QCD and Jets through the Lens of Machine Learning

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Presentation with Frédéric Dreyer

New Physics from Precision at High Energies, KITP, Santa Barbara — March 30, 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]

AI^2: Ab Initio Artificial Intelligence

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

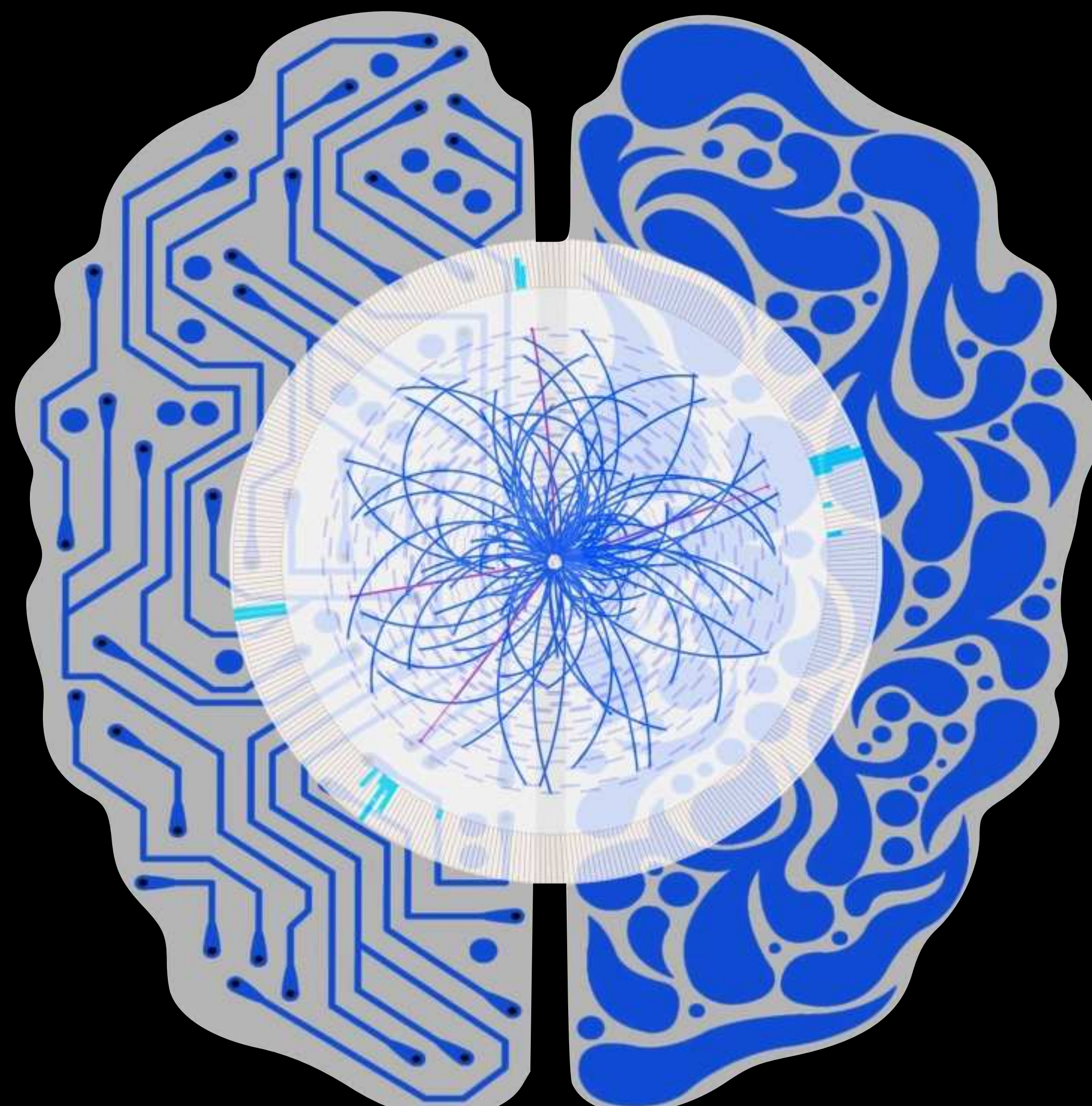
Symmetries, conservation laws, scaling relations, limiting behaviors, locality, causality,
unitarity, gauge invariance, entropy, least action, factorization, unit tests,
exactness, systematic uncertainties, reproducibility, verifiability, …

What aspects of QCD and Jets can be phrased as well-defined optimization problems?

Do we have deep enough physics principles and/or rich enough data sets (real or synthetic) such that machine learning will yield trustable answers?

Apologies that citations/examples in this talk are not (even close to) complete!

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

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

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

[see e.g. D'Agnolo, Wulzer, PRD 2019; simulation-based inference in Cranmer, Brehmer, Louppe, PNAS 2020; relation to f-divergences in Nguyen, Wainwright, Jordan, AoS 2009; 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: $$L = \int \mathrm{d}x \, \mathcal{L}(x)$$

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

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

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

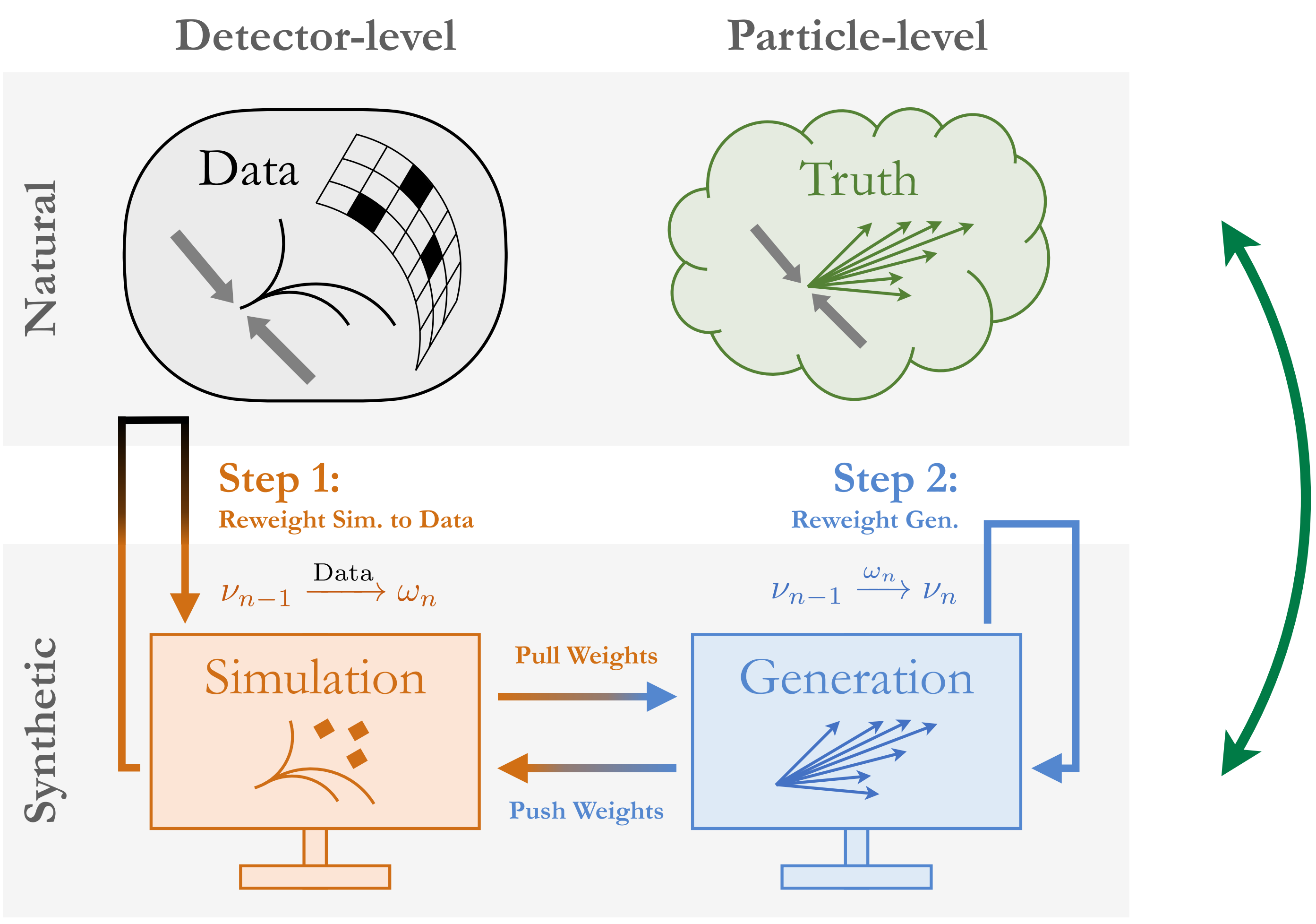
Requires shift in theoretical focus from solving problems to specifying problems

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

E.g. Detector Unfolding

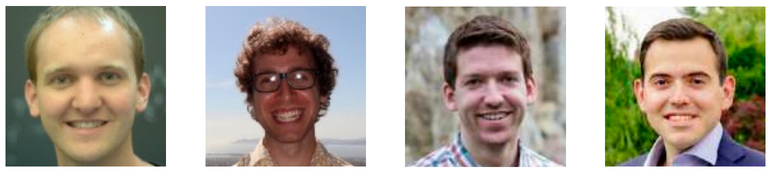
OmniFold

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



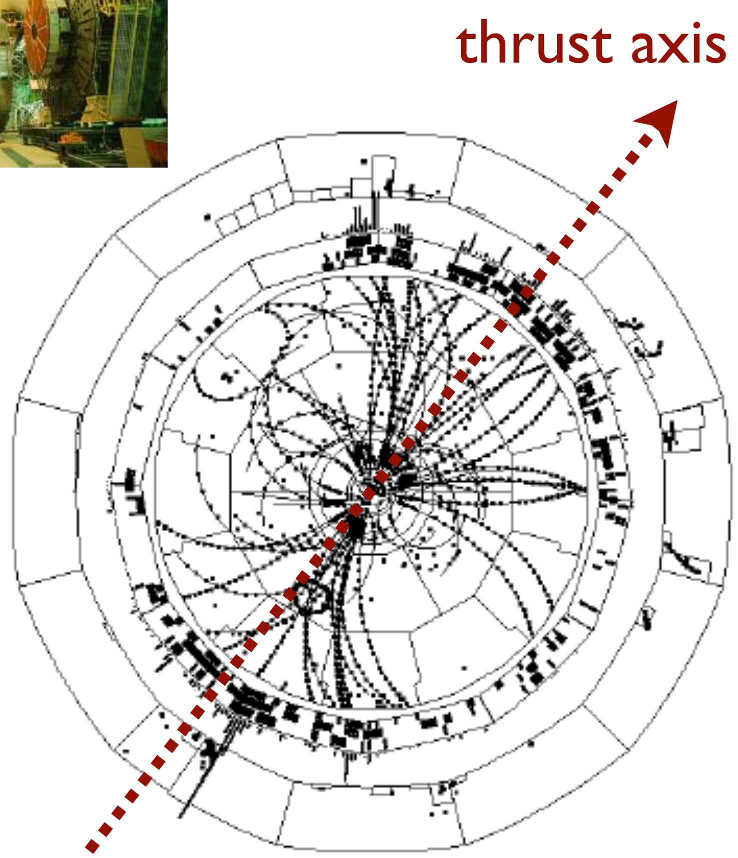
Use ML to compute reweighting factors

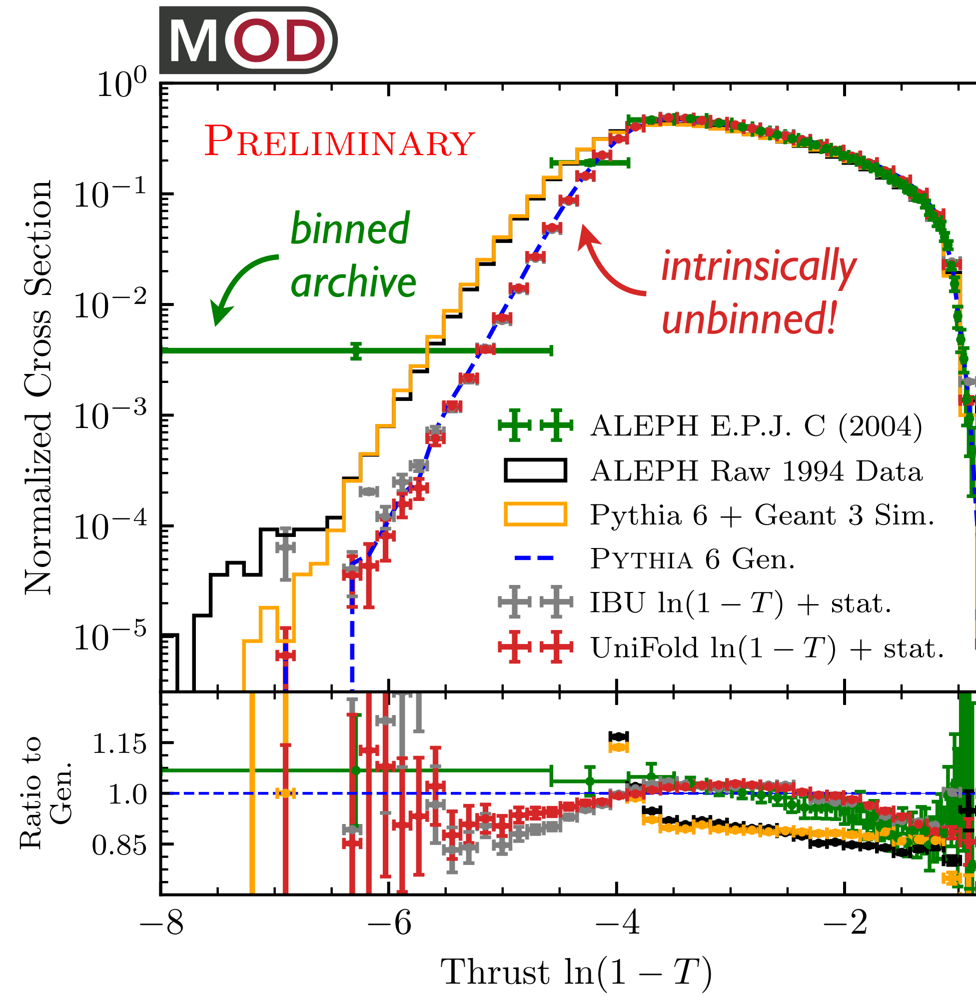
[Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020]

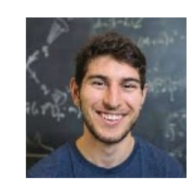


E.g. Detector Unfolding

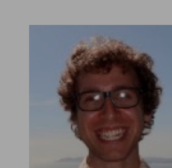
Back to the Future with ALEPH Archival Data





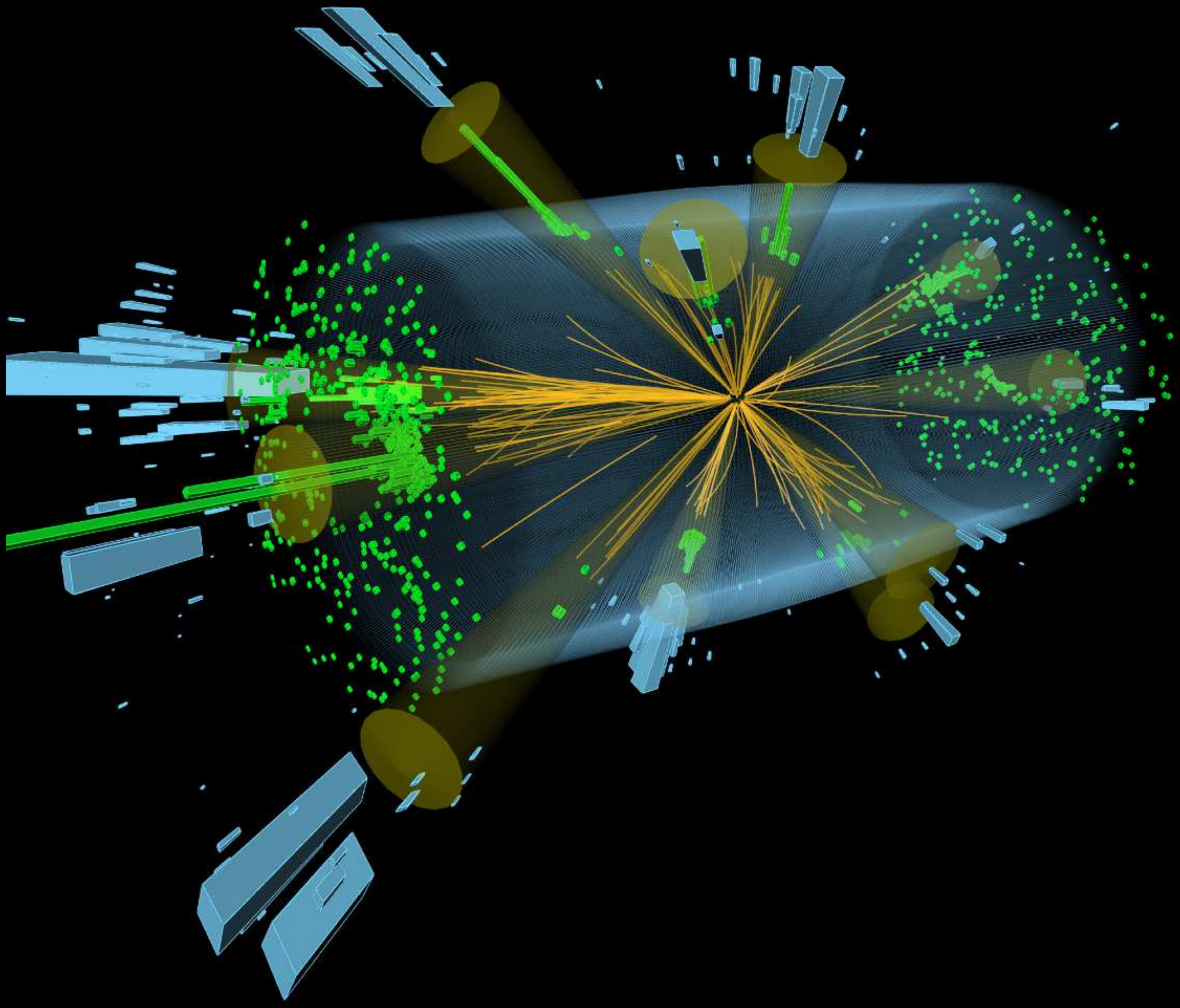


[talk by Badea, ICHEP 2020; cf. ALEPH, EPJC 2004]
[see also Badea, Baty, Chang, Innocenti, Maggi, McGinn, Peters, Sheng, JDT, Lee, PRL 2019]

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

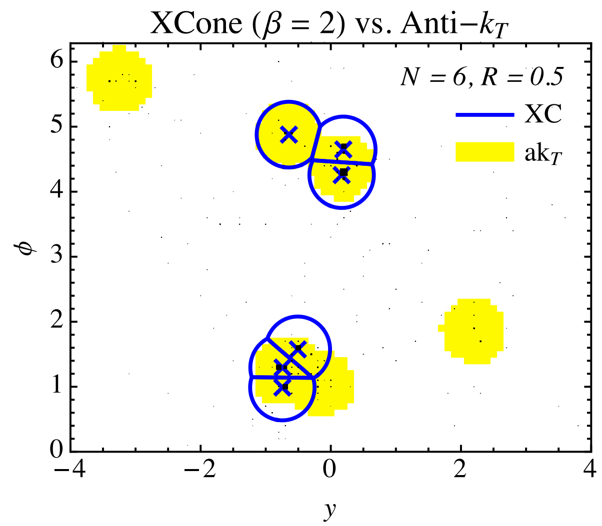
Machine Learning for QCD and Jets



What collider tasks can be phrased as optimization problems?

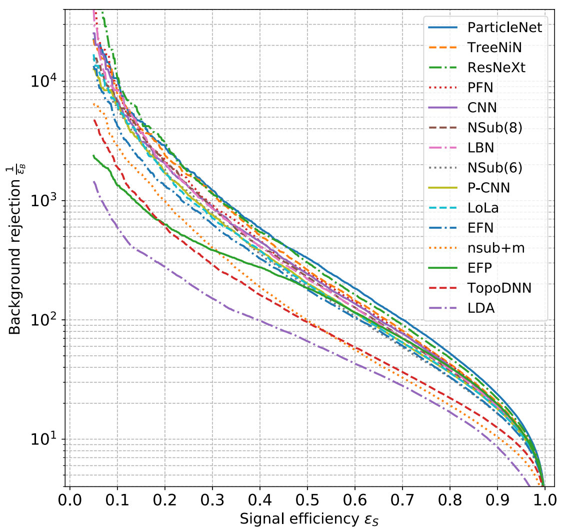
Optimization for QCD and Jets

Jet Algorithms



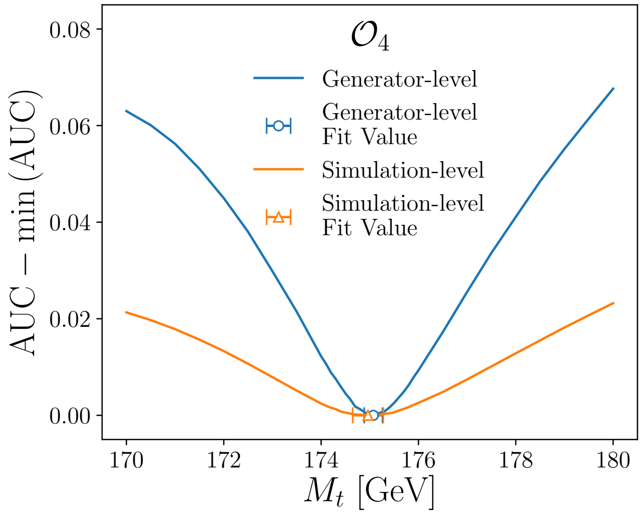
[e.g. Stewart, Tackmann, JDT, Vermilion, Wilkason, JHEP 2015]

Jet Classification



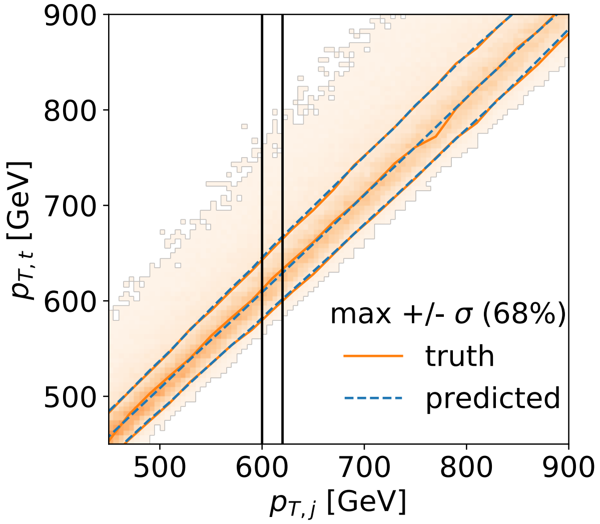
[e.g. Kasieczka, Plehn, et al., SciPost 2019]

Parameter Estimation



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

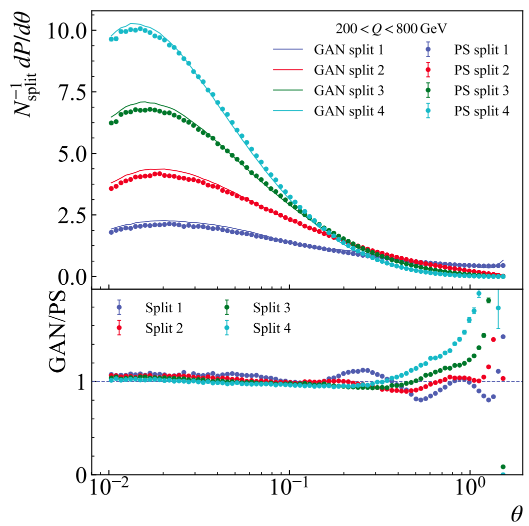
Uncertainty Quantification



[e.g. Kasieczka, Luchmann, Otterpohl, Plehn, SciPost 2020]

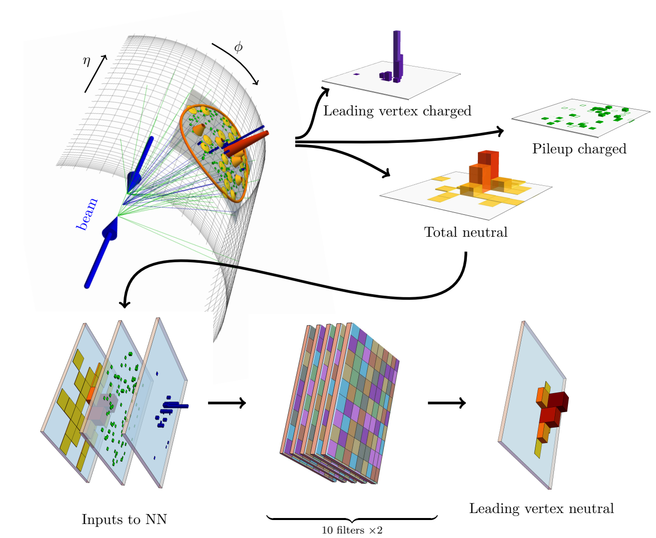
More Optimization for QCD and Jets

Parton Shower Modeling/Tuning



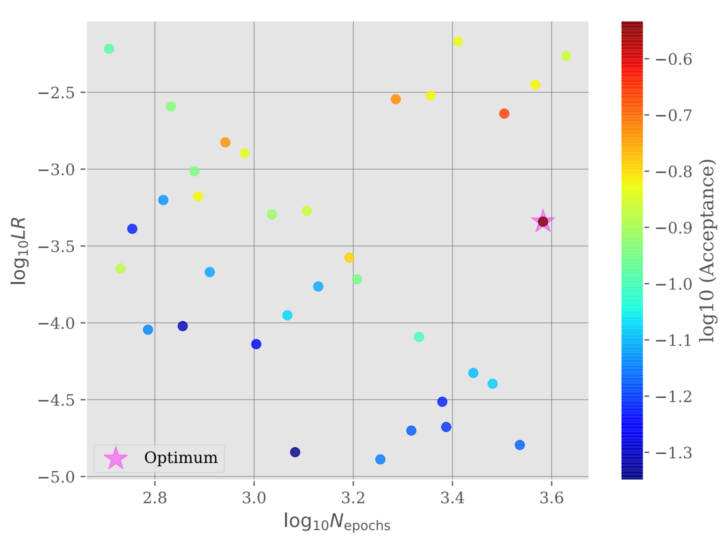
[e.g. Lai, Neill, Płoskoń, Ringer, arXiv 2020]

Pileup Mitigation



[e.g. Komiske, Metodiev, Nachman, Schwartz, JHEP 2017]

Phase Space Integration



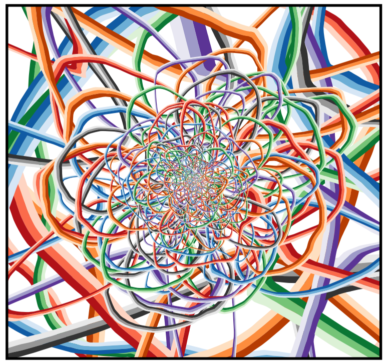
[e.g. Gao, Höche, Isaacson, Krause, Schulz, PRD 2020]

Amplitude Calculations

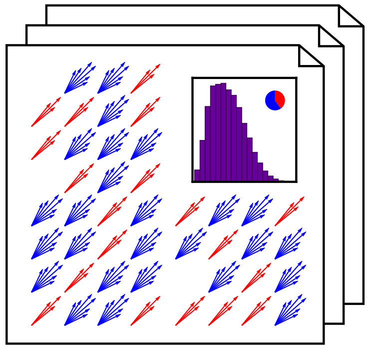
?

From Curmudgeon to Evangelist

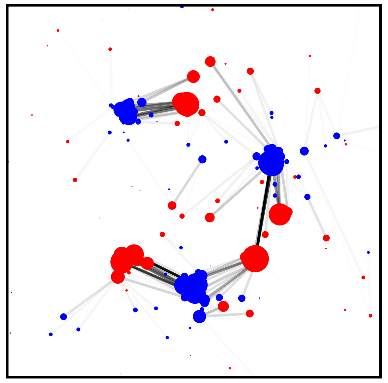
What have been helpful guides in pursing ML ⇔ QCD?



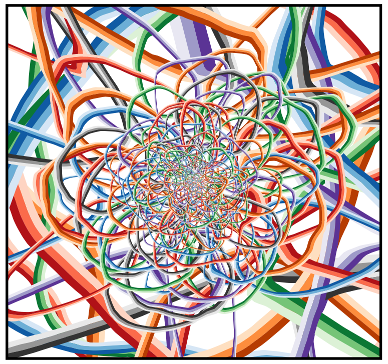
Can theoretical structures be encoded directly?



Can strategy be defined on physical final states?



Can we leverage unsupervised machine learning?



Can theoretical structures be encoded directly?

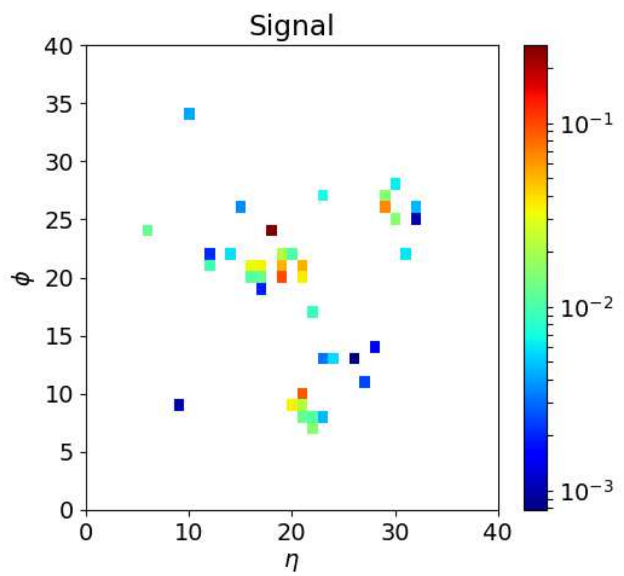
Can strategy be defined on physical final states?

Can we leverage unsupervised machine learning?

Jet Representations

Pixelized Image

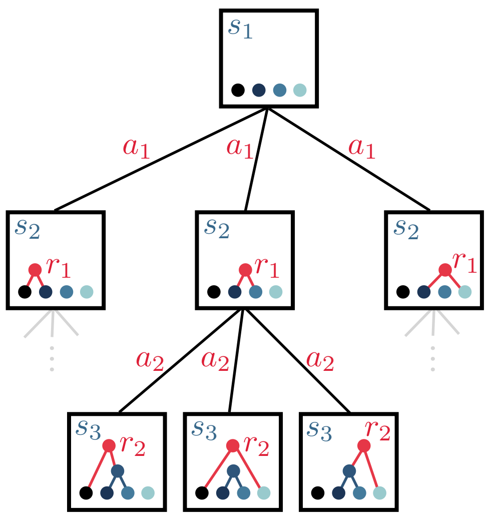
Calorimetry



[review in Kagan, arXiv 2020]

Hierarchical Tree

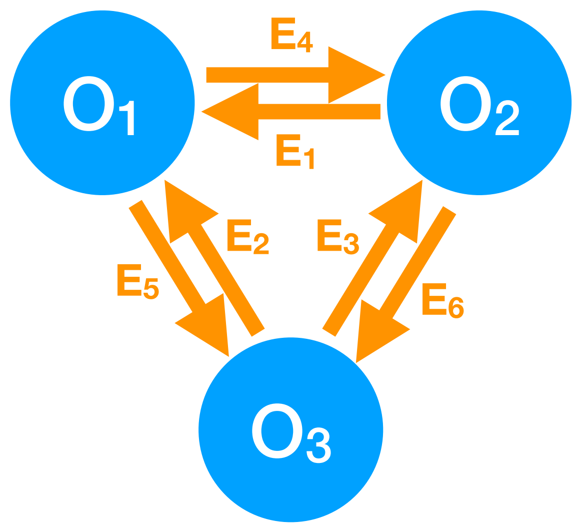
Binary Splittings



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

Graphs

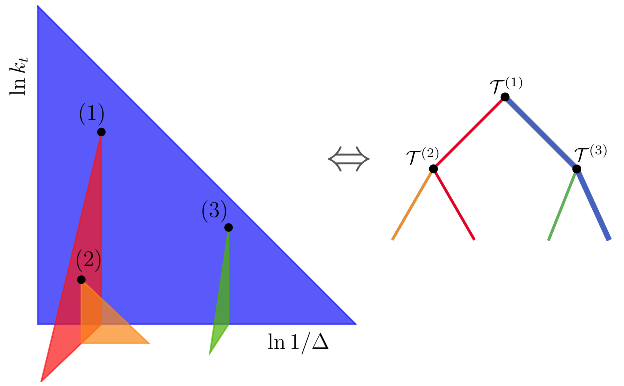
Pairwise Interactions



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

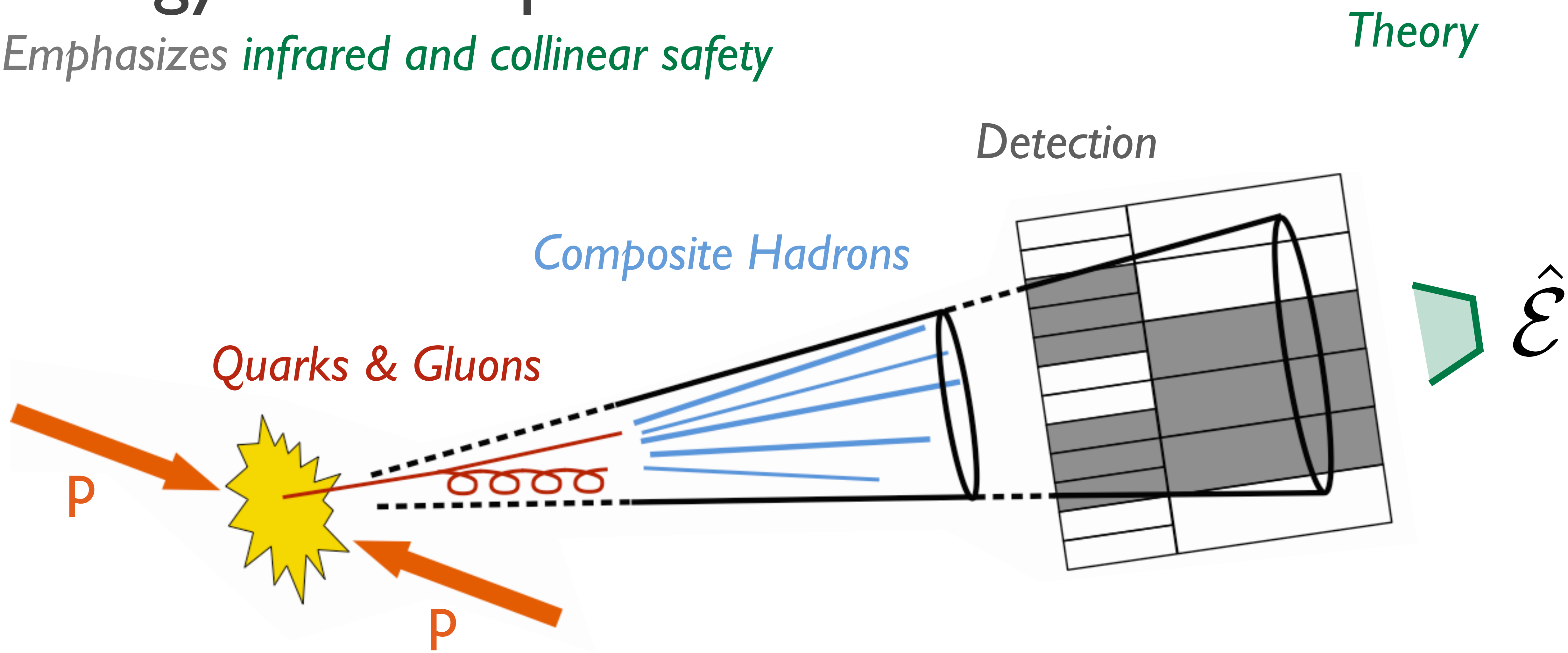
Imposes implicit theoretical prior; affects choice of network architecture

See Frédéric's talk for
Lund Plane + Graph Networks



Energy Flow Representation

Emphasizes infrared and collinear safety



Energy Flow:

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

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

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

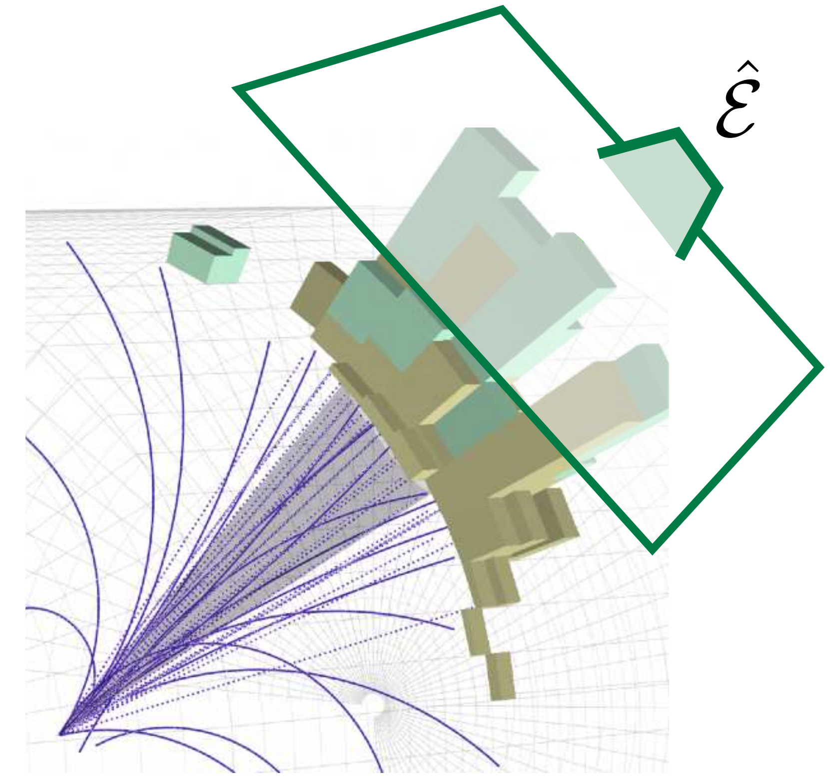
Jets as Weighted Point Clouds

- Energy-Weighted Directions

$$\vec{p} = \{E, \underbrace{\hat{n}_x, \hat{n}_y, \hat{n}_z}_{\text{Direction}}\}$$

Energy

(suppressing "unsafe" charge/flavor information)

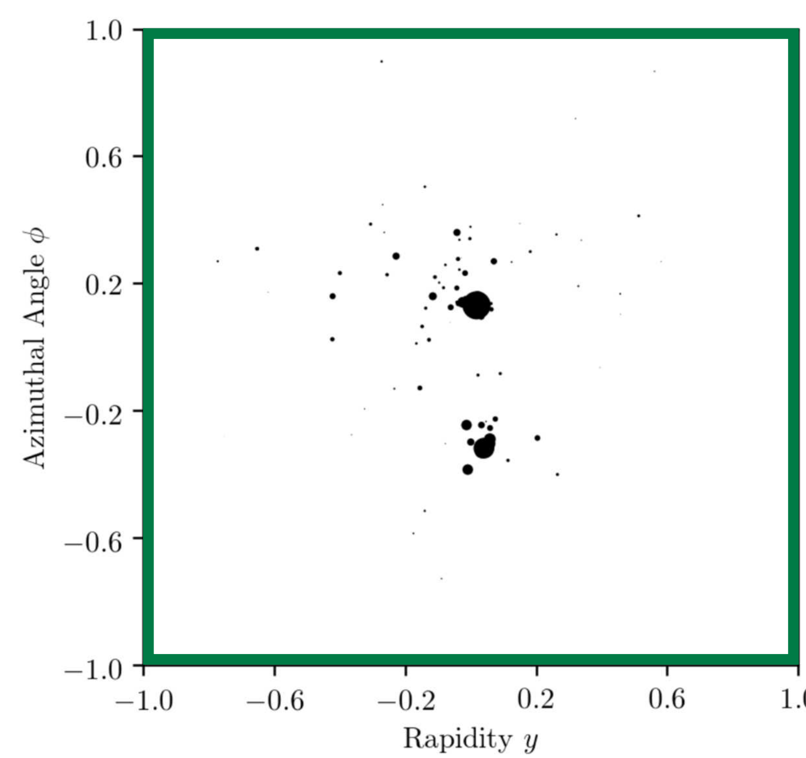


- Equivalently: Energy Density

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

Energy

Direction



Energy Flow Networks

Architecture designed around symmetries and interpretability

Permutation invariant

Linear weights (i.e. safe)

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

Parametrized with Neural Networks

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

[Komiske, Metodiev, JDT, JHEP 2019; see also Komiske, Metodiev, JDT, JHEP 2018; code at energyflow.network; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, NIPS 2017; other set-based architecture in Qu, Gouskos, PRD 2020; Mikuni, Canelli, EPJP 2020; Dolan, Ore, arXiv 2020; Lorentz-equivariant approach in Bogatskiy, Anderson, Offermann, Roussi, Miller, Kondor, arXiv 2020]

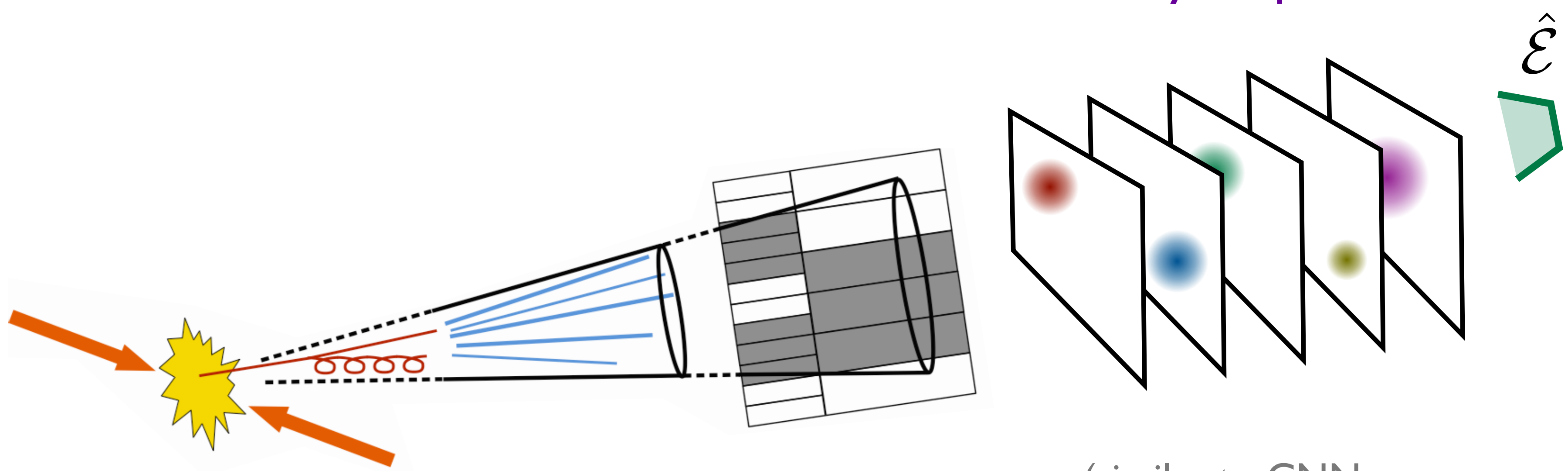
Energy Flow Networks

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

Latent space of dim ℓ

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

Easy to plot!



(similar to CNN filter activation)

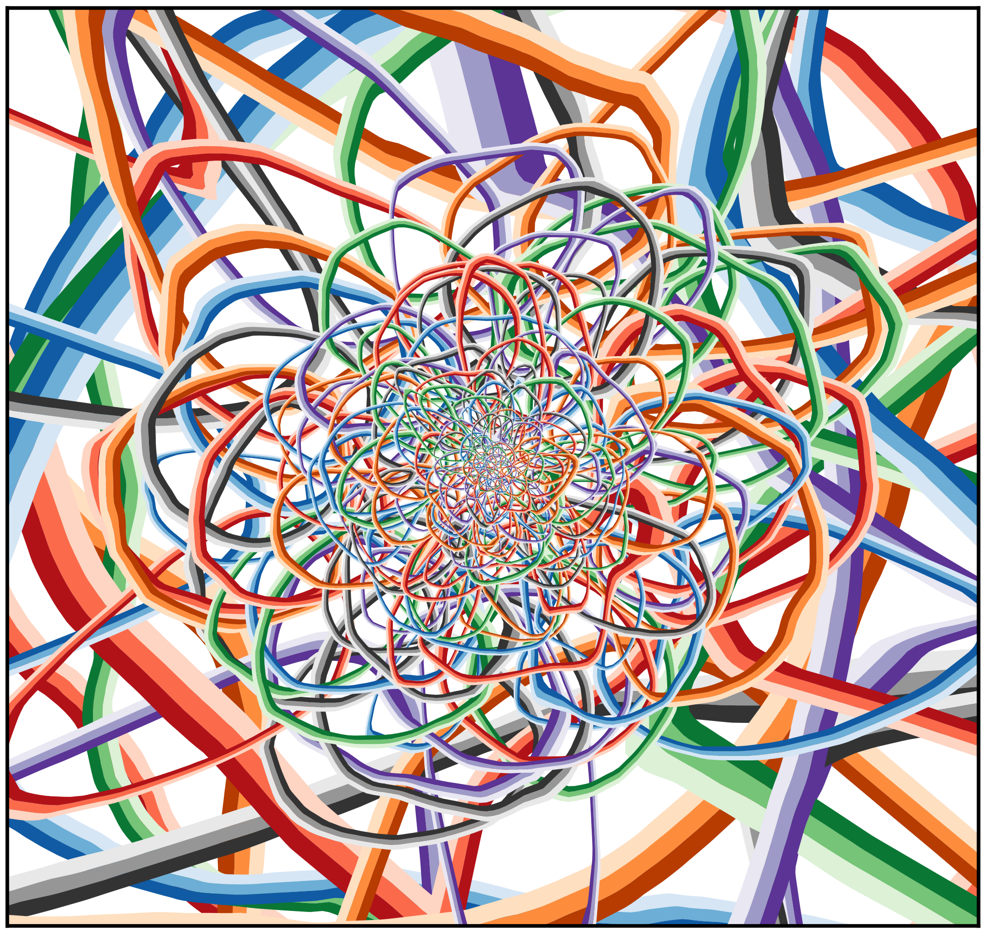
[Komiske, Metodiev, JDT, JHEP 2019; see also Komiske, Metodiev, JDT, JHEP 2018; code at energyflow.network; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, NIPS 2017; other set-based architecture in Qu, Gouskos, PRD 2020; Mikuni, Canelli, EPJP 2020; Dolan, Ore, arXiv 2020; Lorentz-equivariant approach in Bogatskiy, Anderson, Offermann, Roussi, Miller, Kondor, arXiv 2020]

Energy Flow Networks

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

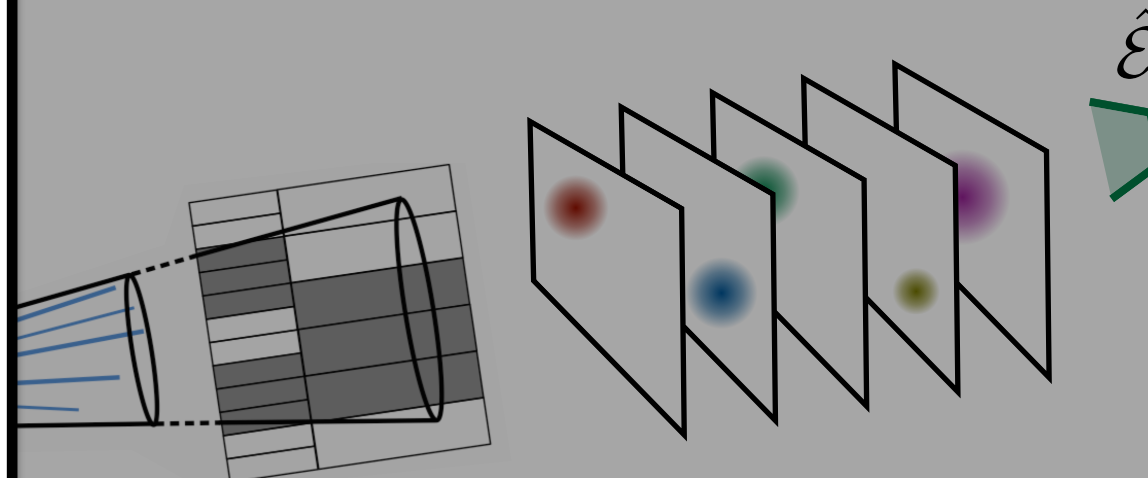
Psychedelic Network Visualization

Latent Dimension 256



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

Easy to plot!



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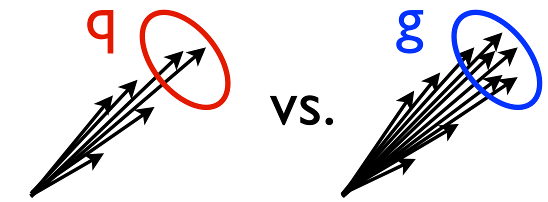
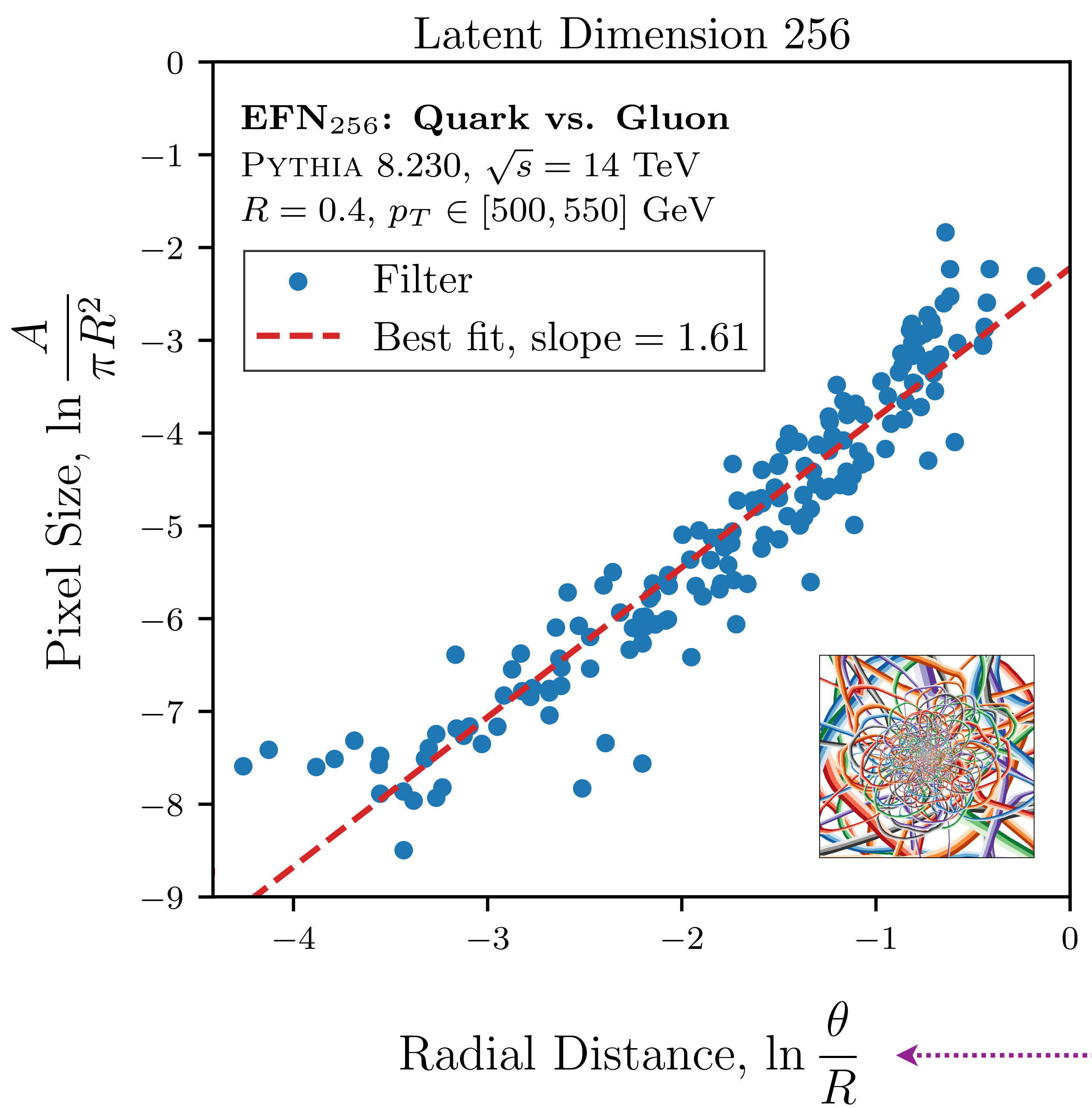
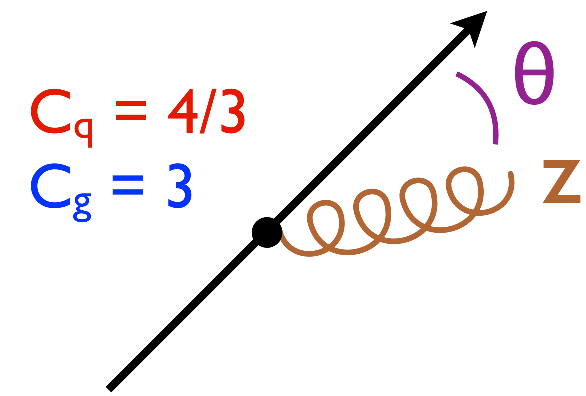
Lorentz-equivariant approach in Bogatskiy, Anderson, Offermann, Roussi, Miller, Kondor, arXiv 2020]

Machine Learning Collinear QCD



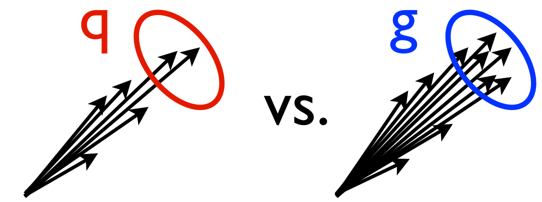


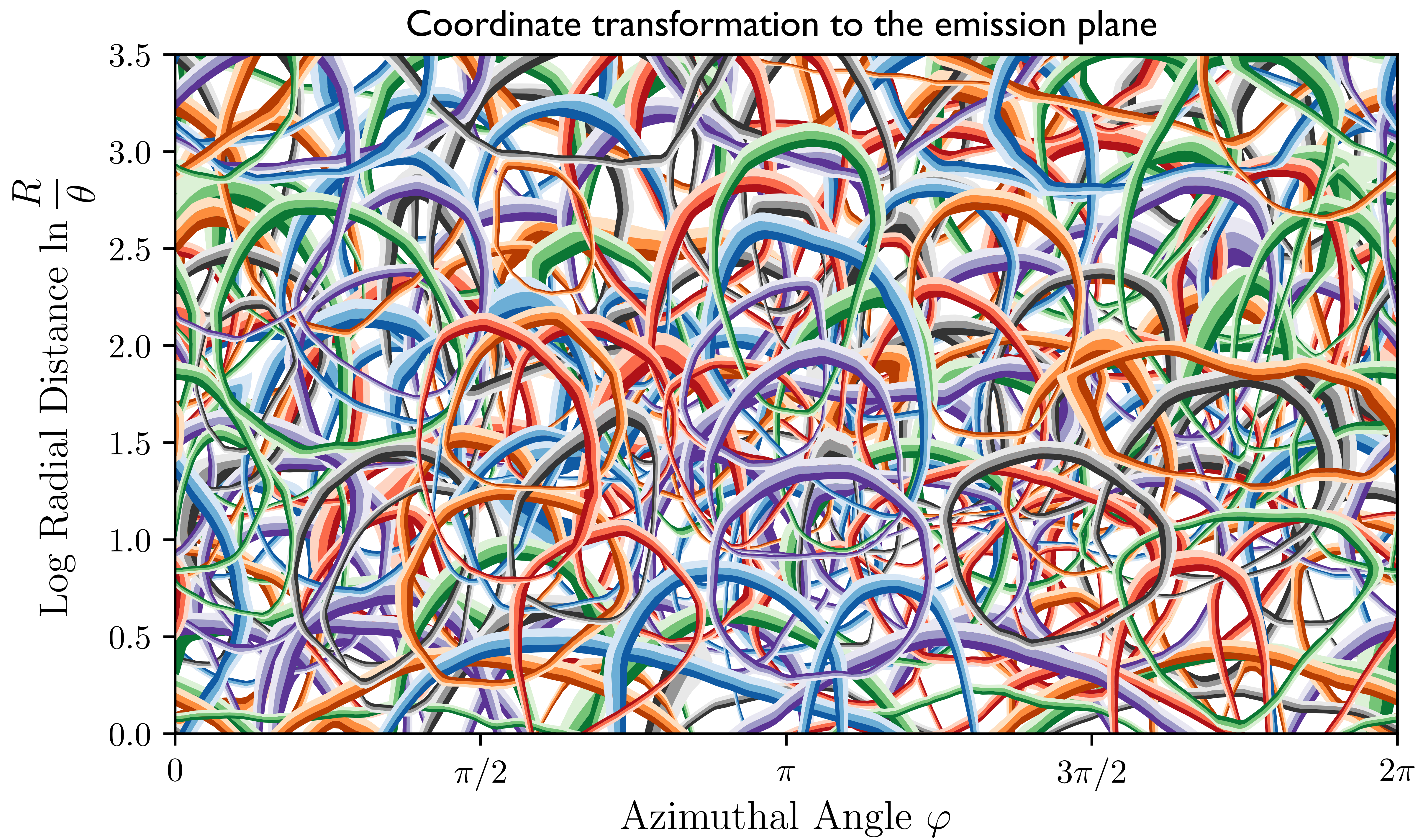


$$\mathrm{d}P_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{\mathrm{d}\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{\mathrm{d}z}{z}}_{\text{Soft}}$$

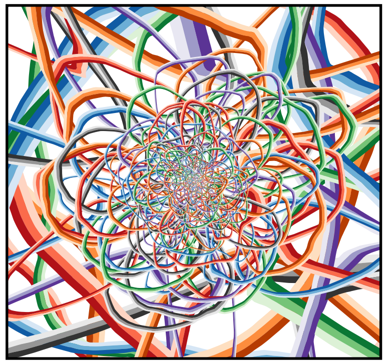
[Komiske, Metodiev, JDT, JHEP 2019]

En Route to the Lund Plane





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



Can theoretical structures be encoded directly?

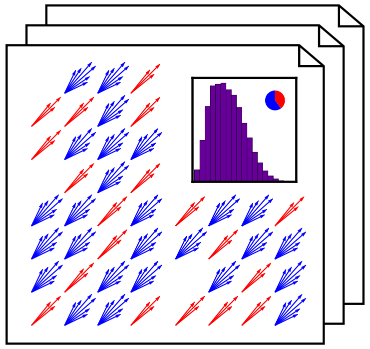
Energy Flow Networks ⇔ IRC Safety + Permutations

Can strategy be defined on physical final states?

Can we leverage unsupervised machine learning?

Can theoretical structures be encoded directly?

Energy Flow Networks ⇔ IRC Safety + Permutations



Can strategy be defined on physical final states?

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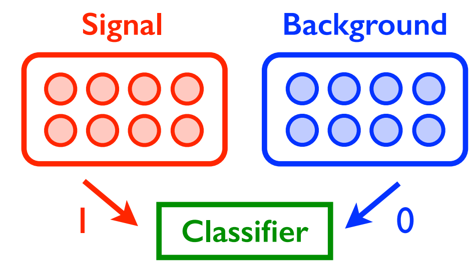
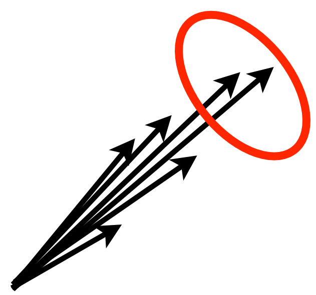
Quark/Gluon Classification

"Hello, World!" of Jet Physics

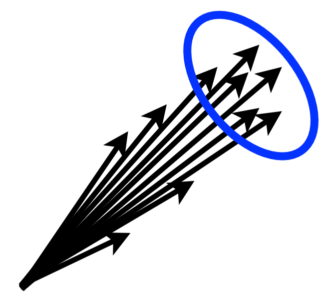


e.g.

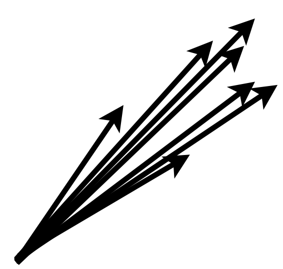


Quark
$C_q = 4/3$

vs.



Gluon
$C_g = 3 = 9/3$

Find $h\Big($  $\Big)$ such that

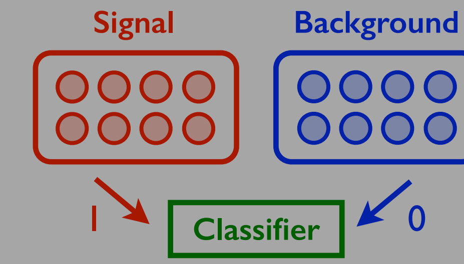
$$h(\text{Quark}) = 1$$

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

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

(Neyman-Pearson lemma)

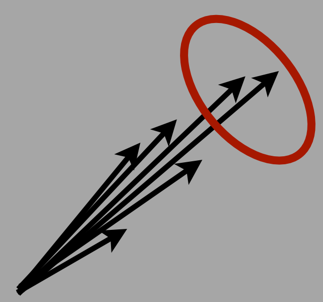
[see e.g. Gras, Höche, Kar, Larkoski, Lönnblad, Plätzer, Siódmok, Skands, Soyez, JDT, JHEP 2017; Komiske, Metodiev, Schwartz, JHEP 2017; Komiske, Metodiev, JDT, JHEP 2018]



Quark/Gluon Classification

“Hello, World!” of Jet Physics

e.g.



Quark
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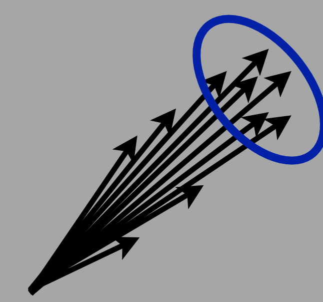


Gluon
$C_g = 3 = 9/3$

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

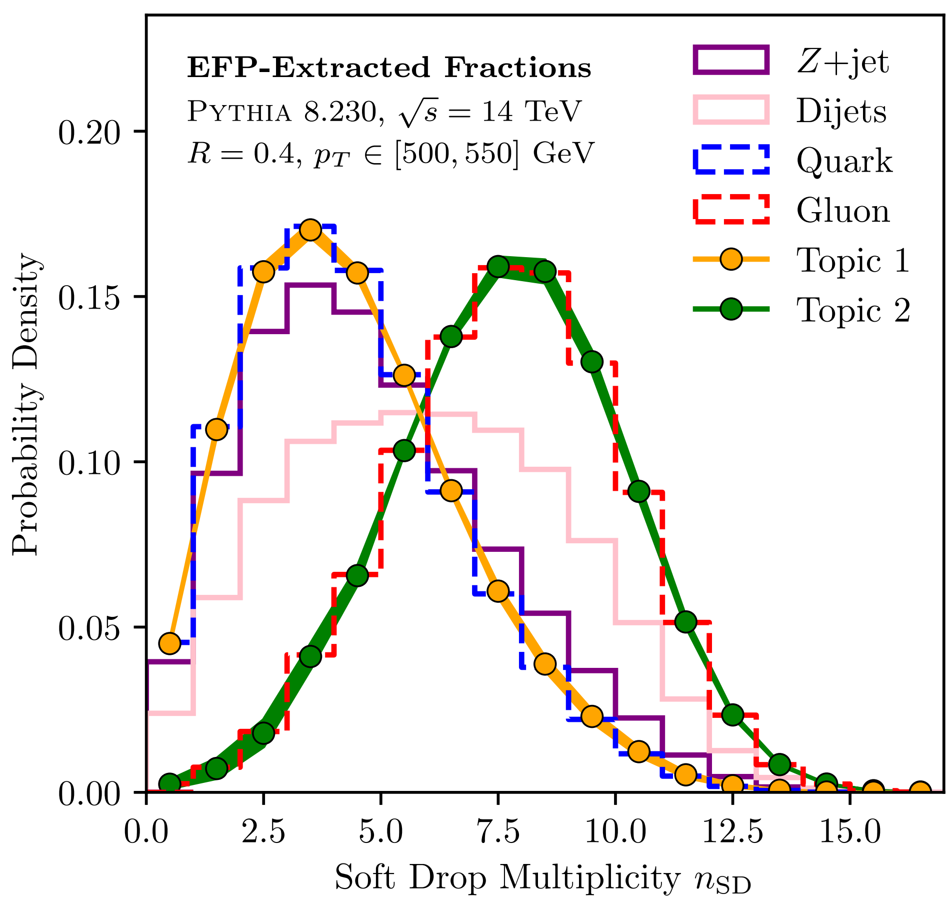
Jets are clusters of colorless hadrons!

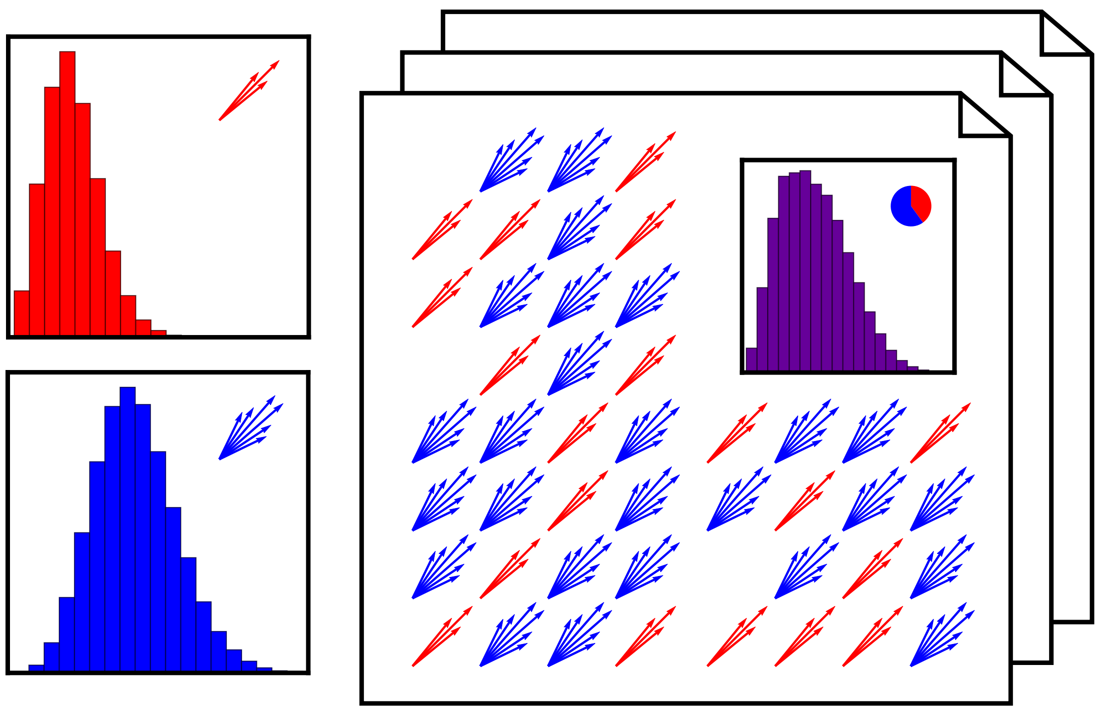
Parton shower “truth” is but a (useful) fiction!

[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



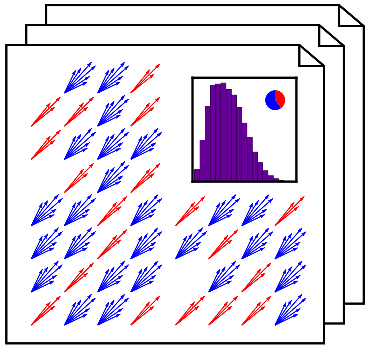


Key concept from natural language processing: "anchor words"

[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 ⇔ IRC Safety + Permutations



Can strategy be defined on physical final states?

Jet Topics ⇔ Hadron-Level Approach to QCD Partons

Can we leverage unsupervised machine learning?

Can theoretical structures be encoded directly?

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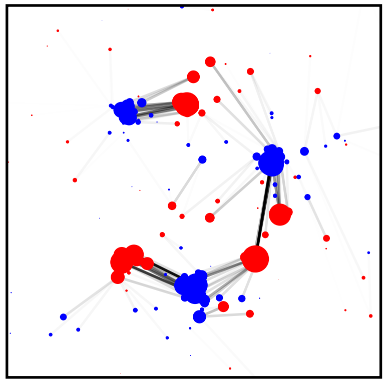

Can we leverage unsupervised machine learning?

The Earth Mover's Distance

Optimal Transport: Minimum "work" (stuff x distance) to make one distribution look like another distribution

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

Déblai

Remblai

[h/t Niles-Weed, ML4Jets 2020; Monge, 1781; Vaseršteĭn, 1969; Wikipedia]

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Additive Weight:

Ground Distance:

⇒ Distance Between Distributions

Déblai Remblai

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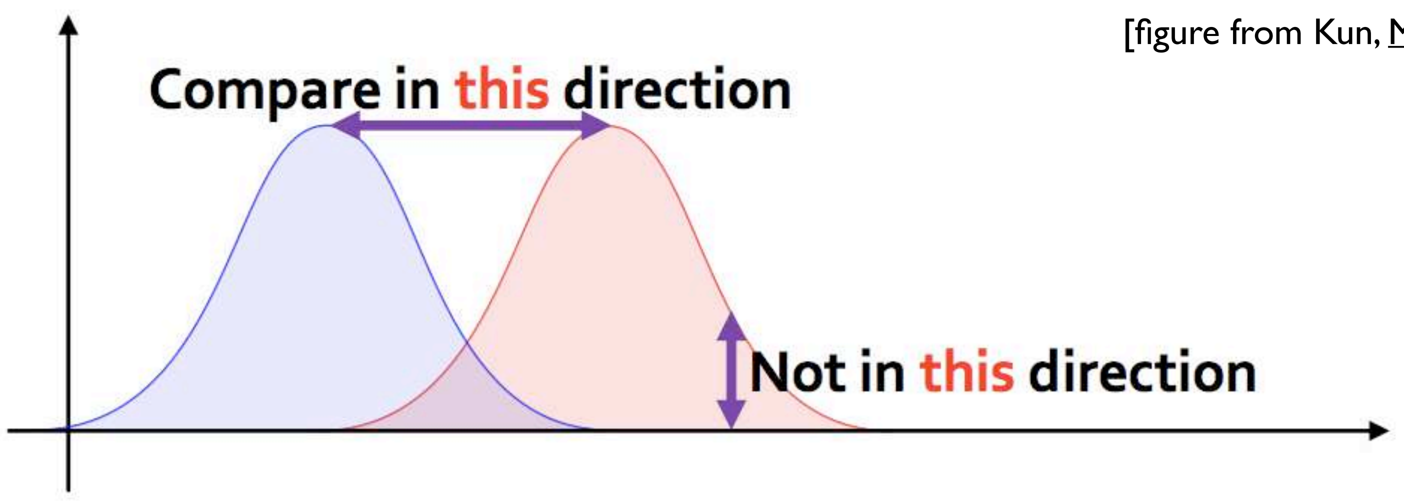
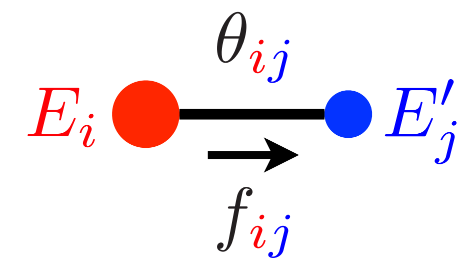
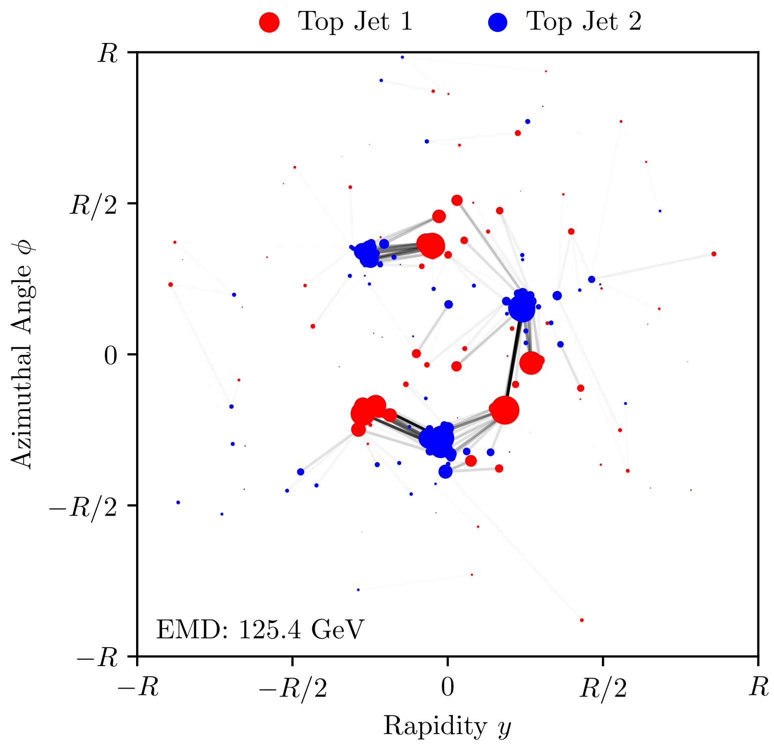


[figure from Kun, Math ∩ Programming]

[h/t Niles-Weed, ML4Jets 2020; Monge, 1781; Vaseršteĭn, 1969; Wikipedia]

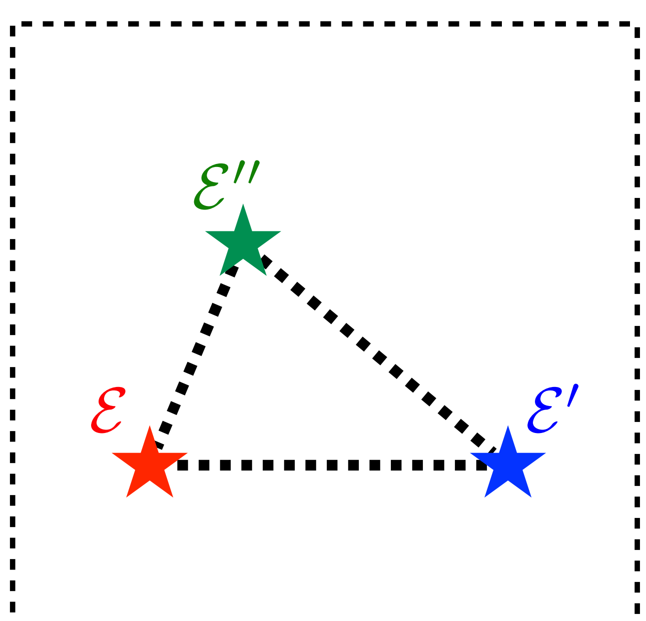
The Energy Mover's Distance





Optimal transport between energy flows…

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



…defines a metric on the space of events

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

(assuming R ≥ θ_{max}/2, i.e. R ≥ jet radius for conical jets)

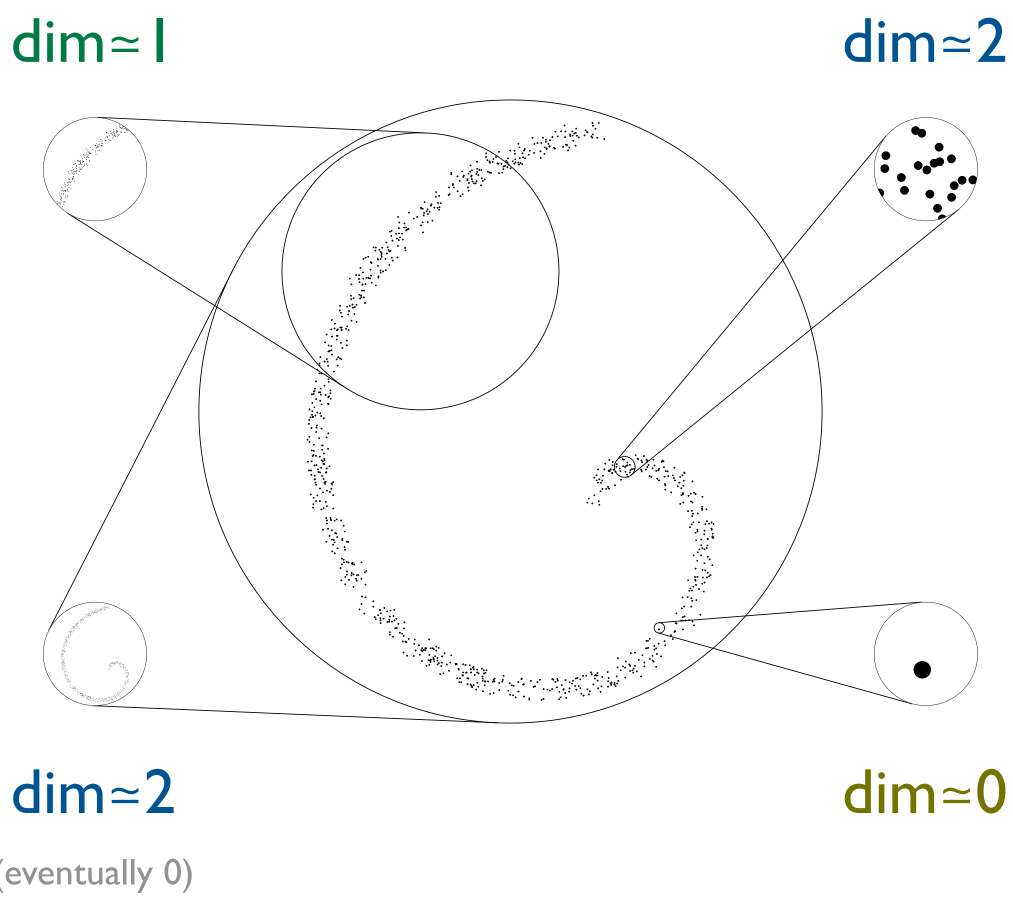
[Komiske, Metodiev, JDT, PRL 2019; see also Pele, Werman, ECCV 2008; Pele, Taskar, GSI 2013]
[see flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, EPJC 2021]
[see computational speed up in Cai, Cheng, Craig, Craig, PRD 2020]
[see graph network approach in Mullin, Pacey, Parker, White, Williams, arXiv 2019]

Dimensionality of Space of Jets

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

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

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



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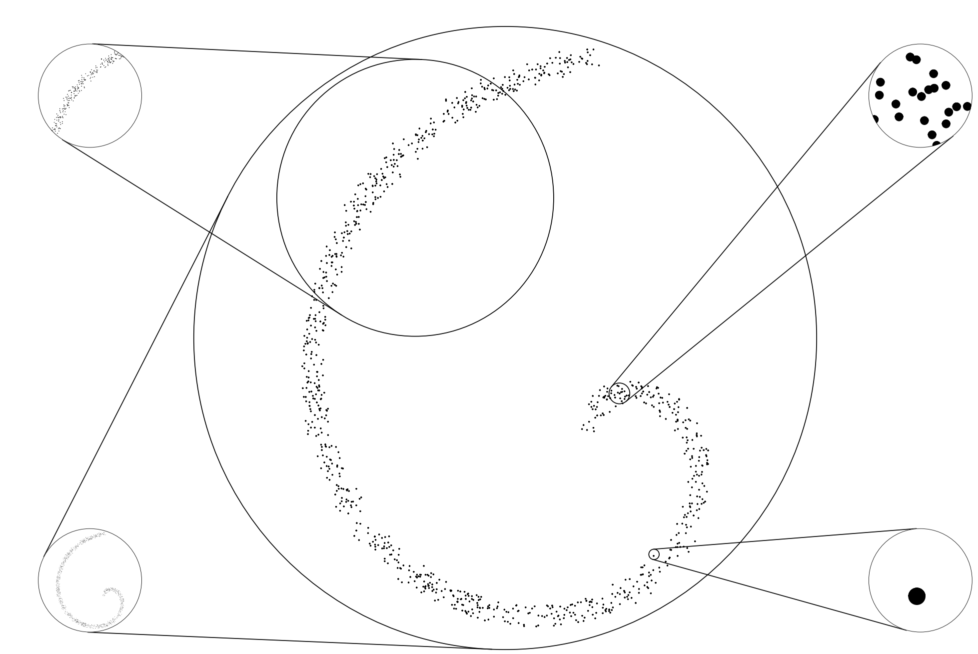
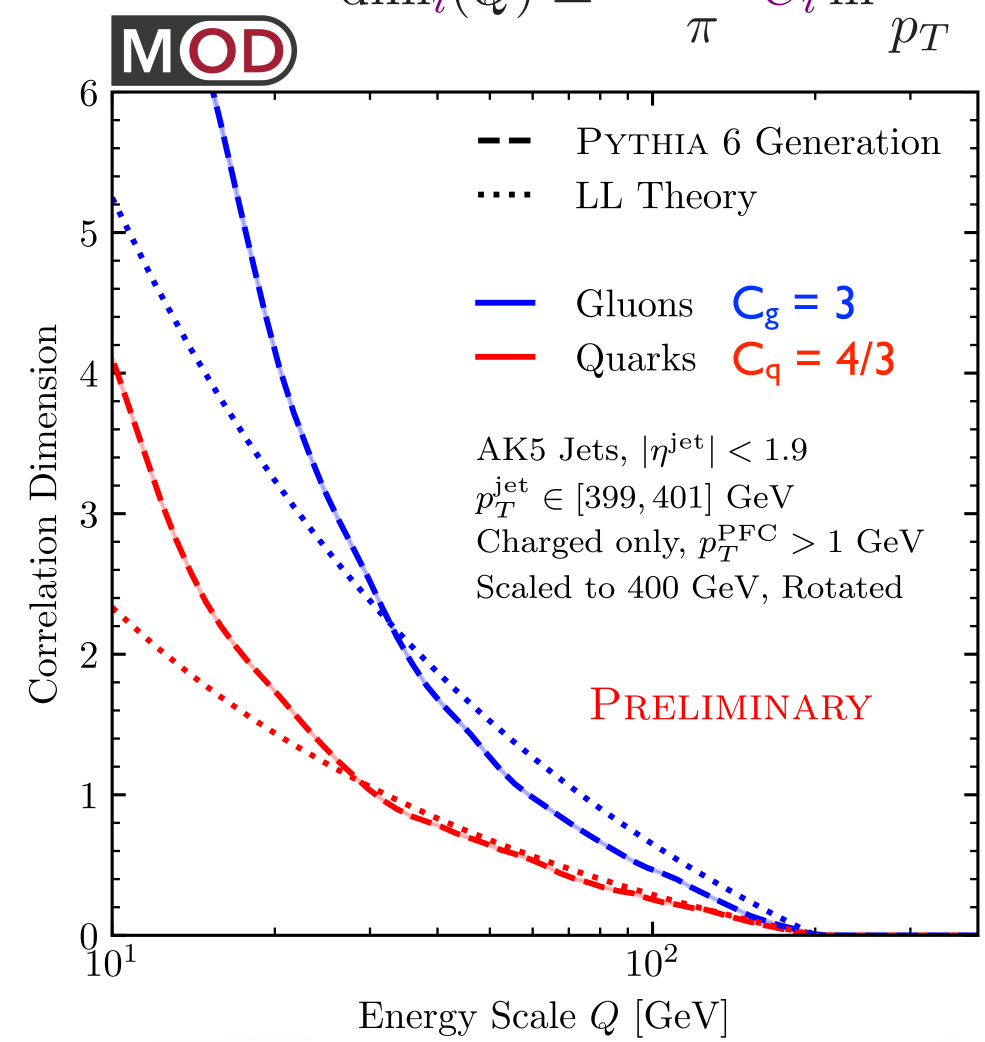
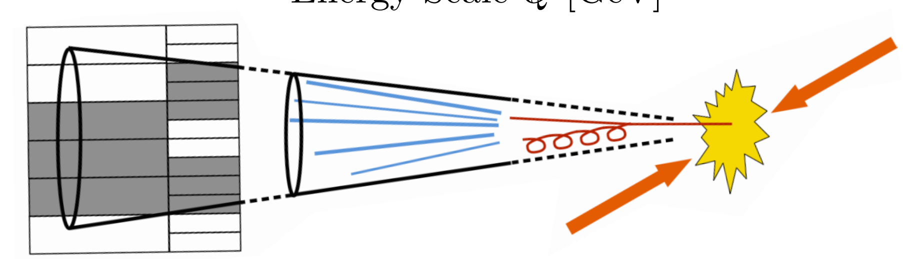


(eventually 0)

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





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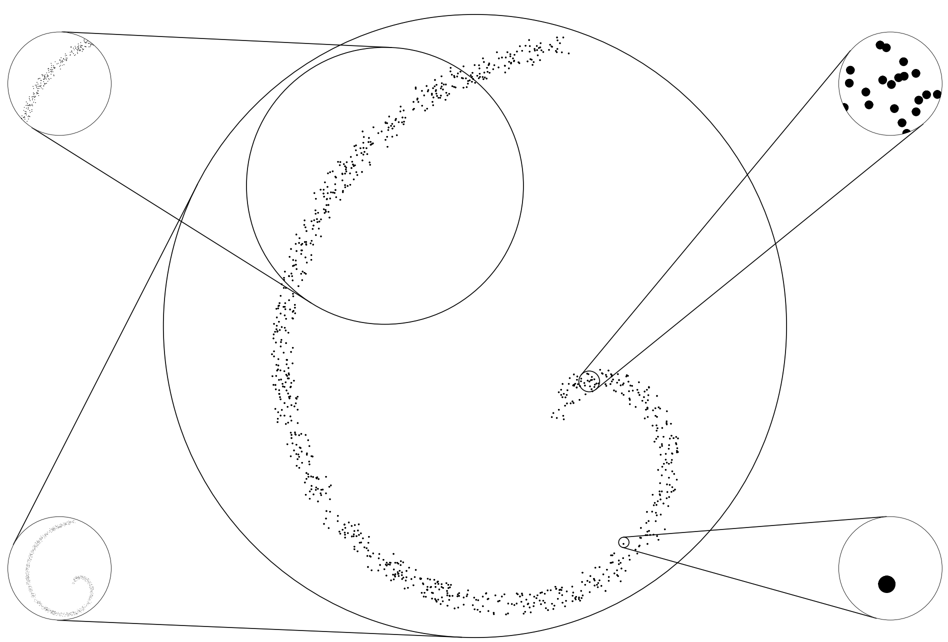
dim≃1

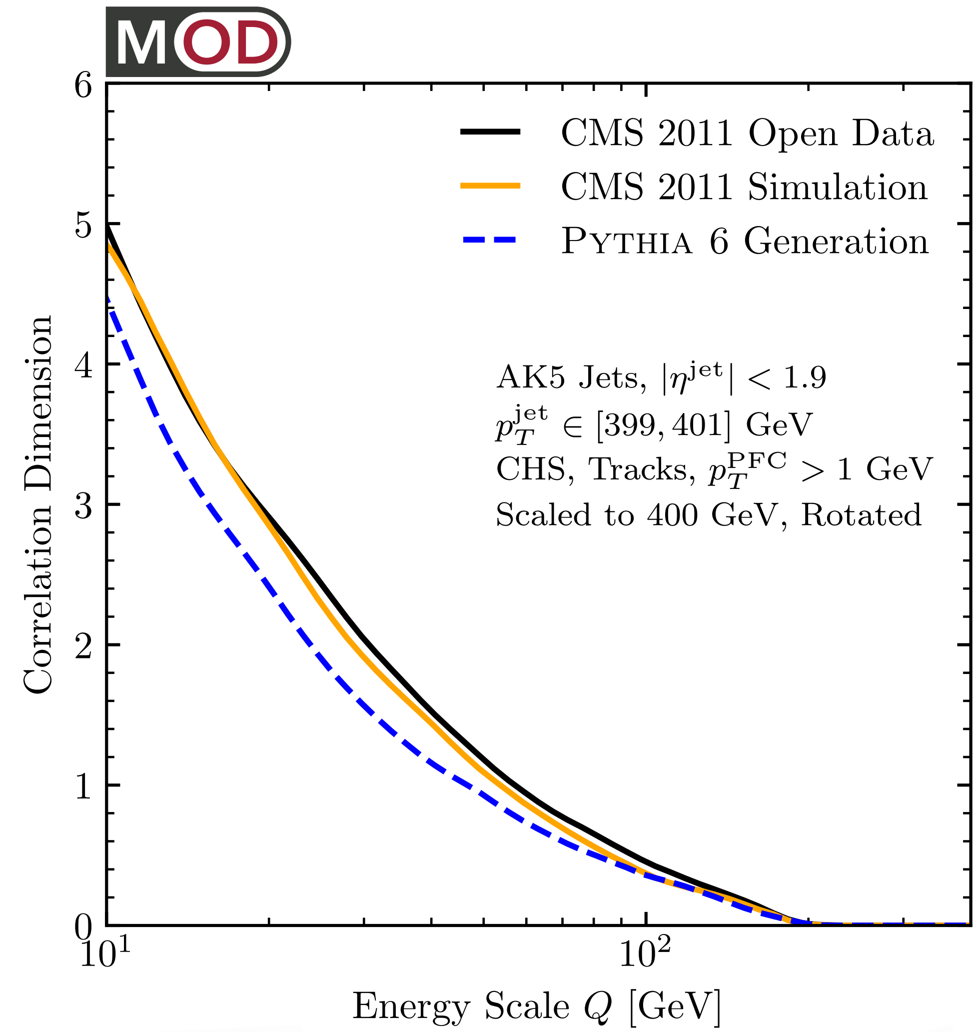
dim≃2

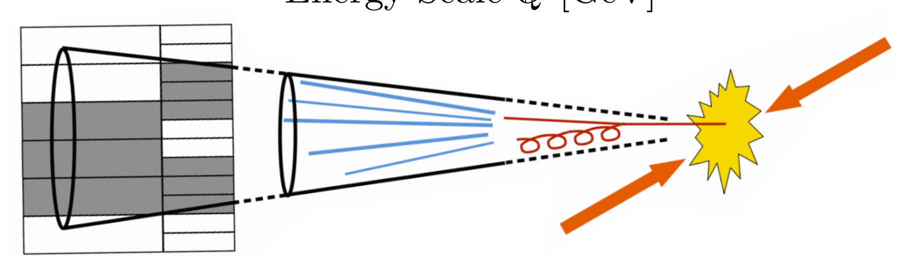


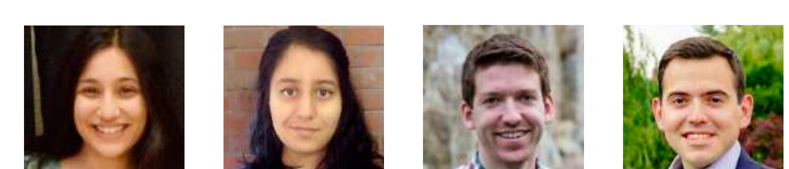
dim≃2

(eventually 0)

dim≃0





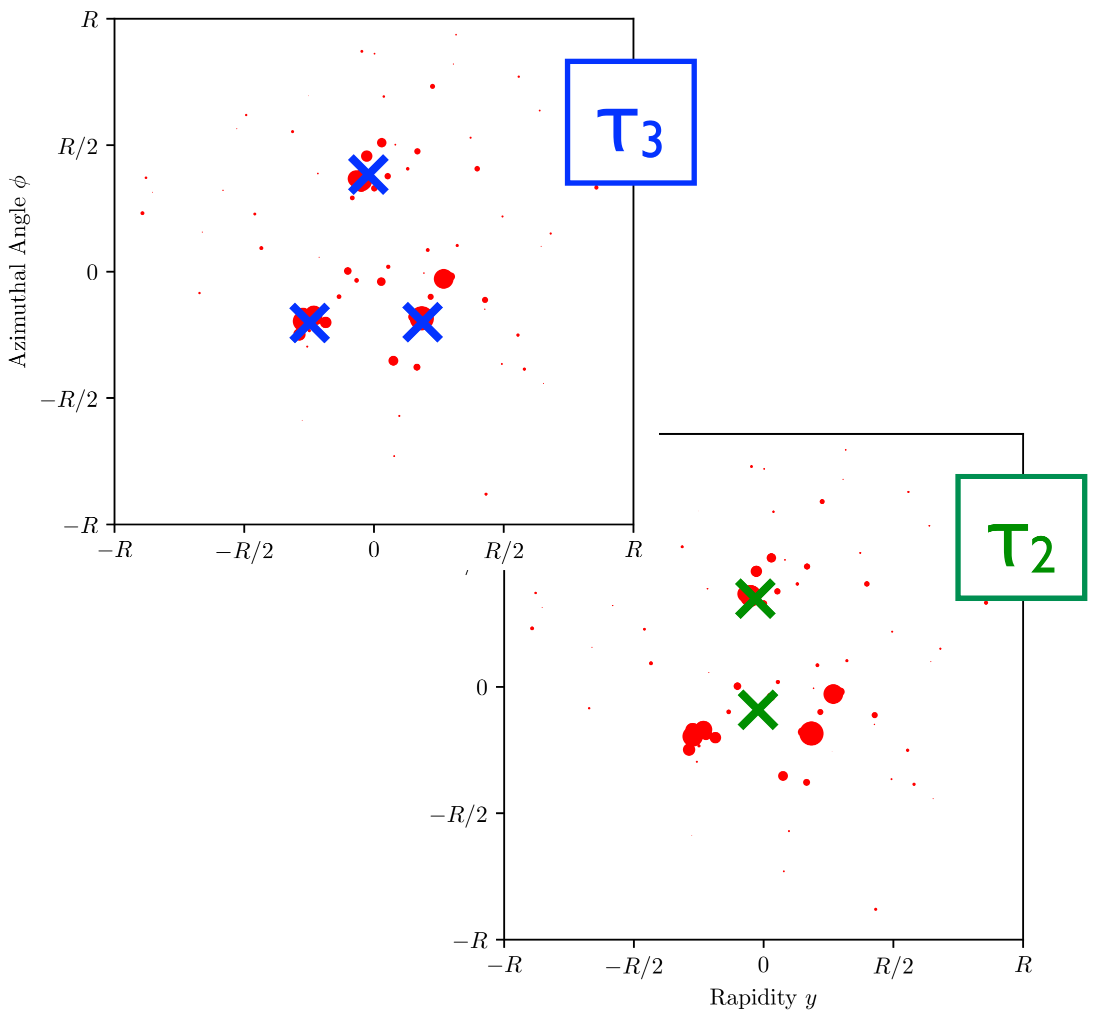


[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using CMS Open Data]

N-subjettiness

Ubiquitous jet substructure observable used for almost a decade…

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

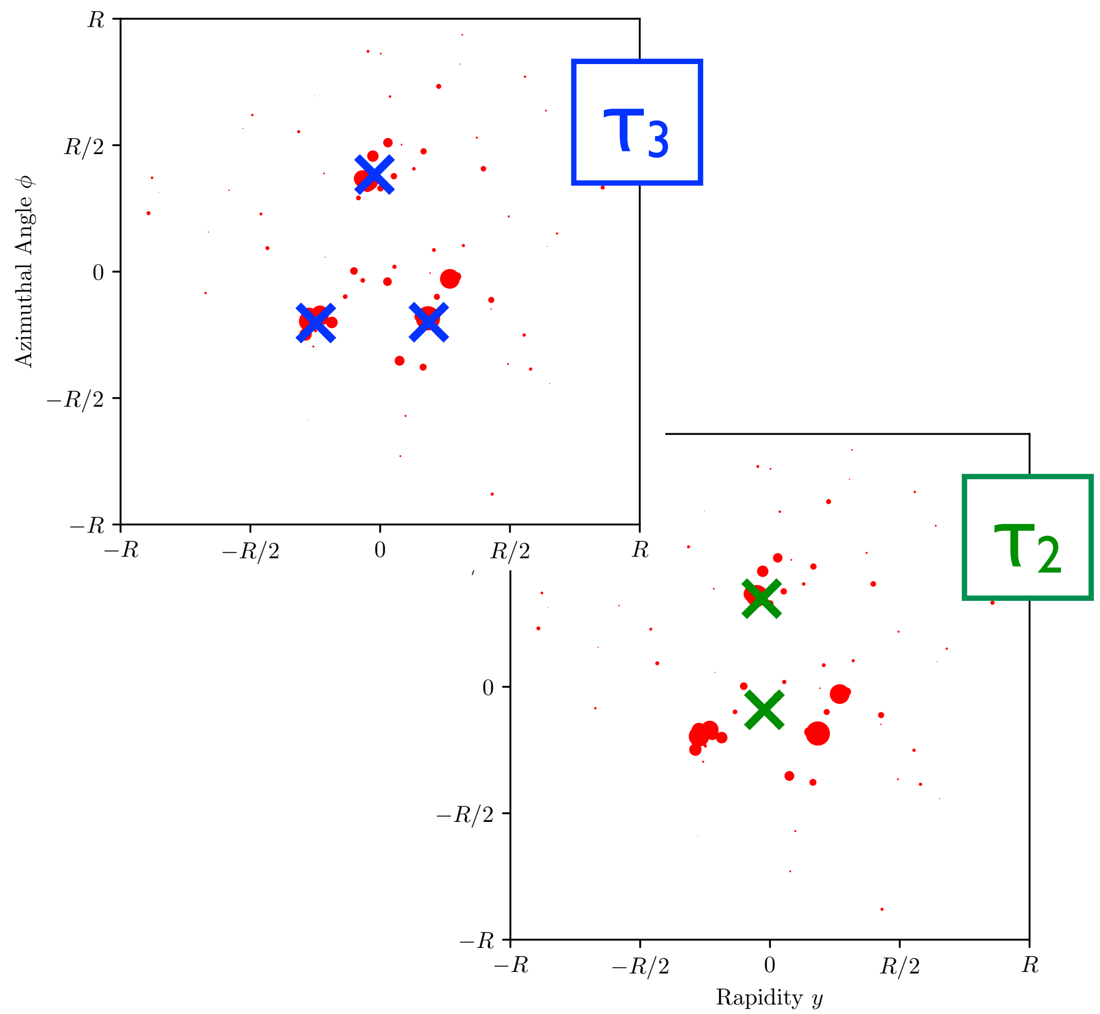


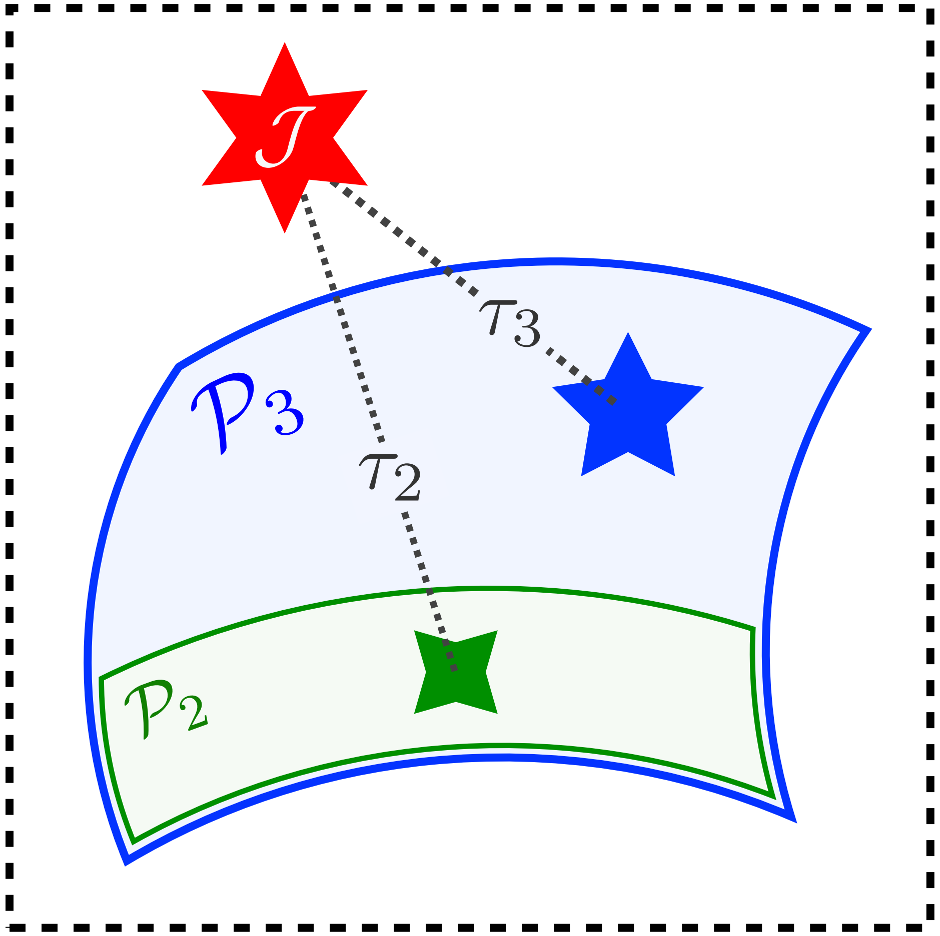
[JDT, Van Tilburg, JHEP 2011, JHEP 2012;
based on Brandt, Dahmen, ZPC 1979; Stewart, Tackmann, Waalewijn, PRL 2010]

N-subjettiness = Point to Manifold EMD

…is secretly an optimal transport problem

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

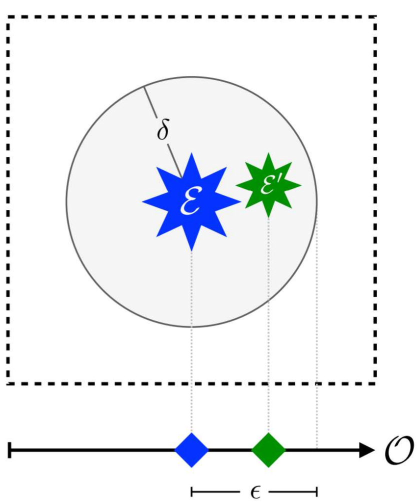




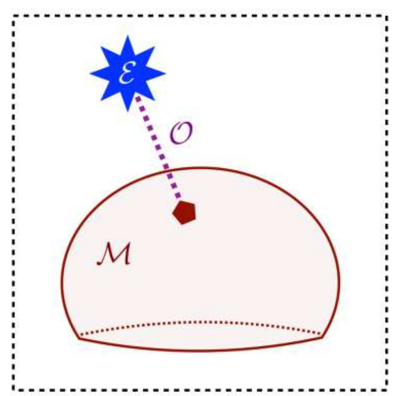
[JDT, Van Tilburg, JHEP 2011, JHEP 2012;
rephrased via Komiske, Metodiev, JDT, JHEP 2020; see opposite limit in Cesarotti, JDT, JHEP 2020]

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

IRC Safety is smoothness in the space of events

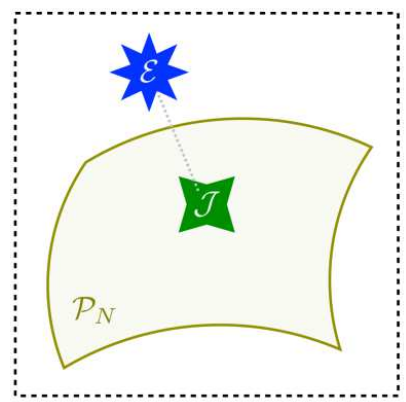


Event shapes are distances from events to manifolds.



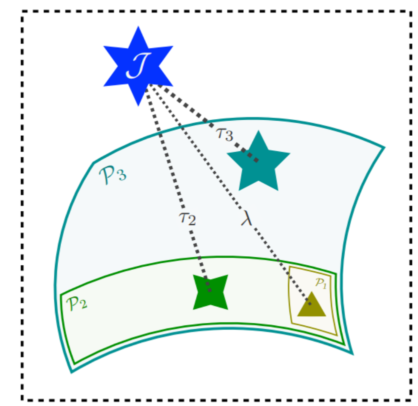
$$\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}'\in\mathcal{M}} \mathrm{EMD}_{\beta,R}(\mathcal{E},\mathcal{E}')$$

Jets are projections to few-particle manifolds.



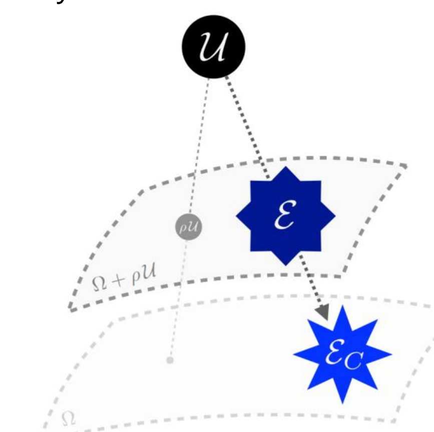
$$\mathcal{J} = \operatorname*{argmin}_{\mathcal{E}'\in\mathcal{P}_N} \mathrm{EMD}_{\beta,R}(\mathcal{E},\mathcal{E}')$$

Substructure resolves emissions within the jet.



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

Pileup mitigation moves away from uniform radiation.



$$\mathcal{E}_C = \arg\min_{\mathcal{E}'} \mathrm{EMD}(\mathcal{E},\mathcal{E}' + \rho\,\mathcal{U})\,.$$

Taming infinities | Event Shapes | Jet Algorithms | Jet Substructure | Pileup

1960 — 2020

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]
[Doskhitzer, Leder, Moretti,Webber, JHEP 1997]

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

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

And many more!

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

Can theoretical structures be encoded directly?

Energy Flow Networks ⇔ IRC Safety + Permutations

Can strategy be defined on physical final states?

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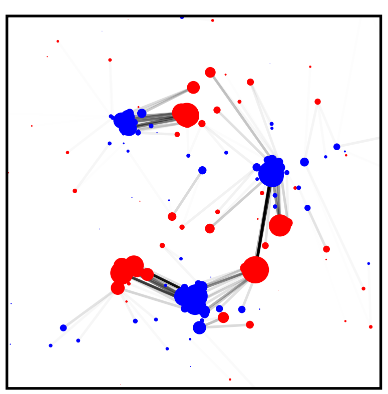
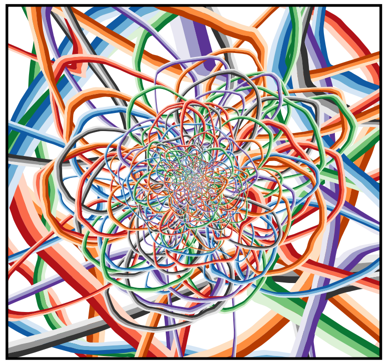


Can we leverage unsupervised machine learning?

Energy Mover's Distance ⇔ Geometric Strategies for Collider Physics

QCD and Jets through the Lens of ML



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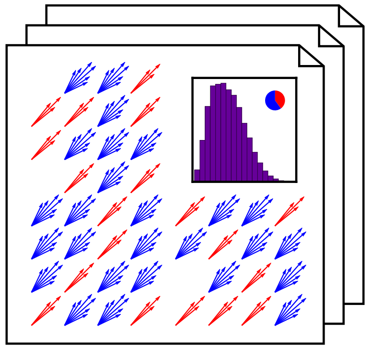

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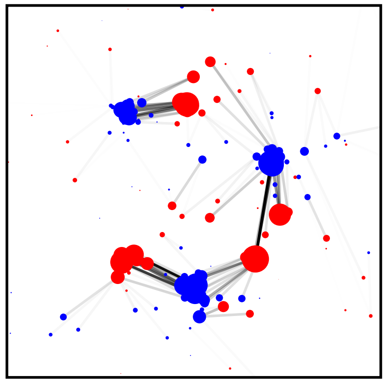

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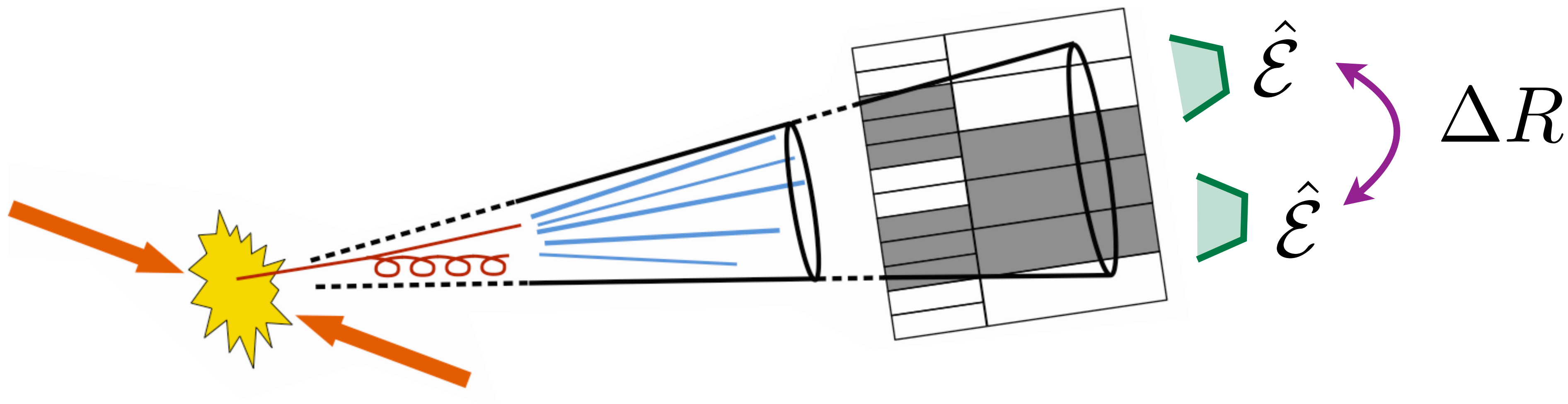
Energy Mover's Distance ⇔ Geometric Strategies for Collider Physics

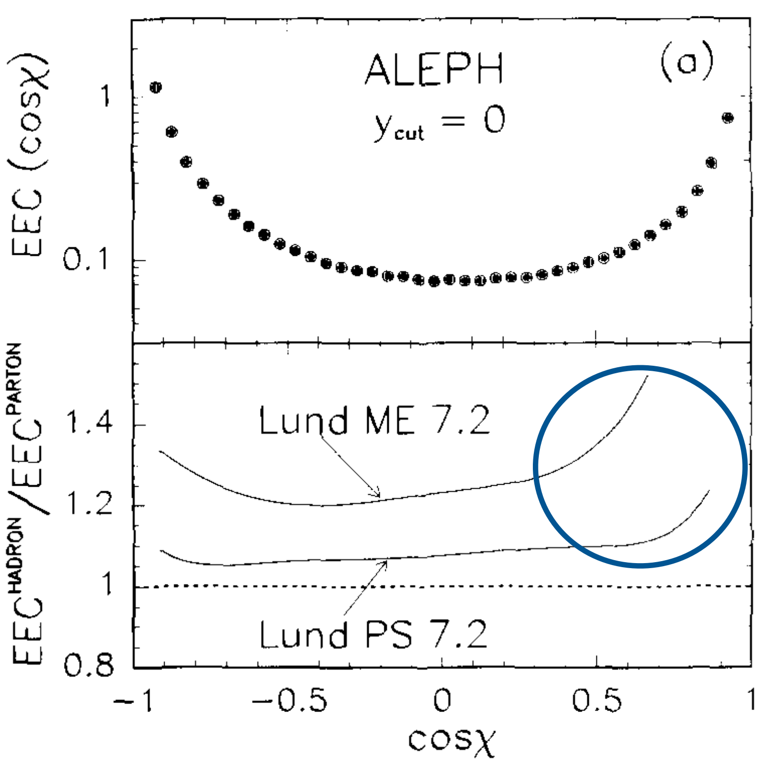
And now… Frédéric's perspective on ML ⇔ QCD!

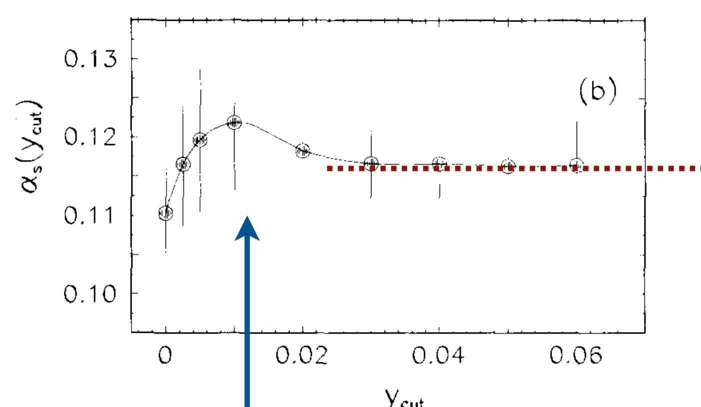
Backup Slides

Energy-Energy Correlators



A long history in probing collinear dynamics of QCD





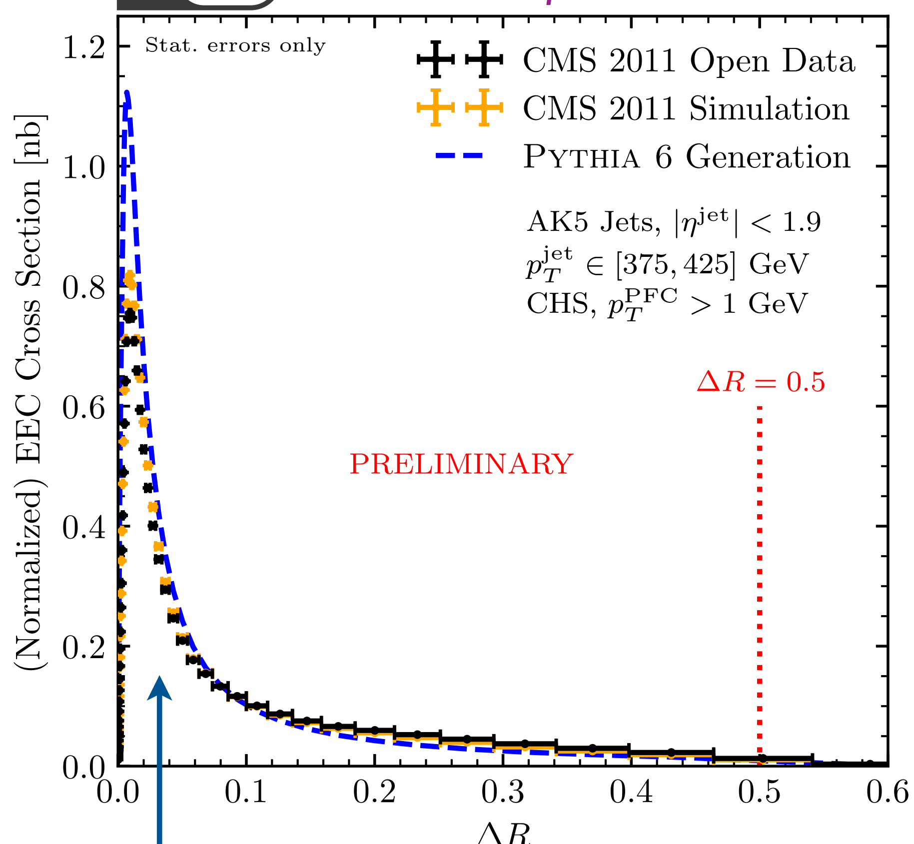
Extracting the strong coupling constant

Theoretical challenges with small angle (collinear) limit

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

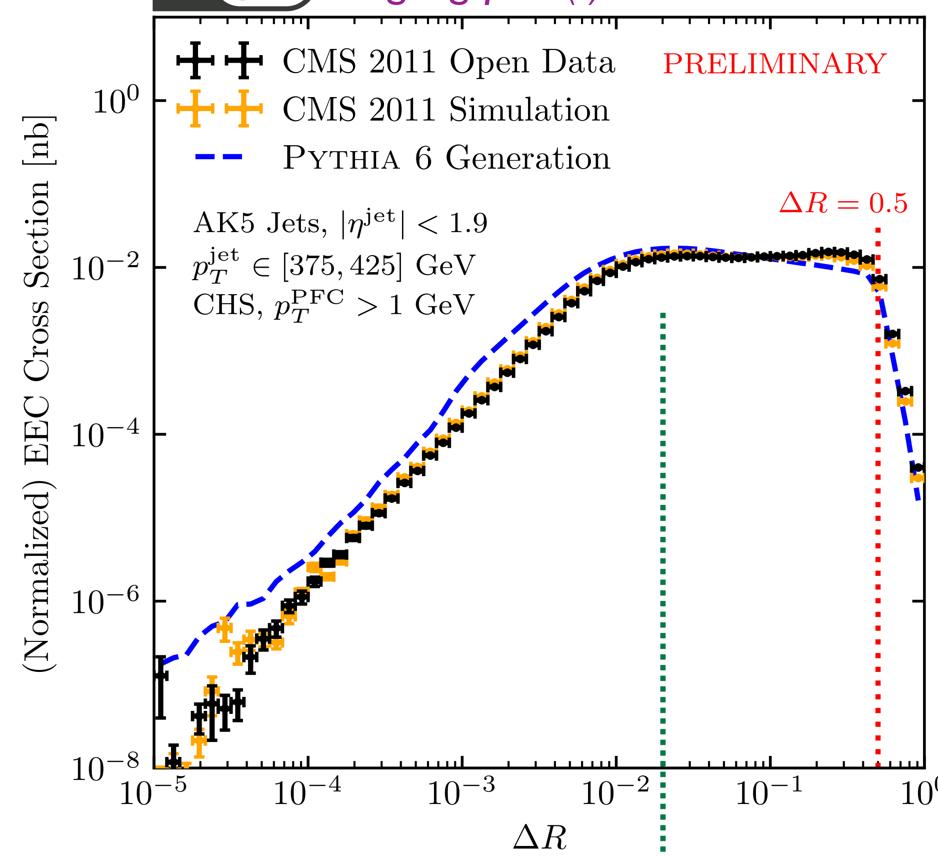
QCD Phase Transition in Jets?

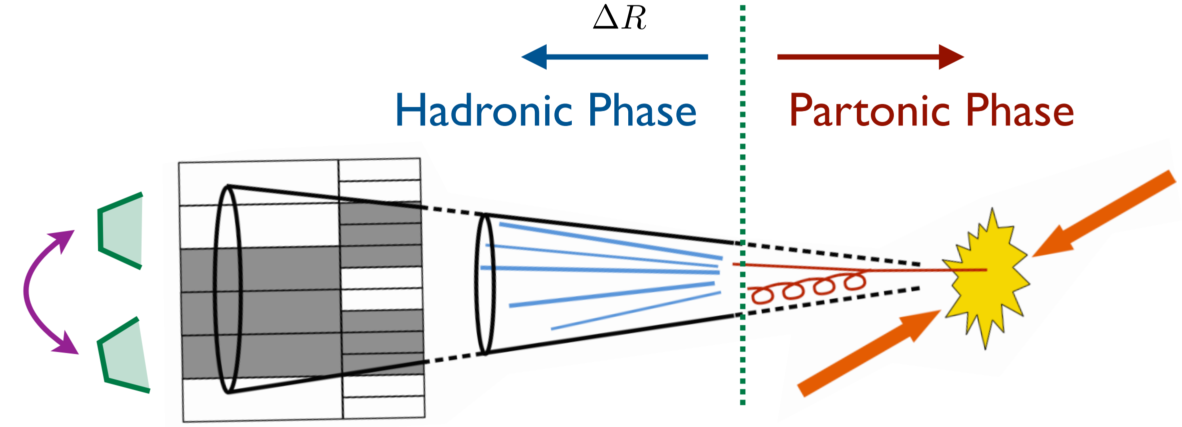
MOD *Linear-linear plot*



Are we learning something about small angle limit of QCD?

MOD *Log-log plot (!)*





First Jet EEC Plot from the LHC (!)


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