

Exploring The (Metric) Space of Collider Events

ATLAS-Theory Lunch Seminar

Eric M. Metodiev

Center for Theoretical Physics

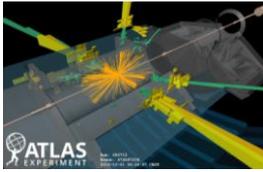
Massachusetts Institute of Technology

Joint work with Patrick Komiske and Jesse Thaler

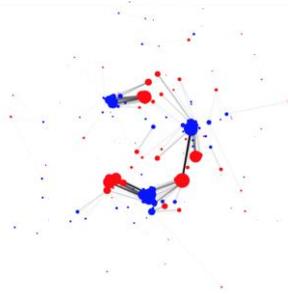
[\[1902.02346\]](#)

April 17, 2019

Outline



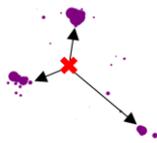
When are two events similar?



The Energy Mover's Distance

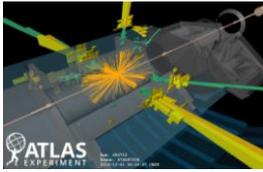


Movie Time



Applications

Outline



When are two events similar?



The Energy Mover's Distance

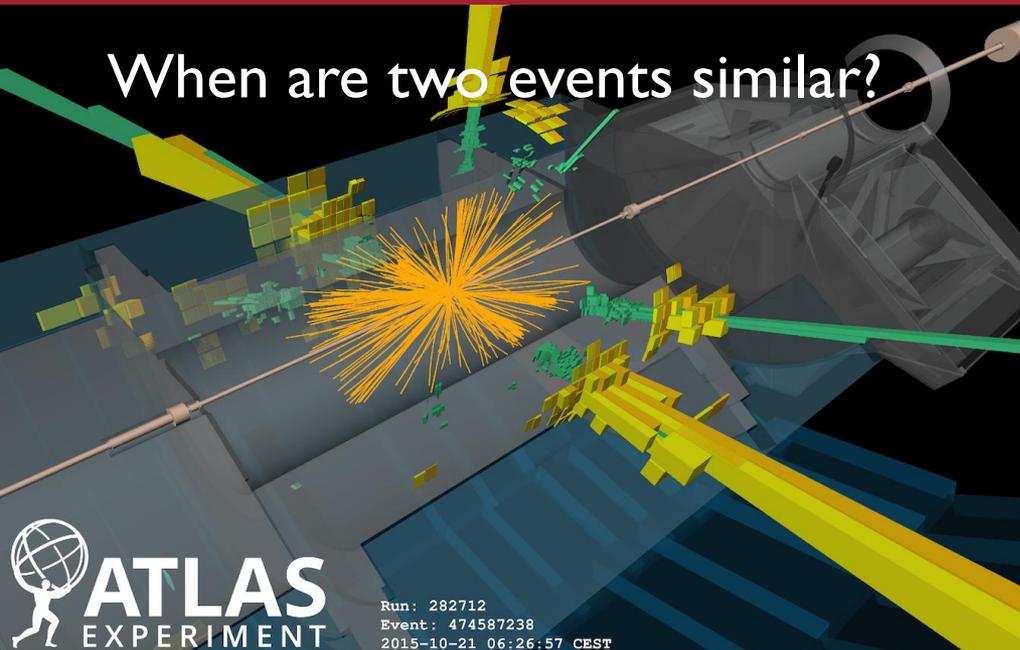


Movie Time

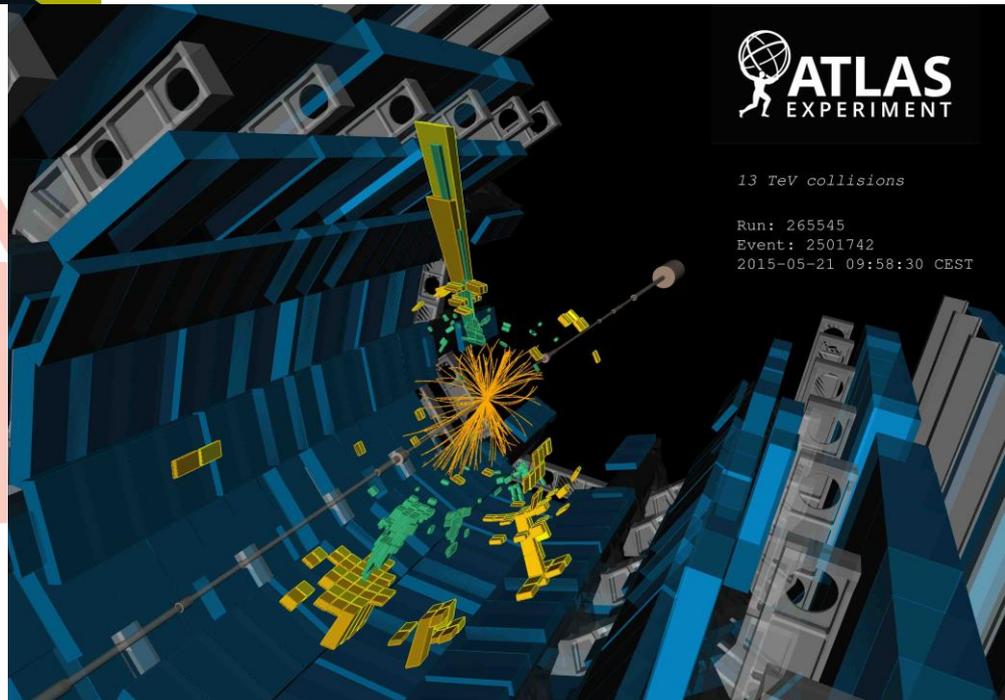
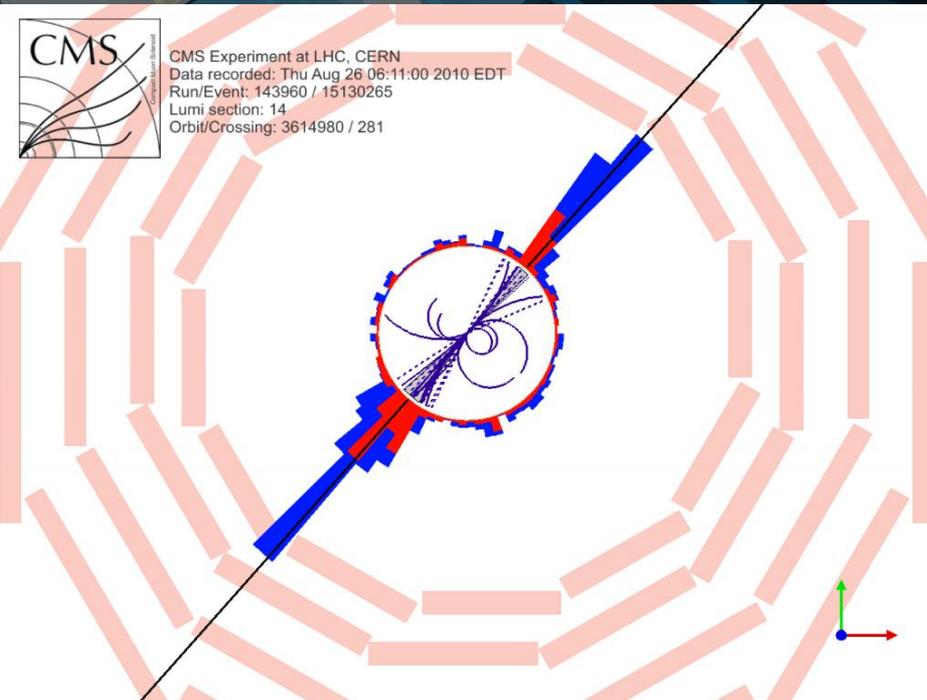
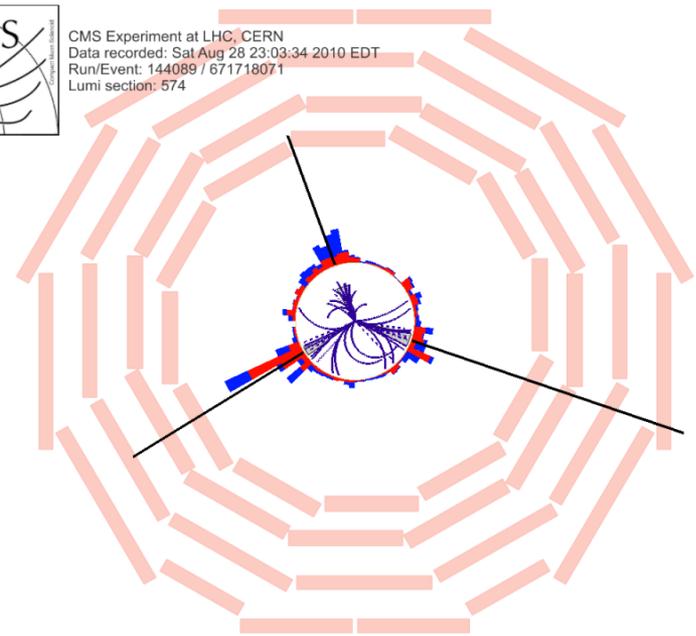


Applications

When are two events similar?

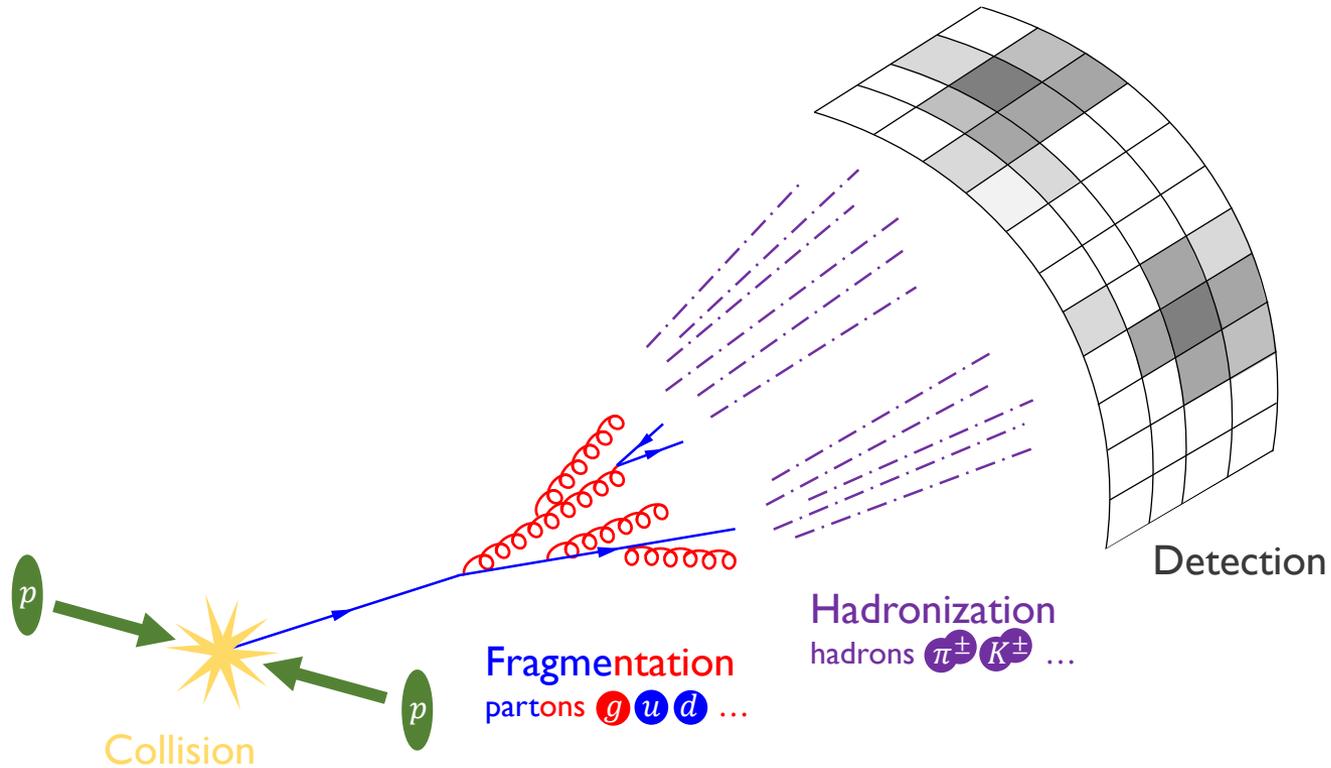


CMS Experiment at LHC, CERN
Data recorded: Sat Aug 28 23:03:34 2010 EDT
Run/Event: 144089 / 671718071
Lumi section: 574



When are two collider events similar?

How an event gets its shape

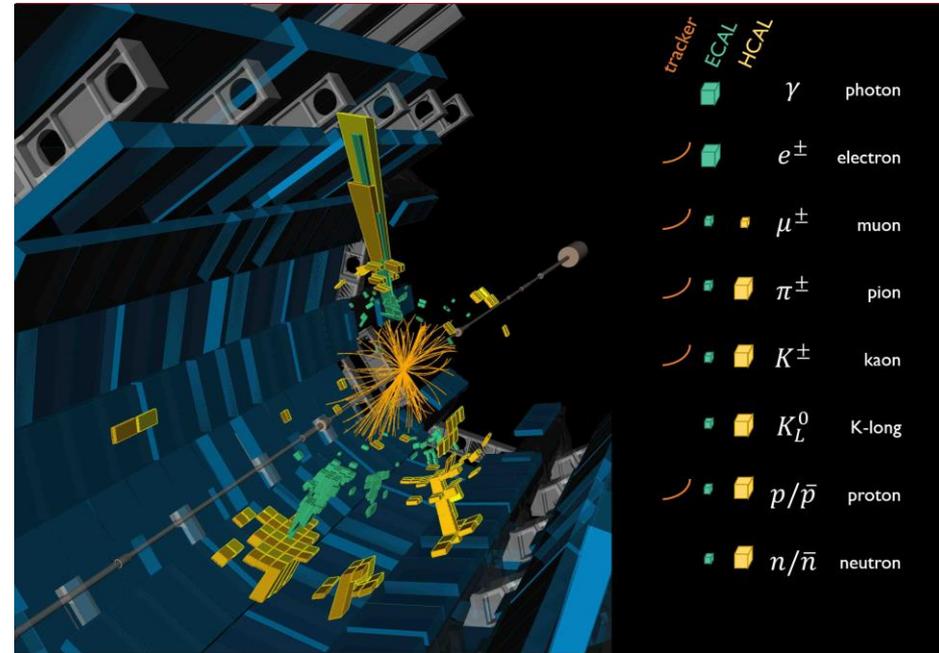
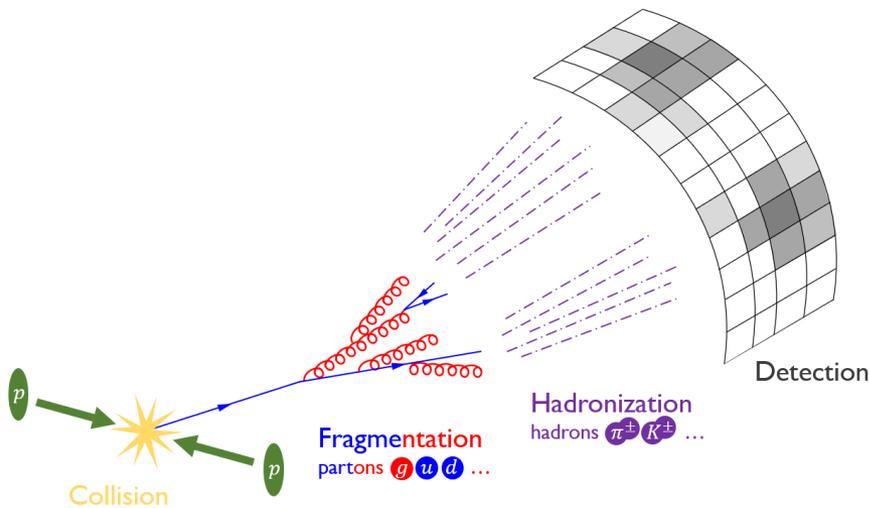


When are two collider events similar?

A collider event is...

Theoretically: very complicated

Experimentally: very complicated



However:

The *energy flow* (distribution of energy) is the information that is robust to:
fragmentation, hadronization, detector effects, ...

[N.A. Sveshnikov, F.V. Tkachov, 9512370]

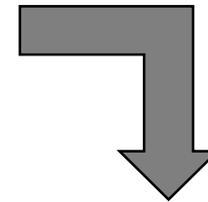
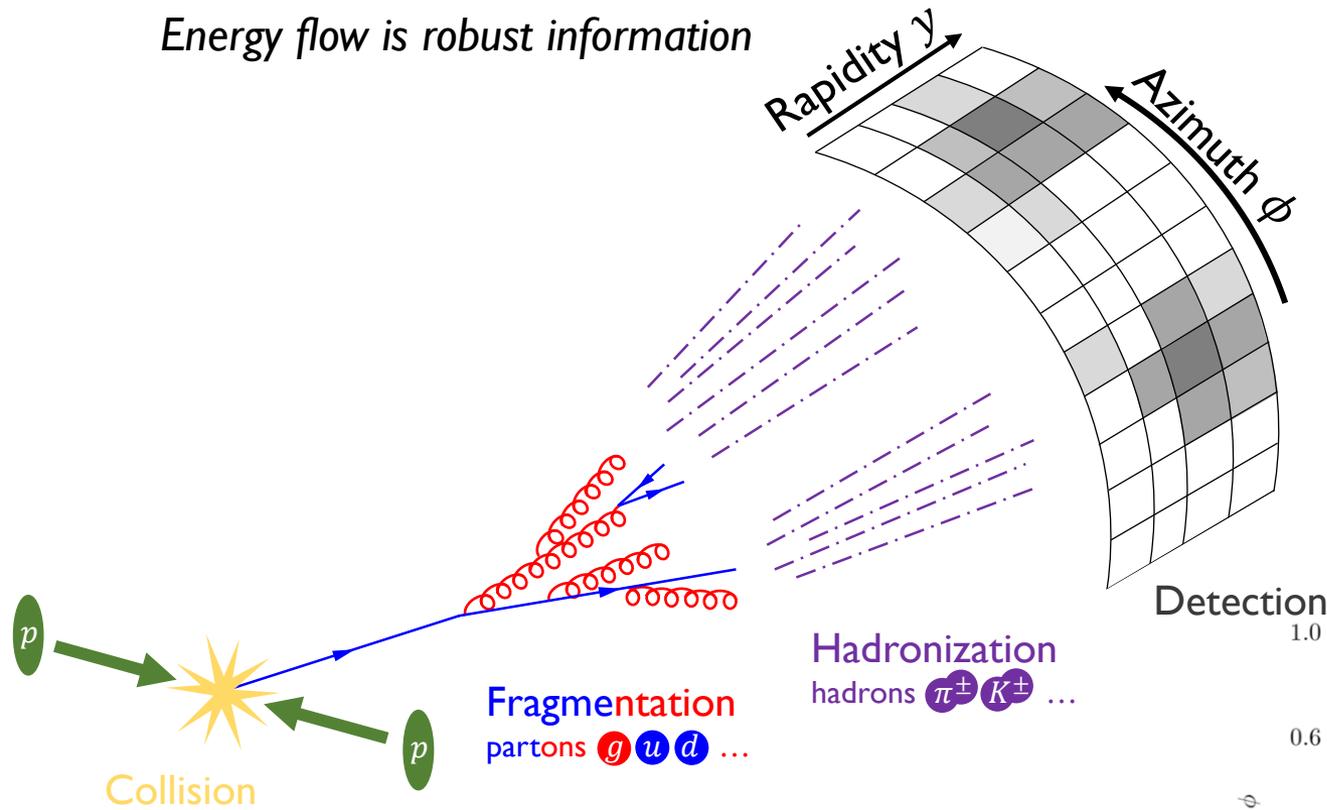
[F.V. Tkachov, 9601308]

[P.S. Cherzor, N.A. Sveshnikov, 9710349]

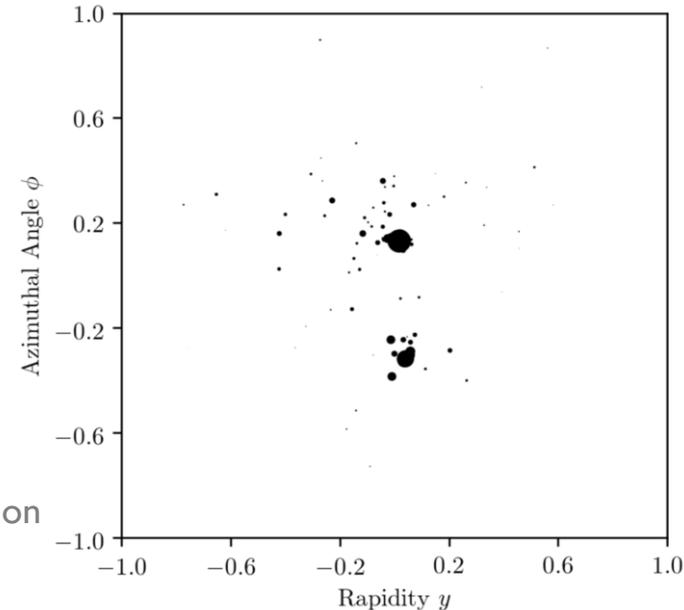
Energy flow \Leftrightarrow Infrared and Collinear (IRC) Safe information

When are two collider events similar?

Energy flow is robust information



Detection



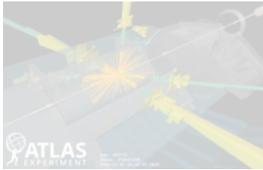
Treat events as distributions of energy:

Ignoring particle flavor, charge...

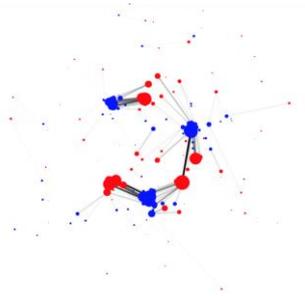
$$\sum_{i=1}^M E_i \delta(\hat{n} - \hat{p}_i)$$

↑
energy
↑
direction

Outline



When are two events similar?



The Energy Mover's Distance



Movie Time



Applications

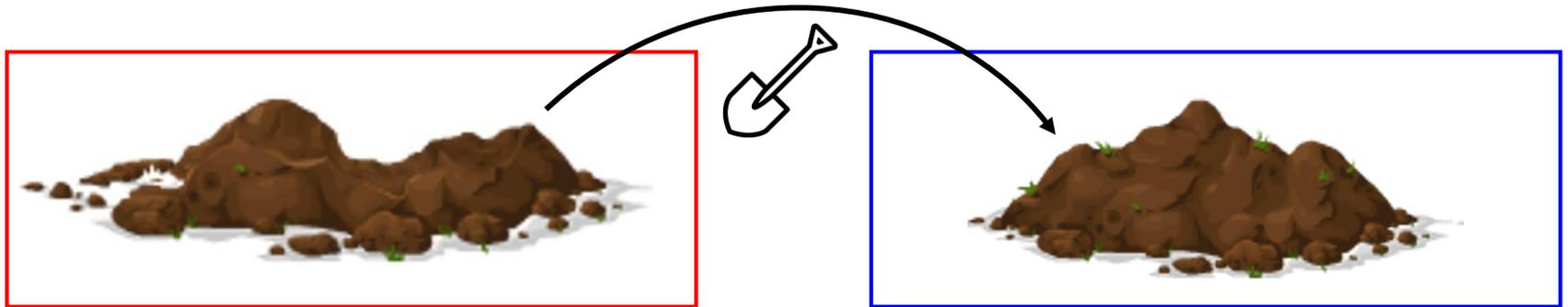
The Energy Mover's Distance

Review: *The Earth Mover's Distance*

Earth Mover's Distance: the minimum “work” (stuff x distance) to rearrange one pile of dirt into another

[\[S. Peleg, M. Werman, H. Rom\]](#)

[\[Y. Rubner, C. Tomasi, and L.J. Guibas\]](#)



Metric on the space of (normalized) distributions: *symmetric, non-negative, triangle inequality*

Distributions are close in EMD \Leftrightarrow their expectation values are close.

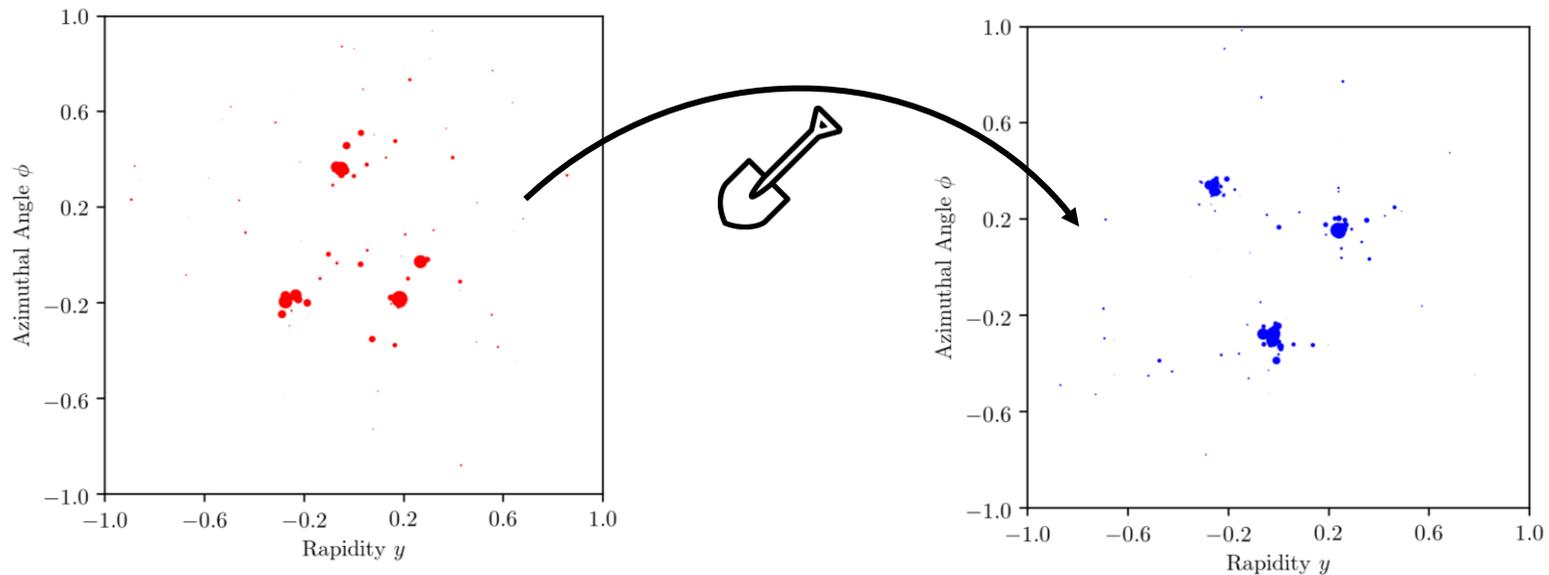
Also known as the 1-Wasserstein metric.

The Energy Mover's Distance

From Earth to Energy

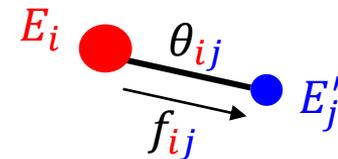
Energy Mover's Distance: the minimum “work” (energy x angle) to rearrange one event (pile of energy) into another

[P.T. Komiske, EMM, J. Thaler, 1902.02346]



$$\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \sum_{i=1}^M \sum_{j=1}^{M'} f_{ij} \frac{\theta_{ij}}{R}$$

Difference in
radiation pattern

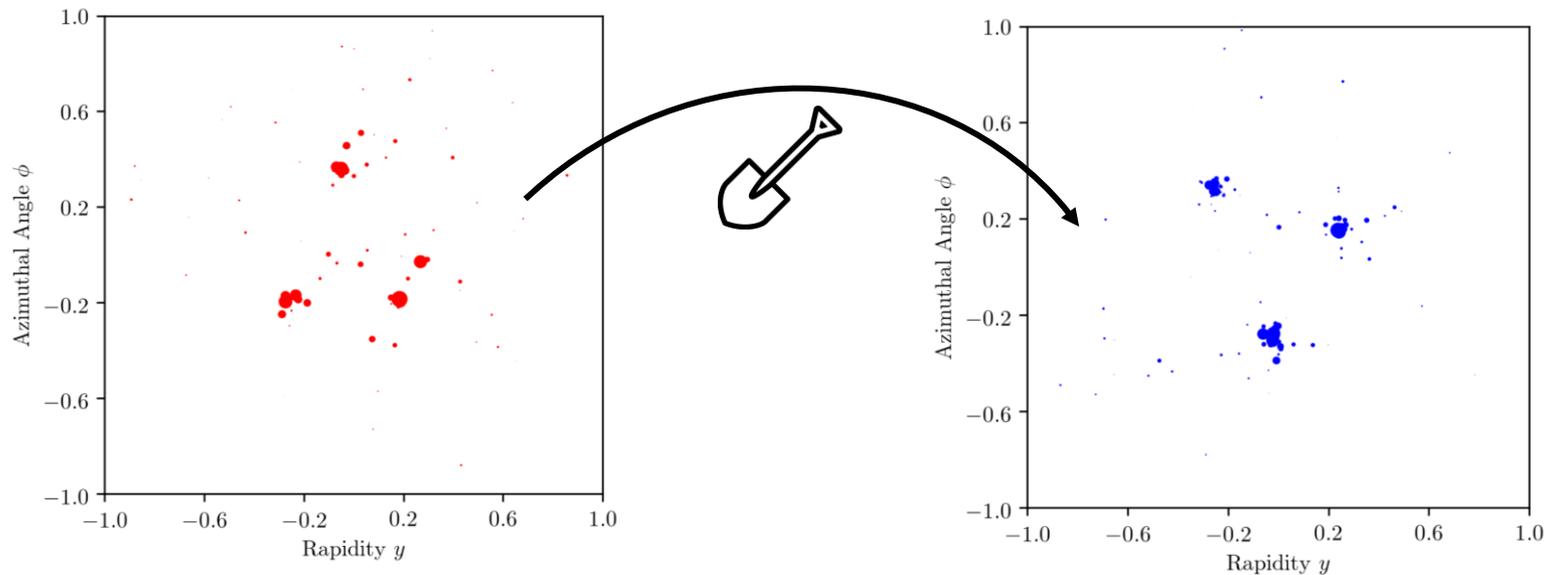


The Energy Mover's Distance

From Earth to Energy

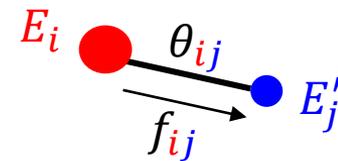
Energy Mover's Distance: the minimum “work” (**energy** x **angle**) to rearrange one event (pile of energy) into another

[P.T. Komiske, EMM, J. Thaler, 1902.02346]



$$\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \sum_{i=1}^M \sum_{j=1}^{M'} f_{ij} \frac{\theta_{ij}}{R} + \left| \sum_{i=1}^M E_i - \sum_{j=1}^{M'} E'_j \right|$$

Difference in radiation pattern
Difference in total energy

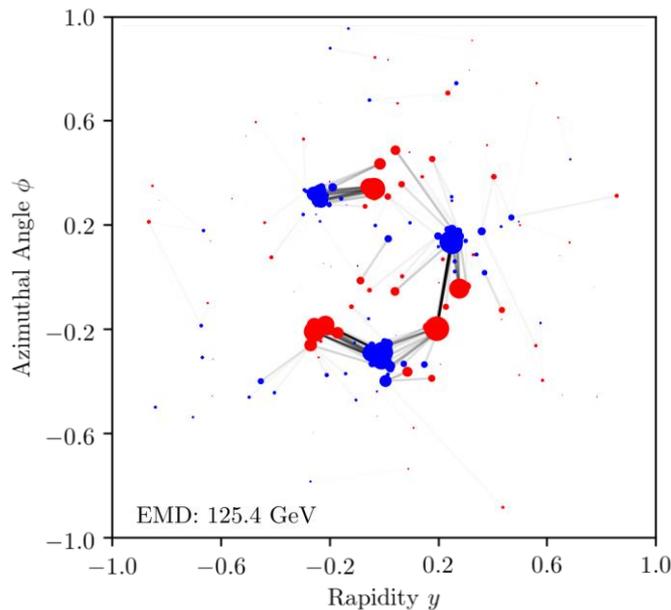


The Energy Mover's Distance

From Earth to Energy

Energy Mover's Distance: the minimum “work” (energy x angle) to rearrange one event (pile of energy) into another

[P.T. Komiske, EMM, J. Thaler, 1902.02346]



EMD has dimensions of energy

True metric as long as $R \geq \frac{1}{2} \theta_{\max}$

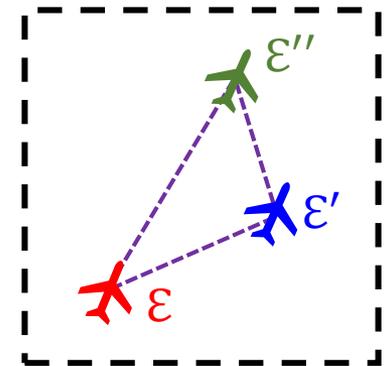
$R \geq$ the jet radius, for conical jets

Solvable via Optimal Transport problem.

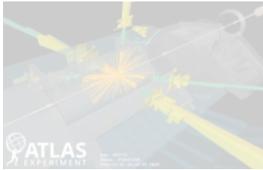
~1ms to compute EMD for two jets with 100 particles.

$$\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \sum_{i=1}^M \sum_{j=1}^{M'} f_{ij} \frac{\theta_{ij}}{R} + \left| \sum_{i=1}^M E_i - \sum_{j=1}^{M'} E'_j \right|$$

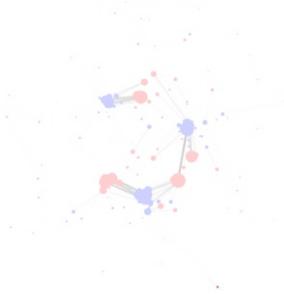
Difference in radiation pattern
Difference in total energy



Outline



When are two events similar?



The Energy Mover's Distance



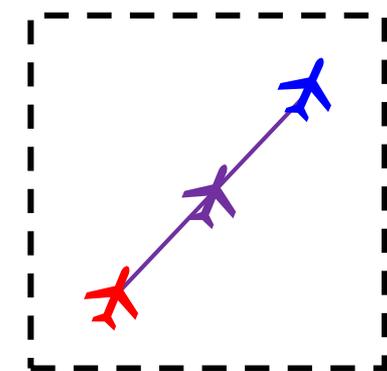
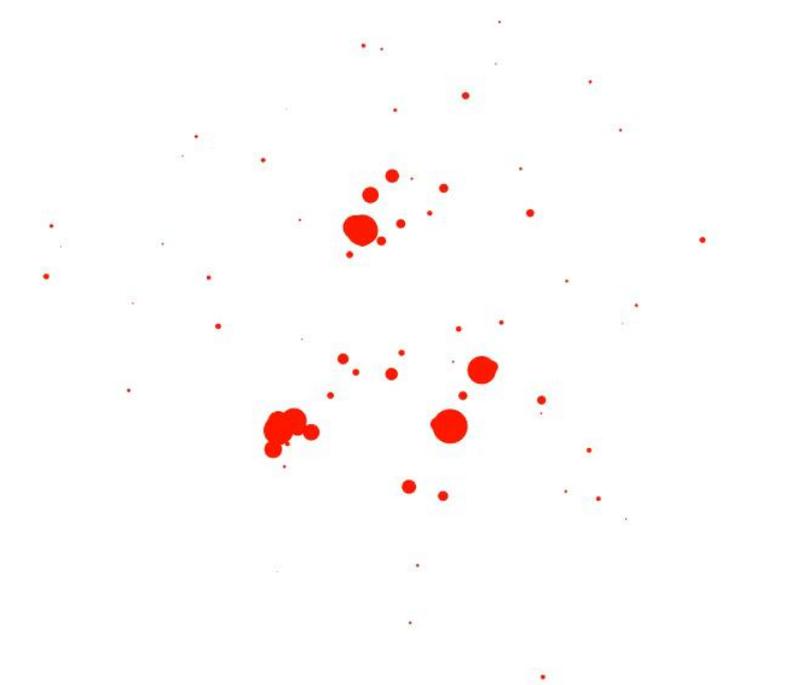
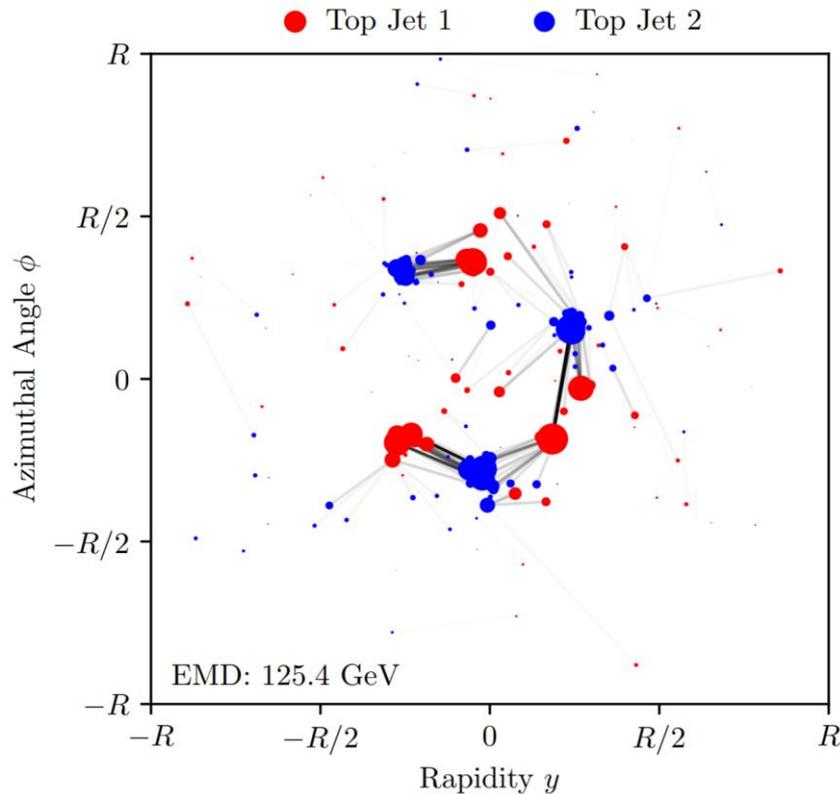
Movie Time



Applications

Movie Time: Visualizing the EMD

Taking a walk in the space of events



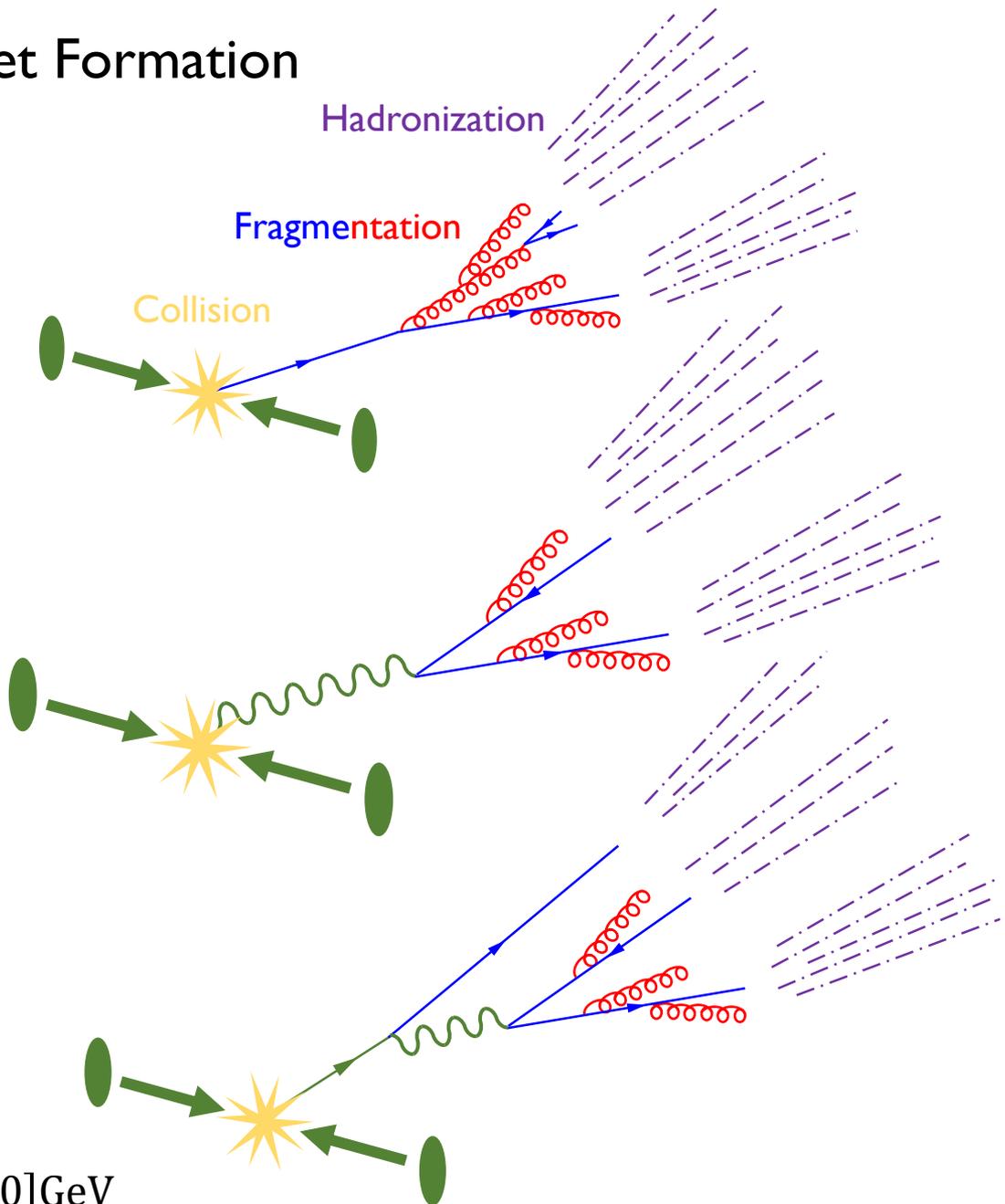
EMD is the cost of an optimal transport problem.

We also get the *shortest path* between the events.

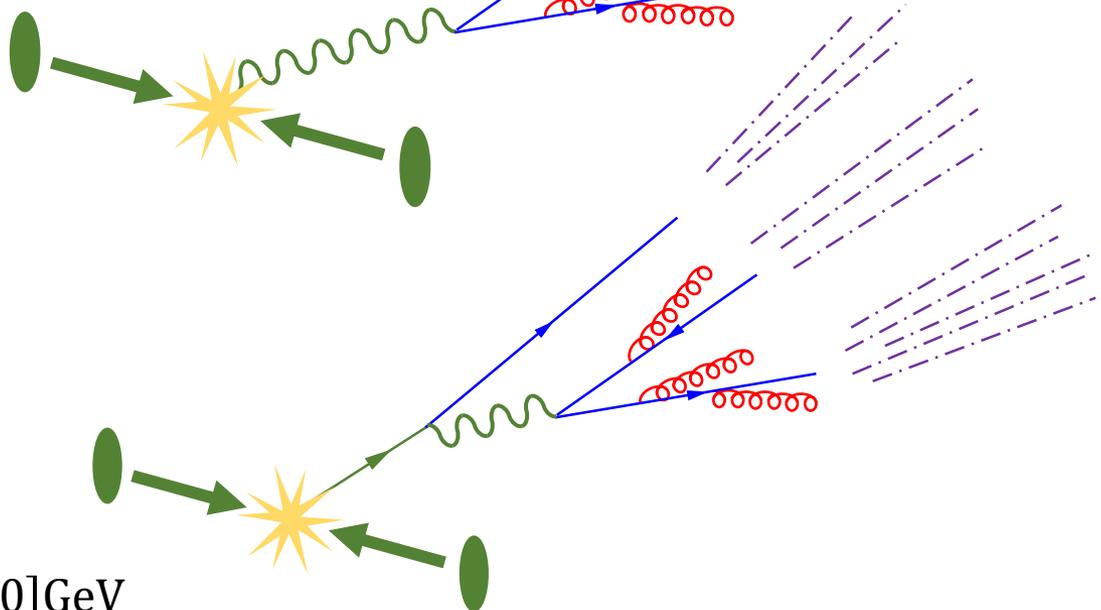
Interpolate along path to visualize!

Movie Time: Visualizing Jet Formation

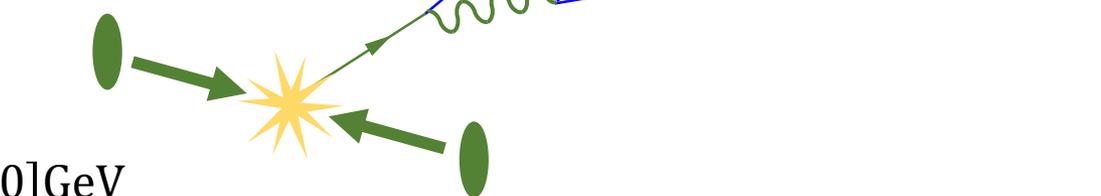
QCD Jets



W Jets

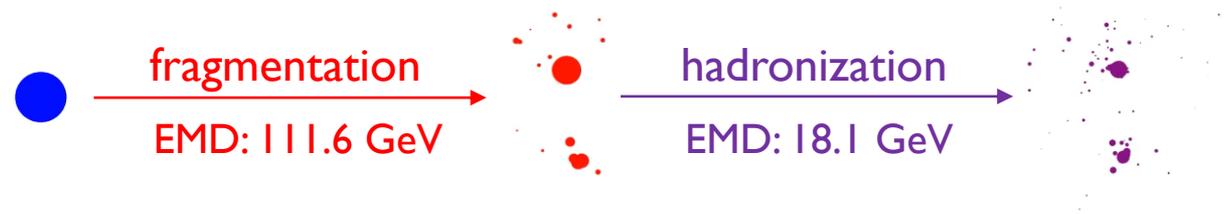
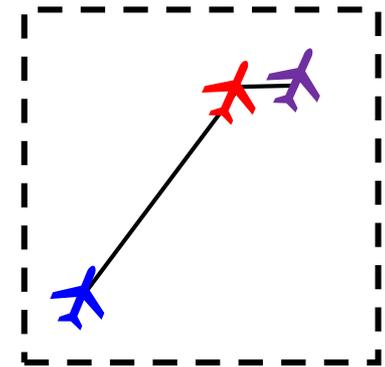
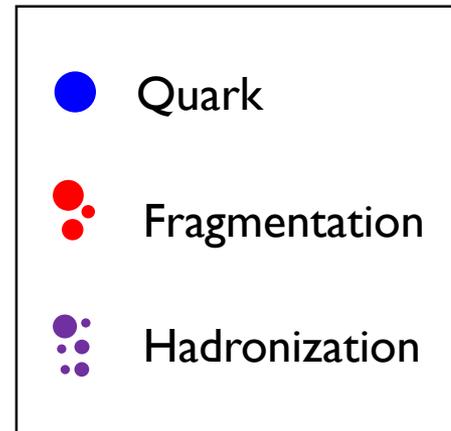
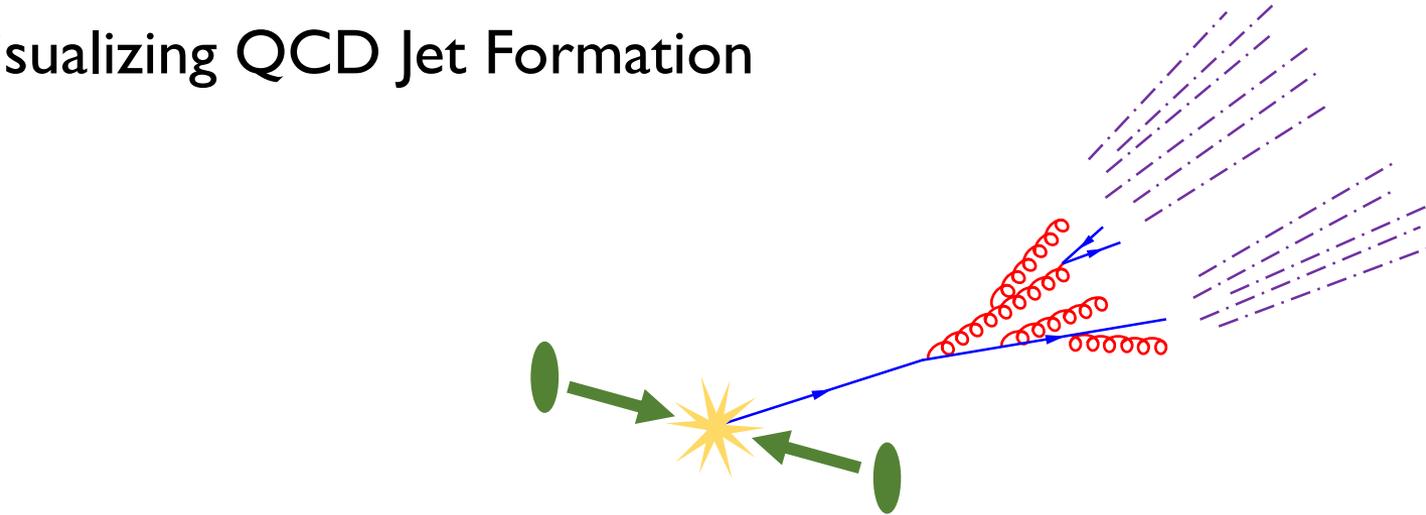


Top Jets

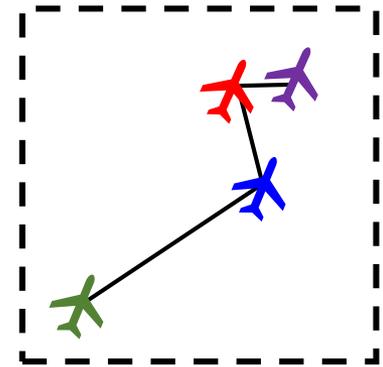
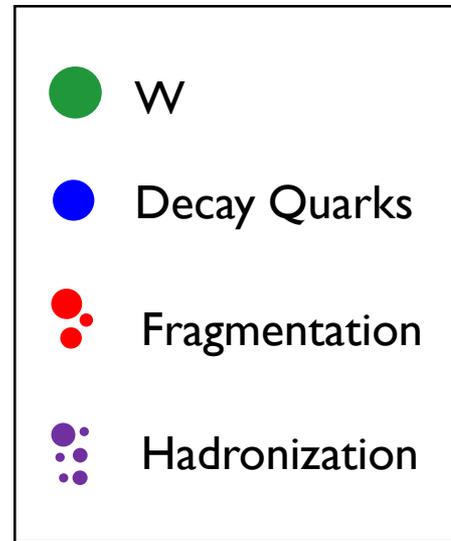
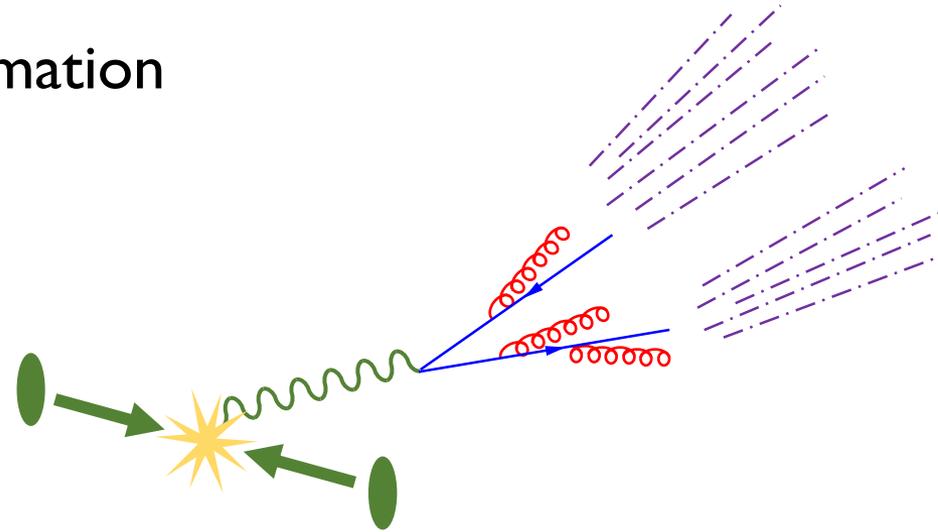


Pythia 8, $R = 1.0$ jets, $p_T \in [500,550]$ GeV

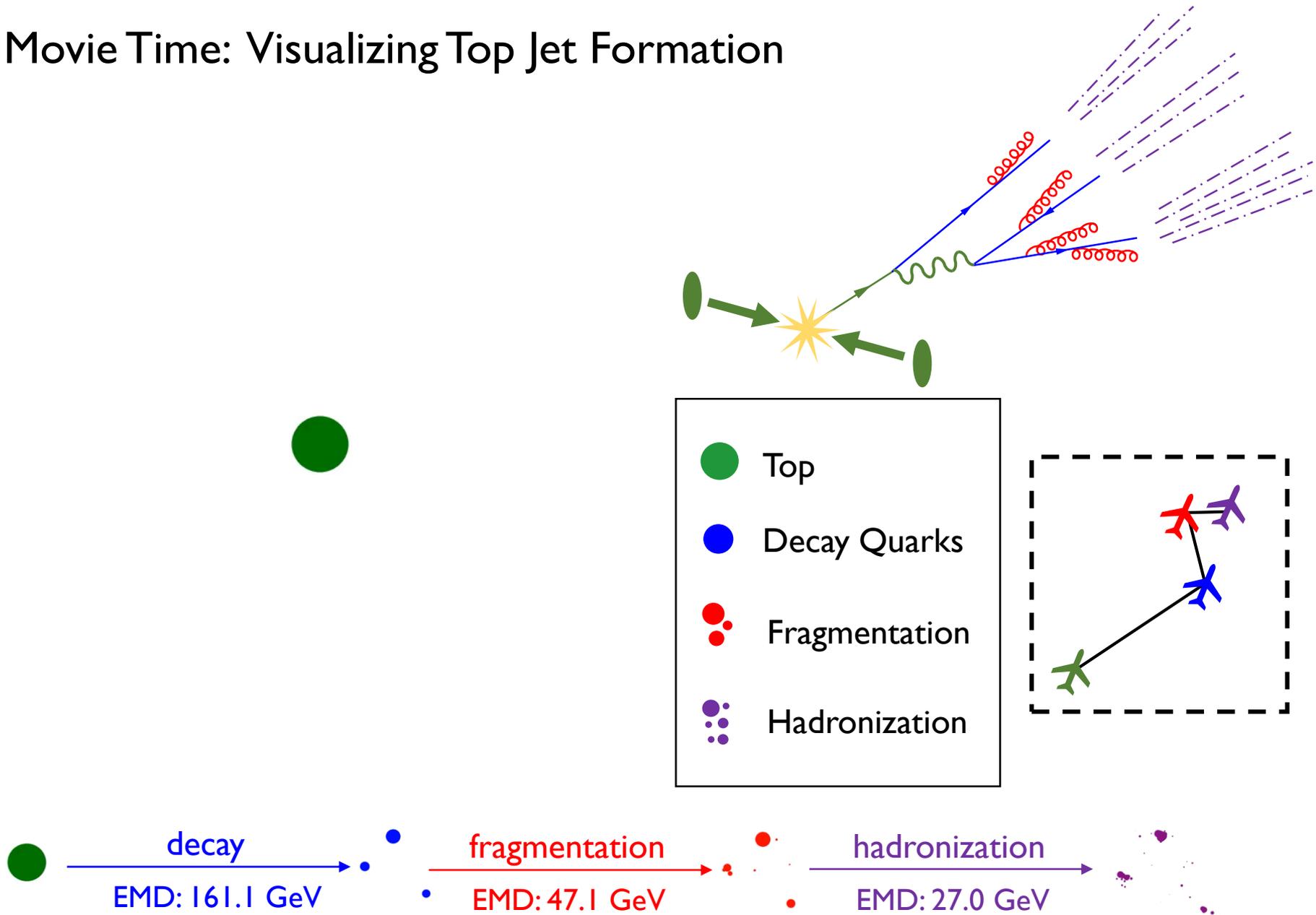
Movie Time: Visualizing QCD Jet Formation



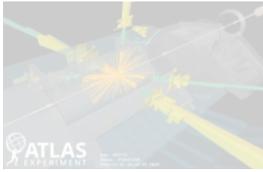
Movie Time: Visualizing W Jet Formation



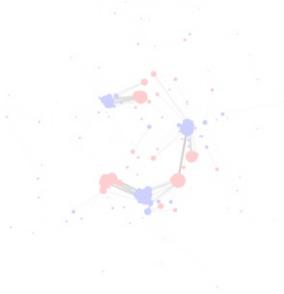
Movie Time: Visualizing Top Jet Formation



Outline



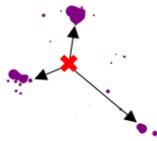
When are two events similar?



The Energy Mover's Distance



Movie Time

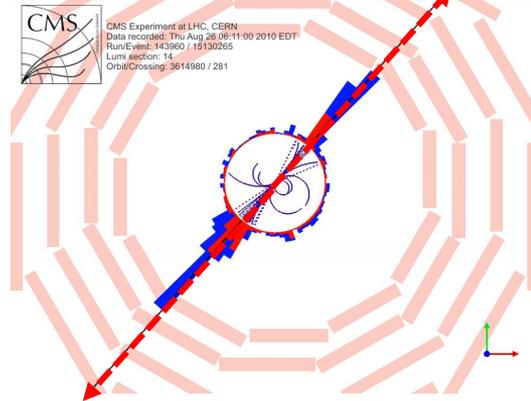


Applications

Old Observables in a New Language

Thrust is the EMD between the event and two back-to-back particles.

$$t = E - \max_{\hat{n}} \sum_i |\vec{p}_i \cdot \hat{n}|$$

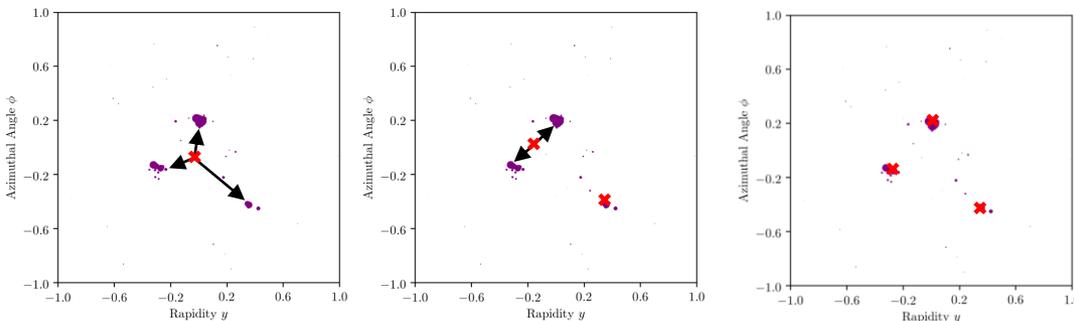


$$t(\mathcal{E}) = \min_{|\mathcal{E}'|=2} \text{EMD}(\mathcal{E}, \mathcal{E}')$$

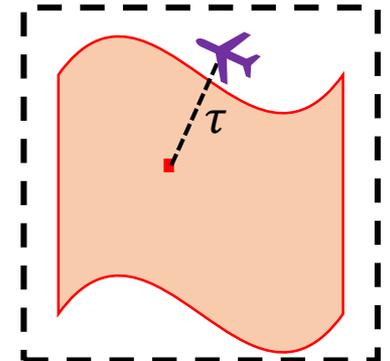
$$\text{with } \theta_{ij} = \hat{p}_i \cdot \hat{p}_j, \quad \hat{p} = \vec{p}/E$$

N -(sub)jettiness is the EMD between the event and the closest N -particle event.

$$\tau_N^{(\beta)} = \min_{N \text{ axes}} \sum_{i=1}^M E_i \min_k \{ \theta_{1,k}^\beta, \theta_{2,k}^\beta, \dots, \theta_{N,k}^\beta \} \longrightarrow \tau_N(\mathcal{E}) = \min_{|\mathcal{E}'|=N} \text{EMD}(\mathcal{E}, \mathcal{E}')$$



$\beta \neq 1$ is p-Wasserstein distance with $p = \beta$.



EMD and IRC-Safe Observables

Events close in EMD are close in any infrared and collinear safe observable

Additive IRC-safe observables:
$$\mathcal{O}(\mathcal{E}) = \sum_{i=1}^M E_i \Phi(\hat{p}_i)$$

Earth Mover's
Distance

$$\text{EMD}(\mathcal{E}, \mathcal{E}') \geq \frac{1}{RL} |\mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}')|$$

Difference in
observable values

“Lipschitz constant” of Φ
i.e. bound on its derivative

e.g. jet angularities:

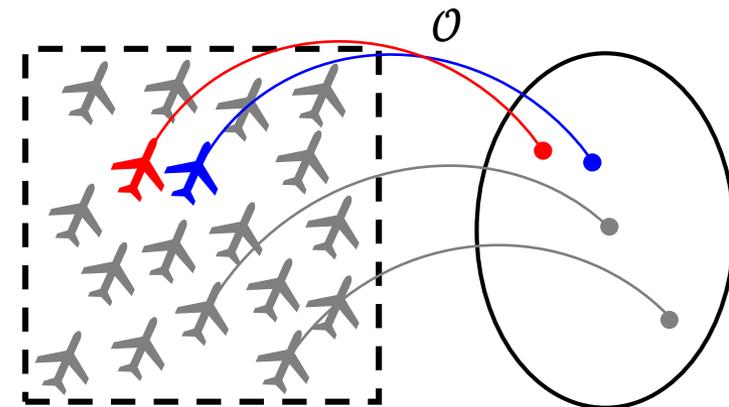
[\[C. Berger, T. Kucs, and G. Sterman, 0303051\]](#)

[\[A. Larkoski, J. Thaler, and W. Waalewijn, 1408.3122\]](#)

For $\beta \geq 1$ jet angularities:

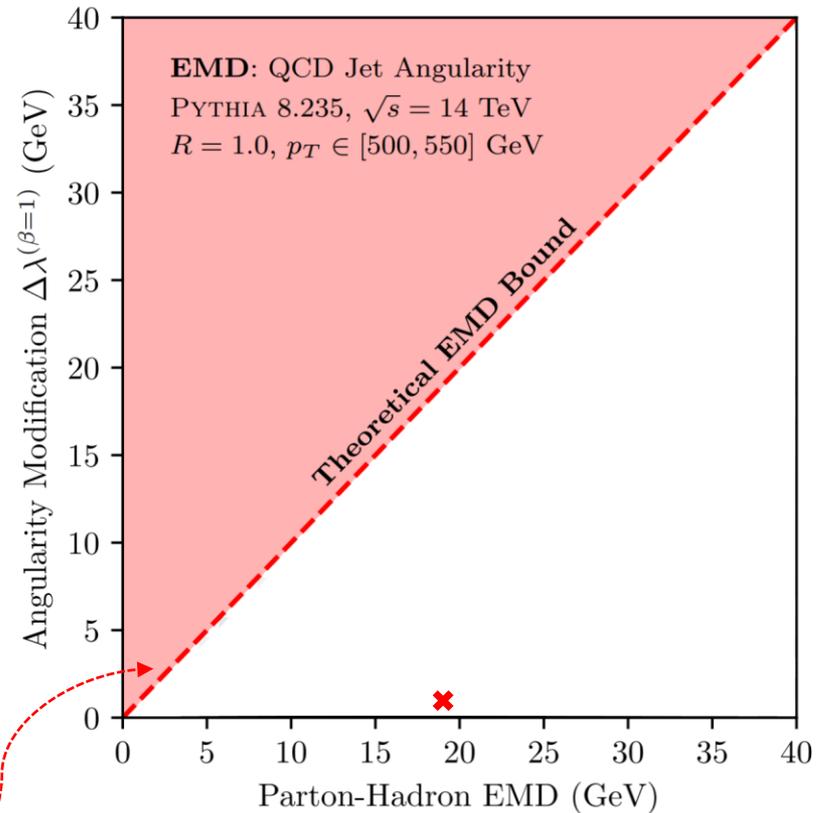
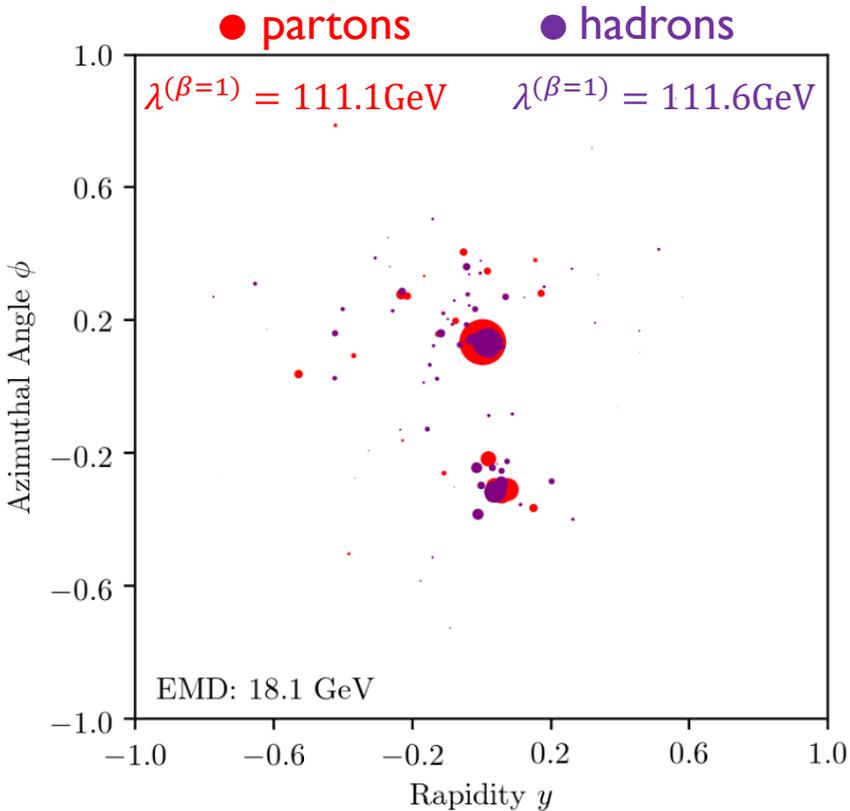
$$\lambda^{(\beta)} = \sum_{i=1}^M E_i \theta_i^\beta$$

$$|\lambda^{(\beta)}(\mathcal{E}) - \lambda^{(\beta)}(\mathcal{E}')| \leq \beta \text{EMD}(\mathcal{E}, \mathcal{E}')$$



Quantifying event modifications: Hadronization

$$\lambda^{(\beta=1)} = \sum_{i=1}^M E_i \theta_i$$



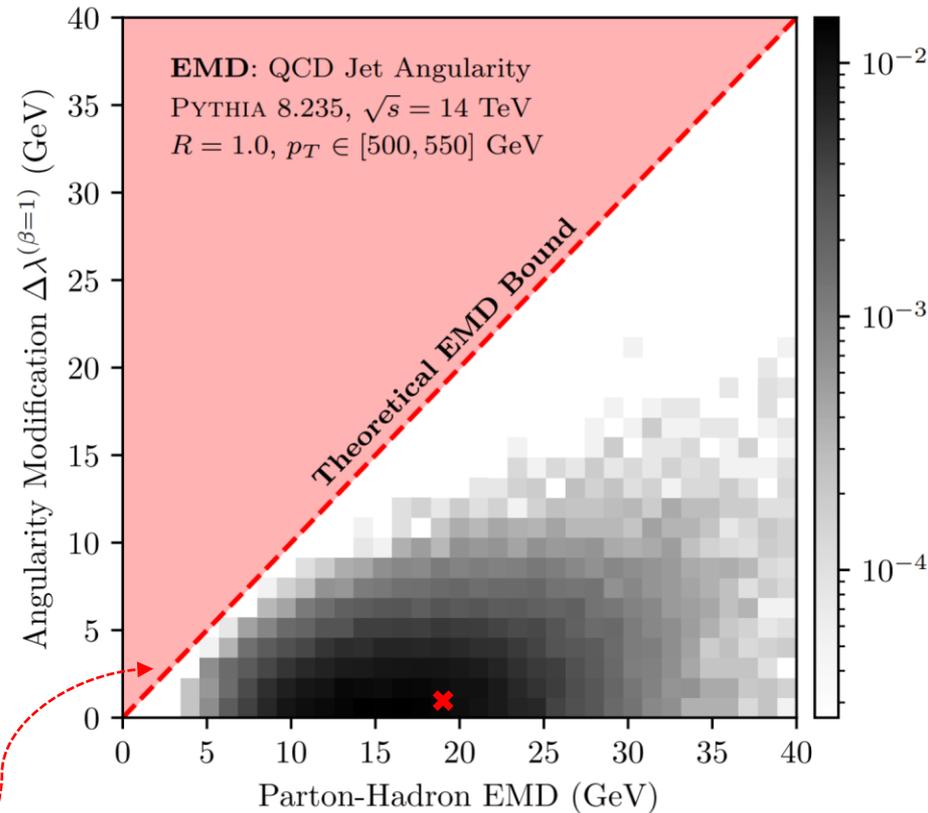
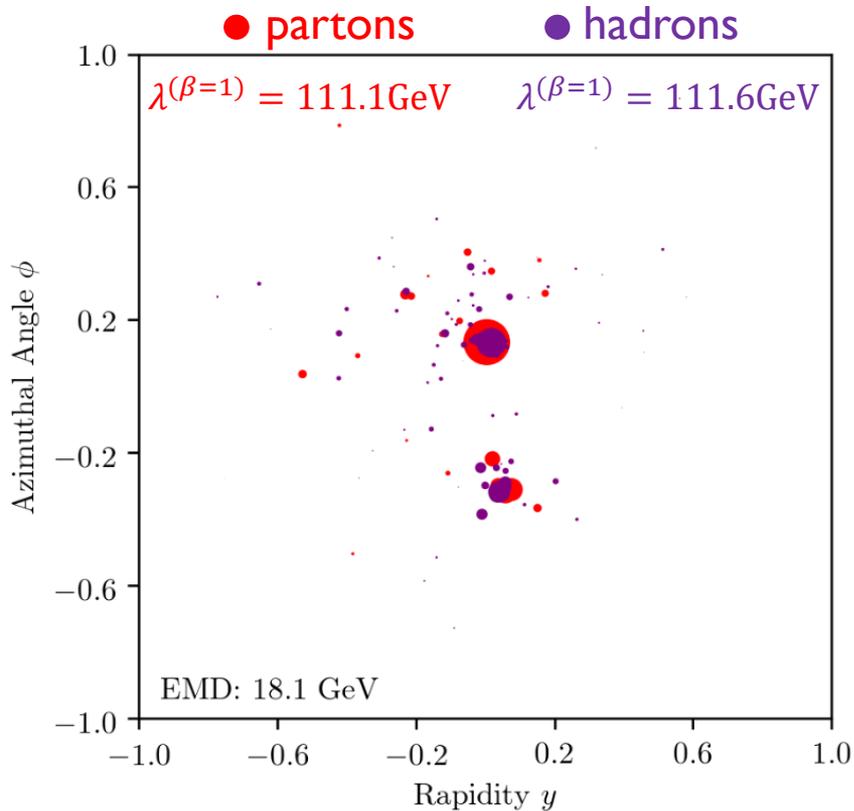
$$\mathcal{E} = \mathcal{E}_{\text{partons}}$$

$$\mathcal{E}' = \mathcal{E}_{\text{hadrons}}$$

$$|\lambda^{(\beta=1)}(\mathcal{E}) - \lambda^{(\beta=1)}(\mathcal{E}')| \leq \text{EMD}(\mathcal{E}, \mathcal{E}')$$

Quantifying event modifications: Hadronization

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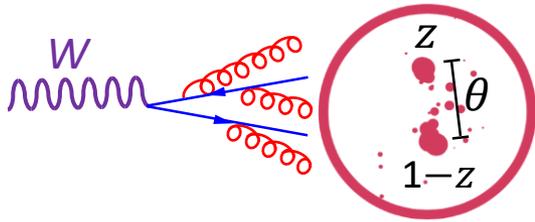


$$\mathcal{E} = \mathcal{E}_{\text{partons}}$$

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$$|\lambda^{(\beta=1)}(\mathcal{E}) - \lambda^{(\beta=1)}(\mathcal{E}')| \leq \text{EMD}(\mathcal{E}, \mathcal{E}')$$

Exploring the Space of Events: W jets



W jets are 2-pronged and constrained by W mass:

$$z(1-z)\theta^2 = \frac{p_{\mu J}^2}{p_T^2} = \frac{m_W^2}{p_T^2}$$

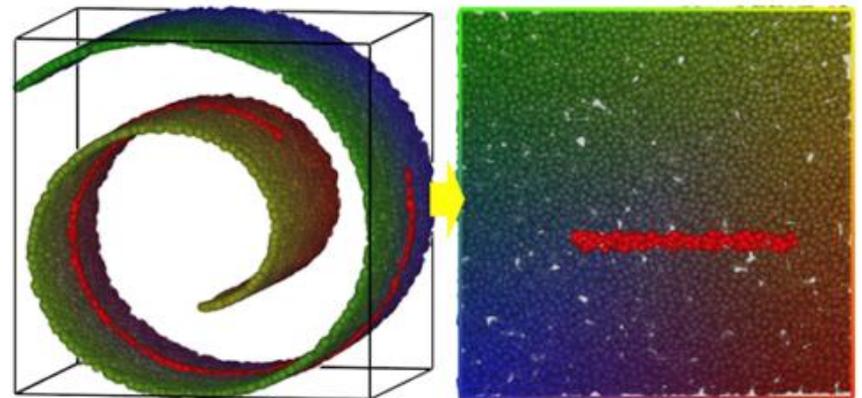
Hence we expect a **two-dimensional** space of W jets: z, φ

After φ rotation, **one-dimensional**: z

Visualize the space of events with t-Distributed Stochastic Neighbor Embedding (t-SNE).

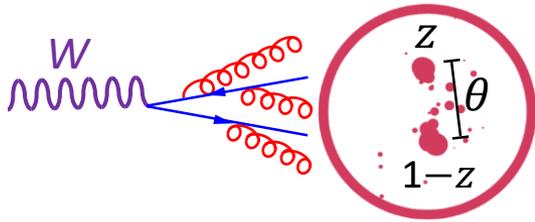
[\[L. van der Maaten, G. Hinton\]](#)

Finds an embedding into a low-dimensional manifold that respects distances.



Src: <http://web-ext.u-aizu.ac.jp/~shigeo/home.html>

Exploring the Space of Events: W jets

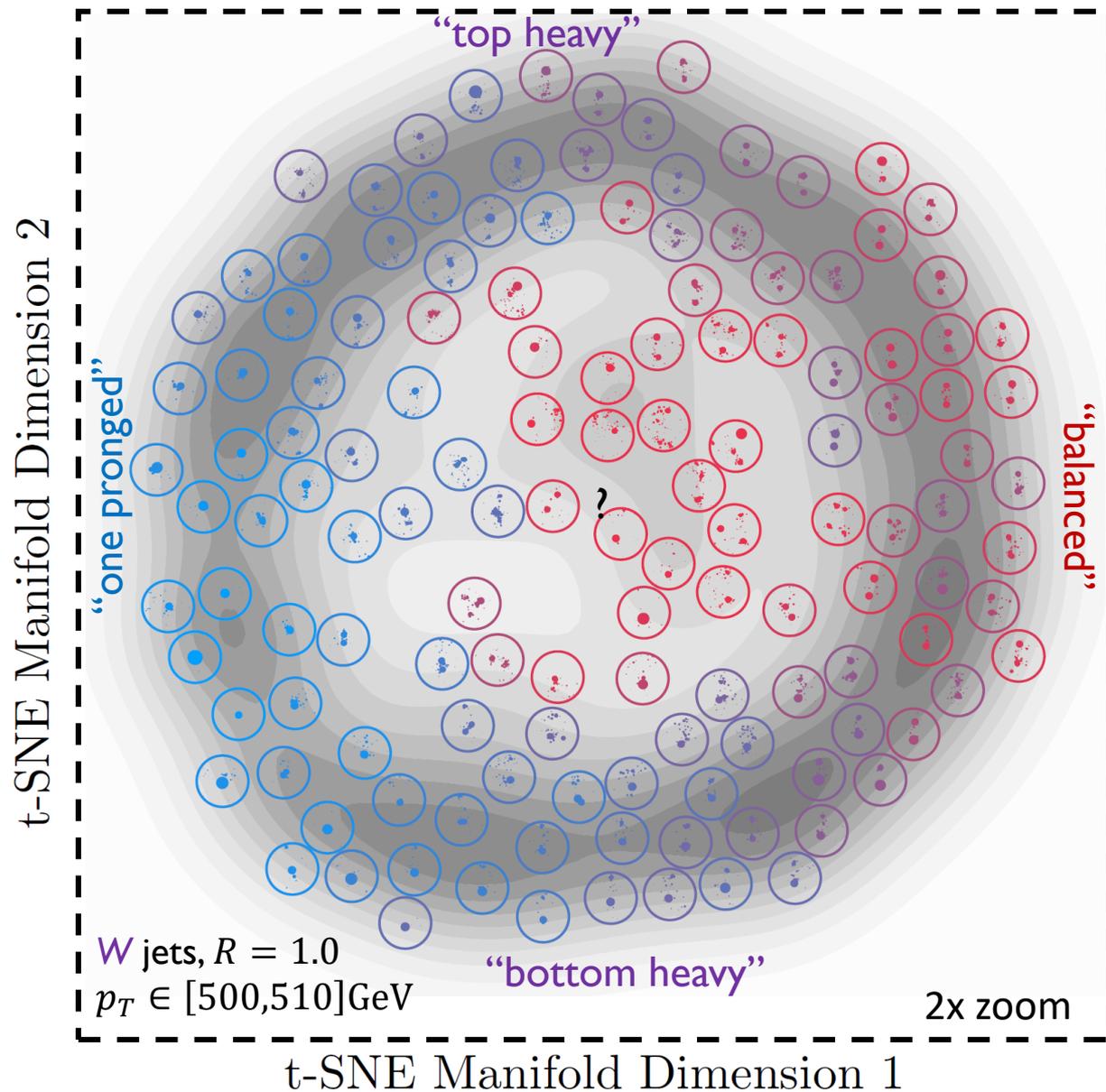


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Hence we expect a **two-dimensional** space of W jets: z, φ

After φ rotation, **one-dimensional**: z



Exploring the Space of Jets: Correlation Dimension

VOLUME 50, NUMBER 5

PHYSICAL REVIEW LETTERS

31 JANUARY 1983

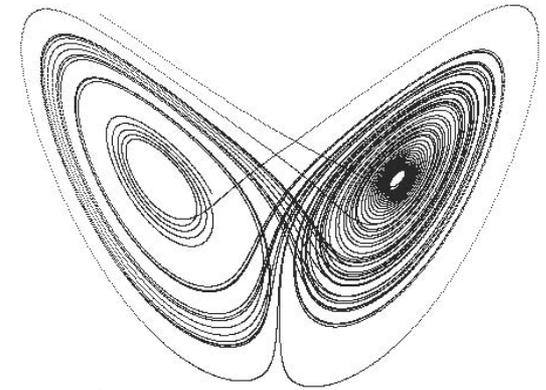
Characterization of Strange Attractors

Peter Grassberger^(a) and Itamar Procaccia

Chemical Physics Department, Weizmann Institute of Science, Rehovot 76100, Israel

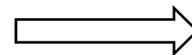
(Received 7 September 1982)

A new measure of strange attractors is introduced which offers a practical algorithm to determine their character from the time series of a single observable. The relation of this new measure to fractal dimension and information-theoretic entropy is discussed.



Intuition:

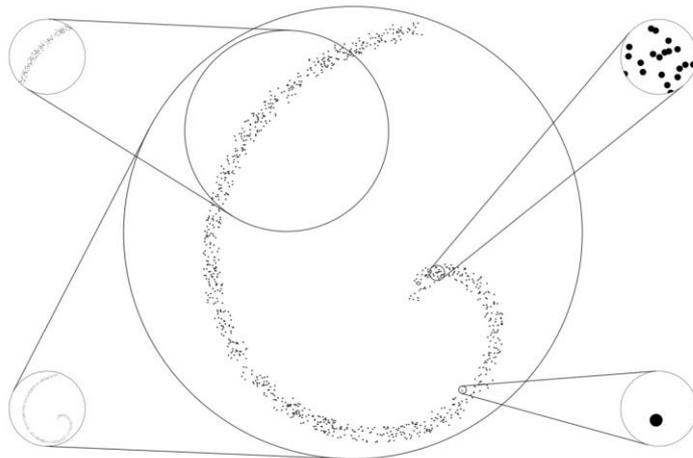
$$N_{\text{neighboring points}}(r) \propto r^{\text{dim}}$$



$$\text{dim}(r) = r \frac{\partial}{\partial r} \ln N_{\text{neighboring}}(r)$$

dim ≈ 1

dim ≈ 2



dim ≈ 2

dim ≈ 0

(eventually 0)

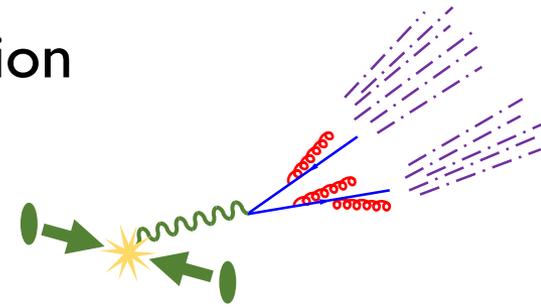
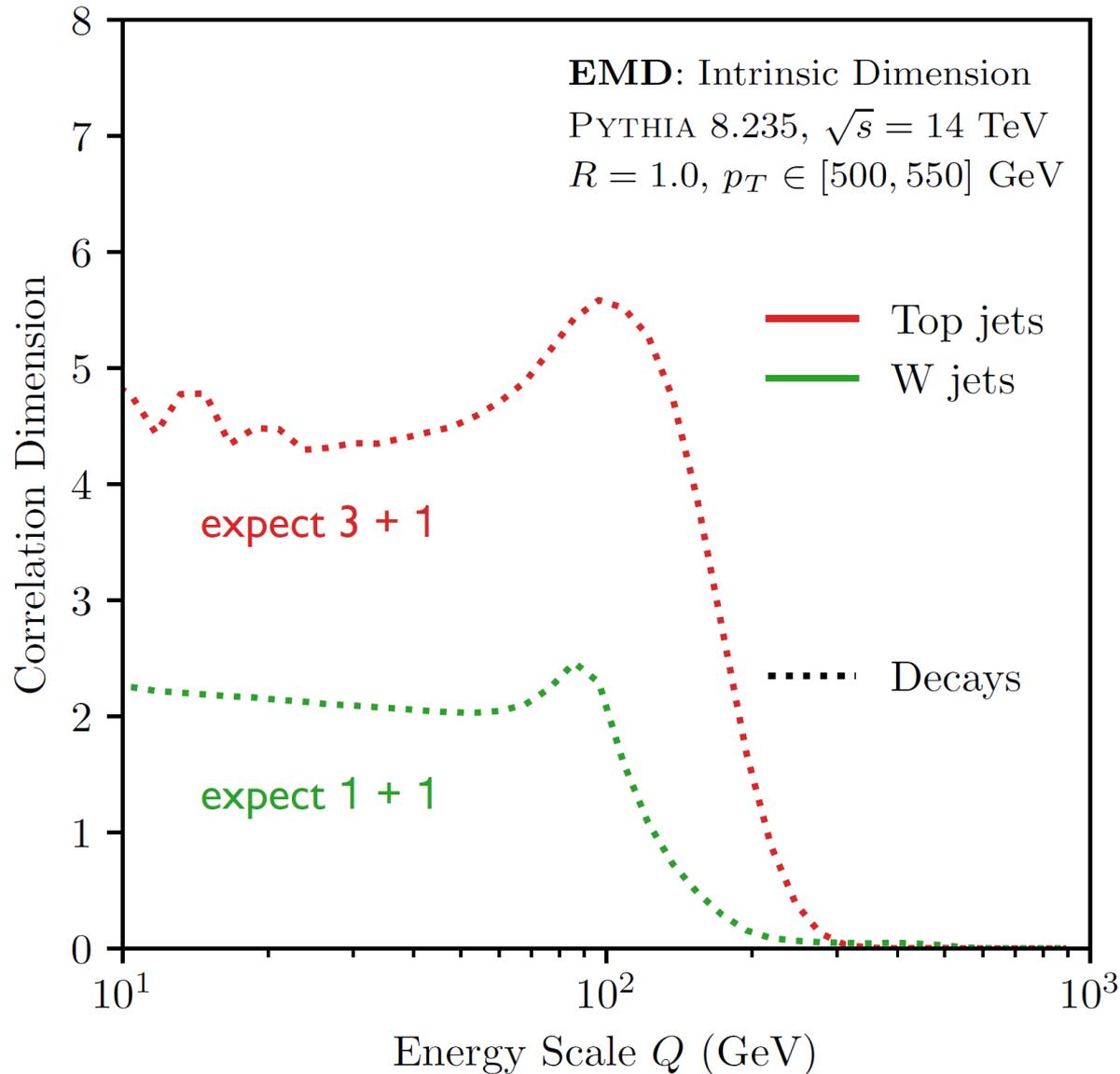
Correlation dimension:

$$\text{dim}(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i=1}^N \sum_{j=1}^N \Theta[\text{EMD}(\epsilon_i, \epsilon_j) < Q]$$

Energy scale Q
dependence

Count neighbors in
ball of radius Q

Exploring the Space of Jets: Correlation Dimension



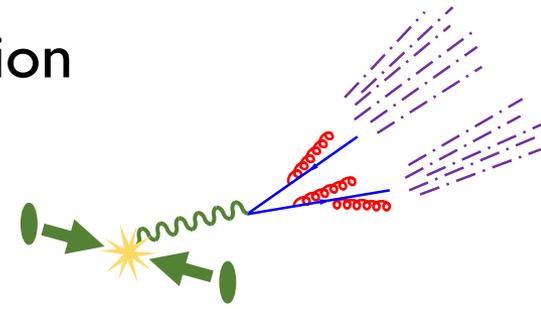
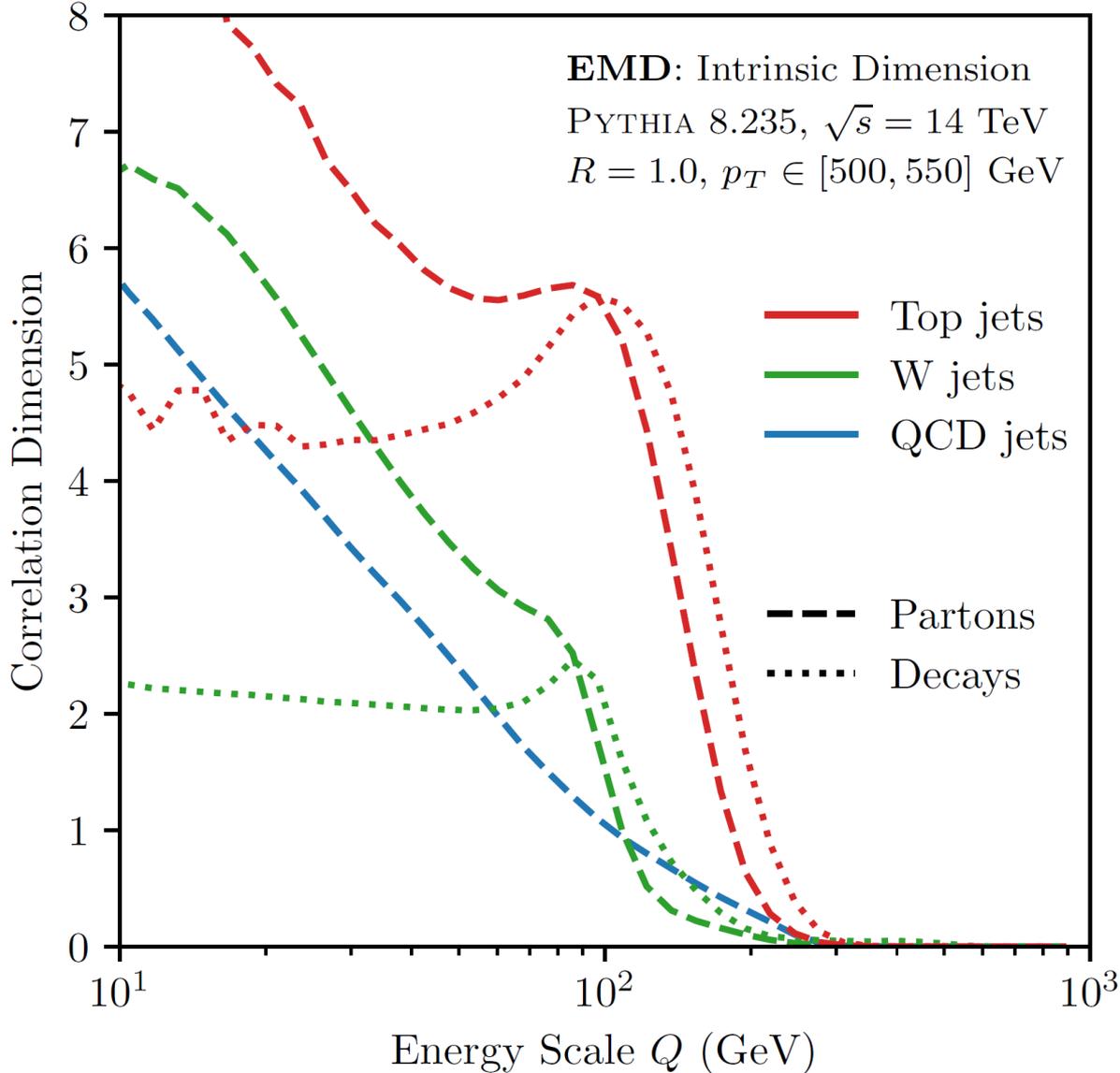
QCD jets are simplest.

W jets are more complicated.

Top jets are most complex.

“Decays” have \sim constant dimension.

Exploring the Space of Jets: Correlation Dimension



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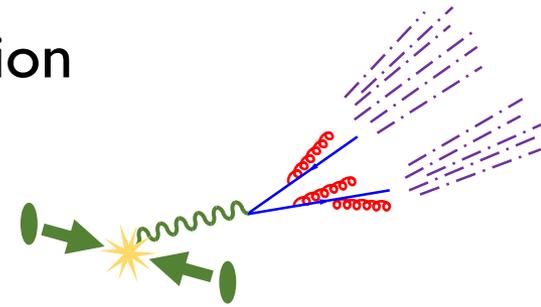
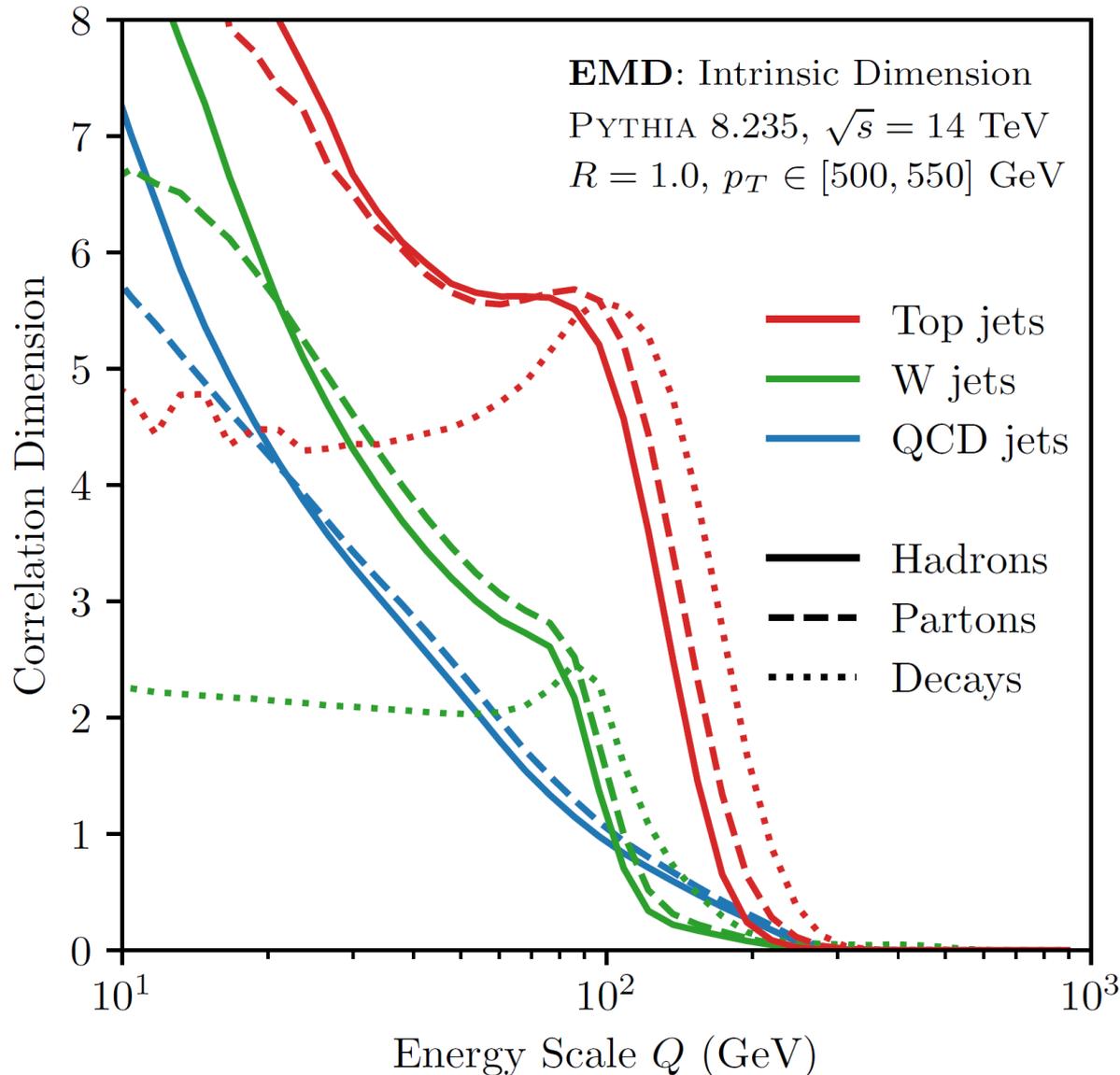
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Exploring the Space of Jets: Correlation Dimension



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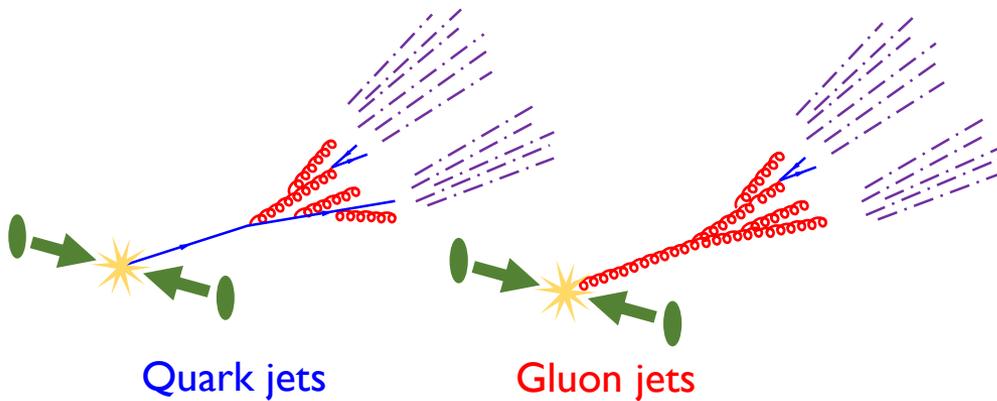
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Hadronization becomes relevant at scales around 20 GeV.

Exploring the Space of Jets: Correlation Dimension

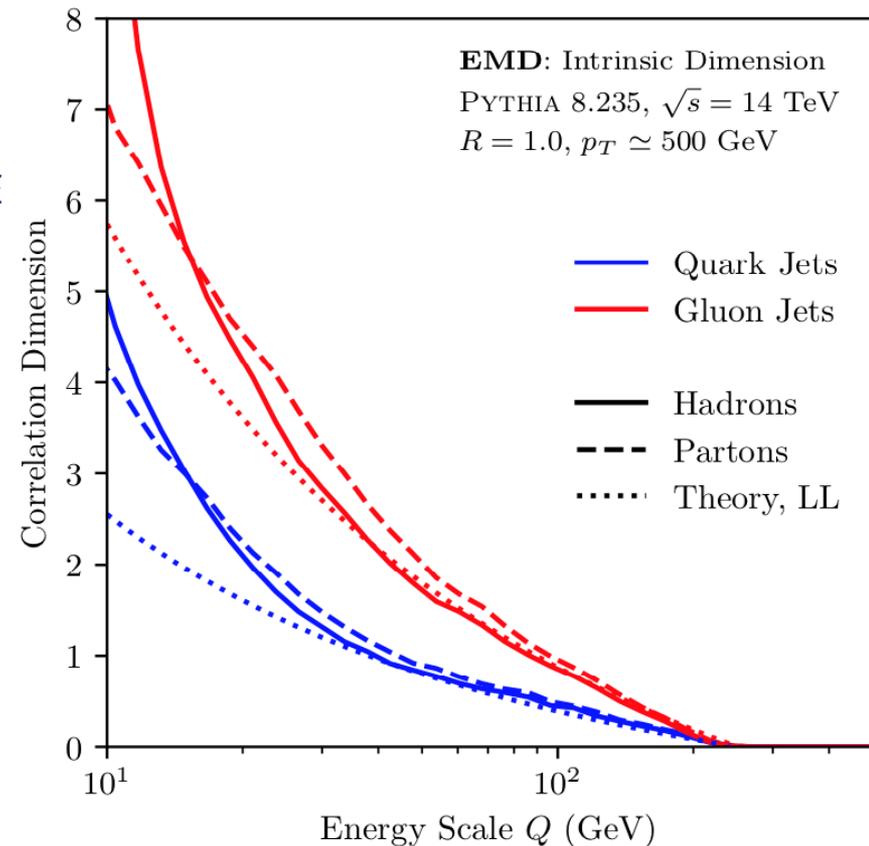


$$\text{At LL: } \dim_{q/g}(Q) = -\frac{8\alpha_s C_{q/g}}{\pi} \ln \frac{Q}{p_T/2}$$

+ 1-loop running of α_s

$$C_q = C_F = \frac{4}{3}$$

$$C_g = C_A = 3$$

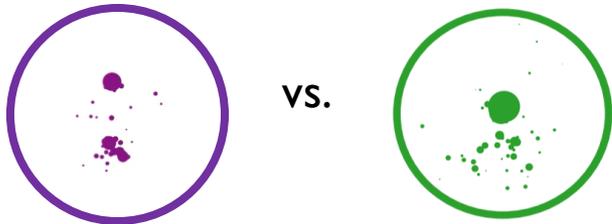


Dimension blows up at low energies.

Jets are “more than fractal”?

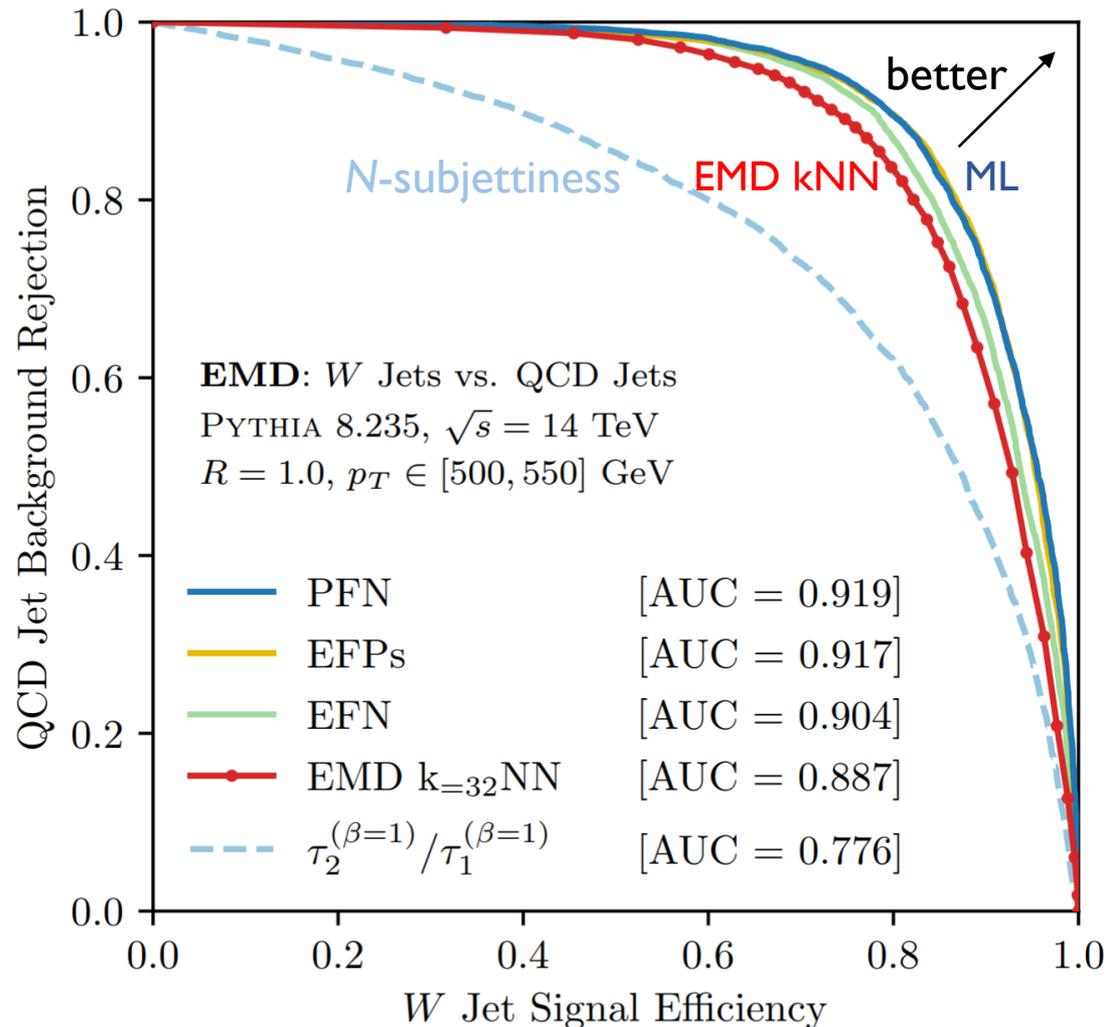
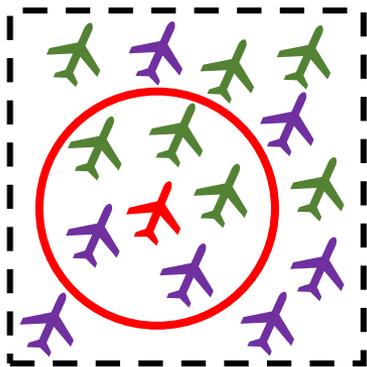
Exploring the Space of Events: Jet Classification

Classify W jets vs. QCD jets

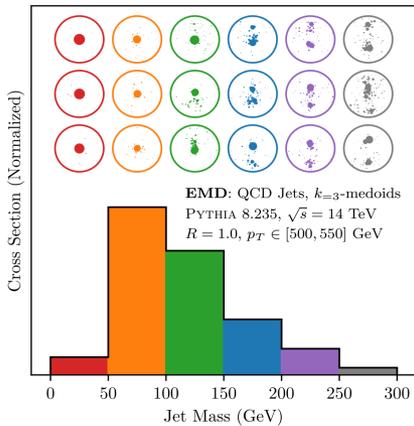


Look at a jet's nearest neighbors (kNN) to predict its class.

Nearing performance of ML.



Going Beyond



Quantifying pileup mitigation

New histogram and data visualizations

Clustering sets of events

New observables through EMD geometry

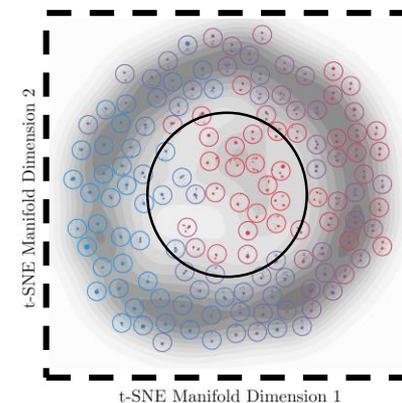
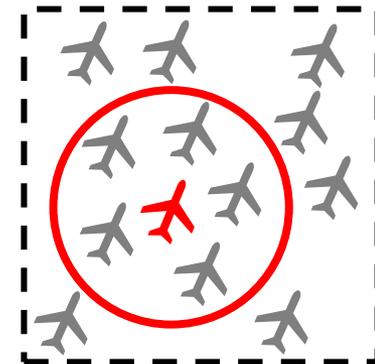
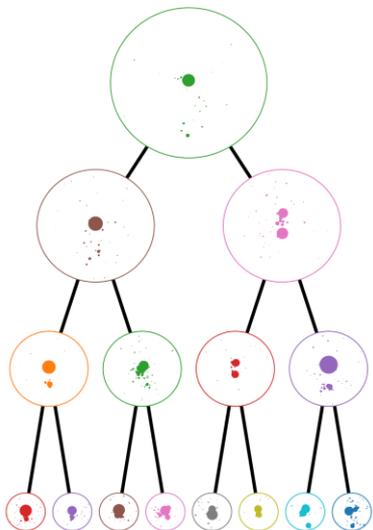
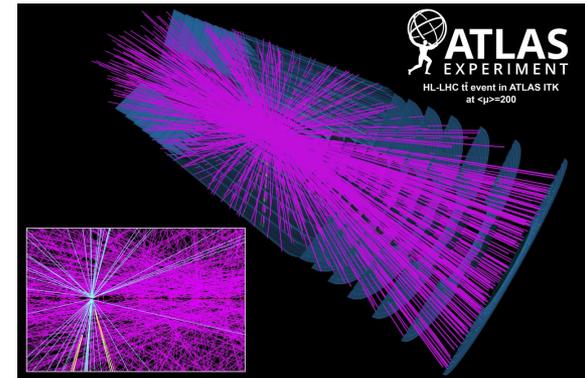
EMD for density estimation (& unfolding?)

“Event” mover’s distance between ensembles?

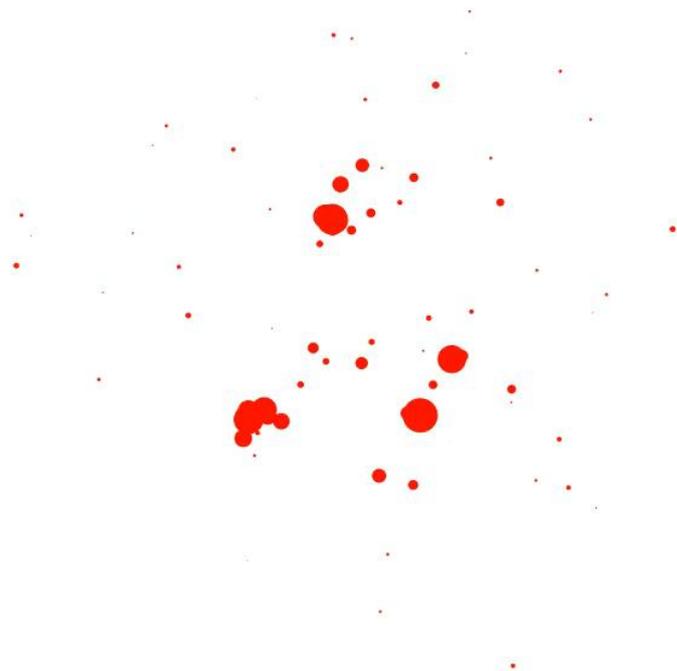
Model (in)dependent anomaly detection?

Train ML models to optimize EMD directly?

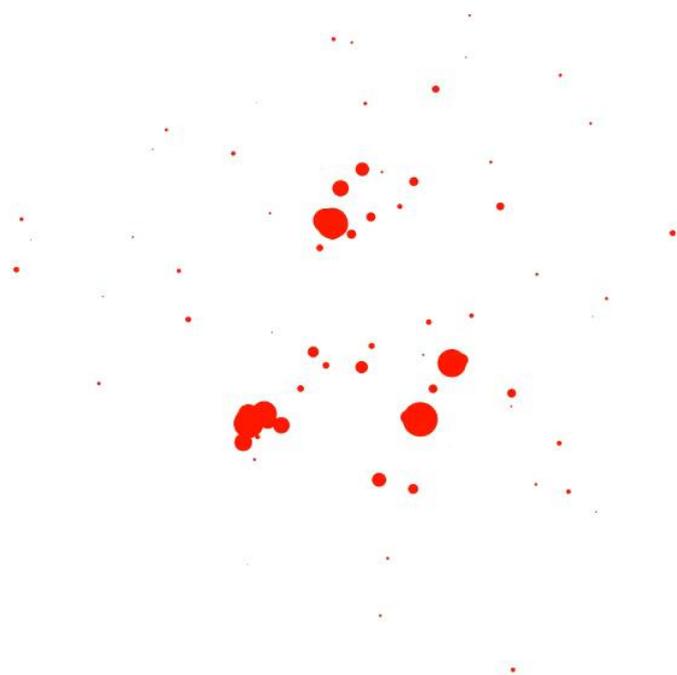
Include flavor information?



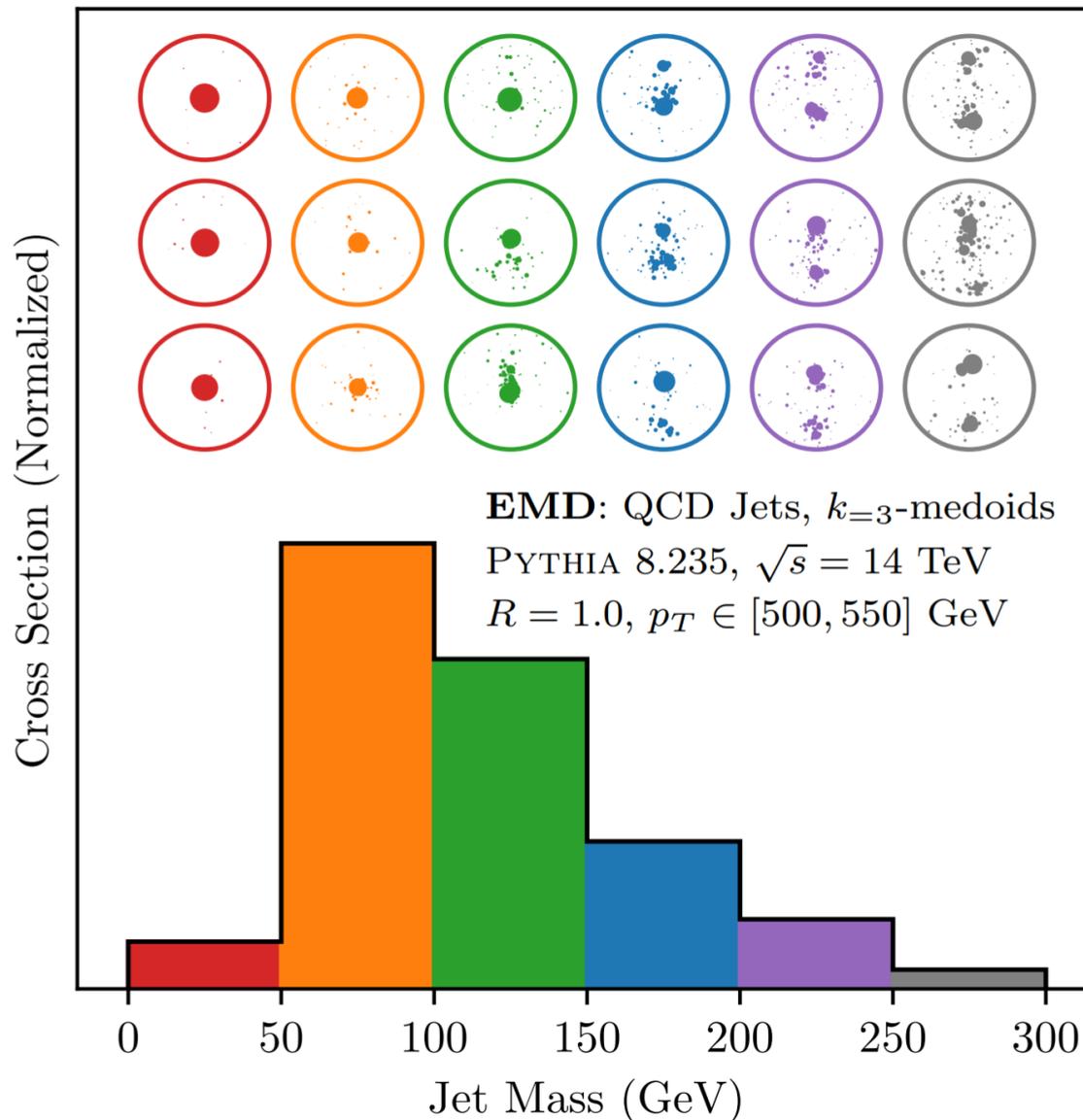
The End
Thank you!



Extra Slides



Exploring the Space of Events: k -medoids



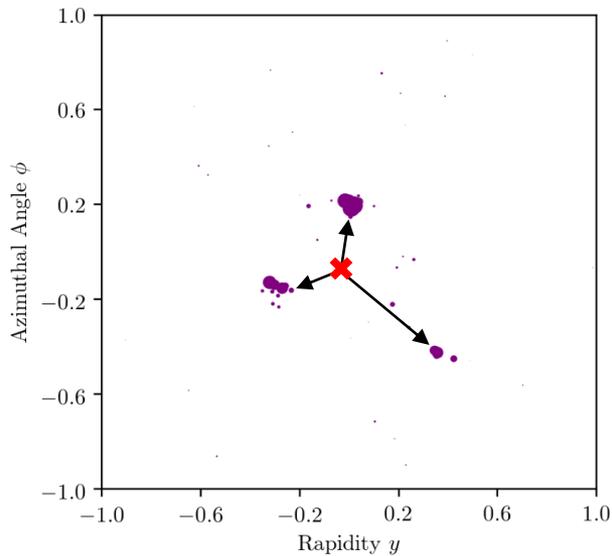
Observables

N -(sub)jettiness:
$$\tau_N^{(\beta)} = \sum_{i=1}^M E_i \min_{N \text{ axes}} \{ \theta_{1,k}^\beta, \theta_{2,k}^\beta, \dots, \theta_{N,k}^\beta \}$$

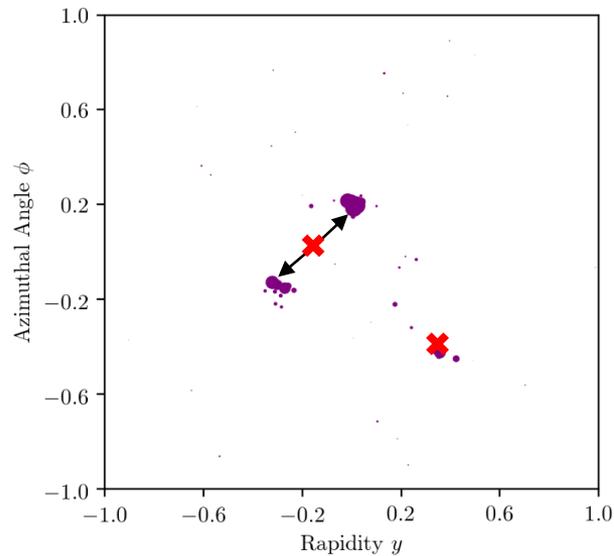
[I. Stewart, F. Tackmann, W. Waalewijn, 1004.2489]
 [J. Thaler, K. Van Tilburg, 1011.2268]
 [J. Thaler, K. Van Tilburg, 1108.2701]

measures how well jet energy is aligned into N (sub)jets

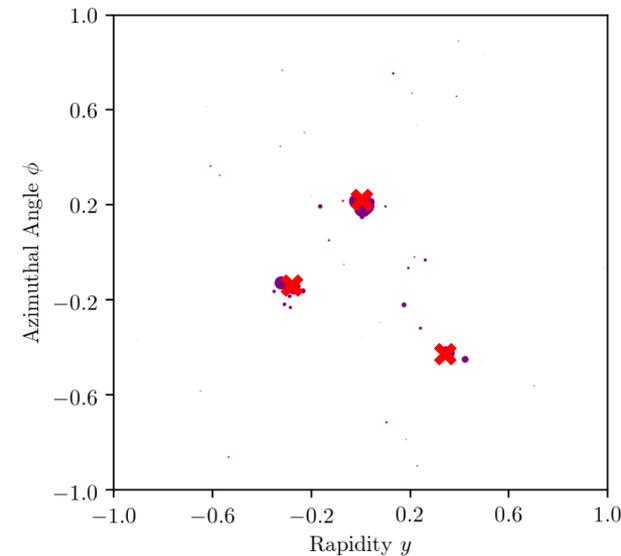
$\tau_1/E \gg 0$



$\tau_1/E > \tau_2/E \gg 0$



$\tau_3/E \simeq 0$



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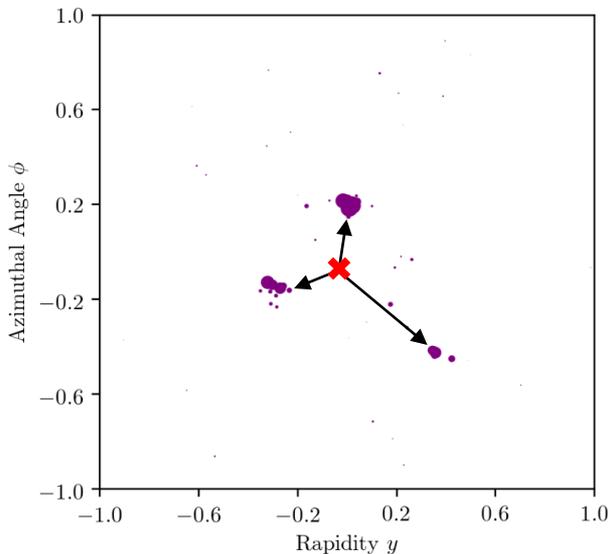
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[J. Thaler, K. Van Tilburg, 1011.2268]

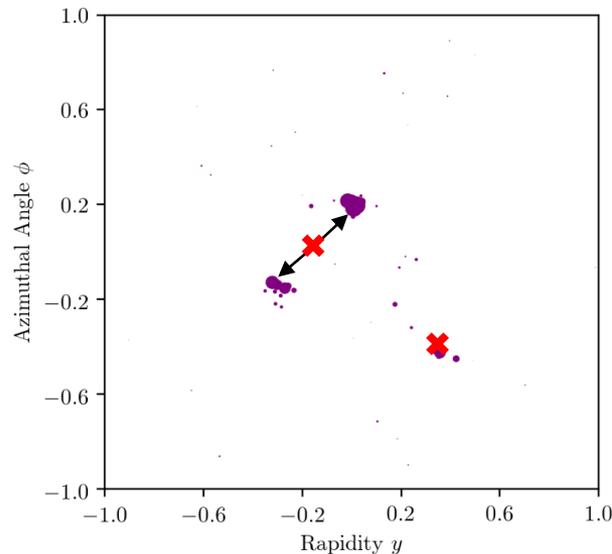
[J. Thaler, K. Van Tilburg, 1108.2701]

measures how well jet energy is aligned into N subjects

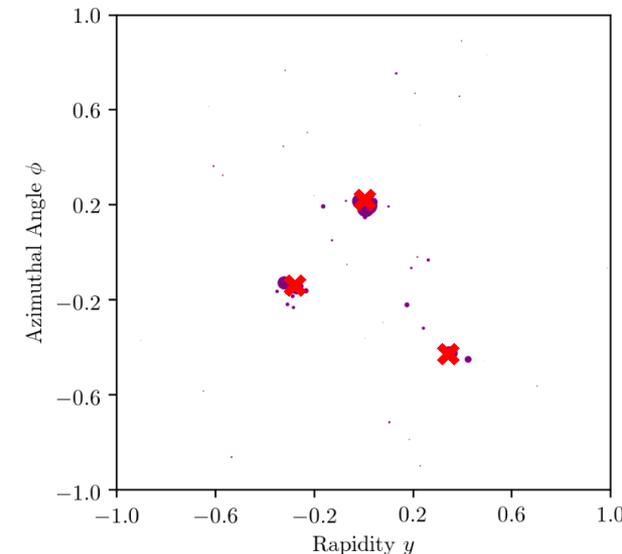
$\tau_1/E \gg 0$



$\tau_1/E > \tau_2/E \gg 0$



$\tau_3/E \simeq 0$



N -subjettiness is the EMD between the event and the closest N -particle event.

$$\tau_N(\mathcal{E}) = \min_{|\mathcal{E}'|=N} \text{EMD}(\mathcal{E}, \mathcal{E}').$$

$\beta \neq 1$ corresponds to other p -Wasserstein distances with $p = \beta$.

Observables

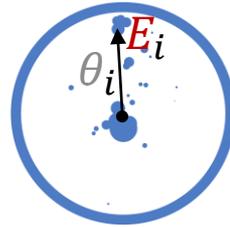
Getting quantitative

Take any additive IRC-safe observable: $\mathcal{O}(\mathcal{E}) = \sum_{i=1}^M E_i \Phi(\hat{p}_i)$

e.g. jet angularities: $\lambda^{(\beta)} = \sum_{i=1}^M E_i \theta_i^\beta$

[\[C. Berger, T. Kucs, and G. Sterman, 0303051\]](#)

[\[A. Larkoski, J. Thaler, and W. Waalewijn, 1408.3122\]](#)



Observables

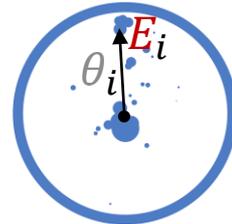
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Via the Kantorovich-Rubinstein dual formulation of EMD:

Earth Mover's
Distance

$$\text{EMD}(\mathcal{E}, \mathcal{E}') \geq \frac{1}{RL} \left| \sum_{i=1}^M E_i \Phi(\hat{p}_i) - \sum_{j=1}^{M'} E'_j \Phi(\hat{p}_j') \right| = \frac{1}{RL} |\mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}')|$$

Difference in
observable values

“Lipschitz constant” of Φ
i.e. bound on its derivative

Observables

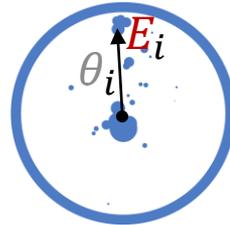
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Difference in
observable values

“Lipschitz constant” of Φ
i.e. bound on its derivative

For $\beta \geq 1$ jet angularities, $L = \beta/R$ over the jet cone, so:

$$|\lambda^{(\beta)}(\mathcal{E}) - \lambda^{(\beta)}(\mathcal{E}')| \leq \beta \text{EMD}(\mathcal{E}, \mathcal{E}')$$

The EMD provides a robust upper bound to any modifications of these observables.

Observables

Key idea: Energy-weighted angular structures contain all the IRC-safe information.

$$\frac{1}{RL} \left| \sum_{i=1}^M E_i \Phi(\hat{p}_i) - \sum_{j=1}^{M'} E'_j \Phi(\hat{p}'_j) \right| \leq \text{EMD}(\mathcal{E}, \mathcal{E}')$$

Theorem: Any infrared and collinear safe observable \mathcal{O} can be approximated arbitrarily well as:

$$\mathcal{O}(p_1, \dots, p_M) = F \left(\sum_{i=1}^M E_i \vec{\Phi}(\hat{p}_i) \right)$$

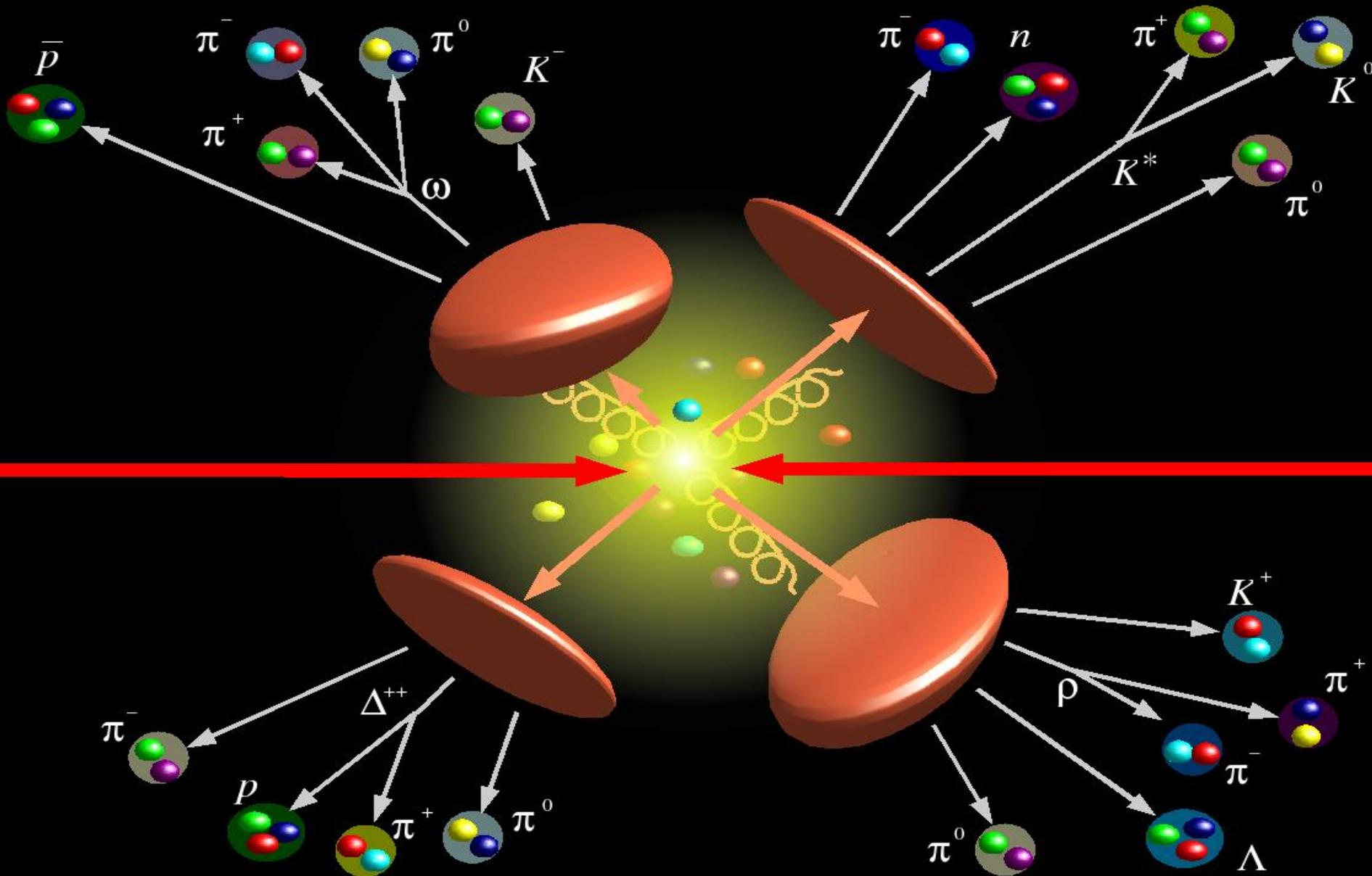
for some $\Phi: \mathbb{R}^2 \rightarrow \mathbb{R}^\ell$ and $F: \mathbb{R}^\ell \rightarrow \mathbb{R}$ and sufficiently large ℓ .

[\[M. Zaheer, et al., 1703.06114\]](#)

[\[P.T. Komiske, EMM, J. Thaler, 1810.05165\]](#)

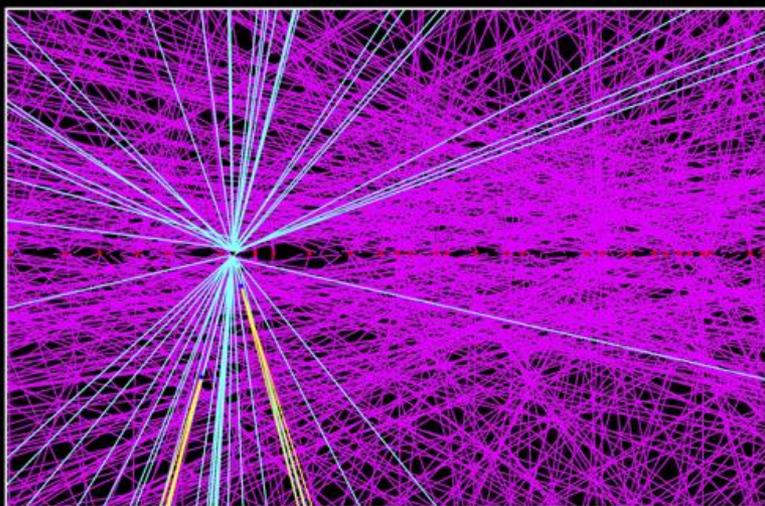
Events close in EMD are close in all infrared and collinear safe information!

Quantifying event modifications: Hadronization



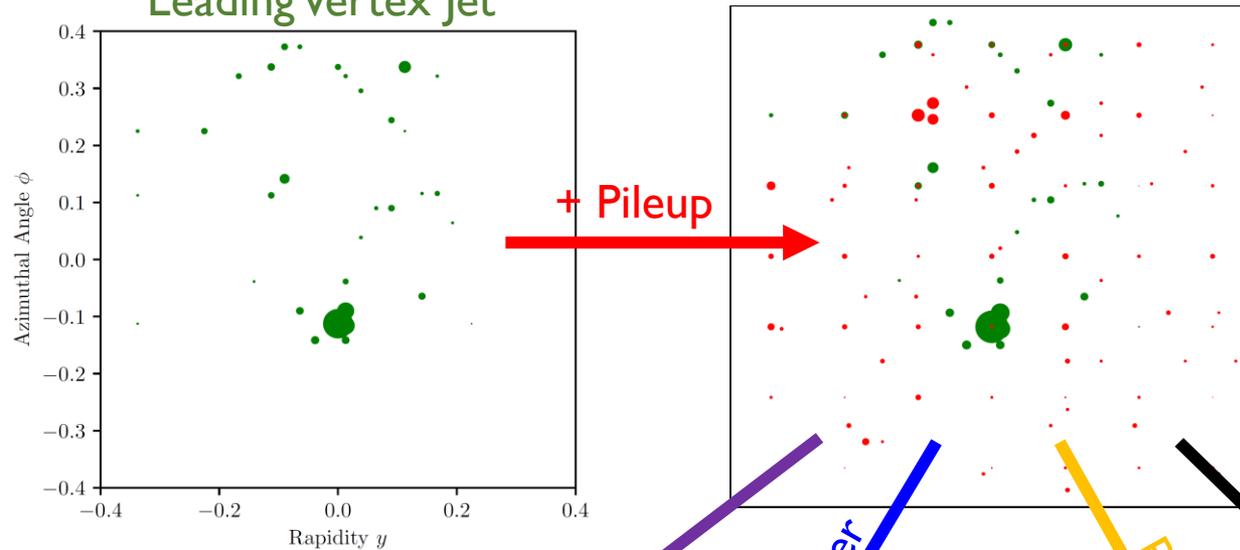
Quantifying event modifications: Pileup

 **ATLAS**
EXPERIMENT
HL-LHC $t\bar{t}$ event in ATLAS ITK
at $\langle\mu\rangle=200$



Quantifying event modifications: Pileup

Leading Vertex Jet



How can we quantify pileup mitigation?

[\[M. Cacciari, G.P. Salam, G. Soyez, 1407.0408\]](#)

[\[D. Bertolini, P. Harris, M. Low, N. Tran, 1407.6013\]](#)

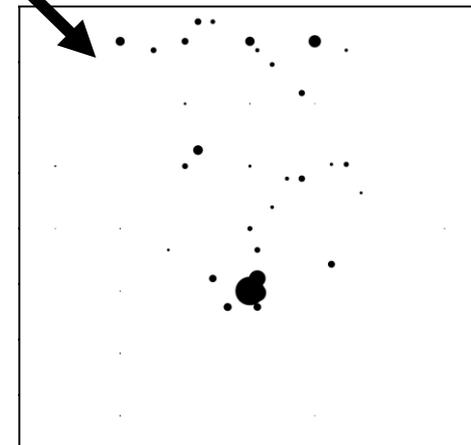
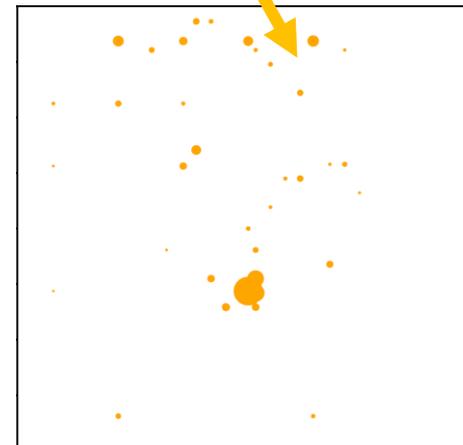
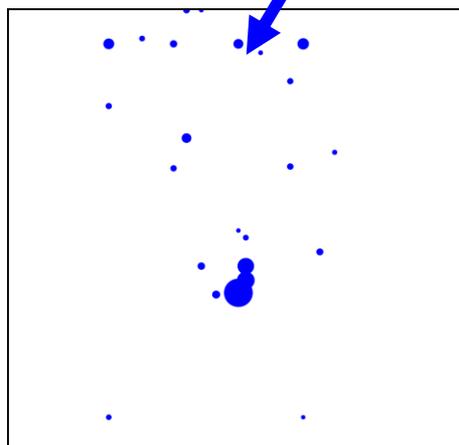
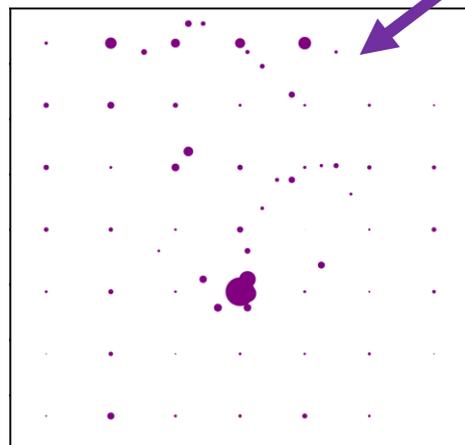
[\[P.T. Komiske, EMM, B. Nachman, M.D. Schwartz, 1707.08600\]](#)

CHS

SoftKiller

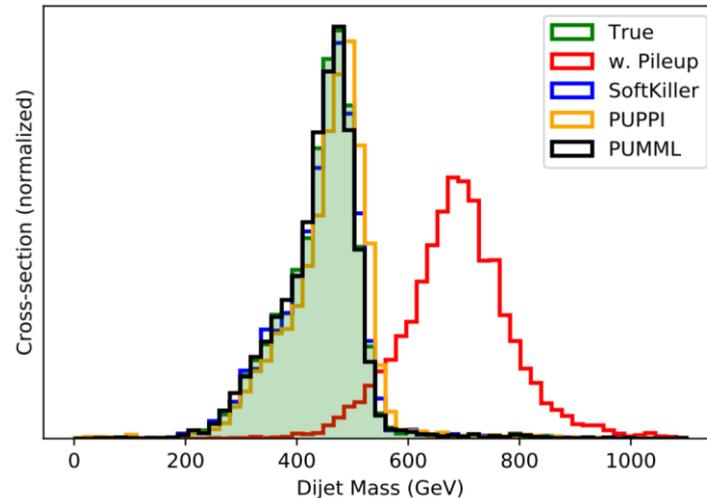
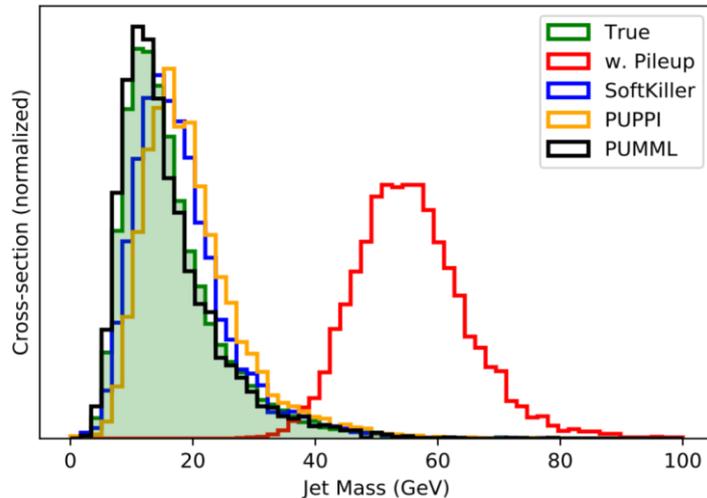
PUPPI

PUMML



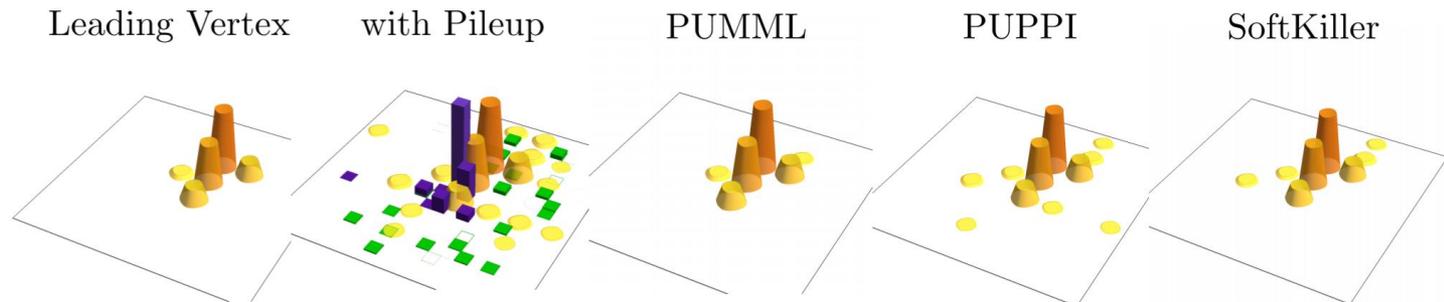
Quantifying event modifications: Pileup

Compare on a collection of observables?



Requires ad hoc choices of observables.

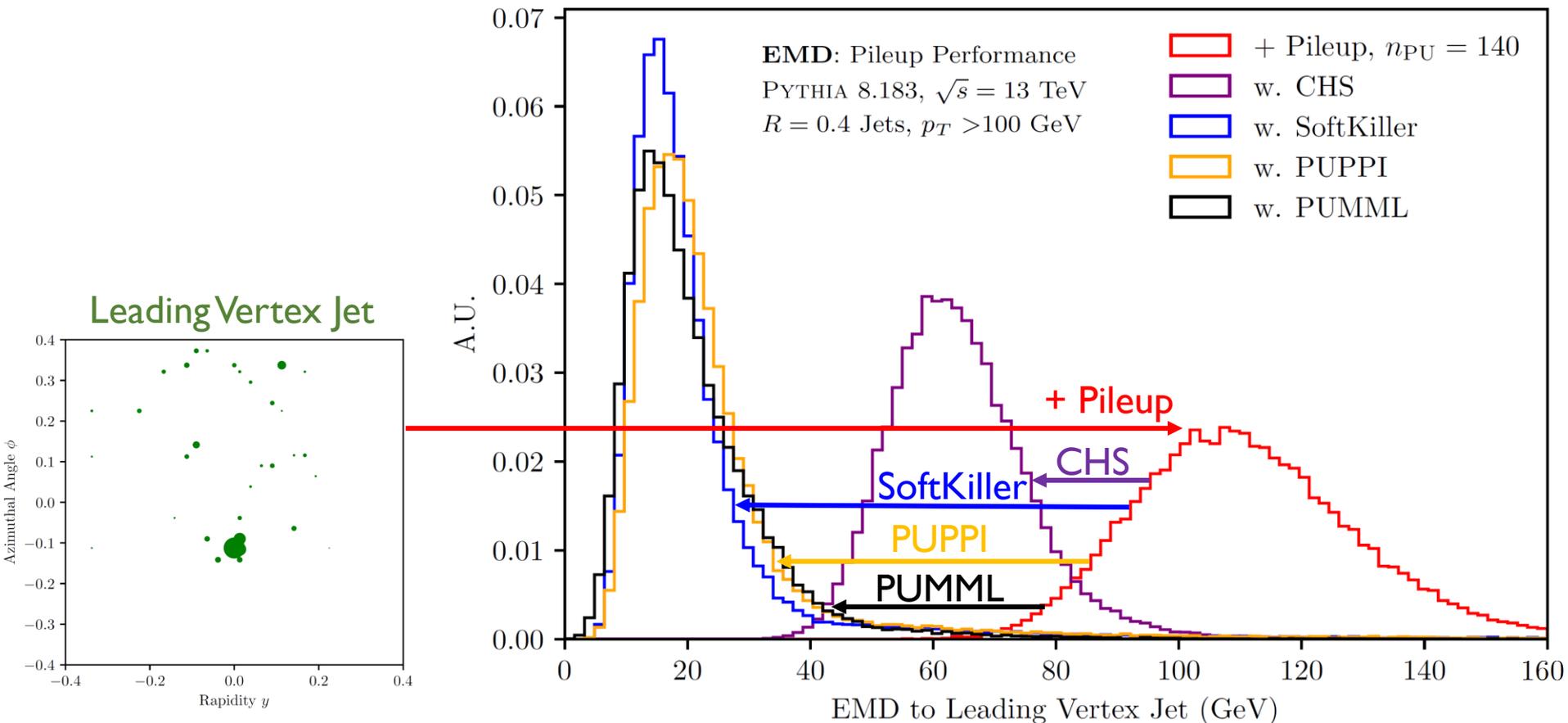
Compare calorimeter images pixel by pixel?



Discontinuous under physically-sensible single-pixel perturbations.
Undesirable behavior with increasing resolution.

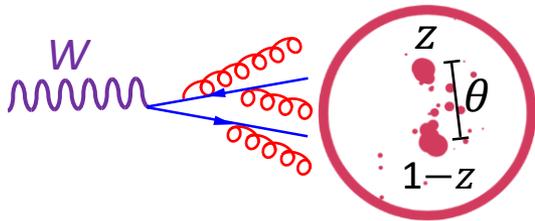
Quantifying event modifications: Pileup

Measure pileup mitigation performance with EMD!



Guarantees performance on IRC safe observables.
Stable under physically-sensible perturbations.
Train to optimize EMD with machine learning?

Exploring the Space of Events: W jets



W jets are 2-pronged:

z : Energy Sharing of Prongs

θ : Angle between Prongs

φ : Azimuthal orientation

Constrained by W mass:

$$z(1-z)\theta^2 = \frac{p_{\mu J}^2}{p_T^2} = \frac{m_W^2}{p_T^2}$$

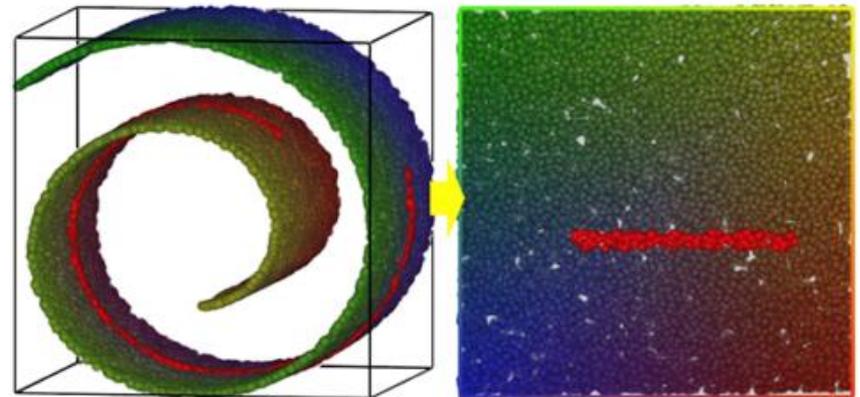
Hence we expect a **two**-dimensional space of W jets.

After φ rotation: **one**-dimensional

Visualize the space of events with t-Distributed Stochastic Neighbor Embedding (t-SNE).

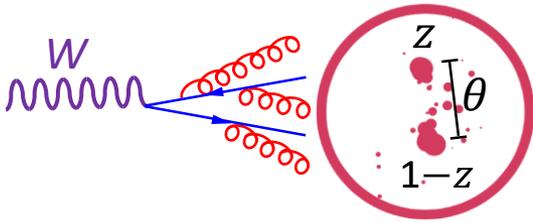
[\[L. van der Maaten, G. Hinton\]](#)

Finds an embedding into a low-dimensional manifold that respects distances.



Src: <http://web-ext.u-aizu.ac.jp/~shigeo/home.html>

Exploring the Space of Events: W jets



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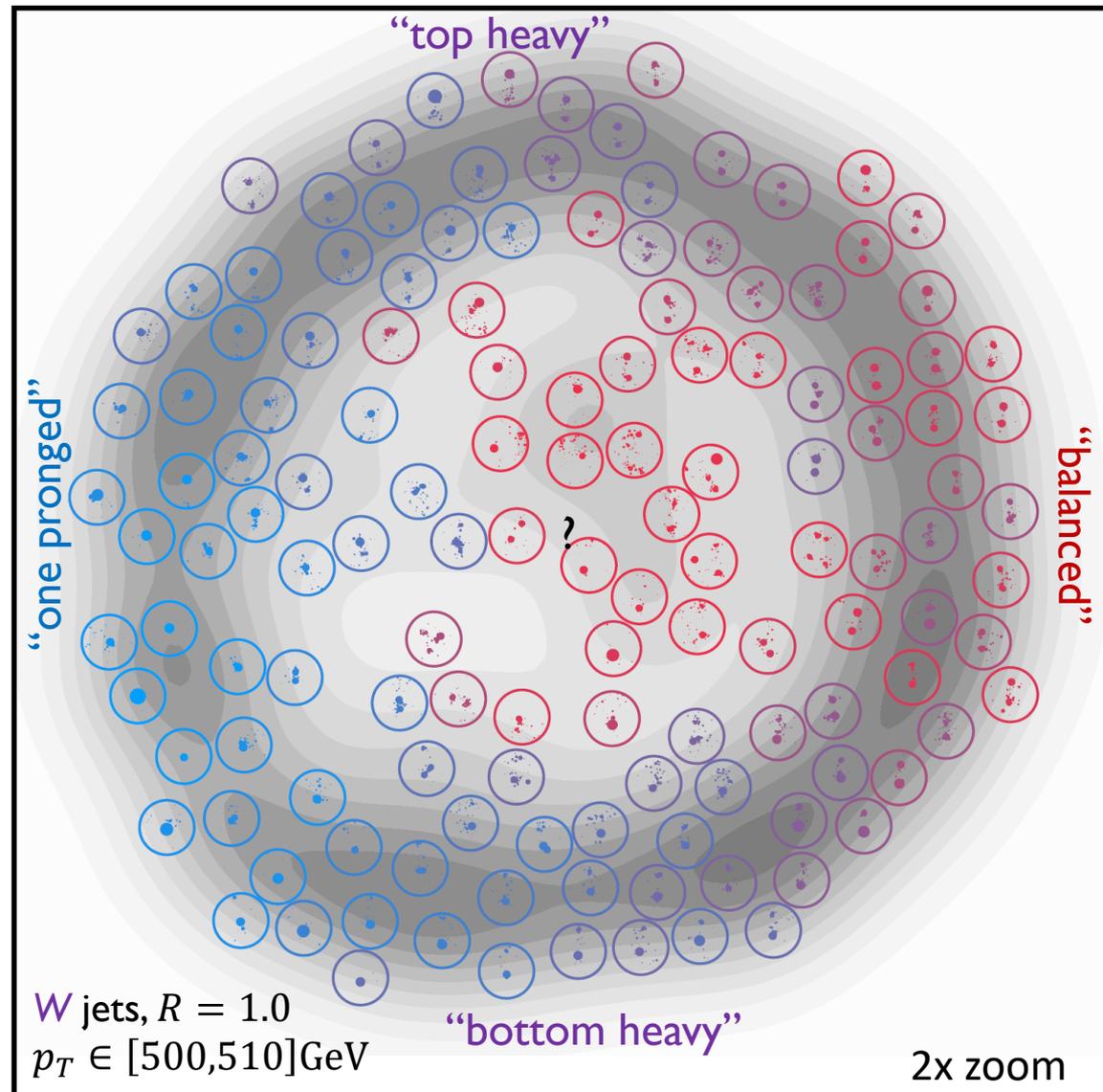
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After φ rotation: **one**-dimensional

t-SNE Manifold Dimension 2



t-SNE Manifold Dimension 1

Exploring the Space of Jets: Correlation Dimension

VOLUME 50, NUMBER 5

PHYSICAL REVIEW LETTERS

31 JANUARY 1983

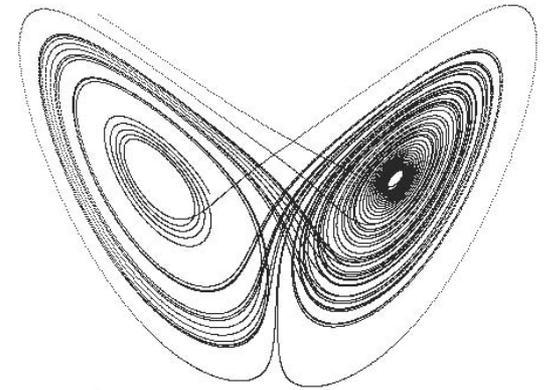
Characterization of Strange Attractors

Peter Grassberger^(a) and Itamar Procaccia

Chemical Physics Department, Weizmann Institute of Science, Rehovot 76100, Israel

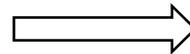
(Received 7 September 1982)

A new measure of strange attractors is introduced which offers a practical algorithm to determine their character from the time series of a single observable. The relation of this new measure to fractal dimension and information-theoretic entropy is discussed.

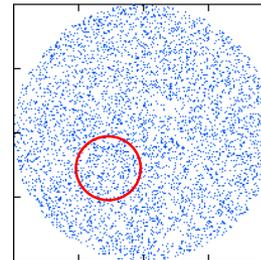
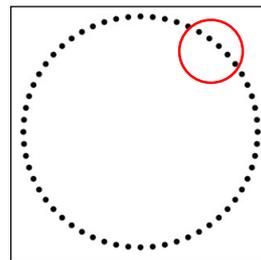


Intuition:

$$N_{\text{neighboring points}}(r) \propto r^{\text{dim}}$$



$$\text{dim}(r) = r \frac{\partial}{\partial r} \ln N_{\text{neighboring}}(r)$$



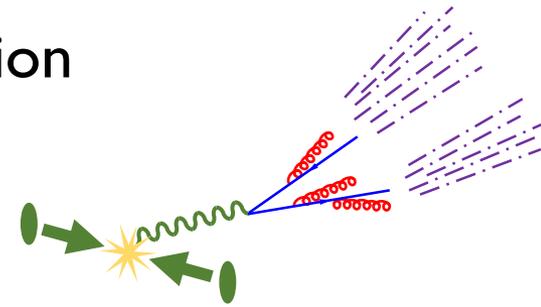
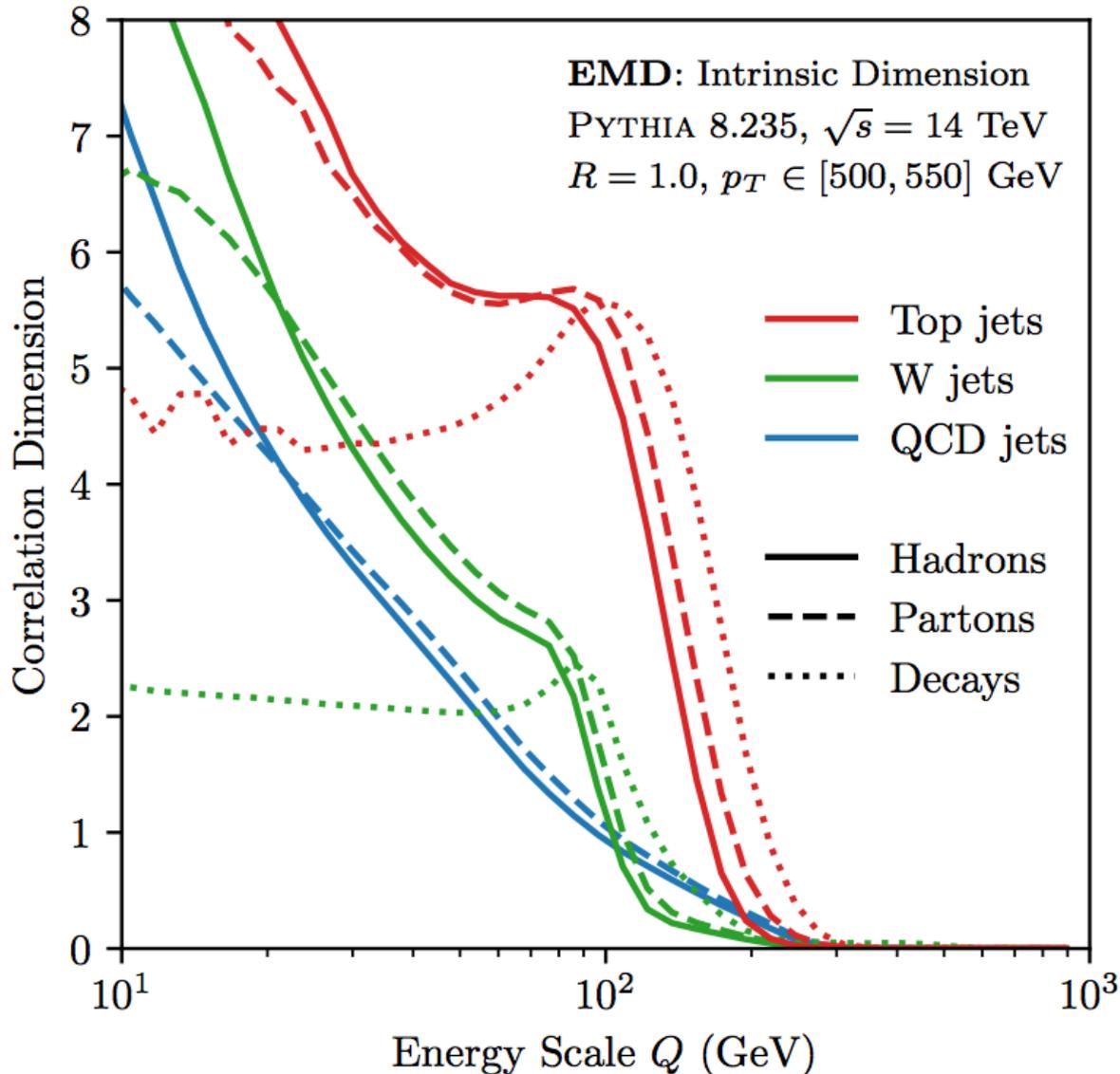
Correlation dimension:

$$\text{dim}(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i=1}^N \sum_{j=1}^N \Theta[\text{EMD}(\epsilon_i, \epsilon_j) < Q]$$

Energy scale Q
dependence

Count neighbors in
ball of radius Q

Exploring the Space of Jets: Correlation Dimension



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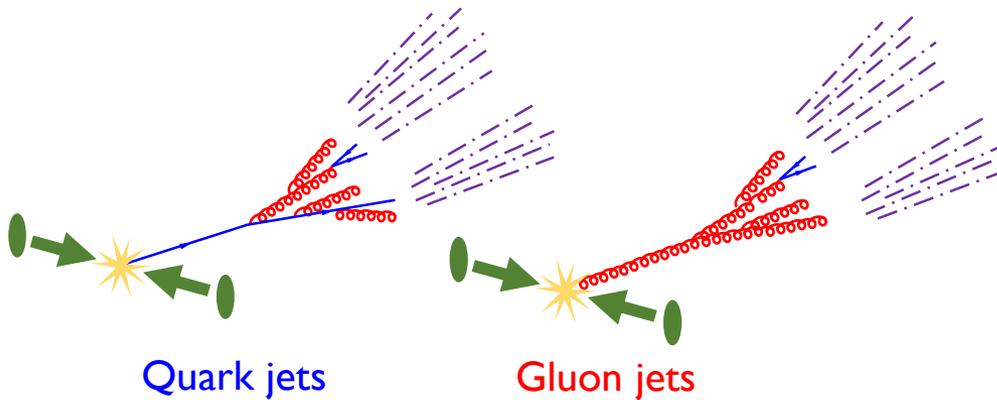
“Decays” have \sim constant dimension.

Fragmentation becomes more complex at lower energy scales.

Hadronization becomes relevant at scales around 20 GeV.

Can we understand this analytically?

Exploring the Space of Jets: Correlation Dimension

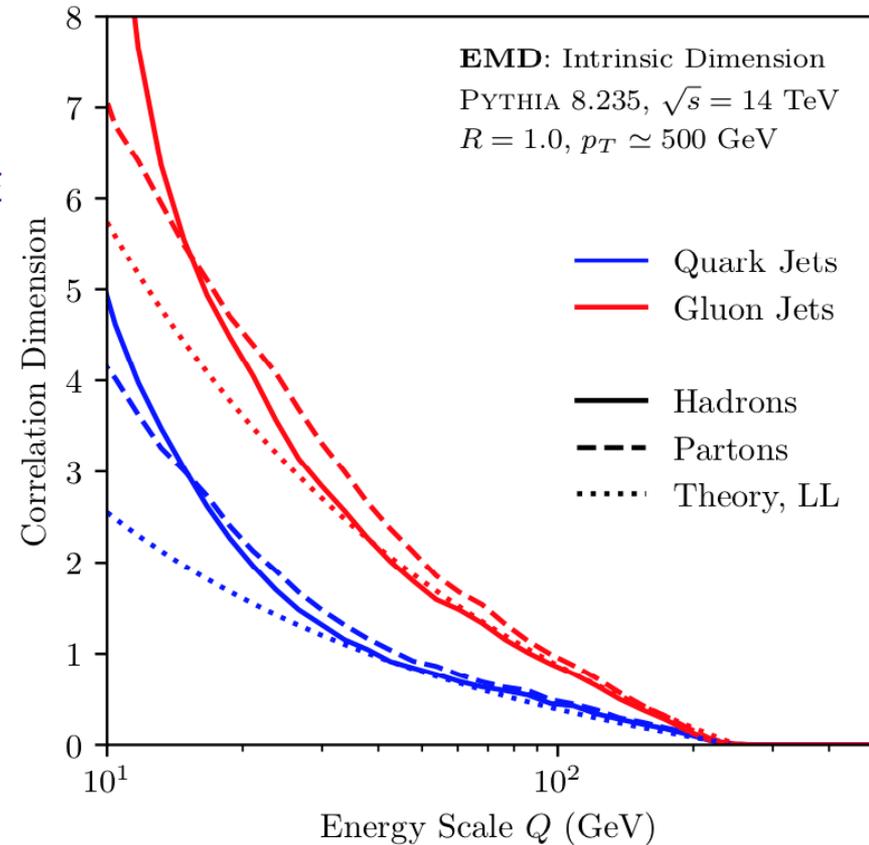


$$\text{At LL: } \dim_{q/g}(Q) = -\frac{8\alpha_s C_{q/g}}{\pi} \ln \frac{Q}{p_T/2}$$

+ 1-loop running of α_s

$$C_q = C_F = \frac{4}{3}$$

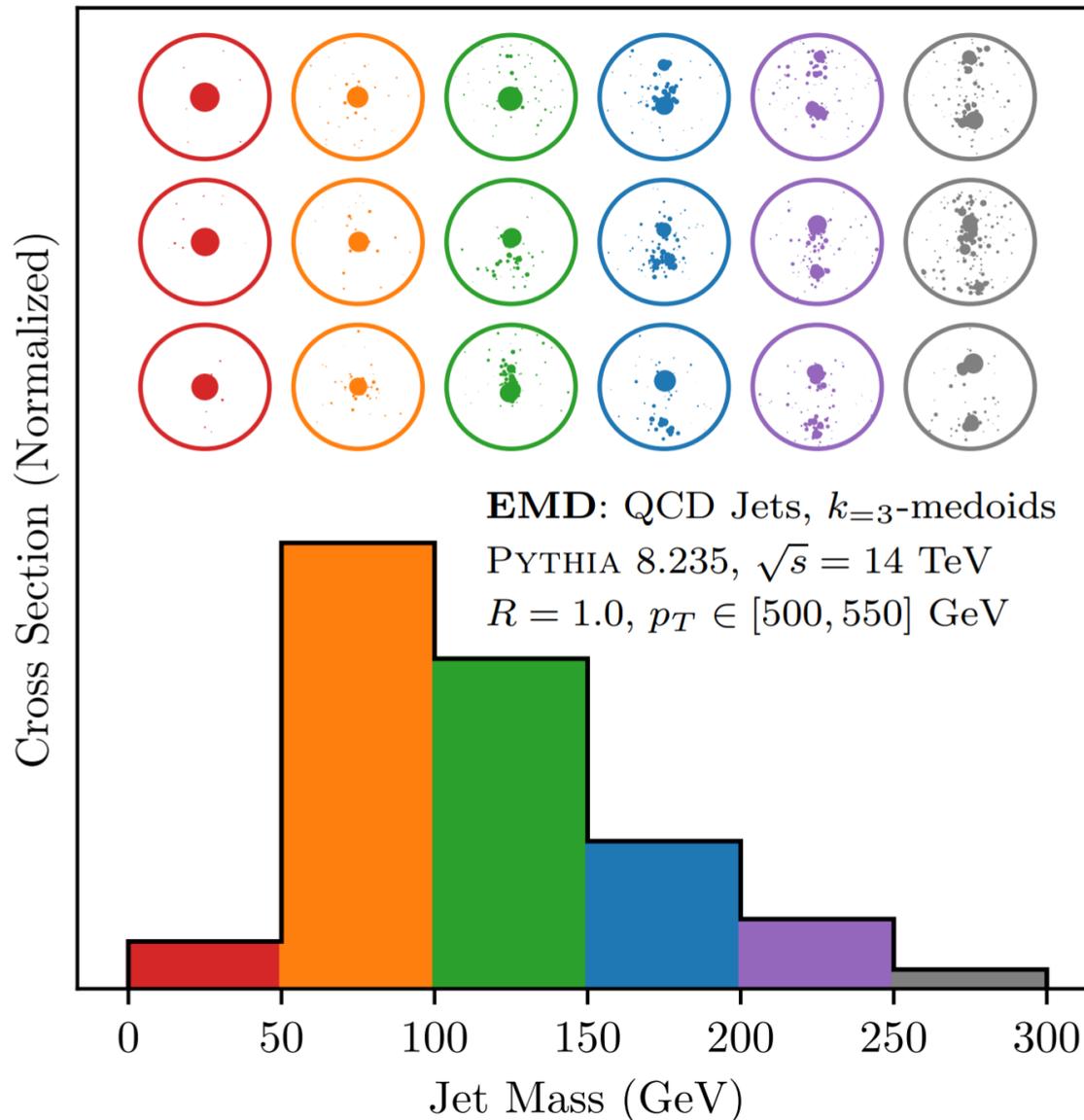
$$C_g = C_A = 3$$



Dimension blows up at low energies.

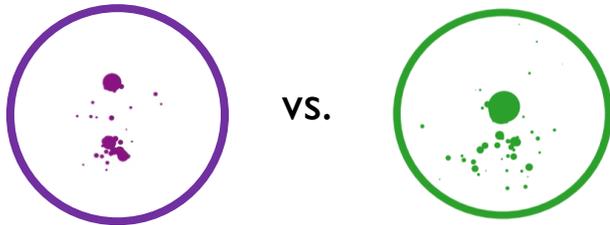
Jets are “more than fractal”?

Exploring the Space of Events: k -medoids



Exploring the Space of Events: Jet Classification

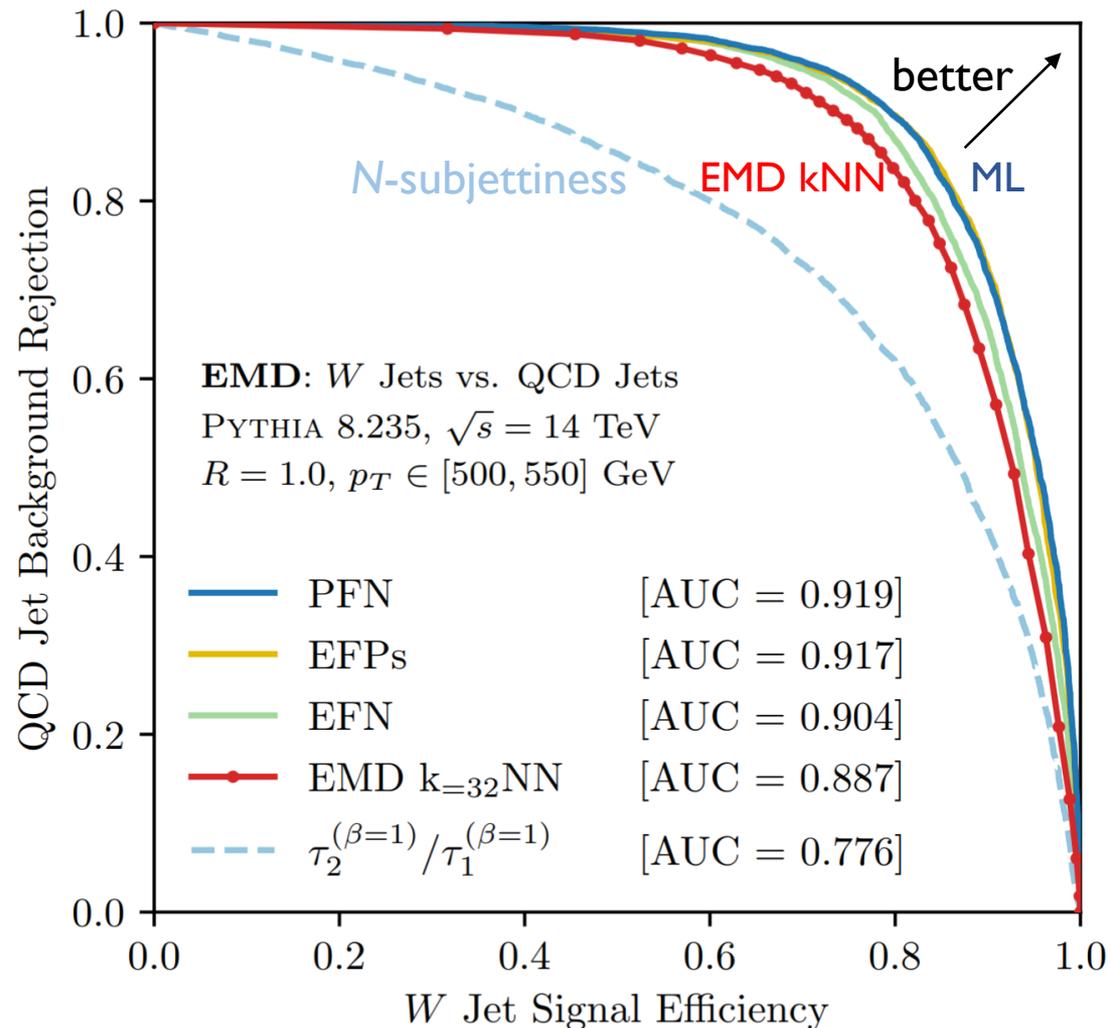
Classify W jets vs. QCD jets



Look at a jet's nearest neighbors (kNN) to predict its class.

Optimal IRC-safe classifier with enough data.

Nearing performance of ML.



Exploring the Space of Events

Use EMD as a measure of event similarity

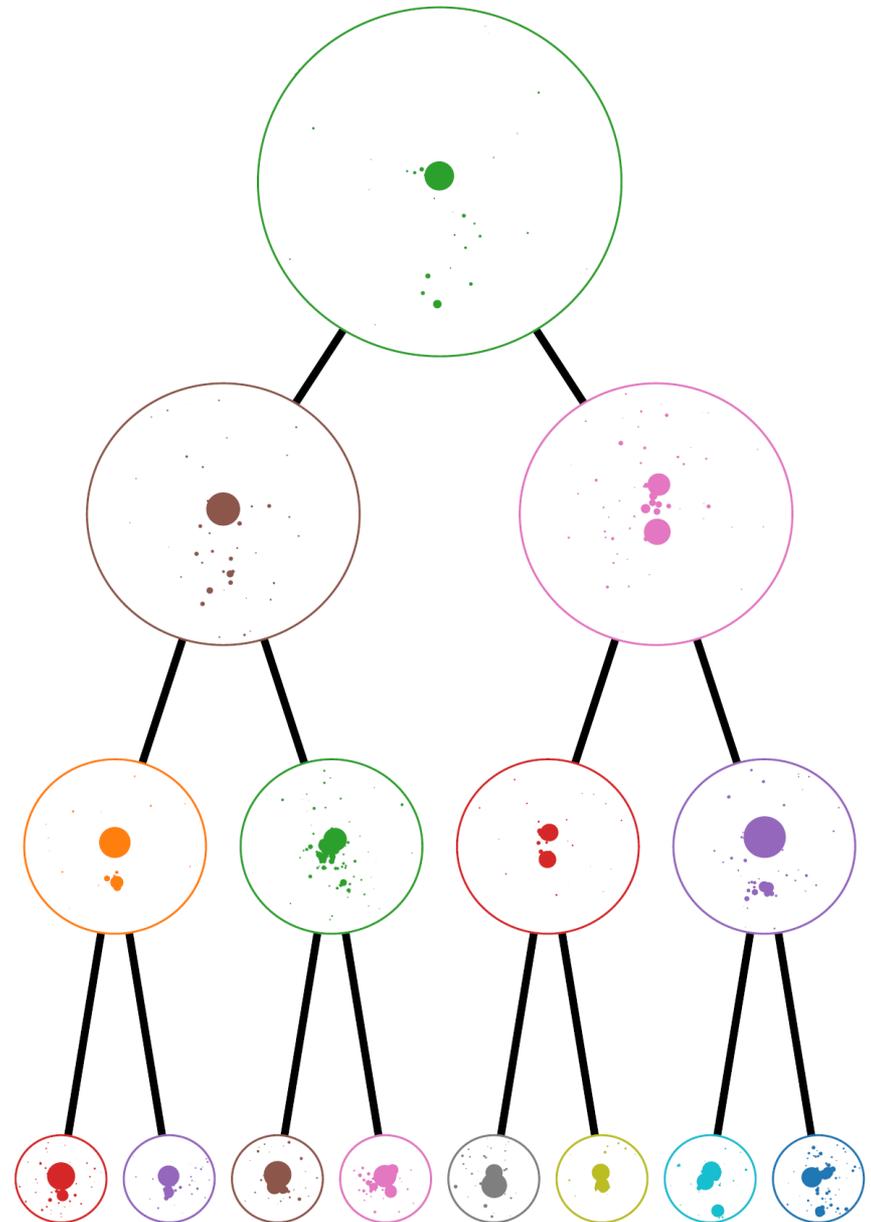
Unsupervised clustering algorithms can be used to cluster events

Jets are clusters of particles
???? are clusters of jets

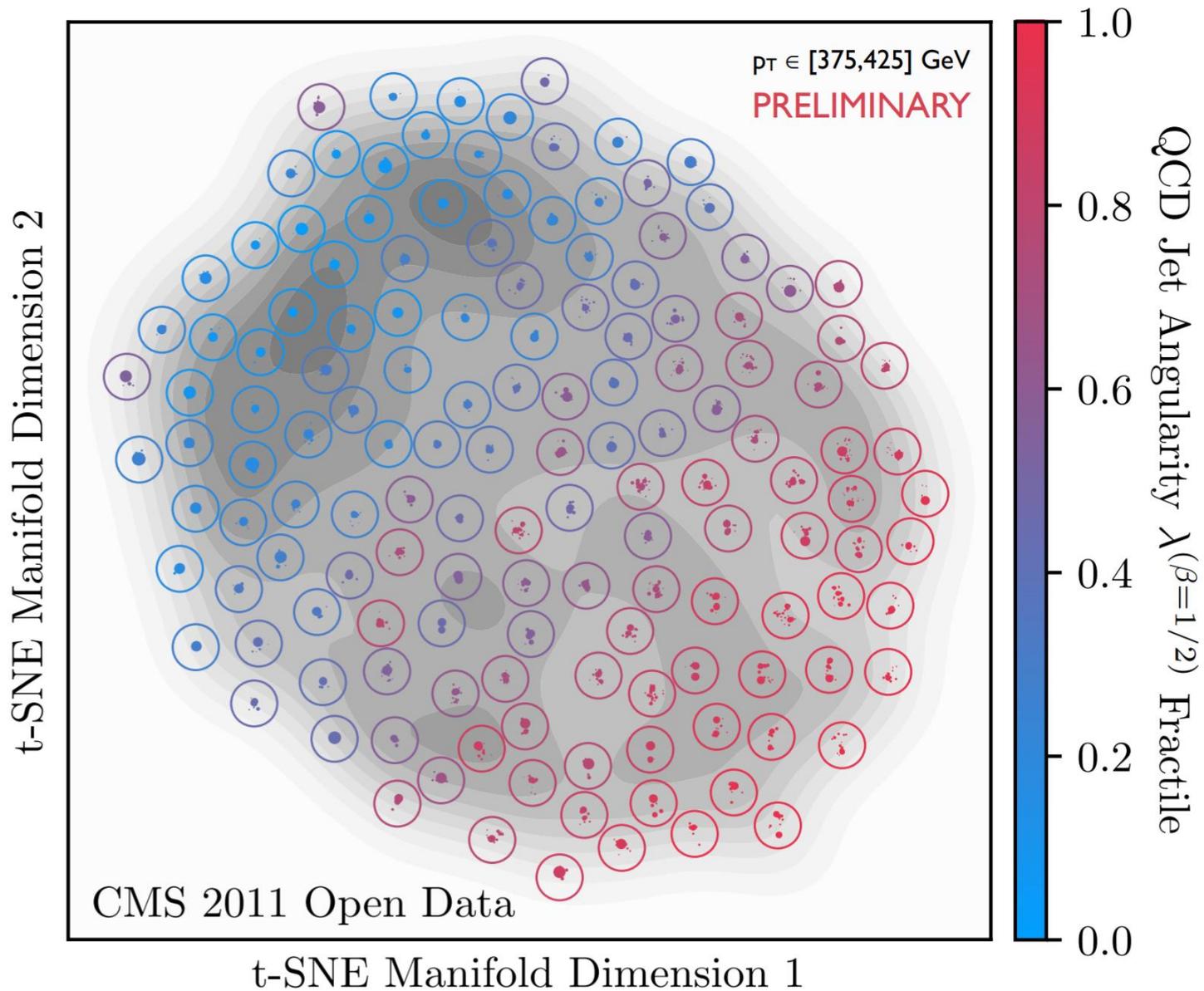
VP Tree: $O(\log(N))$ neighbor query time

Much more to explore.

Vantage Point (VP) Tree



Exploring the Space of Events: QCD Jets



Exploring the Space of Jets: Correlation Dimension

Sketch of leading log (one emission) calculation:

$$\dim_{q/g}(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i=1}^N \sum_{j=1}^N \Theta[\text{EMD}(\boldsymbol{\varepsilon}_i, \boldsymbol{\varepsilon}_j) < Q]$$

$$= Q \frac{\partial}{\partial Q} \ln \text{Pr} [\text{EMD} < Q]$$

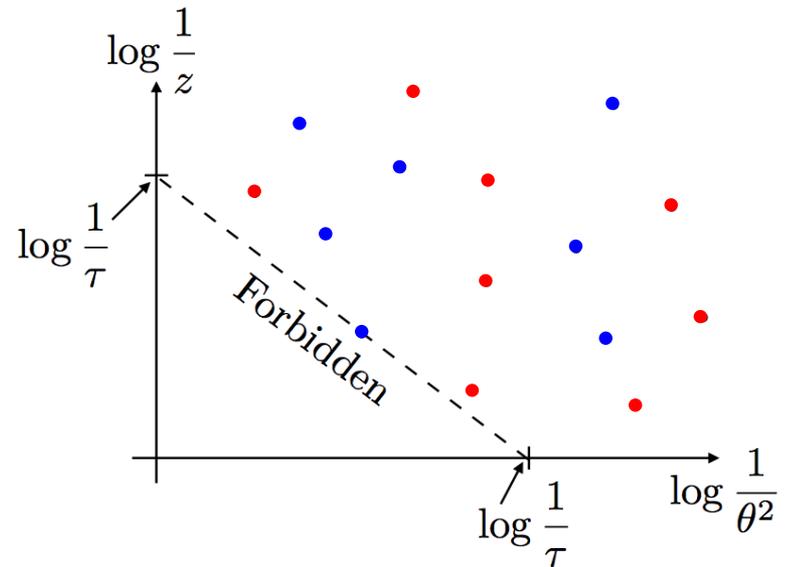
$$= Q \frac{\partial}{\partial Q} \ln \text{Pr} [\lambda^{(\beta=1)} < Q; C_{q/g} \rightarrow 2 C_{q/g}]$$

$$= Q \frac{\partial}{\partial Q} \ln \exp \left(-\frac{4\alpha_s C_{q/g}}{\pi} \ln^2 \frac{Q}{p_T/2} \right)$$

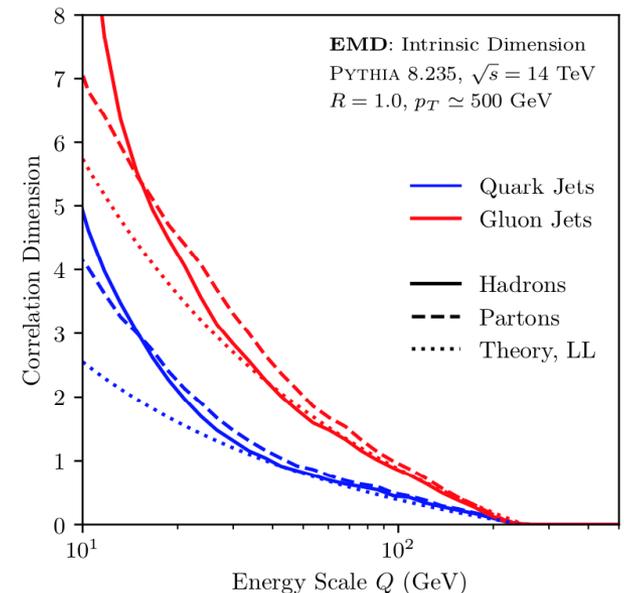
$$= -\frac{8\alpha_s C_{q/g}}{\pi} \ln \frac{Q}{p_T/2} \quad C_q = C_F = \frac{4}{3}$$

$$C_g = C_A = 3$$

+ 1-loop running of α_s

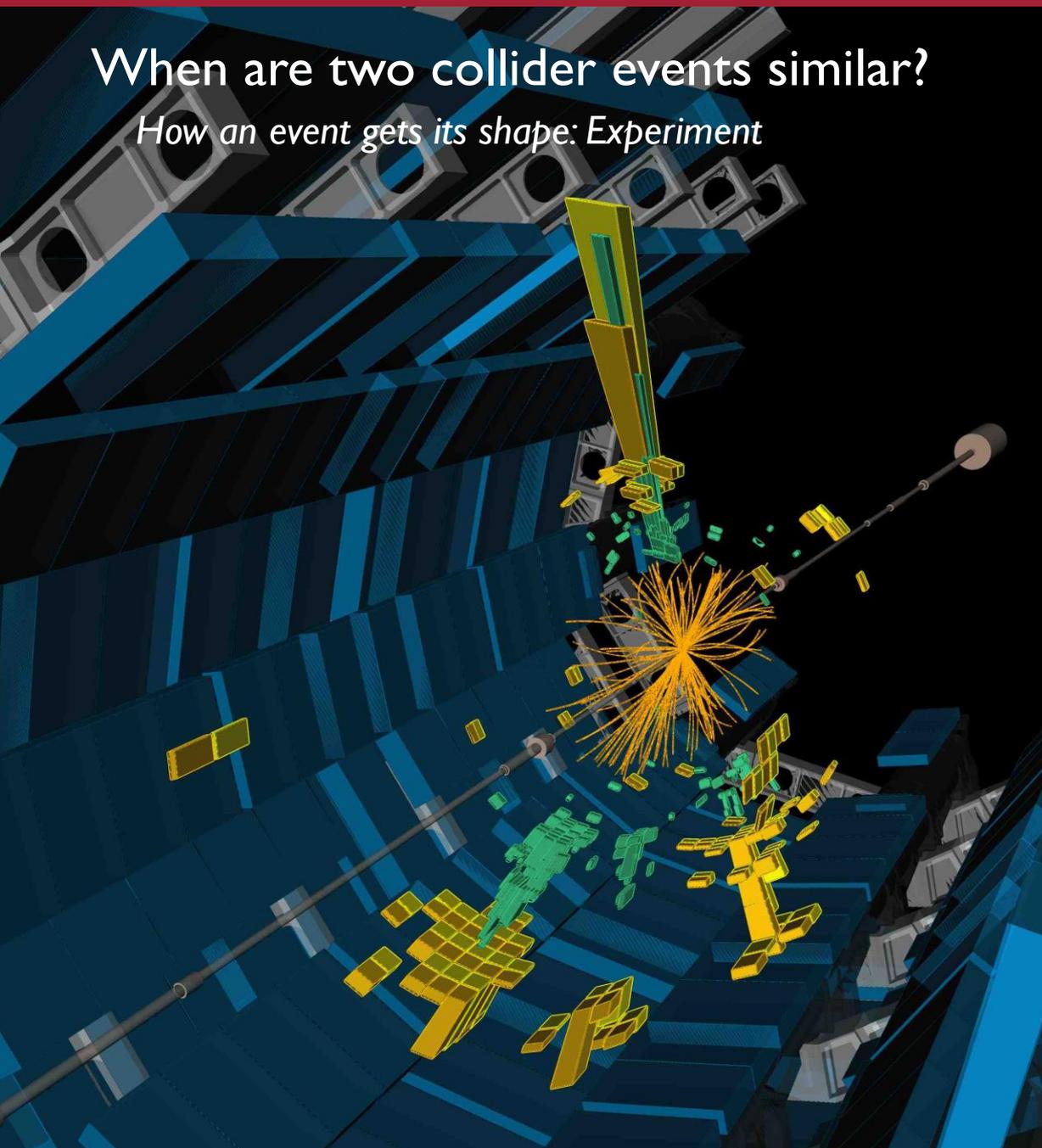


[A. Larkoski, 1709.06195]



When are two collider events similar?

How an event gets its shape: Experiment



| tracker | ECAL | HCAL | | |
|---------|------|------|-------------|----------|
| | | | γ | photon |
| | | | e^{\pm} | electron |
| | | | μ^{\pm} | muon |
| | | | π^{\pm} | pion |
| | | | K^{\pm} | kaon |
| | | | K_L^0 | K-long |
| | | | p/\bar{p} | proton |
| | | | n/\bar{n} | neutron |

Pileup Mitigation with PUMML

