QCD and Jets through the Lens of Machine Learning

Jesse Thaler

Machine Learning Techniques in Lattice QCD, MITP Virtual Workshop — May 26, 2021

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

Next speaker (Di Luo) is one of the inaugural IAIFI Fellows!

Advance physics knowledge — from the smallest building blocks of nature to the largest structures in the universe — and galvanize AI research innovation

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

Can we teach a machine to "think" like a physicist?

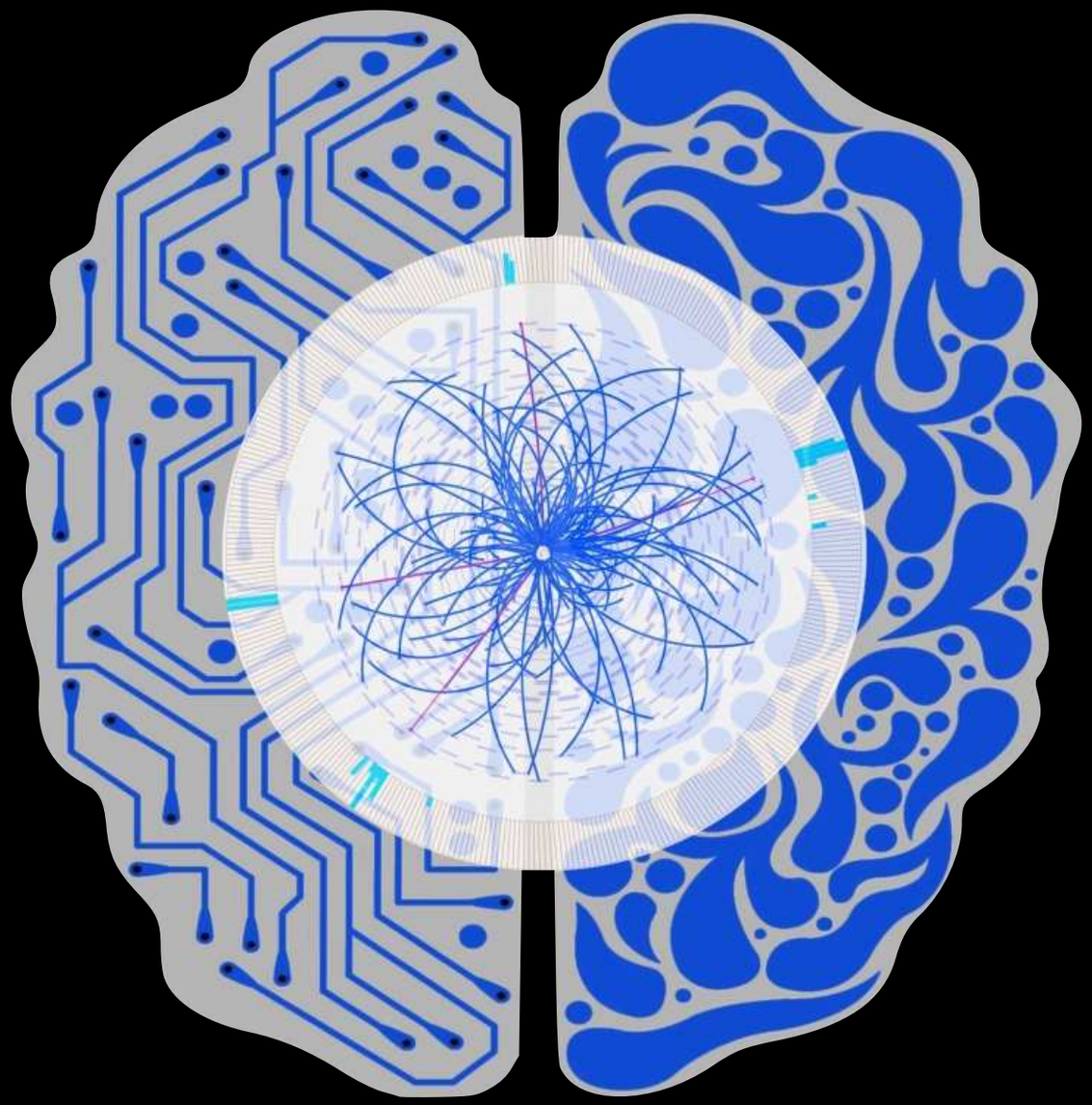
The New York Times By Dennis Overbye Nov. 23, 2020

Can a Computer Devise a Theory of Everything?

Deep Learning meets "Deep Thinking"

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

The Lens of Machine Learning



What formalisms are needed to leverage ML for QCD?

Likelihood Ratio Trick

Many QCD/collider problems can be expressed in this form!

Key example of simulation-based inference

Goal: Estimate p(x) / q(x)

Training Data: Finite samples P and Q

Learnable Function: f(x) parametrized by, e.g., neural networks

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

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

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

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

Likelihood Ratio Trick

Many QCD/collider 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: $$f(x) = \frac{p(x)}{q(x)}$$

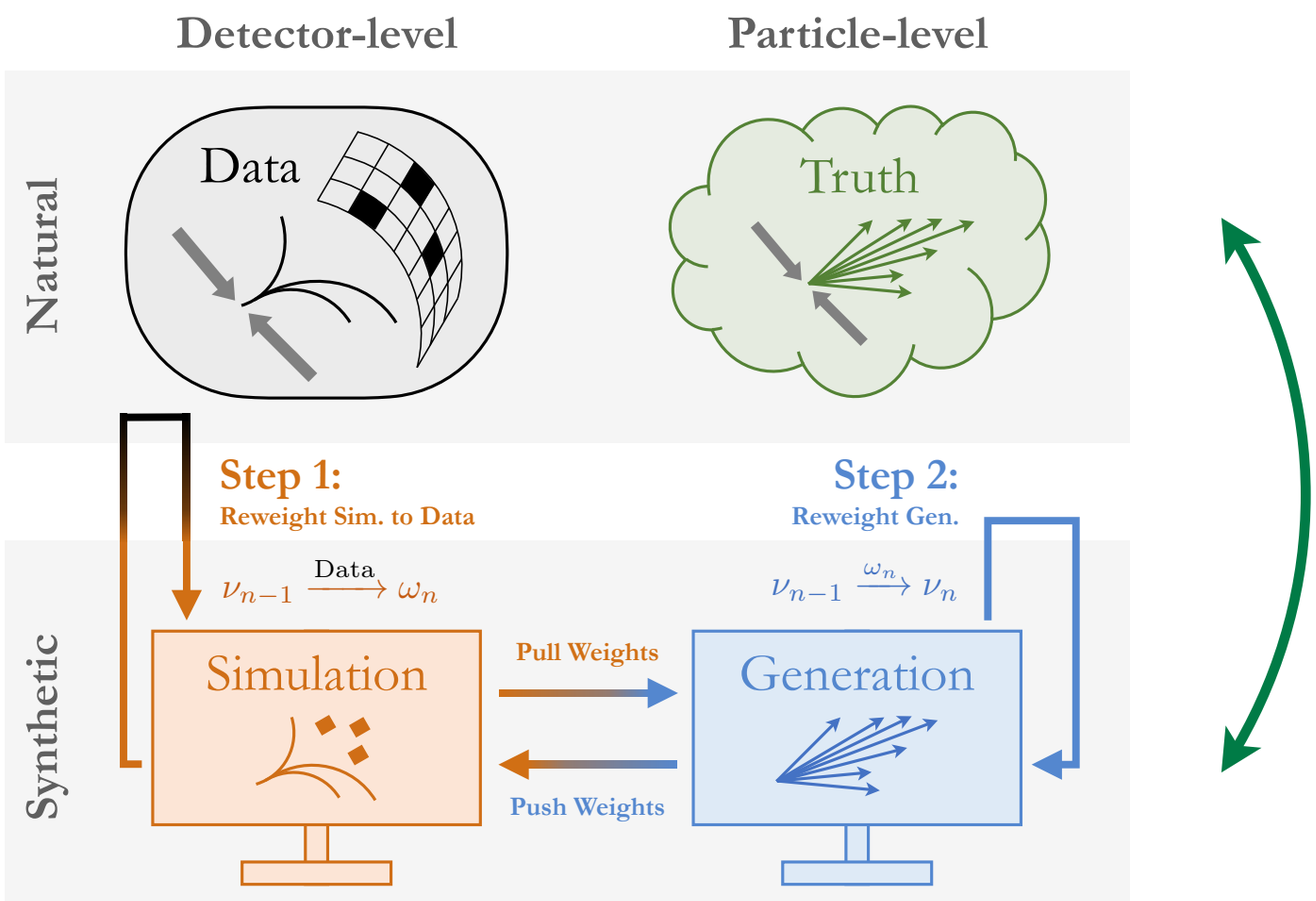
Requires shift in focus from solving problems to specifying problems

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

E.g. Detector Unfolding

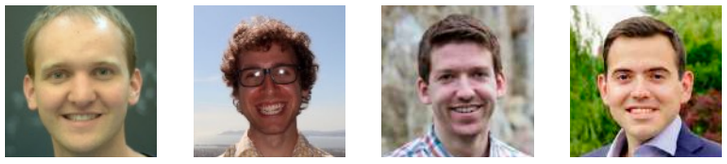
OmniFold

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



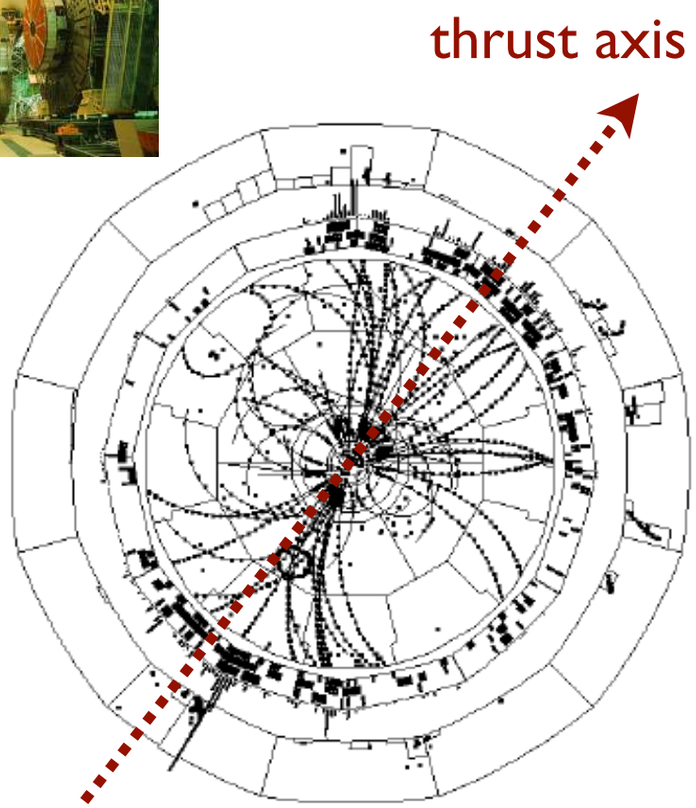
Use ML to compute reweighting factors

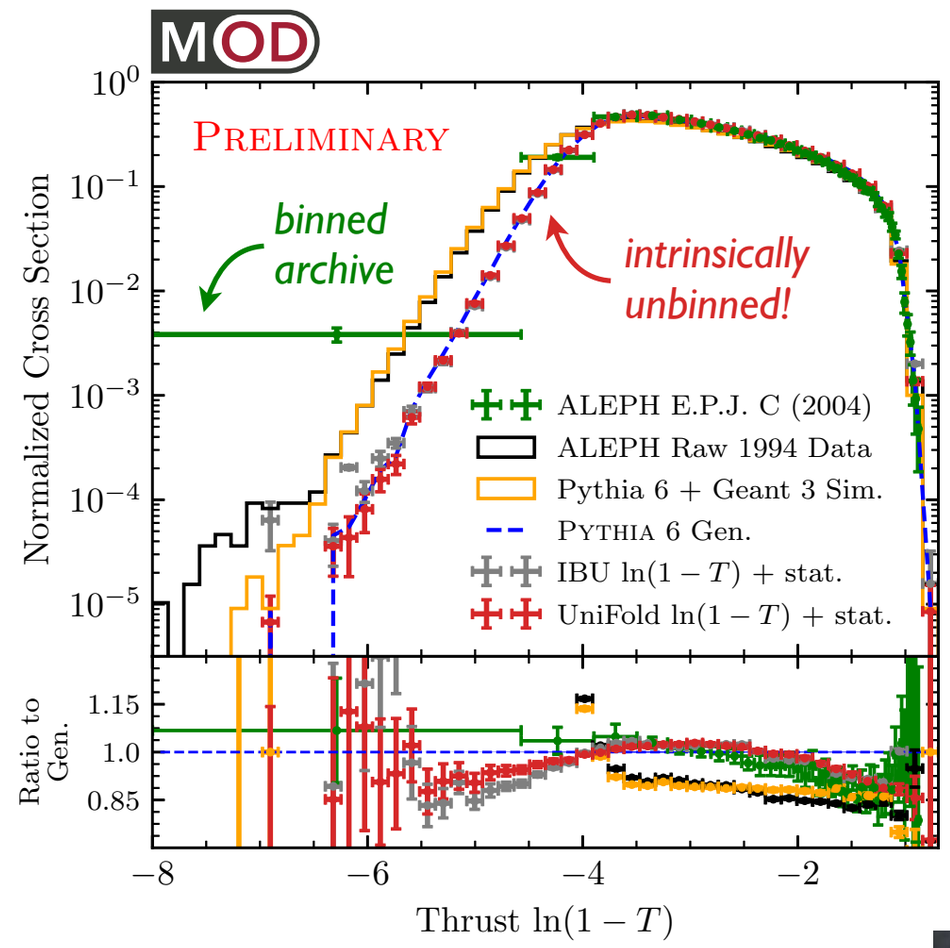
[Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020; + Suresh, ICLR SimDL 2021; Komiske, McCormack, Nachman, arXiv 2021; see unfolding comparison in Petr Baron, arXiv 2021]

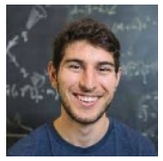


E.g. Detector Unfolding

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; H1, DIS2021]

[Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020; + Suresh, ICLR SimDL 2021;
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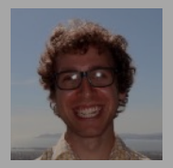


Machine Learning Requirements

If you have in hand…

Well-specified loss
Reliable training data
Learnable function

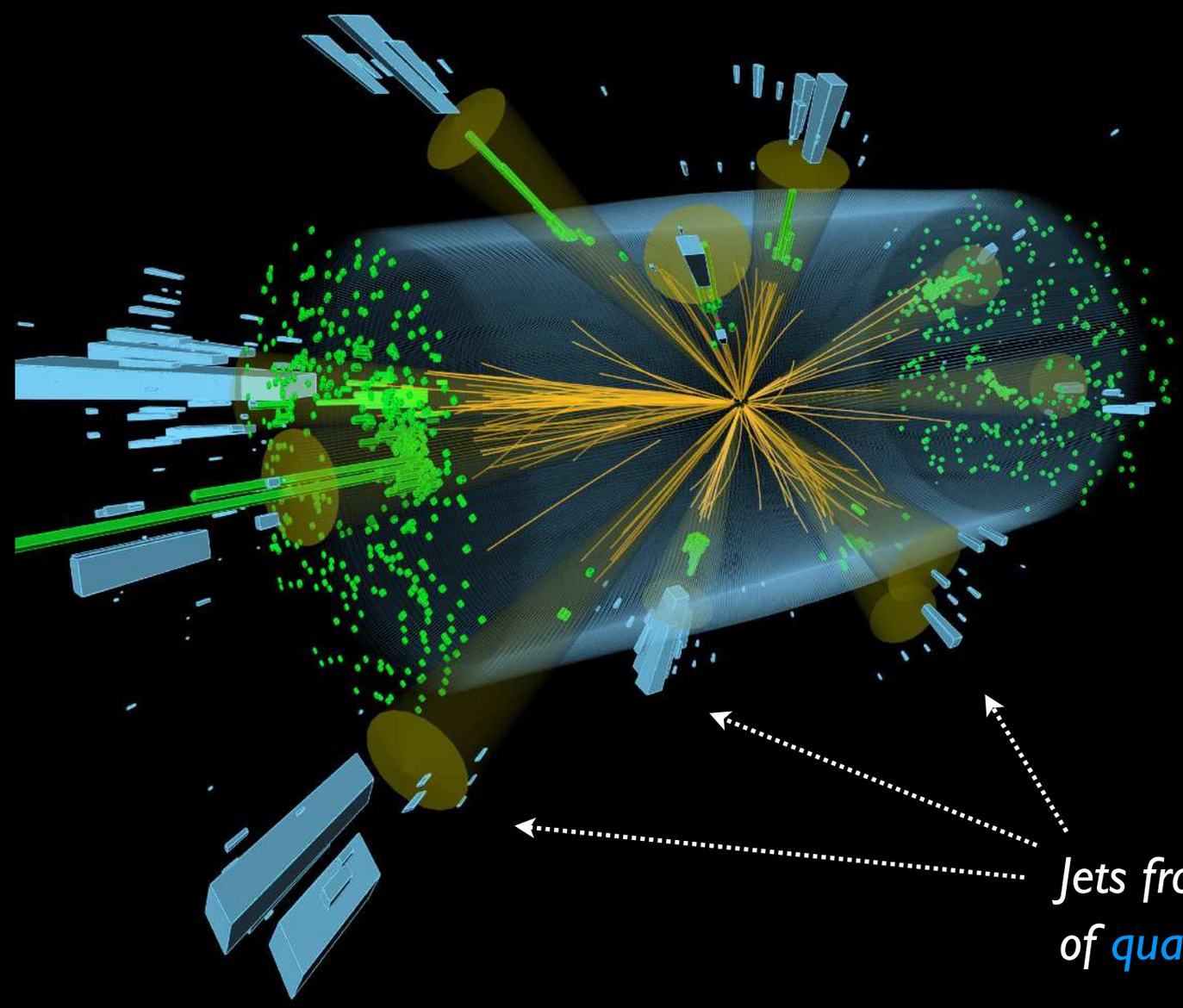
…then you can leverage ML!

Many QCD/collider tasks can be phrased in this language

Theory input essential for robust usage of these tools

[see HEPML-LivingReview for extensive bibliography]

Machine Learning for QCD and Jets



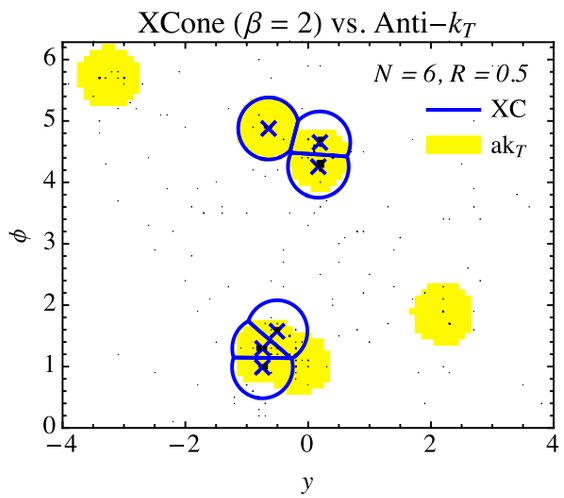
Jets from fragmentation of quarks and gluons

What collider tasks are amendable to a machine learned approach?

Optimization for QCD and Jets

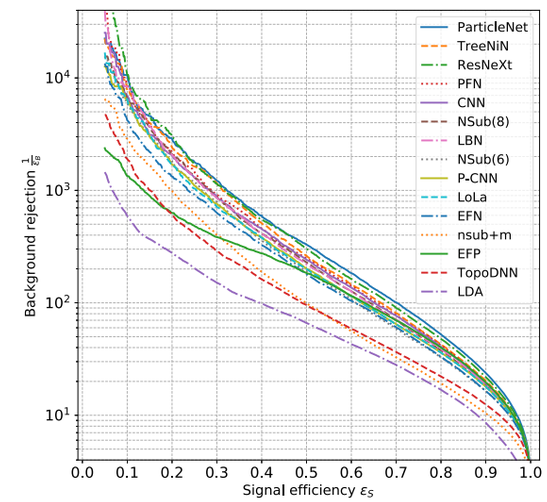
These slides are far from exhaustive

Jet Algorithms



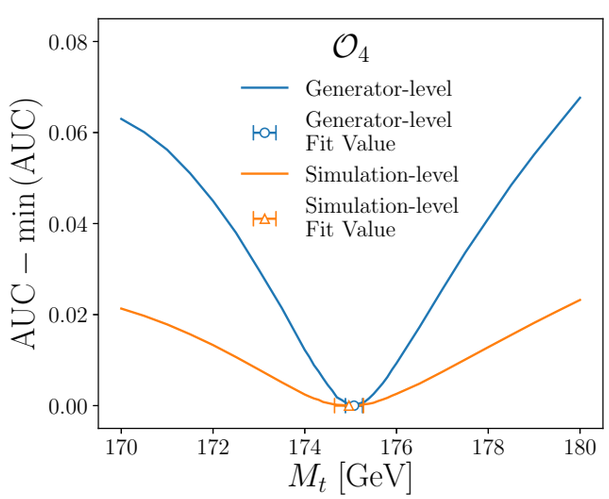
[e.g. Stewart, Tackmann, JDT, Vermilion, Wilkason, JHEP 2015]

Jet Classification



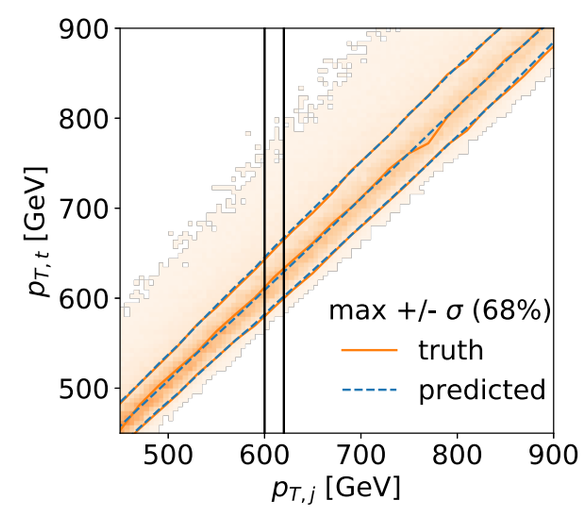
[e.g. Kasieczka, Plehn, et al., SciPost 2019]

Parameter Estimation



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

Uncertainty Quantification



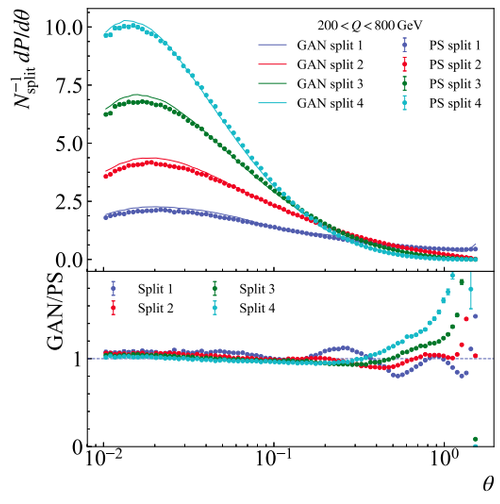
[e.g. Kasieczka, Luchmann, Otterpohl, Plehn, SciPost 2020]

...

More Optimization for QCD and Jets

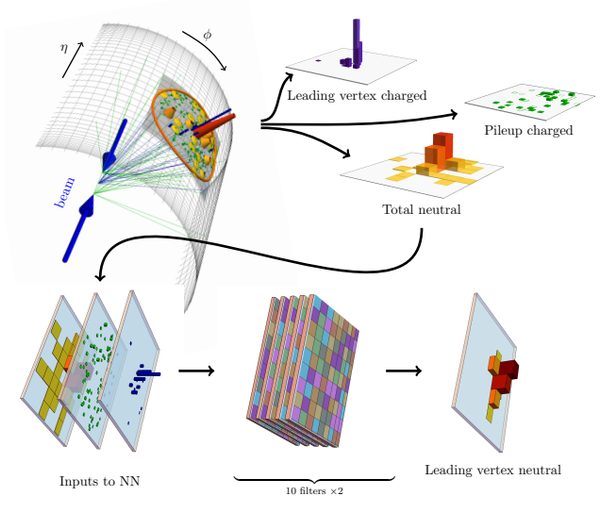
These slides are far from exhaustive

Parton Shower Modeling/Tuning



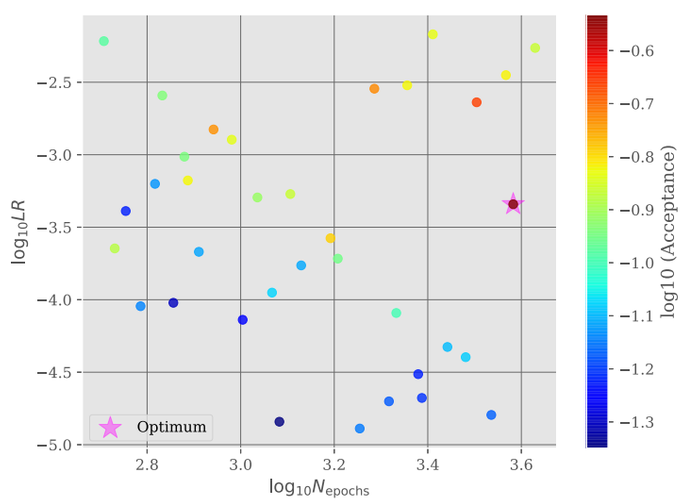
[e.g. Lai, Neill, Płoskoń, Ringer, arXiv 2020]

Pileup Mitigation



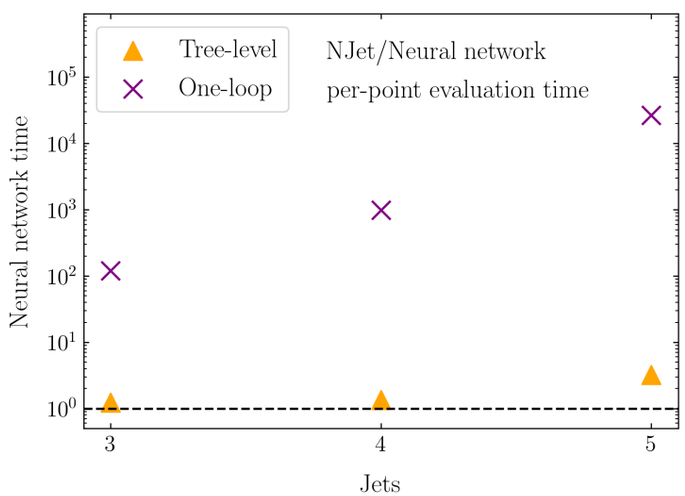
[e.g. Komiske, Metodiev, Nachman, Schwartz, JHEP 2017]

Phase Space Integration



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

Amplitude Calculations



[e.g. Badger, Bullock, JHEP 2020]

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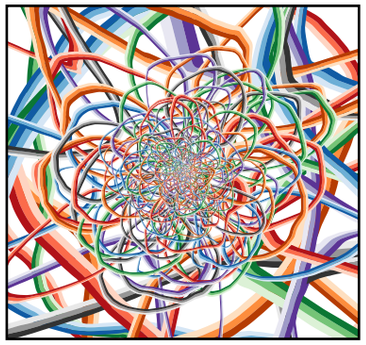
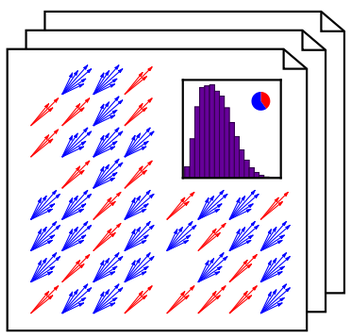
From Curmudgeon to Evangelist

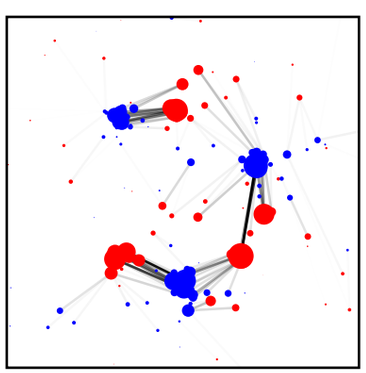
What have been helpful guides in pursing ML ⇔ QCD?



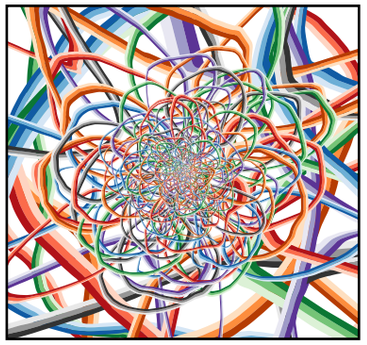
Can theoretical structures be encoded directly?



Can strategy be defined on physical quantities?



Can we leverage unsupervised machine learning?



Can theoretical structures be encoded directly?

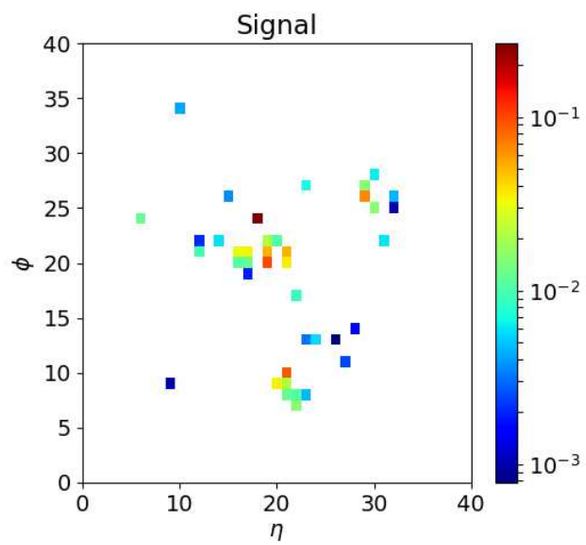
Can strategy be defined on physical quantities?

Can we leverage unsupervised machine learning?

Jet Representations

Pixelized Image

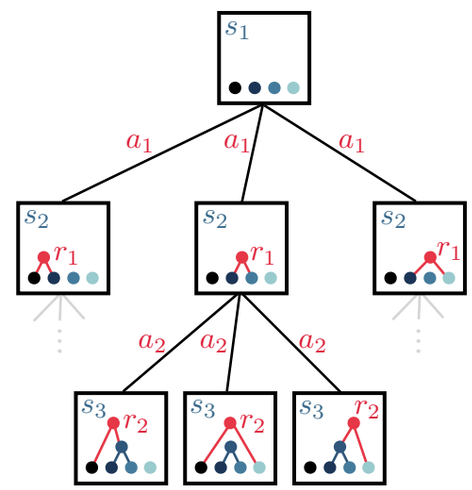
Calorimetry



[review in Kagan, arXiv 2020]

Hierarchical Tree

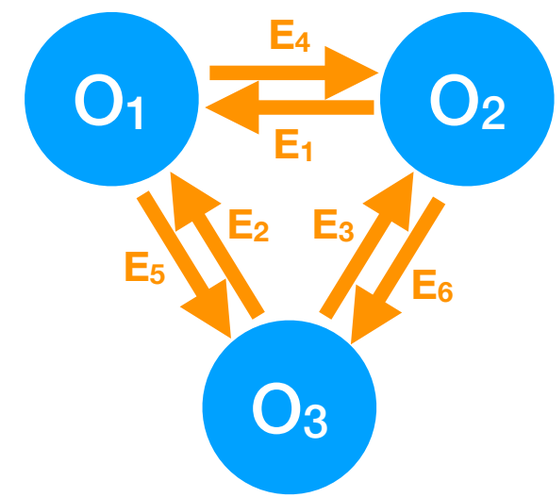
Binary Splittings



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

Graphs

Pairwise Interactions

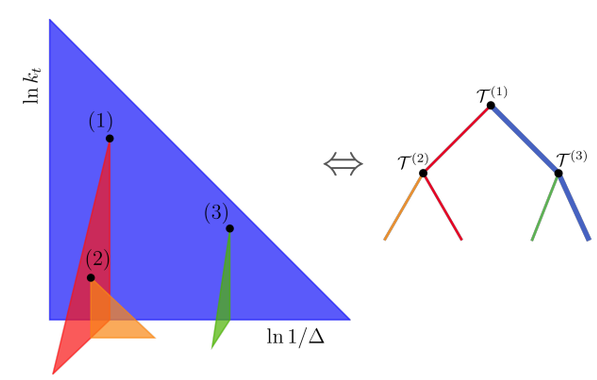


[e.g. Moreno, Cerri, Duarte, Newman, Nguyen, Periwal, Pierini, Serikova, Spiropulu, Vlimant, EPJC 2020]

Imposes implicit theoretical prior; affects choice of network architecture

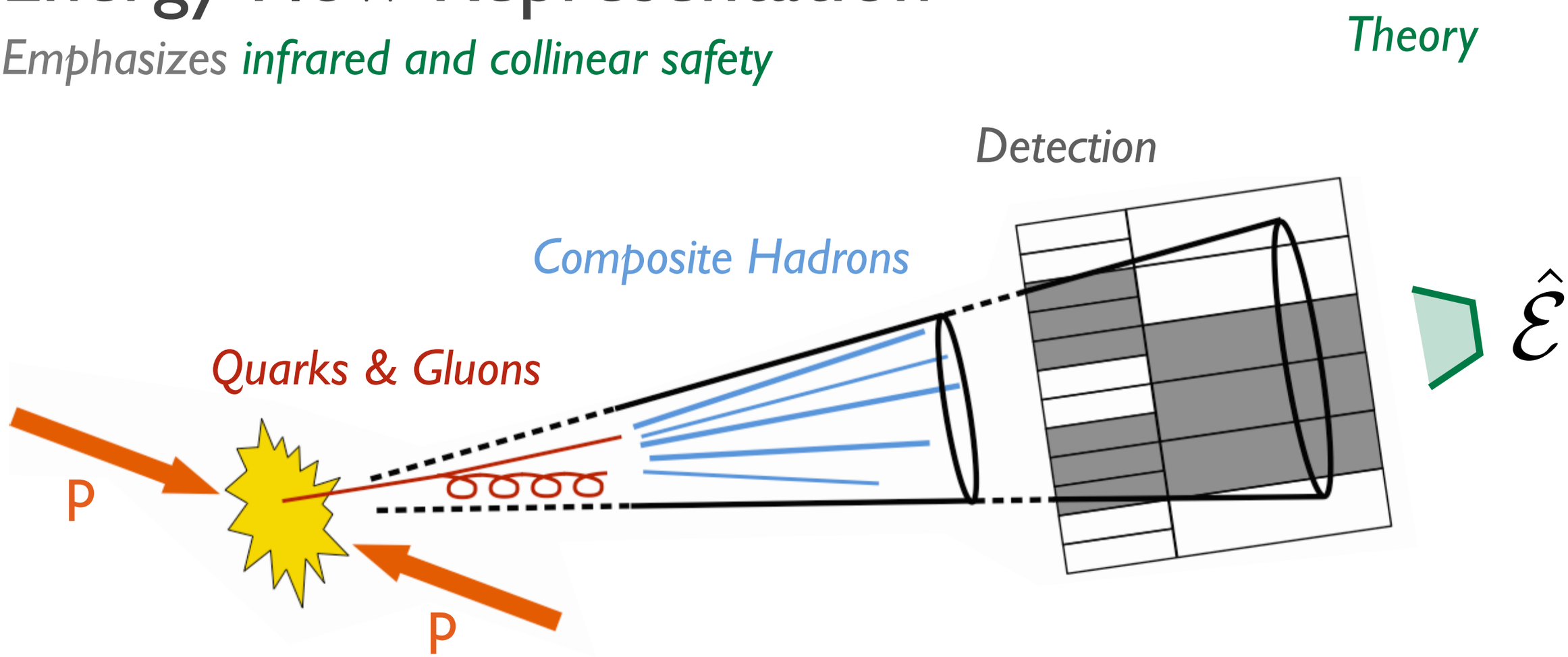
E.g. recent progress with
Lund Plane + Graph Networks

[Dreyer, Qu, JHEP 2021]



Energy Flow Representation

Emphasizes infrared and collinear safety



Energy Flow:

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

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

[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]

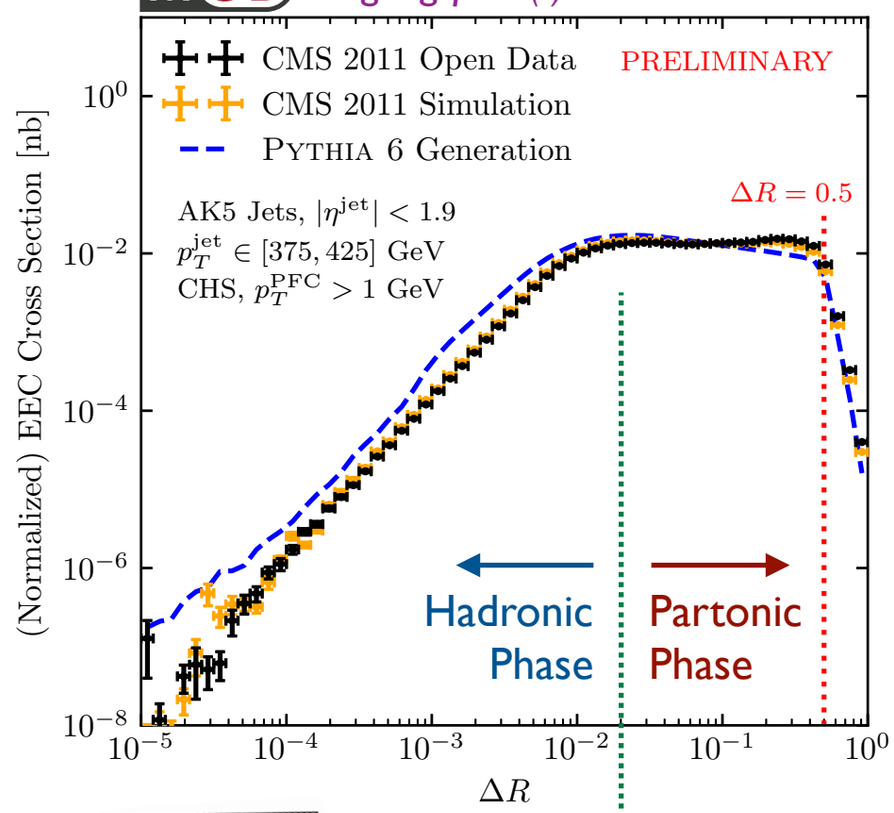
Energy Flow Representation

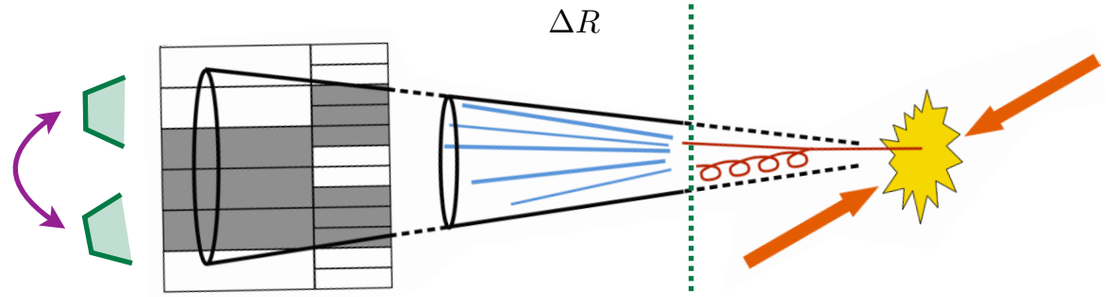
Emphasizes

Theory

Revisiting Energy^2 Correlators

MOD *Log-log plot (!)*





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

Q

P

Robust to
Well-d

$t, vt\hat{n})$

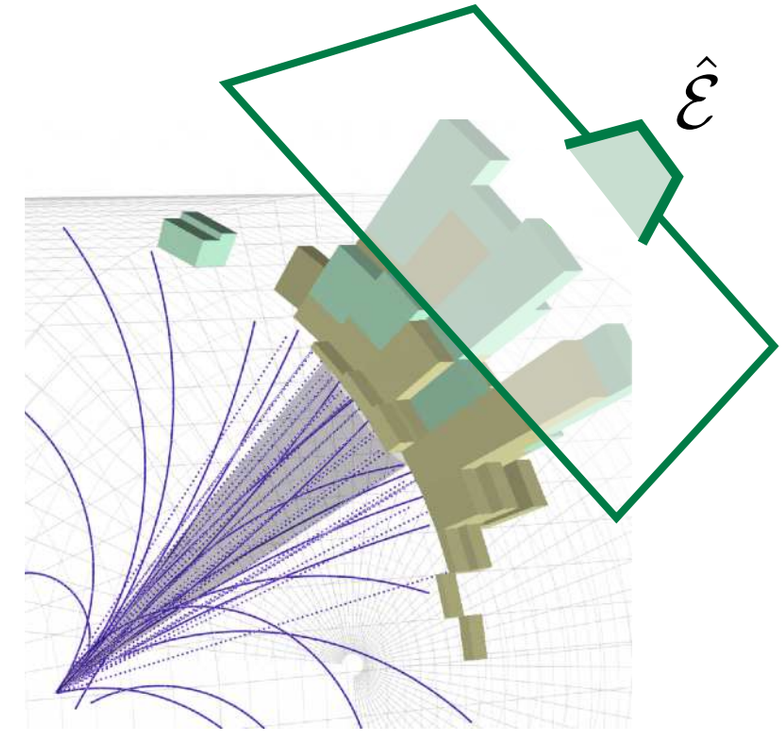
teu, Stewart, JDT, PRD 2013;
oult, Zhang, Zhu, PRD 2020]
Nojiri, Takeuchi, JHEP 2020]

Jets as Weighted Point Clouds

- Energy-Weighted Directions

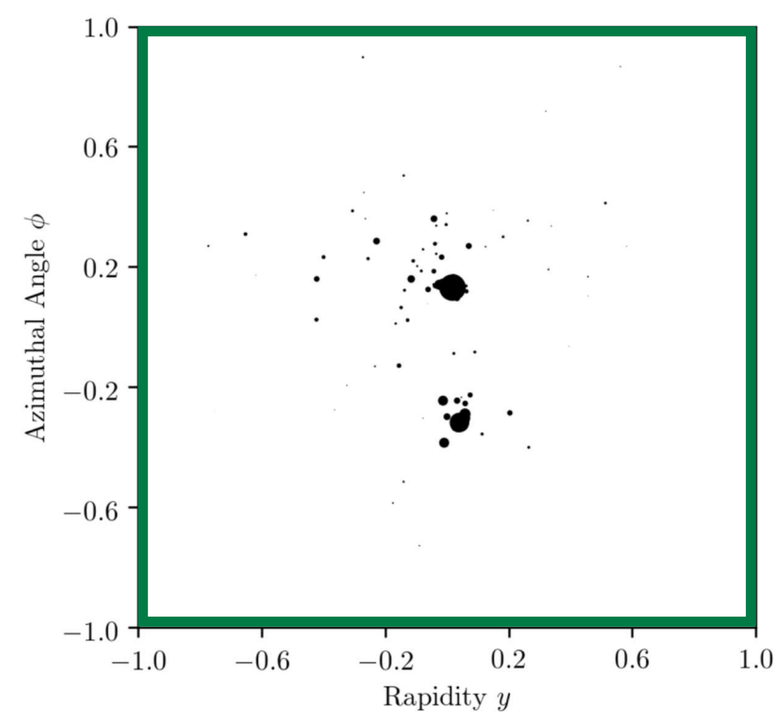
$$\vec{p} = \{\underbrace{E}_{\text{Energy}}, \underbrace{\hat{n}_x, \hat{n}_y, \hat{n}_z}_{\text{Direction}}\}$$

(suppressing "unsafe" charge/flavor information)



- Equivalently: Energy Density

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



Energy Flow Networks

Architecture designed around symmetries and interpretability

Permutation invariant

Linear weights (i.e. safe)

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

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, PRD 2021;
Lorentz-equivariant approach in Bogatskiy, Anderson, Offermann, Roussi, Miller, Kondor, arXiv 2020;
histogram pooling in Cranmer, Kreisch, Pisani, Villaescusa-Navarro, Spergel, Ho, ICLR SimDL 2021]

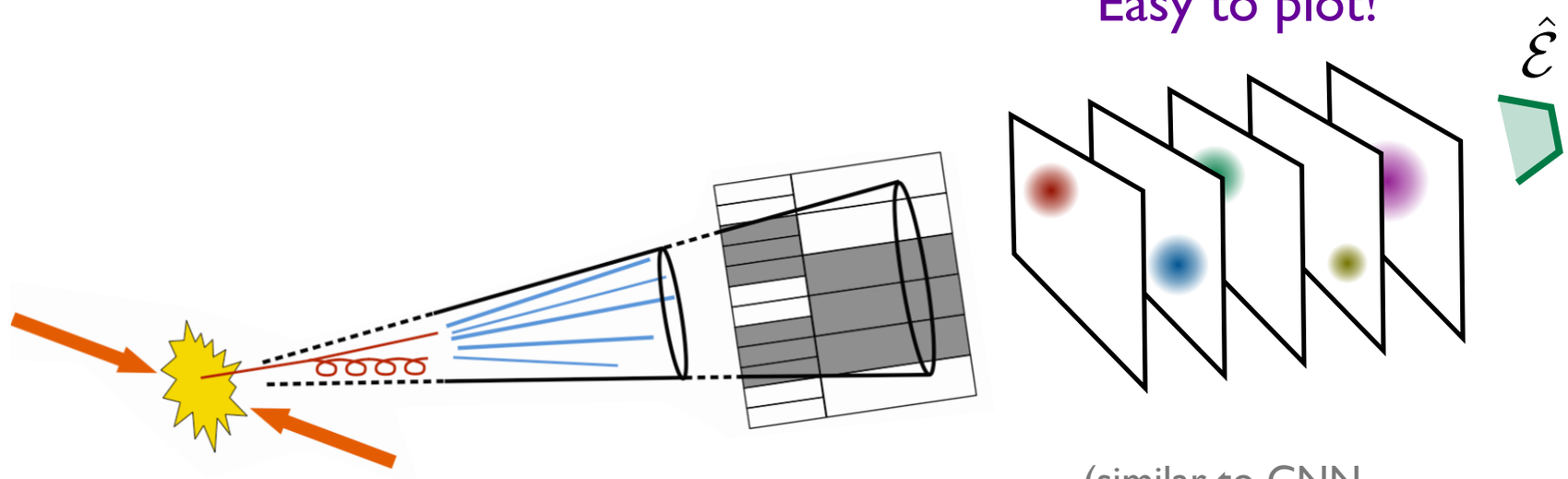

Energy Flow Networks

Architecture designed around symmetries and interpretability

Latent space of dim ℓ

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

Easy to plot!



(similar to CNN filter activation)

[Komiske, Metodiev, JDT, JHEP 2019; see also Komiske, Metodiev, JDT, JHEP 2018; code at energyflow.network;
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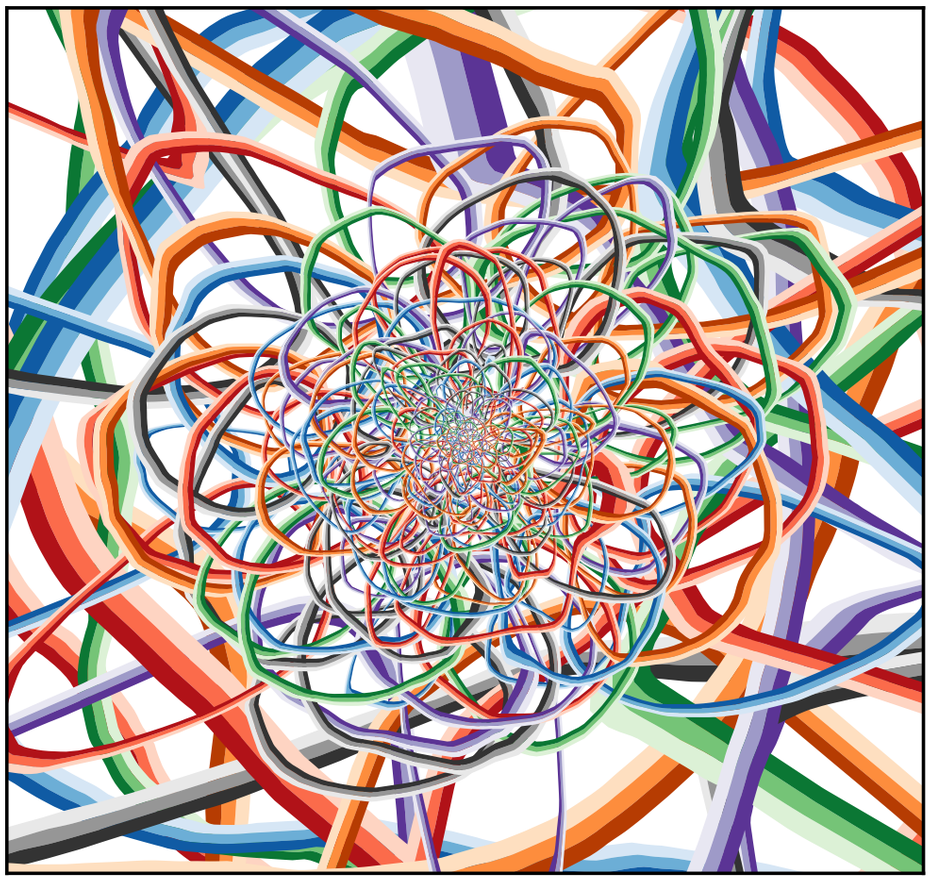
Energy Flow Networks

Architecture designed around symmetries and interpretability

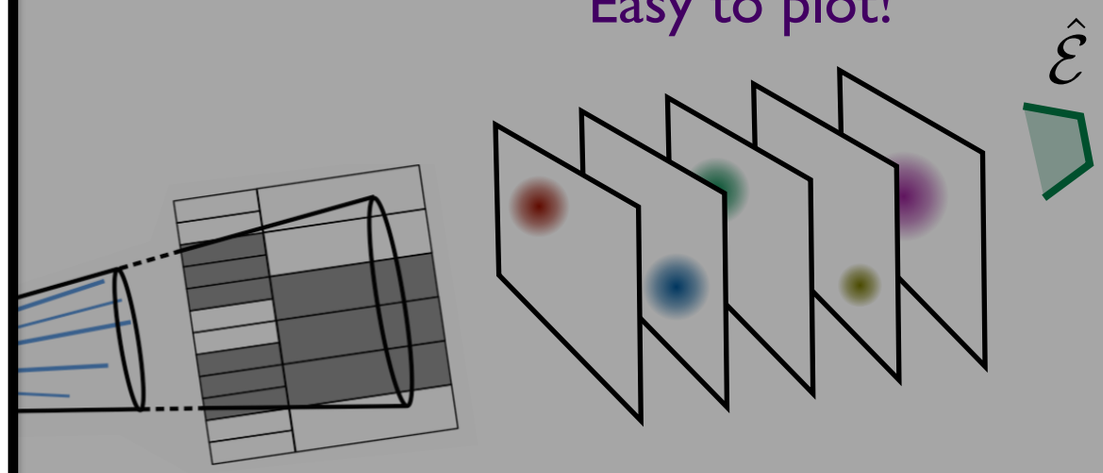
Psychedelic Network Visualization

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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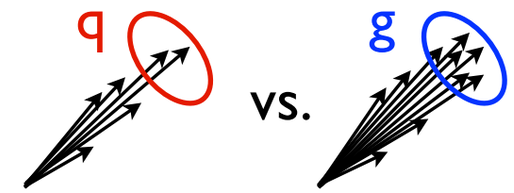
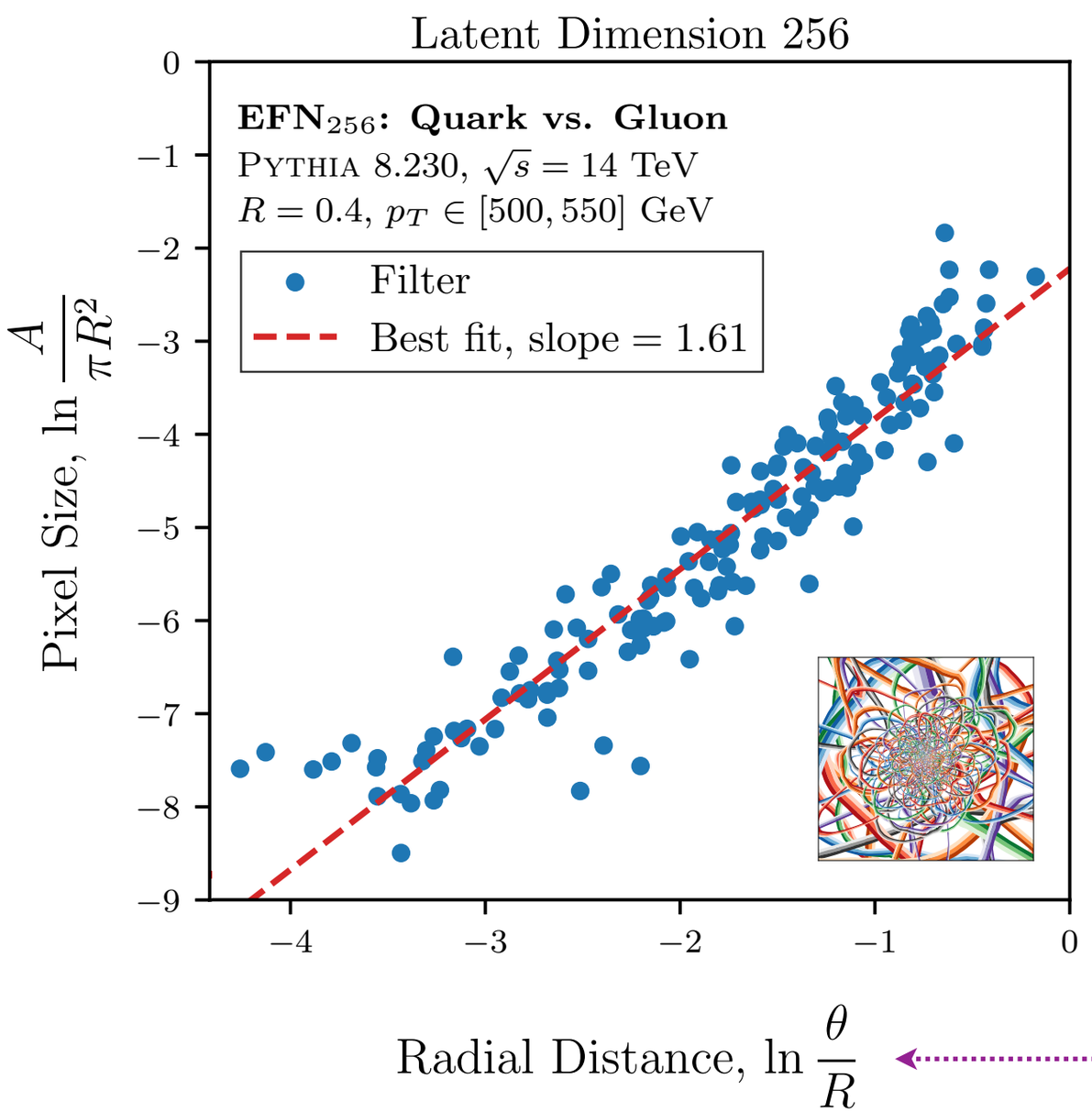
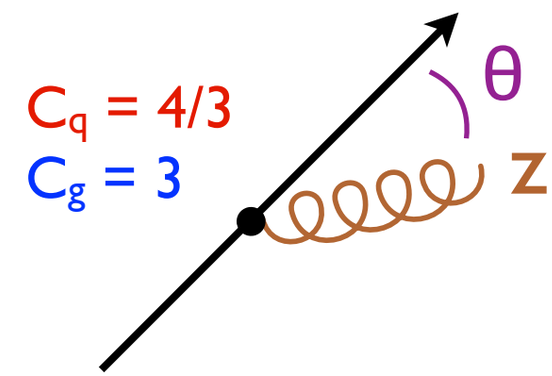
Machine Learning Collinear QCD

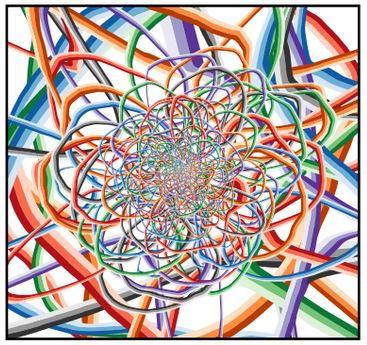






$$\mathrm{d}P_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{\mathrm{d}\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{\mathrm{d}z}{z}}_{\text{Soft}}$$

[Komiske, Metodiev, JDT, JHEP 2019]



Can theoretical structures be encoded directly?

Energy Flow Networks ⇔ IRC Safety + Permutations

Can strategy be defined on physical quantities?

Can we leverage unsupervised machine learning?

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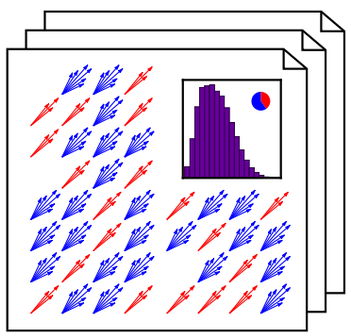
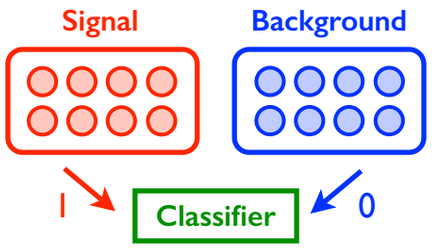


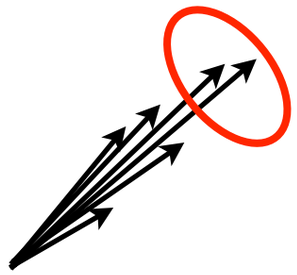
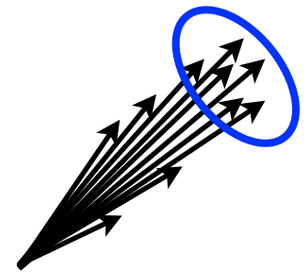
Can strategy be defined on physical quantities?

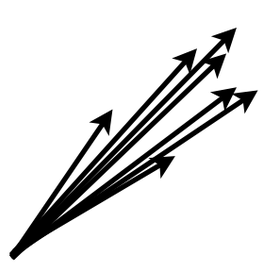
Can we leverage unsupervised machine learning?

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

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

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

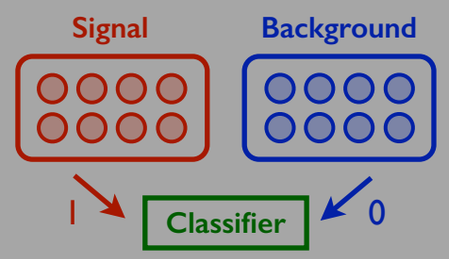
Best you can do: $h(\mathcal{J}) = \dfrac{p(\mathcal{J}|\mathrm{Q})}{p(\mathcal{J}|\mathrm{Q}) + p(\mathcal{J}|\mathrm{G})}$

(Neyman-Pearson lemma)

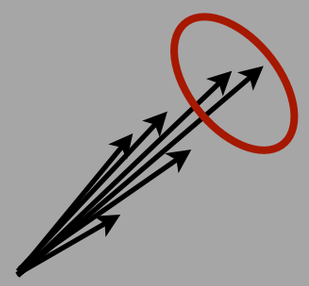
[see e.g. Gras, Höche, Kar, Larkoski, Lönnblad, Plätzer, Siódmok, Skands, Soyez, JDT, JHEP 2017; Komiske, Metodiev, Schwartz, JHEP 2017; Komiske, Metodiev, JDT, JHEP 2018]

Quark/Gluon Classification

"Hello, World!" of Jet Physics

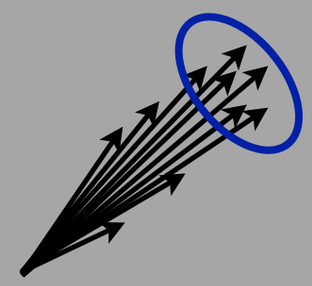


e.g.



Quark
$C_q = 4/3$

vs.



Gluon
$C_g = 3 = 9/3$

What do you mean by "quark" and "gluon"?

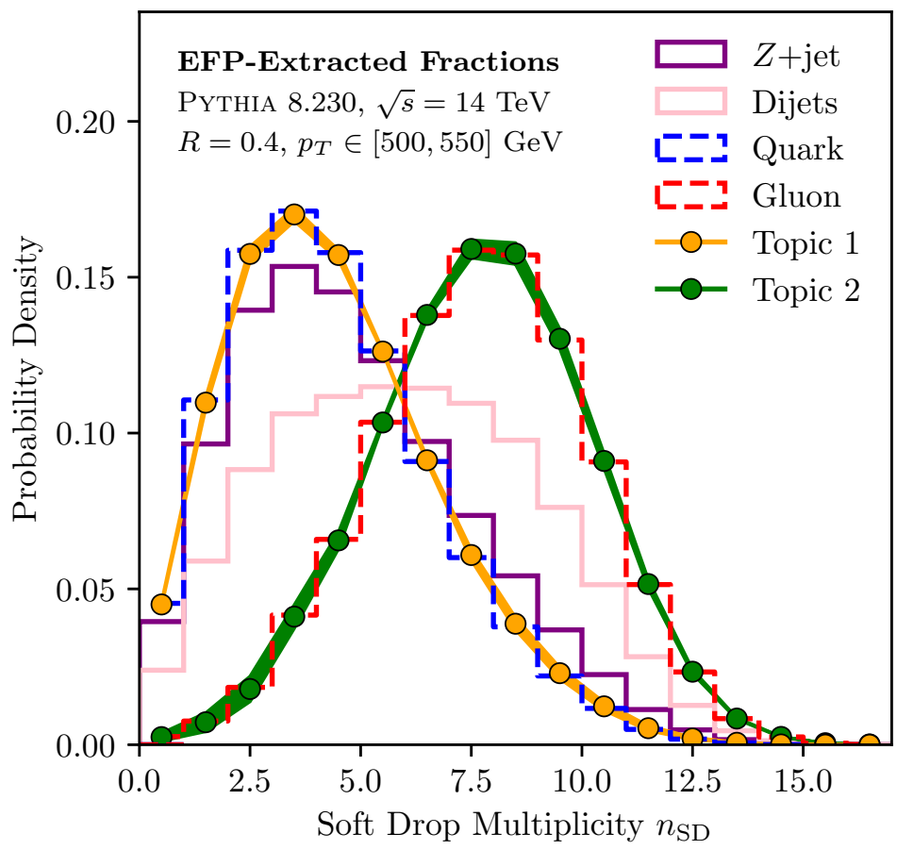
Jets are clusters of colorless hadrons!

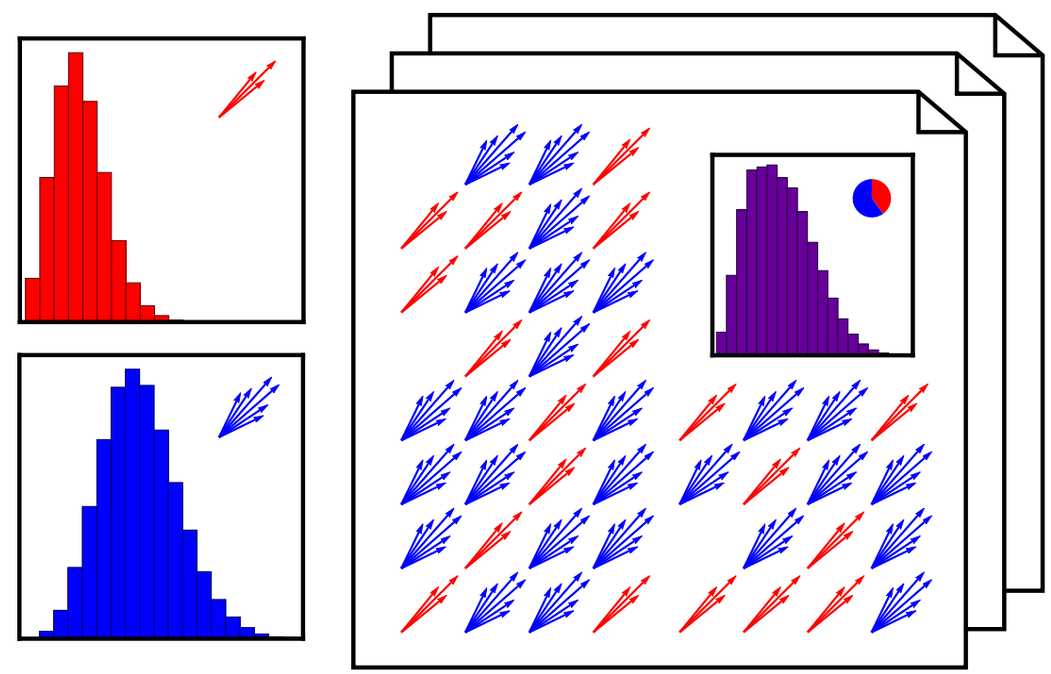
Parton shower "truth" is but a (useful) fiction!

[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



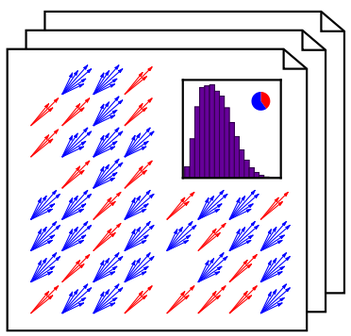


Key concept from natural language processing: "anchor words"

[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 quantities?

Jet Topics ⇔ Hadron-Level Approach to QCD Partons

Can we leverage unsupervised machine learning?

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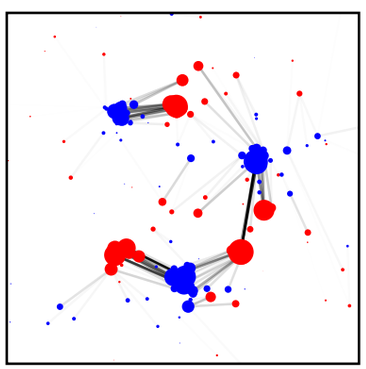

Can we leverage unsupervised machine learning?

The Earth Mover's Distance

Optimal Transport:

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

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

Déblai

Remblai

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

The Earth Mover's Distance

Optimal Transport:

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

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

Additive Weight:

Ground Distance:

$\Rightarrow$ Distance Between Distributions

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

The Earth Mover's Distance

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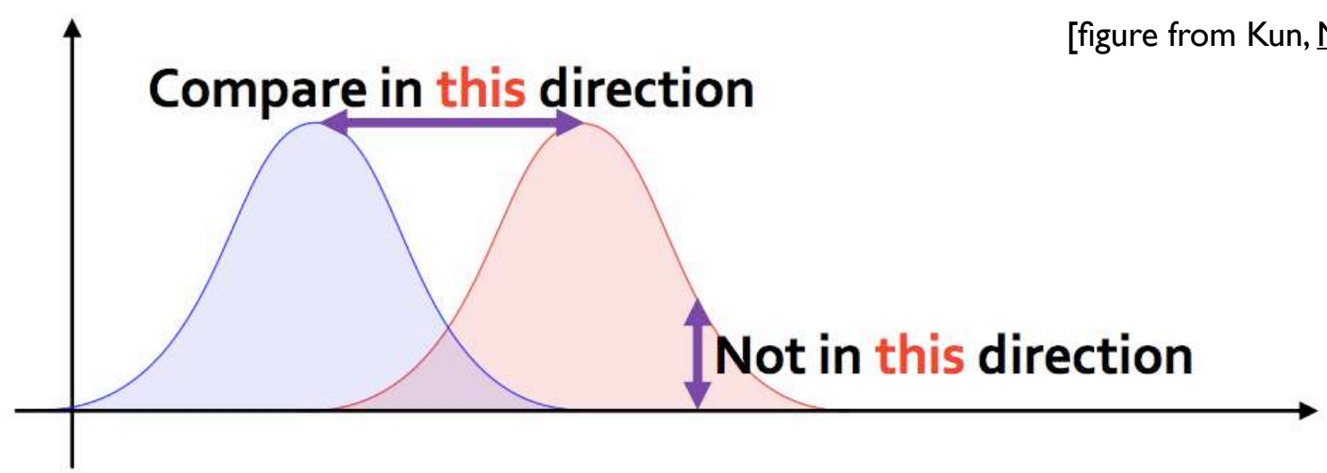
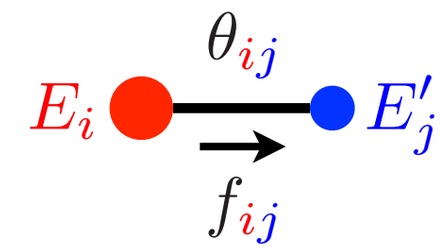
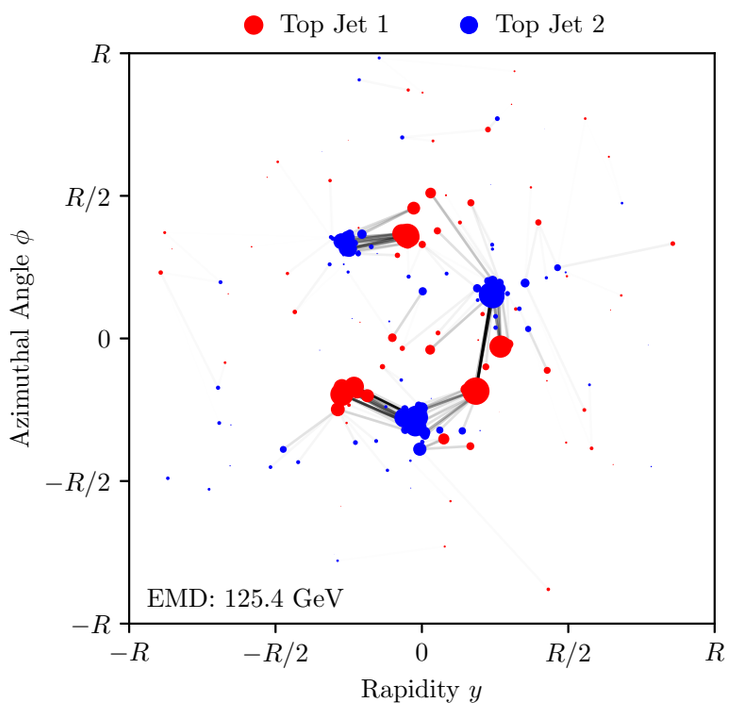


[figure from Kun, Math ∩ Programming]

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

The Energy Mover's Distance





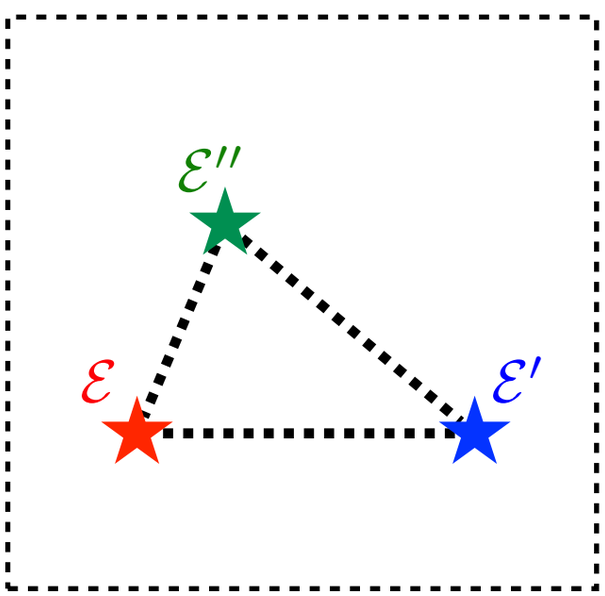
Optimal transport between energy flows…

$$\mathrm{EMD}(\mathcal{E},\mathcal{E}') = \min_{\{f\}} \sum_i \sum_j f_{ij} \frac{\theta_{ij}}{R} + \left| \sum_i E_i - \sum_j E'_j \right|$$

in GeV

Cost to move energy

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 $R \geq \theta_{max}/2$, i.e. $R \geq$ jet radius for conical jets)

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

Dimensionality of Space of Jets

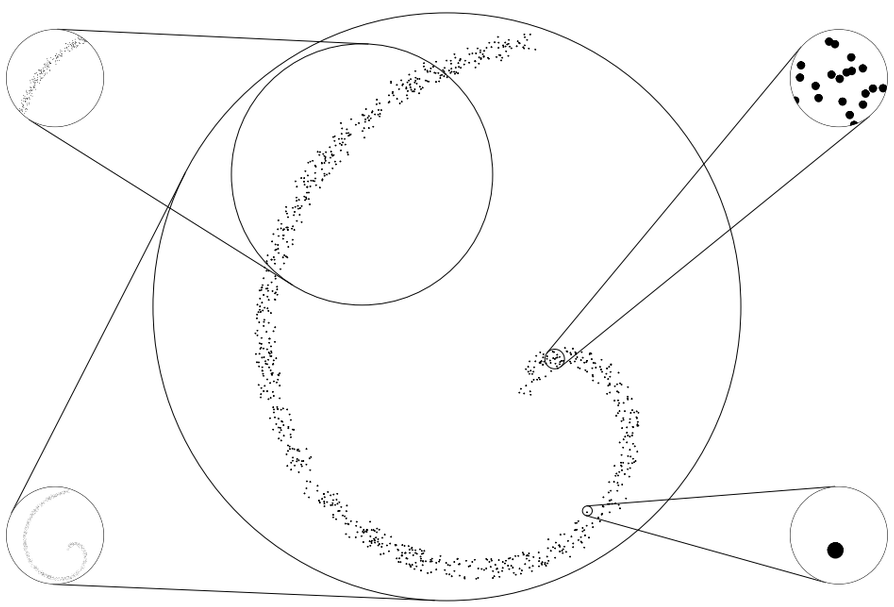
$$N_{\text{neighbors}}(r) \sim r^{\dim}$$

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

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

dim≃1

dim≃2



dim≃2

(eventually 0)

dim≃0

Dimensionality of Space of Jets

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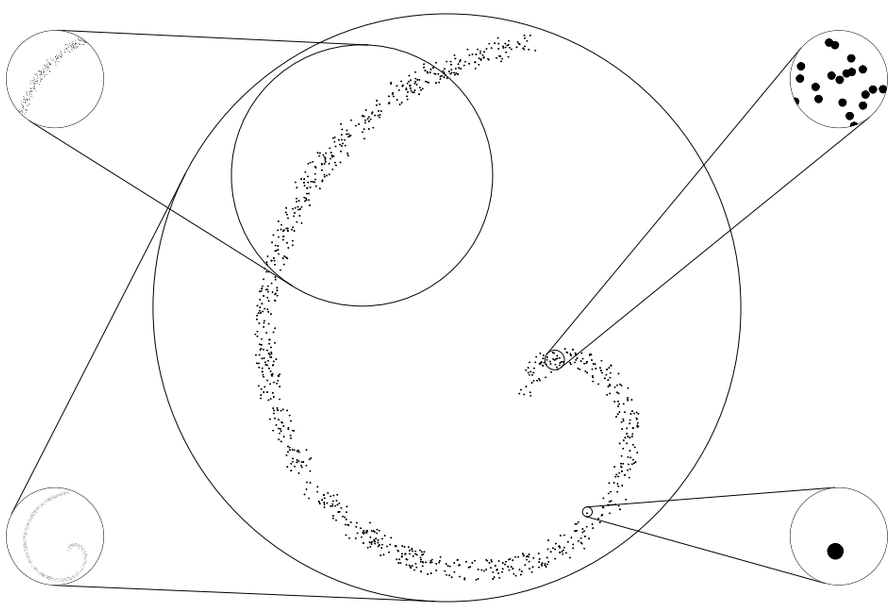
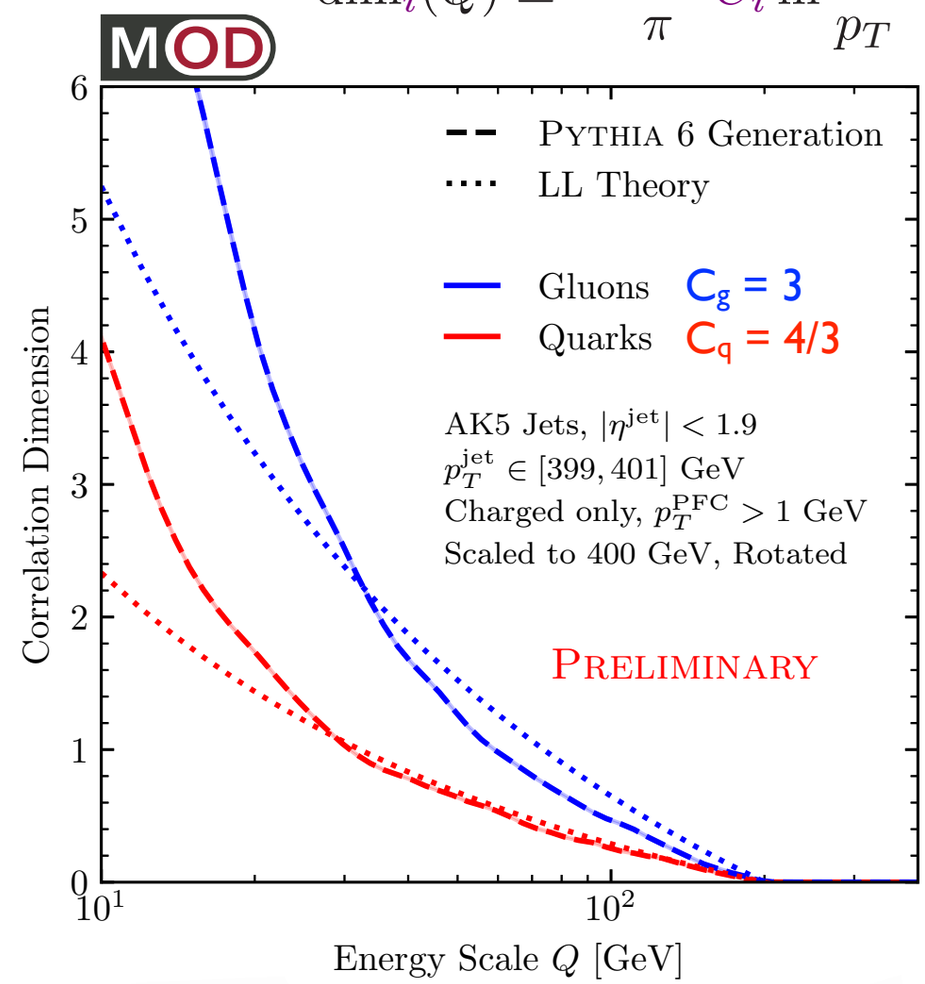
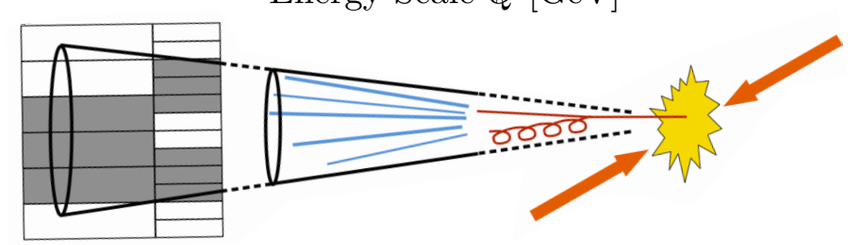


dim≃2 dim≃0

(eventually 0)

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





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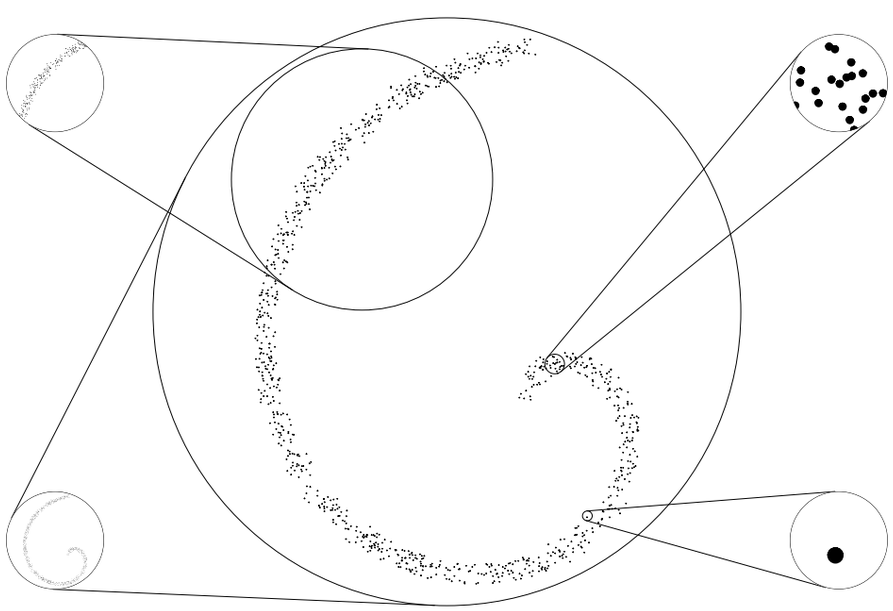
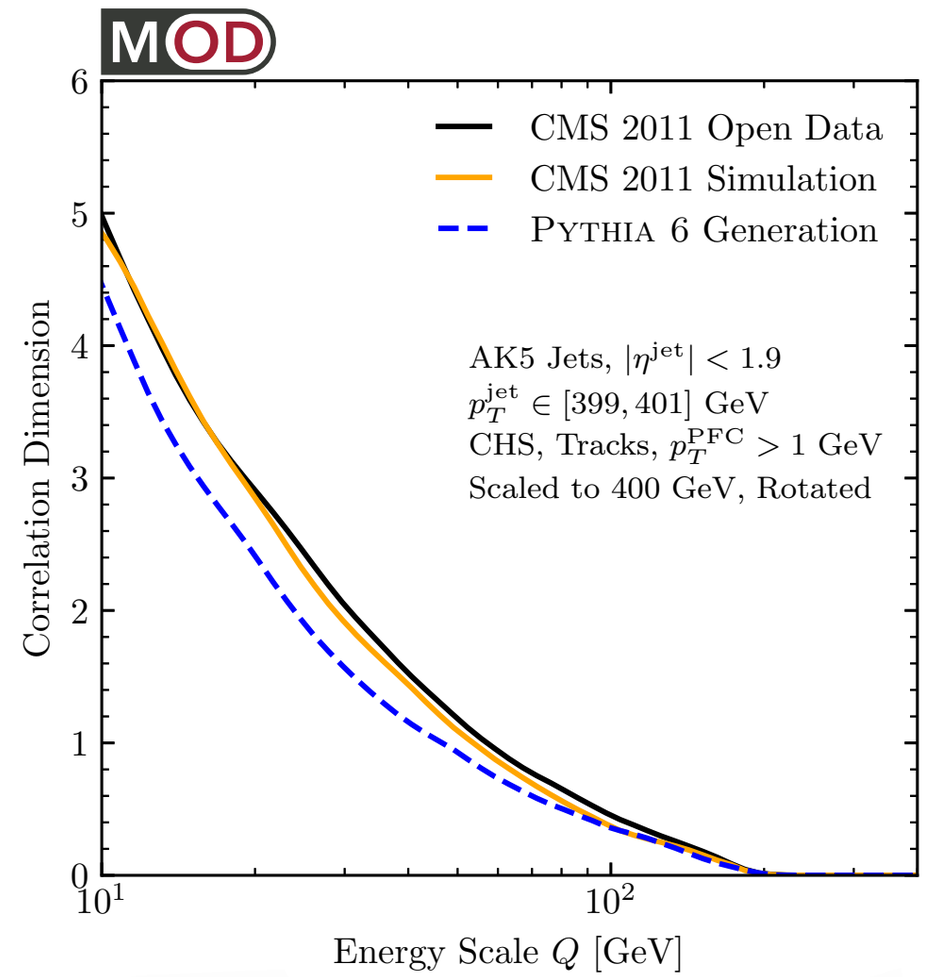
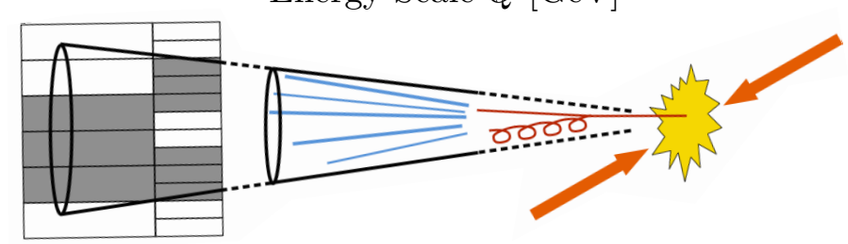


dim≃2 dim≃0

(eventually 0)





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

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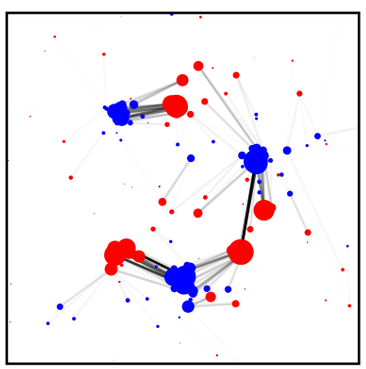
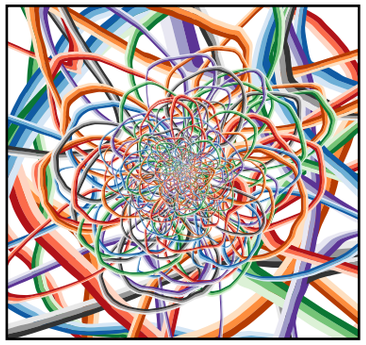


Can we leverage unsupervised machine learning?

Energy Mover's Distance ⇔ Geometric Strategies for Collider Physics

QCD and Jets through the Lens of ML



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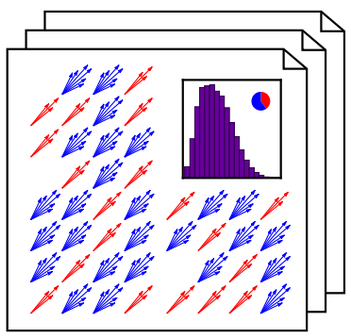

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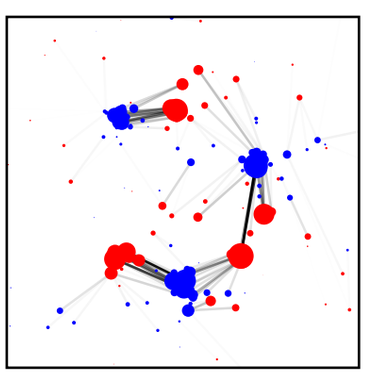


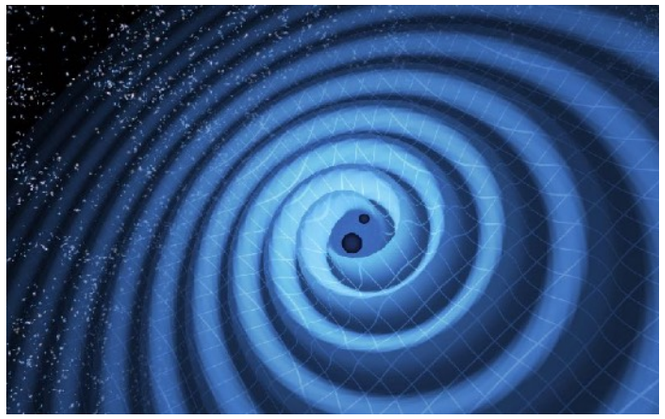
Can we leverage unsupervised machine learning?

Energy Mover's Distance ⇔ Geometric Strategies for Collider Physics

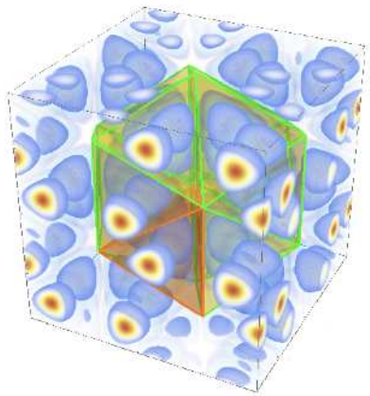
Theory insights essential for developing these tools

Artificial Intelligence ⇔ *Fundamental Interactions*

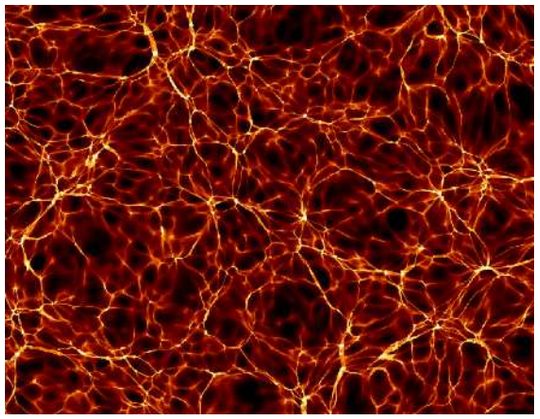
Gravitational Waves



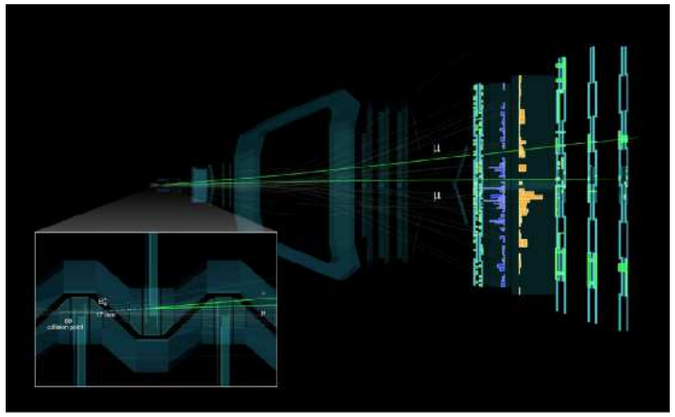
Nuclear Physics



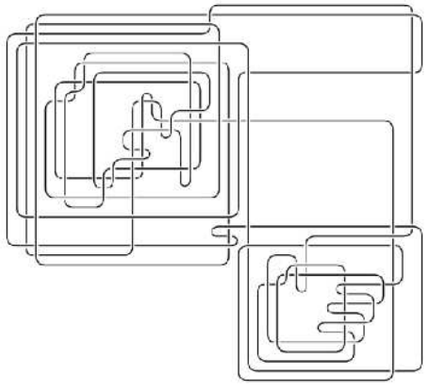
Dark Matter



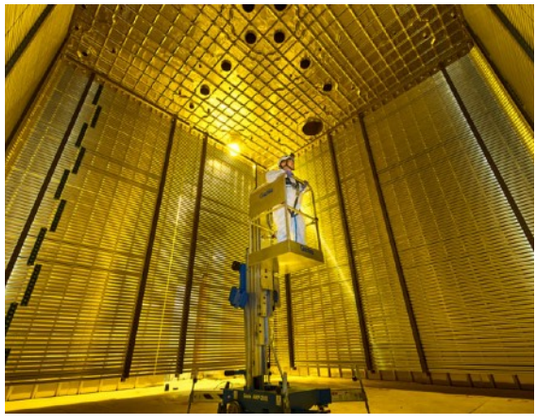
Particle Colliders



Mathematical Physics



Neutrino Detection



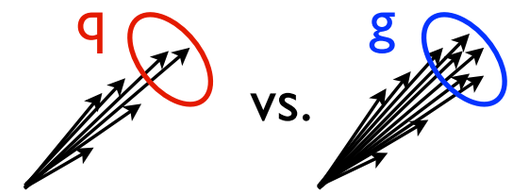
…

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

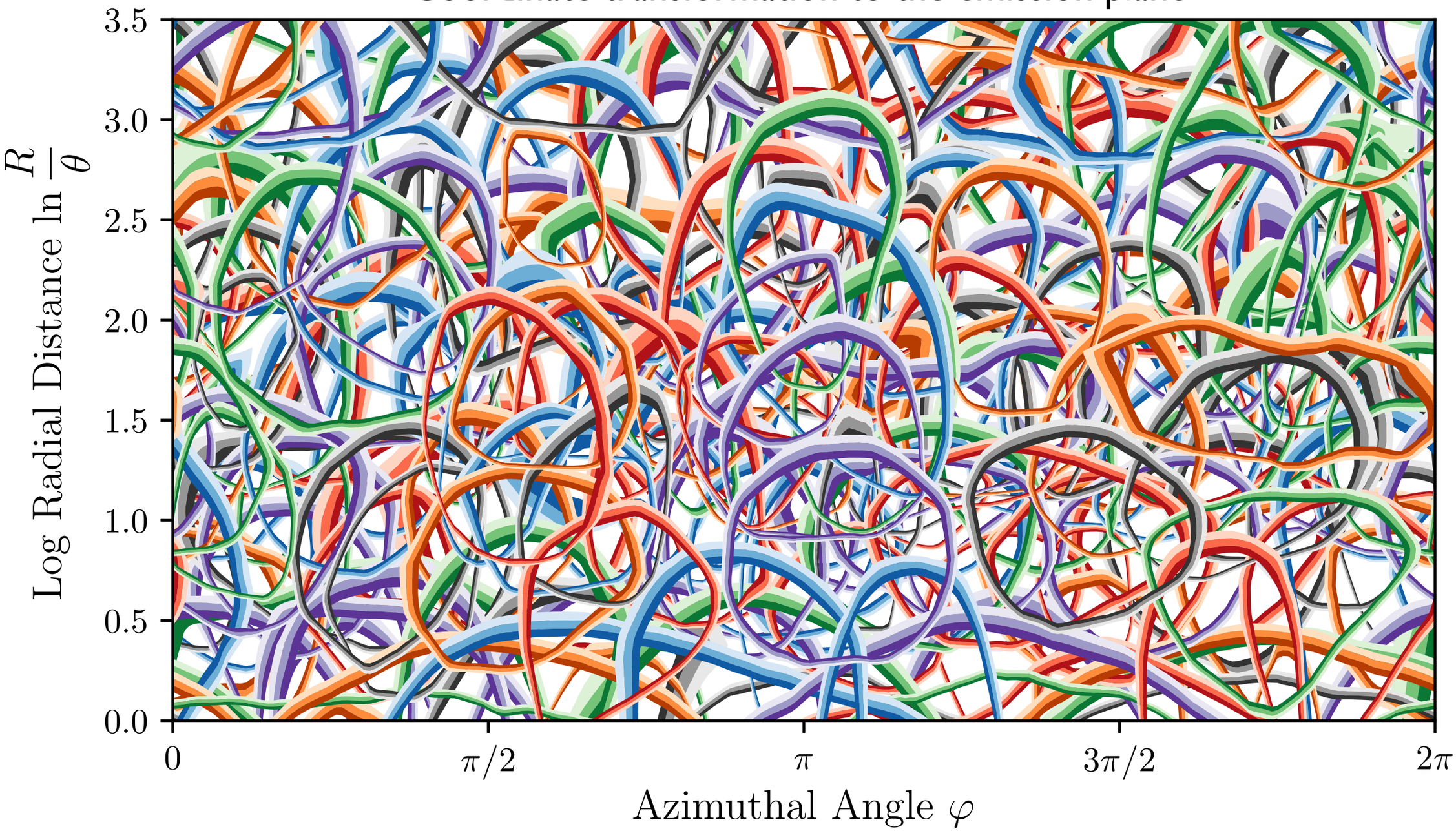
[http://iaifi.org]

Backup Slides

En Route to the Lund Plane



Coordinate transformation to the emission plane

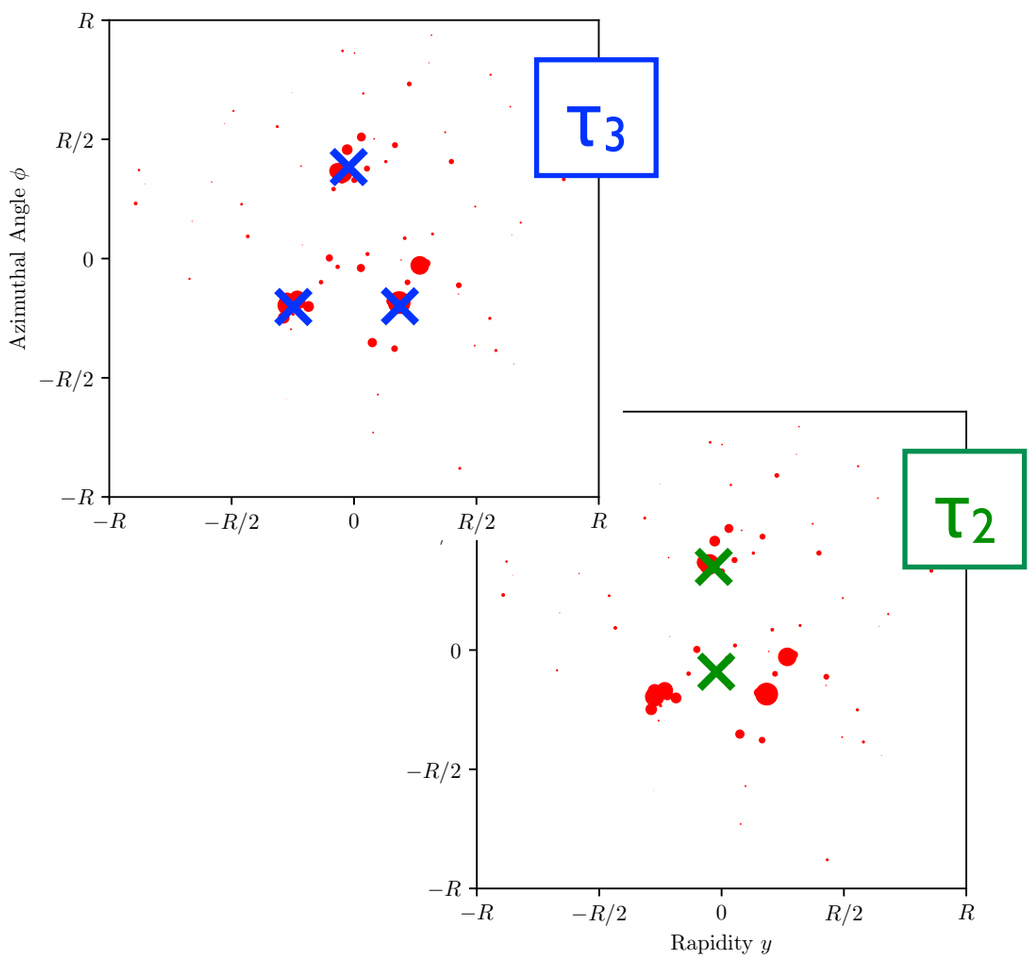


[Komiske, Metodiev, JDT, JHEP 2019; see also Dreyer, Salam, Soyez, JHEP 2018]

N-subjettiness

Ubiquitous jet substructure observable used for almost a decade…

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

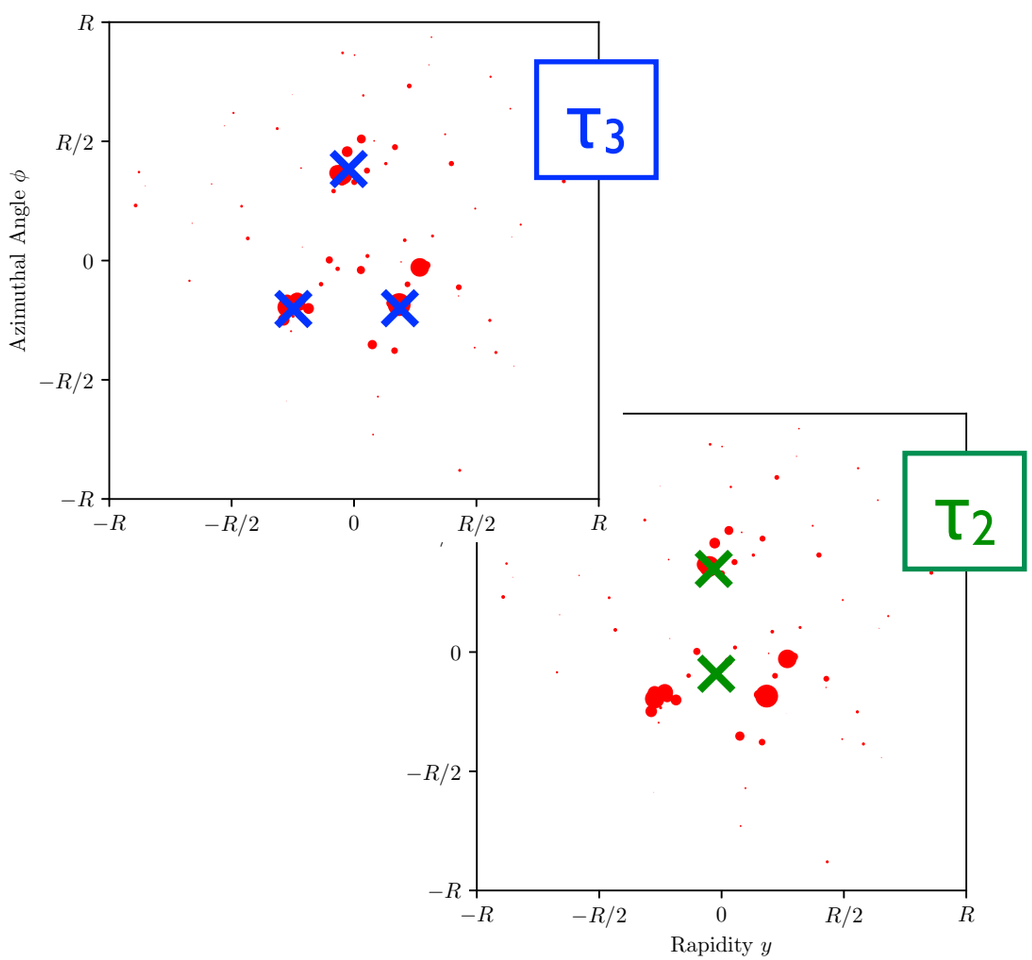


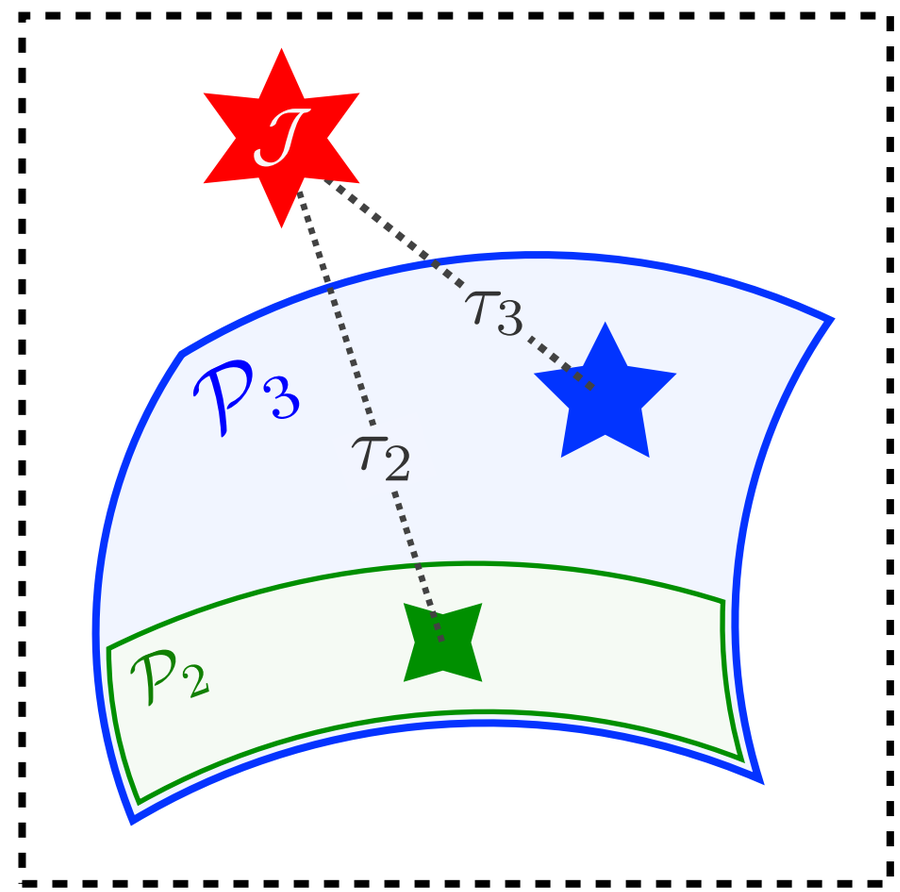
[JDT, Van Tilburg, JHEP 2011, JHEP 2012;
based on Brandt, Dahmen, ZPC 1979; Stewart, Tackmann, Waalewijn, PRL 2010]

N-subjettiness = Point to Manifold EMD

…is secretly an optimal transport problem

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

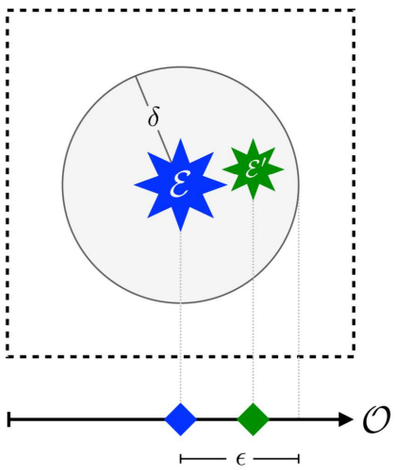




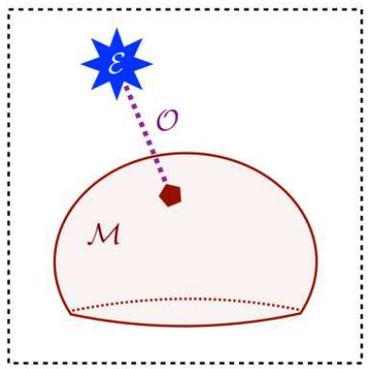
[JDT, Van Tilburg, JHEP 2011, JHEP 2012;
rephrased via Komiske, Metodiev, JDT, JHEP 2020; see opposite limit in Cesarotti, JDT, JHEP 2020]

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

IRC Safety is smoothness in the space of events

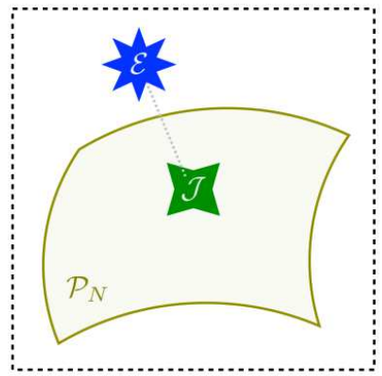


Event shapes are distances from events to manifolds.



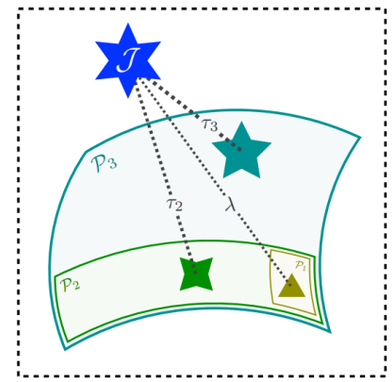
$$\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{M}} \mathrm{EMD}_{\beta,R}(\mathcal{E}, \mathcal{E}')$$

Jets are projections to few-particle manifolds.



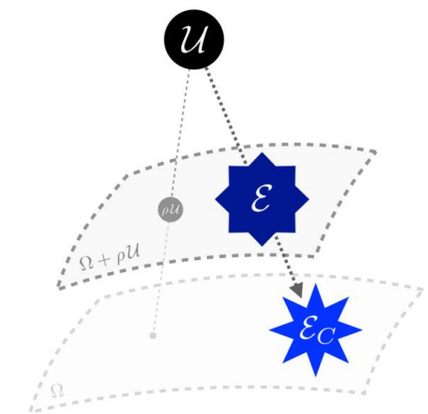
$$\mathcal{J} = \operatorname*{argmin}_{\mathcal{E}' \in \mathcal{P}_N} \mathrm{EMD}_{\beta,R}(\mathcal{E}, \mathcal{E}')$$

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]