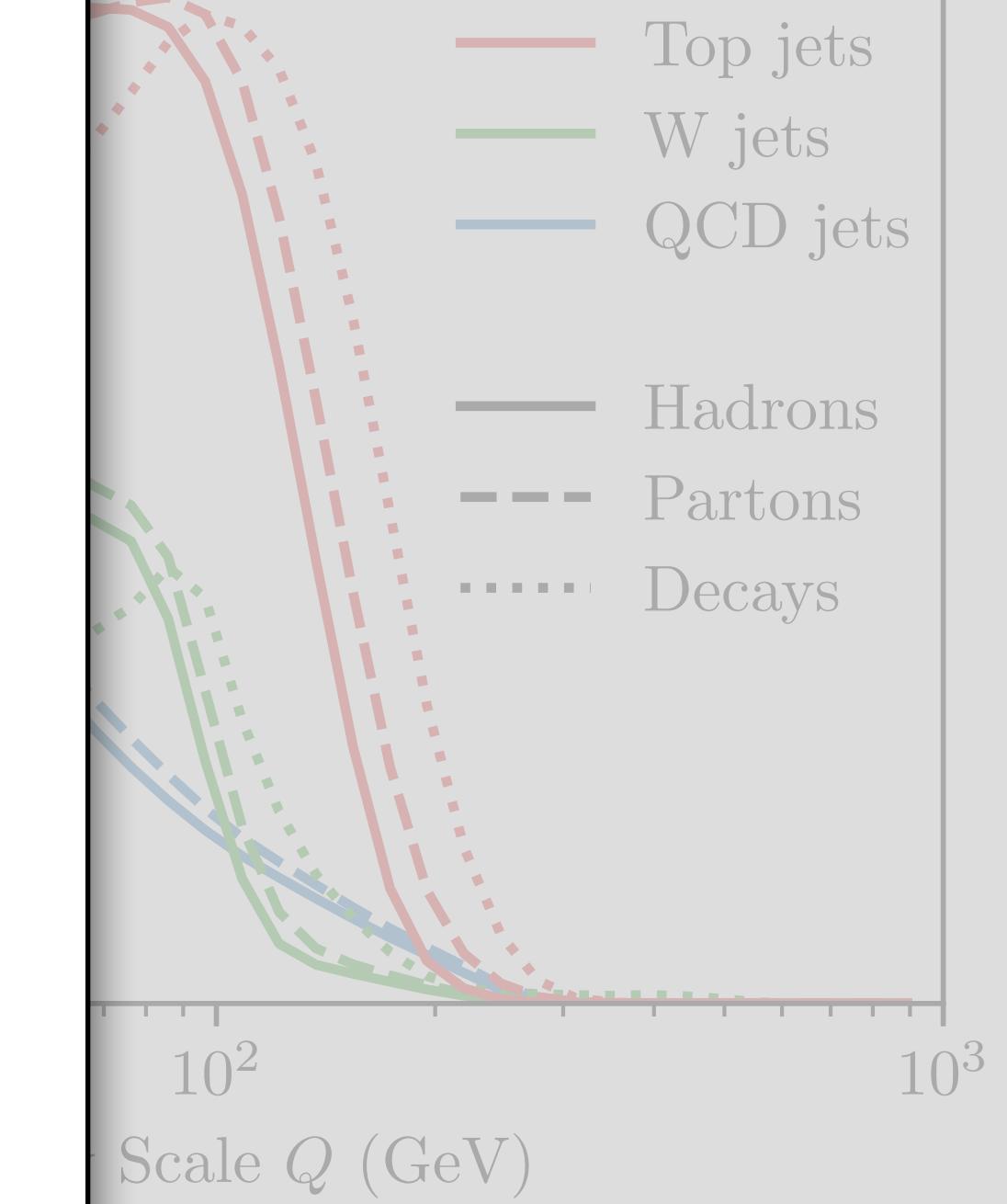
Correlation dimension
Decays are "constant"
Complexity hierarchy
Fragmentation increases
Hadronization important

... in CMS Open Data



$$\sum_j \Theta(\text{EMD}(\mathcal{E}_i, \mathcal{E}'_j) < Q)$$

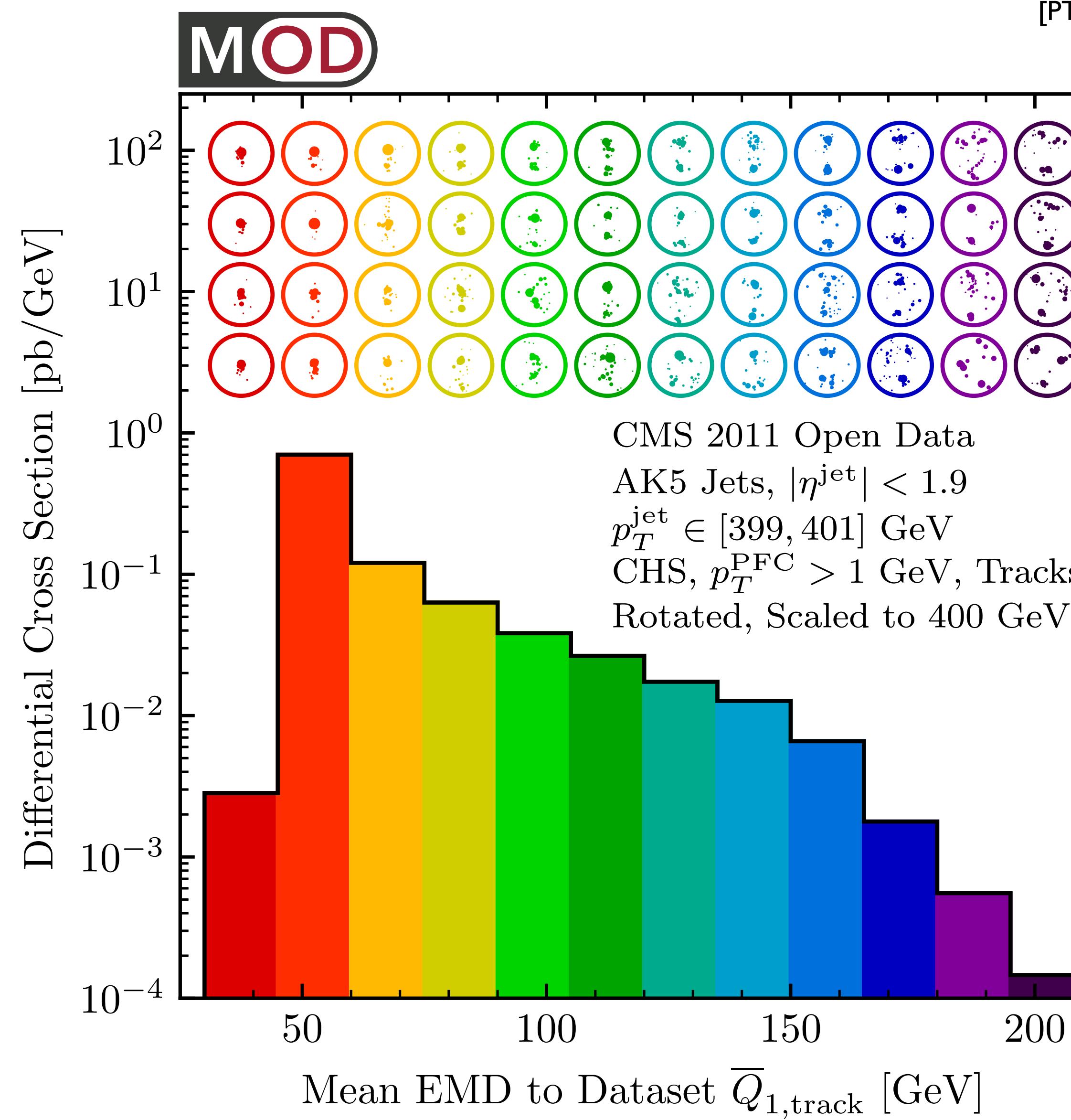
EMD: Intrinsic Dimension
PYTHIA 8.235, $\sqrt{s} = 14$ TeV
 $R = 1.0$, $p_T \in [500, 550]$ GeV



[Bocca, PRL 1983; PTK, Metodiev, Thaler, PRL 2019]

Visualizing Geometry in CMS Open Data

[PTK, Mastandrea, Metodiev, Naik, Thaler, PRD 2019; code and datasets at energyflow.network]



EMD for anomaly detection

4 medoids in each bin of anomaliness \bar{Q}_1

n^{th} moment of EMD distribution for a dataset

$$\bar{Q}_n(\mathcal{I}) = \sqrt[n]{\frac{1}{N} \sum_{k=1}^N (\text{EMD}(\mathcal{I}, \mathcal{J}_k))^n}$$

How far does this go?

$$\mathcal{V}_k = \frac{1}{N} \sum_{i=1}^N \min \{ \text{EMD}(\mathcal{J}_i, \mathcal{K}_1), \dots, \text{EMD}(\mathcal{J}_i, \mathcal{K}_k) \}$$

k-eventiness?

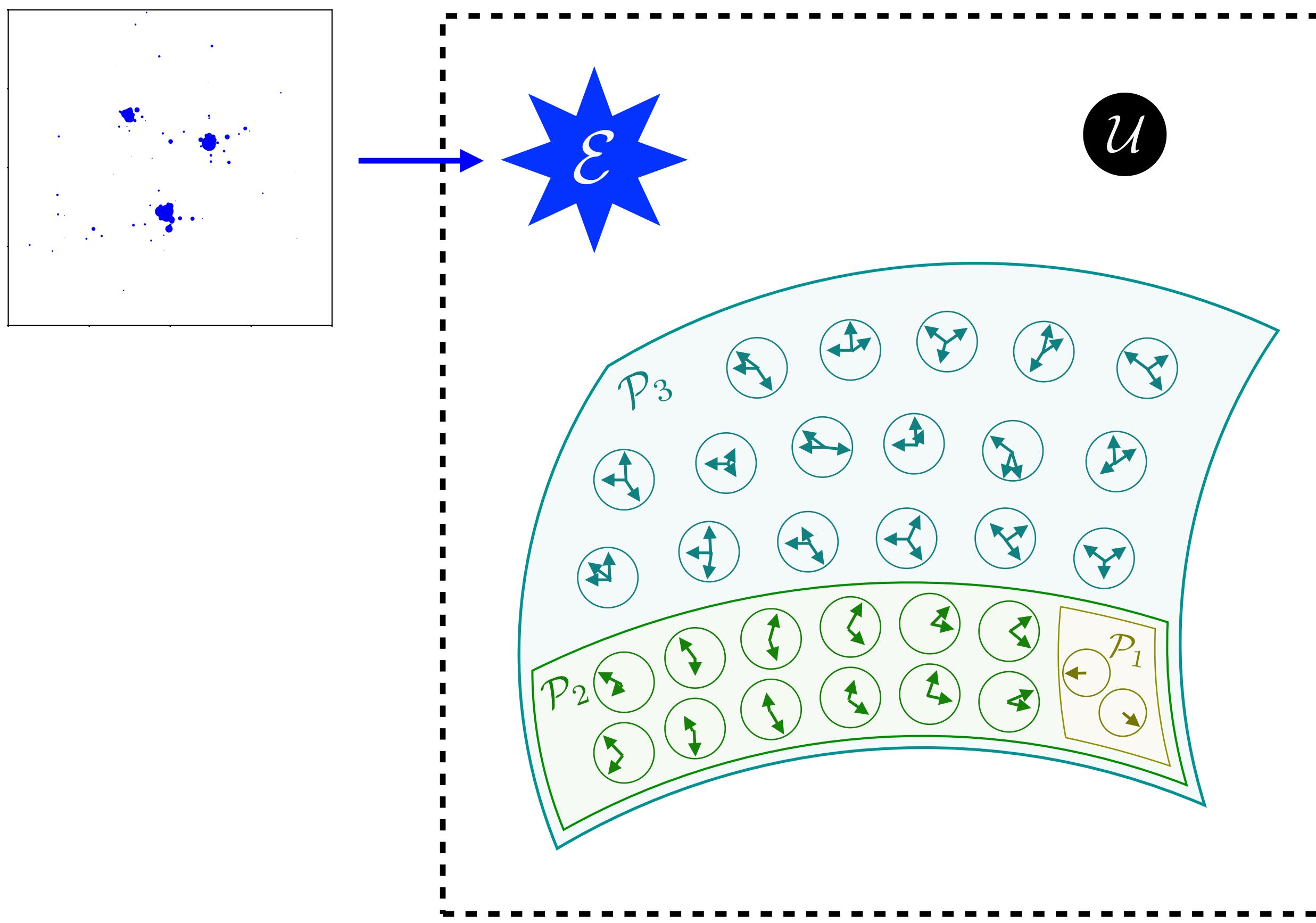
jet from dataset

medoids

N-particle Manifolds in the Space of Events

[PTK, Metodiev, Thaler, 2004.04.159]

$$\mathcal{P}_N = \text{set of all N-particle configurations} = \left\{ \sum_{i=1}^N E_i \delta(\hat{n} - \hat{n}_i) \mid E_i \geq 0 \right\}$$



\mathcal{P}_1 : manifold of events with one particle

\mathcal{P}_2 : manifold of events with two particles

\mathcal{P}_3 : manifold of events with three particles

⋮

$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \dots \supset \mathcal{P}_3 \supset \mathcal{P}_2 \supset \mathcal{P}_1$

by soft and collinear limits

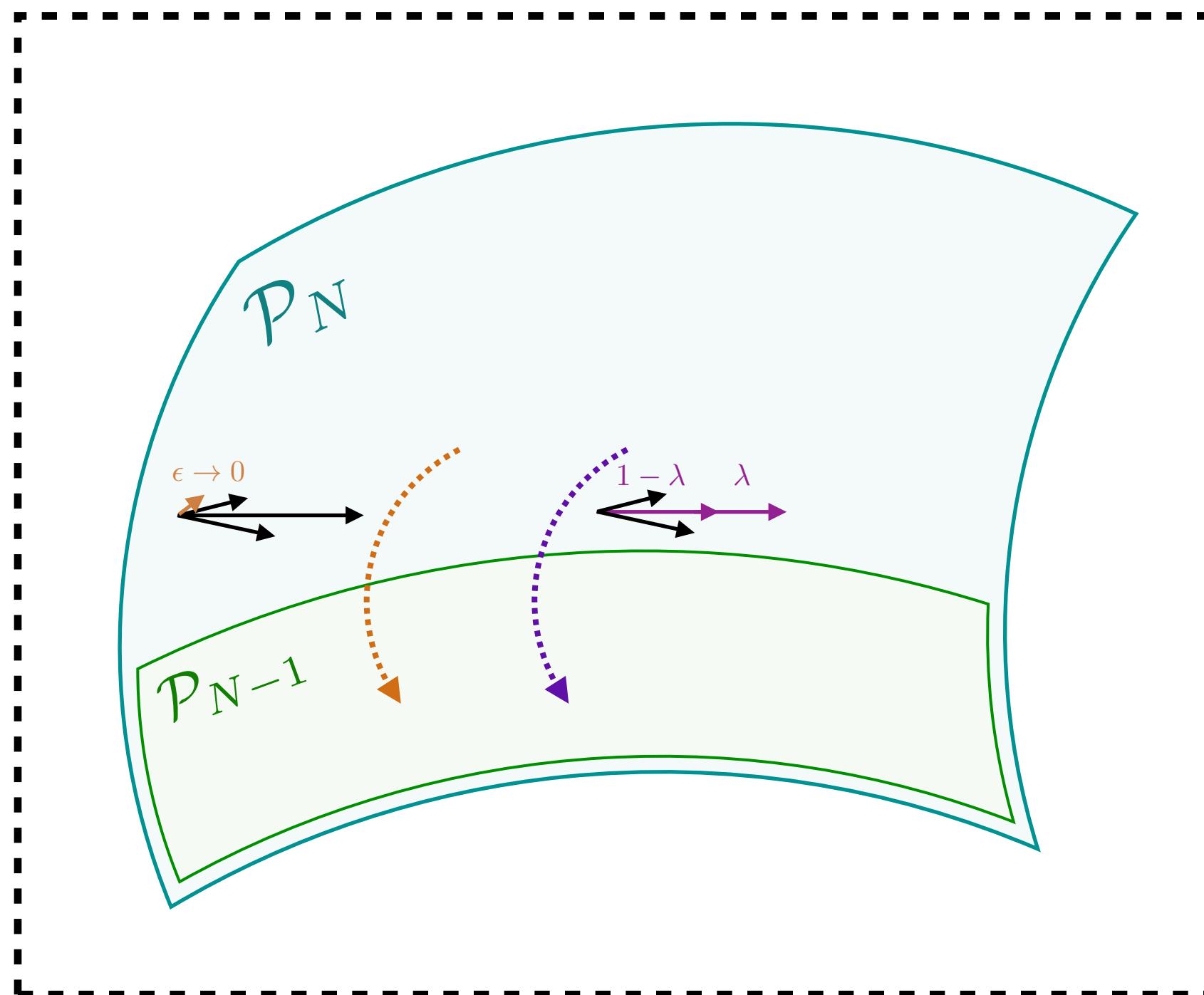


Uniform event, not contained in any \mathcal{P}_N

N-particle Manifolds in the Space of Events – Infrared Divergences

[PTK, Metodiev, Thaler, 2004.04.159]

$$\mathcal{P}_N = \text{set of all } N\text{-particle configurations} = \left\{ \sum_{i=1}^N E_i \delta(\hat{n} - \hat{n}_i) \mid E_i \geq 0 \right\}$$



Energy flow is unchanged by exact soft/collinear emissions

$$\longleftrightarrow = \xrightarrow{\epsilon \rightarrow 0} = \xrightarrow{1-\lambda \quad \lambda}$$

Functions of energy flow automatically satisfy exact IRC invariance!

Real and virtual divergences appear naturally together

$$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \cdots \supset \mathcal{P}_3 \supset \mathcal{P}_2 \supset \mathcal{P}_1$$

by soft and collinear limits

Defining IRC Safety Precisely

[Sterman, Weinberg, [PRL 1997](#); Sterman, [PRD 1978](#); Banfi, Salam, Zanderighi, [JHEP 2005](#)]

Infrared and collinear safety is a proxy for perturbative calculability of an observable

Exact **IRC** invariance

$$\mathcal{O}(p_1^\mu, \dots, p_M^\mu) = \mathcal{O}(0p_0^\mu, p_1^\mu, \dots, p_M^\mu)$$

$$\mathcal{O}(p_1^\mu, \dots, p_M^\mu) = \mathcal{O}(\lambda p_1^\mu, (1 - \lambda)p_1^\mu, \dots, p_M^\mu)$$

Guarantees observable is well-defined on **energy** flows

Allows for pathological observables, e.g. pseudo-multiplicity

Smooth **IRC** invariance

$$\mathcal{O}(p_1^\mu, \dots, p_M^\mu) = \lim_{\epsilon \rightarrow 0} \mathcal{O}(\epsilon p_0^\mu, p_1^\mu, \dots, p_M^\mu)$$

$$\mathcal{O}(p_1^\mu, \dots, p_M^\mu) = \lim_{p_0^\mu \rightarrow p_1^\mu} \mathcal{O}(\lambda p_0^\mu, (1 - \lambda)p_1^\mu, \dots, p_M^\mu)$$

Eliminates common observables with hard boundaries

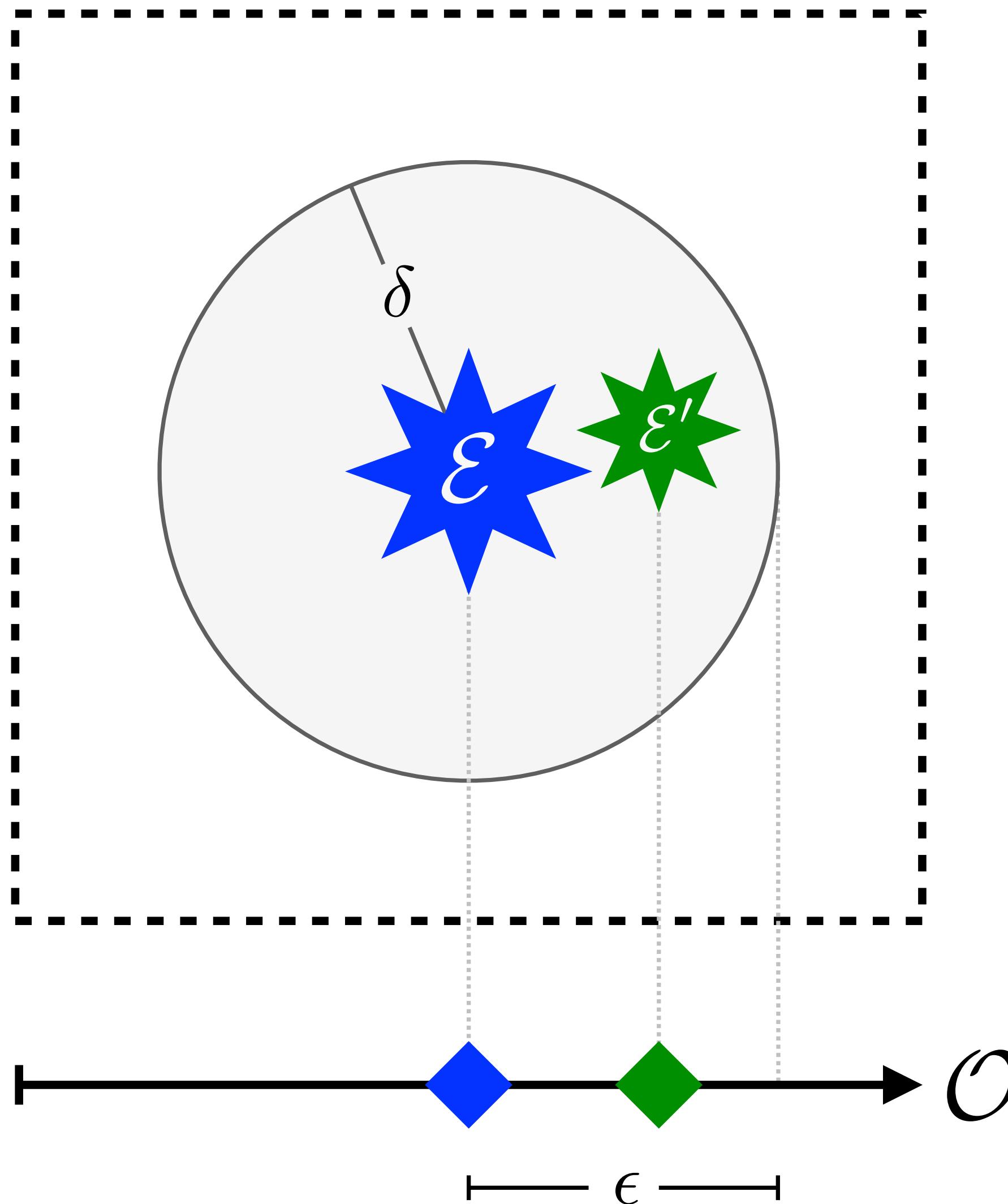
All Observables	Comments
Multiplicity ($\sum_i 1$)	IR unsafe and C unsafe
Momentum Dispersion [65] ($\sum_i E_i^2$)	IR safe but C unsafe
Sphericity Tensor [66] ($\sum_i p_i^\mu p_i^\nu$)	IR safe but C unsafe
Number of Non-Zero Calorimeter Deposits	C safe but IR unsafe

Defined on Energy Flows	
Pseudo-Multiplicity ($\min\{N \mid \mathcal{T}_N = 0\}$)	Robust to exact IR or C emissions

Infrared & Collinear Safe	
Jet Energy ($\sum_i E_i$)	Disc. at jet boundary
Heavy Jet Mass [67]	Disc. at hemisphere boundary
Soft-Dropped Jet Mass [38, 68]	Disc. at grooming threshold
Calorimeter Activity [69] (N_{95})	Disc. at cell boundary

More EMD Geometry – Continuity in the Space of Events

[PTK, Metodiev, Thaler, 2004.04.159]



Classic $\epsilon - \delta$ definition of continuity in a metric space

An observable \mathcal{O} is **EMD continuous** at an event \mathcal{E} if, for any $\epsilon > 0$, there exists a $\delta > 0$ such that for all events \mathcal{E}' :

$$\text{EMD}(\mathcal{E}, \mathcal{E}') < \delta \implies |\mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}')| < \epsilon.$$

Towards a geometric definition of **IRC Safety**

IRC Safety = EMD Continuity*

*on all but a negligible set[‡] of events

[‡]a negligible set is one that contains no positive-radius EMD-ball

⋮

Perturbation Theory in the Space of Events

[PTK, Metodiev, Thaler, 2004.04.159]

Sudakov safety

[Larkoski, Thaler, JHEP 2014; Larkoski, Marzani, Thaler, PRD 2015]

Some observables have discontinuities on P_N for some N

A resummed **IRC-safe companion** can mitigate the divergences

$$p(\mathcal{O}_{\text{Sudakov}}) = \int d\mathcal{O}_{\text{Comp.}} p(\mathcal{O}_{\text{Sudakov}} | \mathcal{O}_{\text{Comp.}}) p(\mathcal{O}_{\text{Comp.}})$$

Event geometry suggests N -(sub)jettiness as universal companion

Fixed-order calculability

[Sterman, PRD 1979; Banfi, Salam, Zanderighi, JHEP 2005]

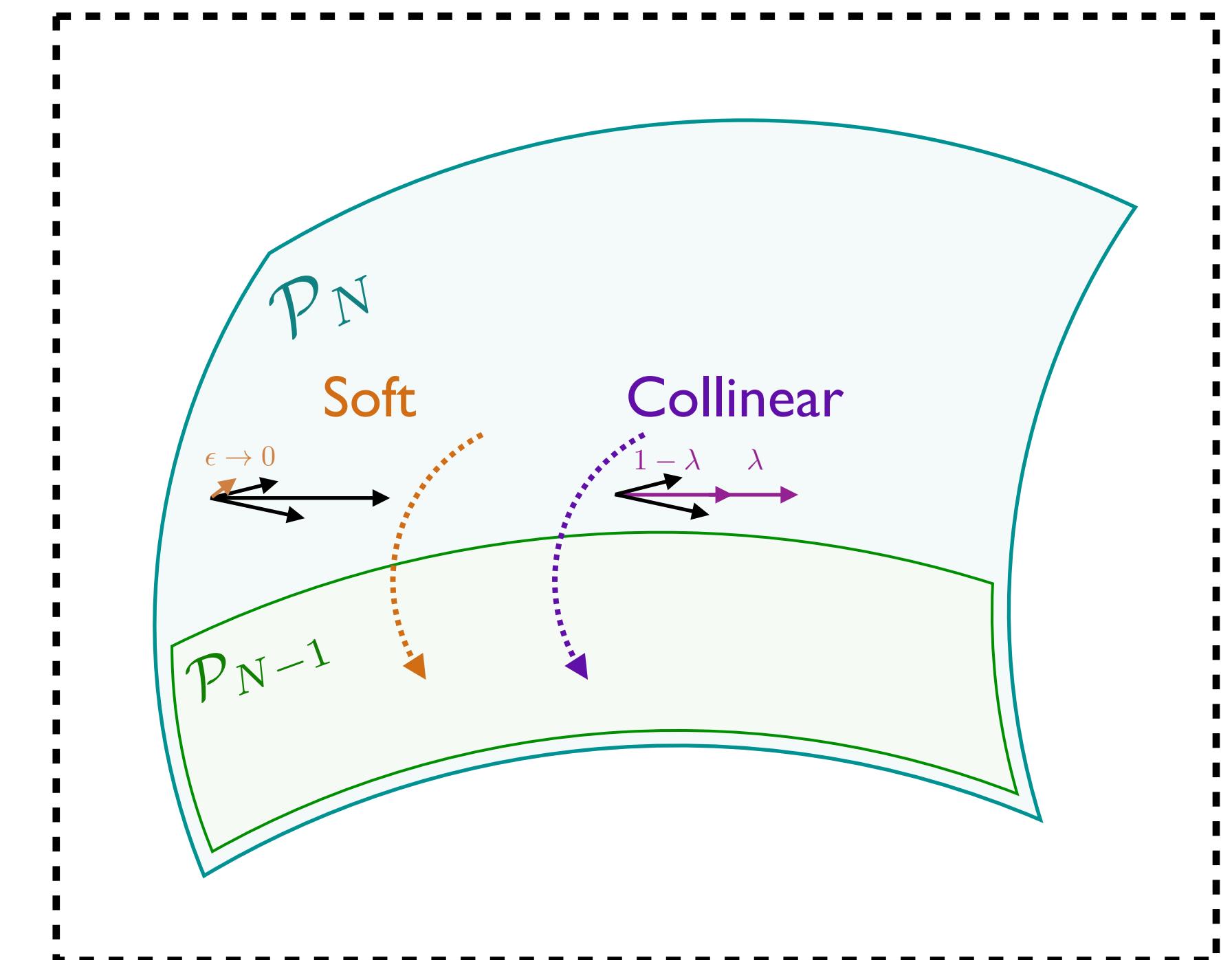
Is a statement of integrability on each P_N

EMD continuity must be upgraded to EMD-Hölder continuity on each P_N

$$\lim_{\mathcal{E} \rightarrow \mathcal{E}'} \frac{\mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}')}{\text{EMD}(\mathcal{E}, \mathcal{E}')^c} = 0, \quad c > 0$$

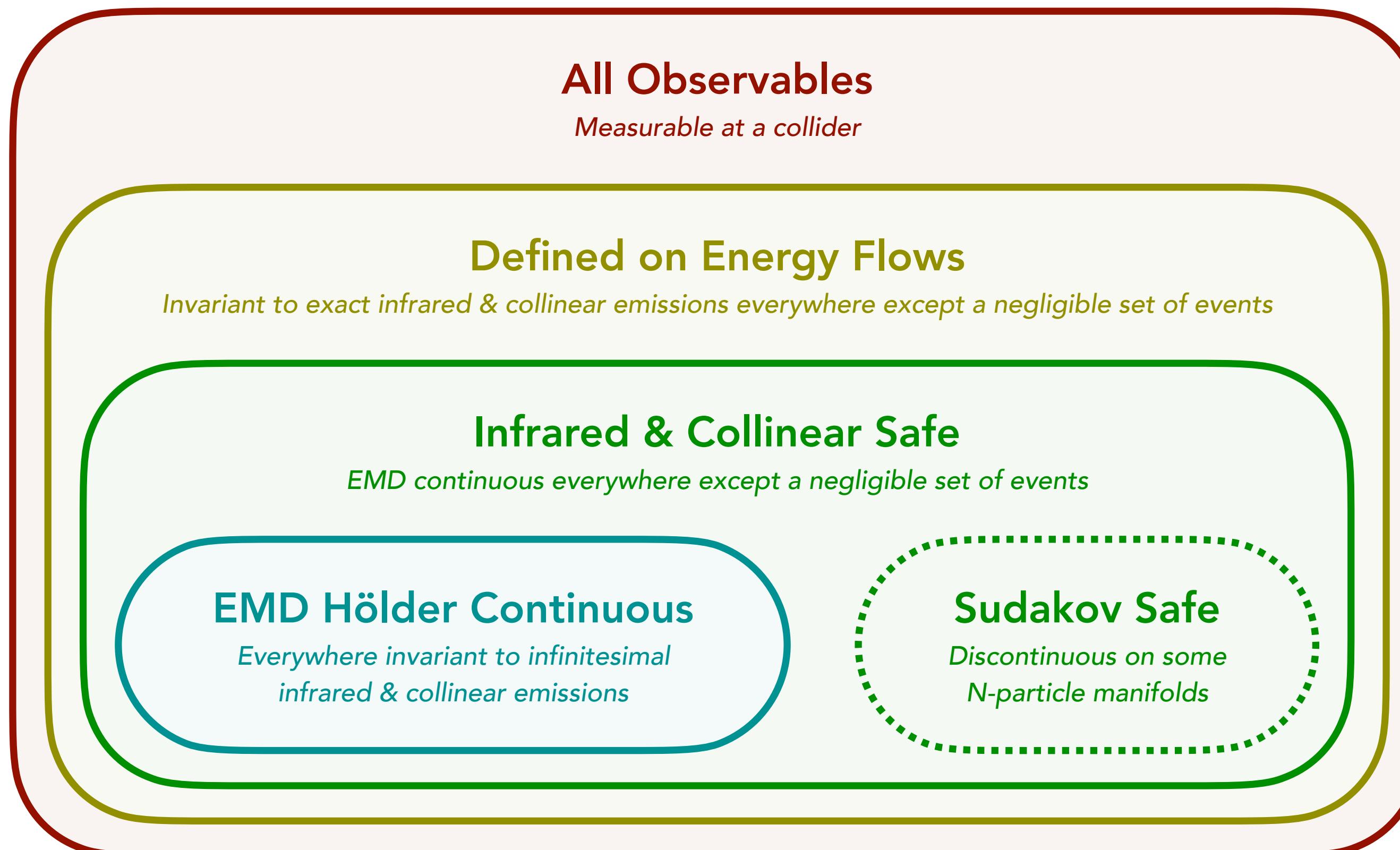
Example: $V(\mathcal{E}) = \mathcal{T}_2(\mathcal{E}) \left(1 + \frac{1}{\ln E(\mathcal{E})/\mathcal{T}_3(\mathcal{E})} \right)$ is EMD continuous but not EMD Hölder continuous (it is Sudakov safe)

Infrared singularities of massless gauge theories appear on each P_N



Hierarchy of IRC Safety Definitions

[PTK, Metodiev, Thaler, 2004.04.159]



All Observables	Comments
Multiplicity ($\sum_i 1$)	IR unsafe and C unsafe
Momentum Dispersion [65] ($\sum_i E_i^2$)	IR safe but C unsafe
Sphericity Tensor [66] ($\sum_i p_i^\mu p_i^\nu$)	IR safe but C unsafe
Number of Non-Zero Calorimeter Deposits	C safe but IR unsafe
Defined on Energy Flows	
Pseudo-Multiplicity ($\min\{N \mid \mathcal{T}_N = 0\}$)	Robust to exact IR or C emissions
Infrared & Collinear Safe	
Jet Energy ($\sum_i E_i$)	Disc. at jet boundary
Heavy Jet Mass [67]	Disc. at hemisphere boundary
Soft-Dropped Jet Mass [38, 68]	Disc. at grooming threshold
Calorimeter Activity [69] (N_{95})	Disc. at cell boundary
Sudakov Safe	
Groomed Momentum Fraction [39] (z_g)	Disc. on 1-particle manifold
Jet Angularity Ratios [37]	Disc. on 1-particle manifold
N -subjettiness Ratios [47, 48] (τ_{N+1}/τ_N)	Disc. on N -particle manifold
V parameter [36] (Eq. (2.11))	Hölder disc. on 3-particle manifold
EMD Hölder Continuous Everywhere	
Thrust [40, 41]	
Sphericity [42]	
Angularities [70]	
N -jettiness [44] (\mathcal{T}_N)	
C parameter [71–74]	Resummation beneficial at $C = \frac{3}{4}$
Linear Sphericity [72] ($\sum_i E_i n_i^\mu n_i^\nu$)	
Energy Correlators [36, 75–77]	
Energy Flow Polynomials [15, 17]	