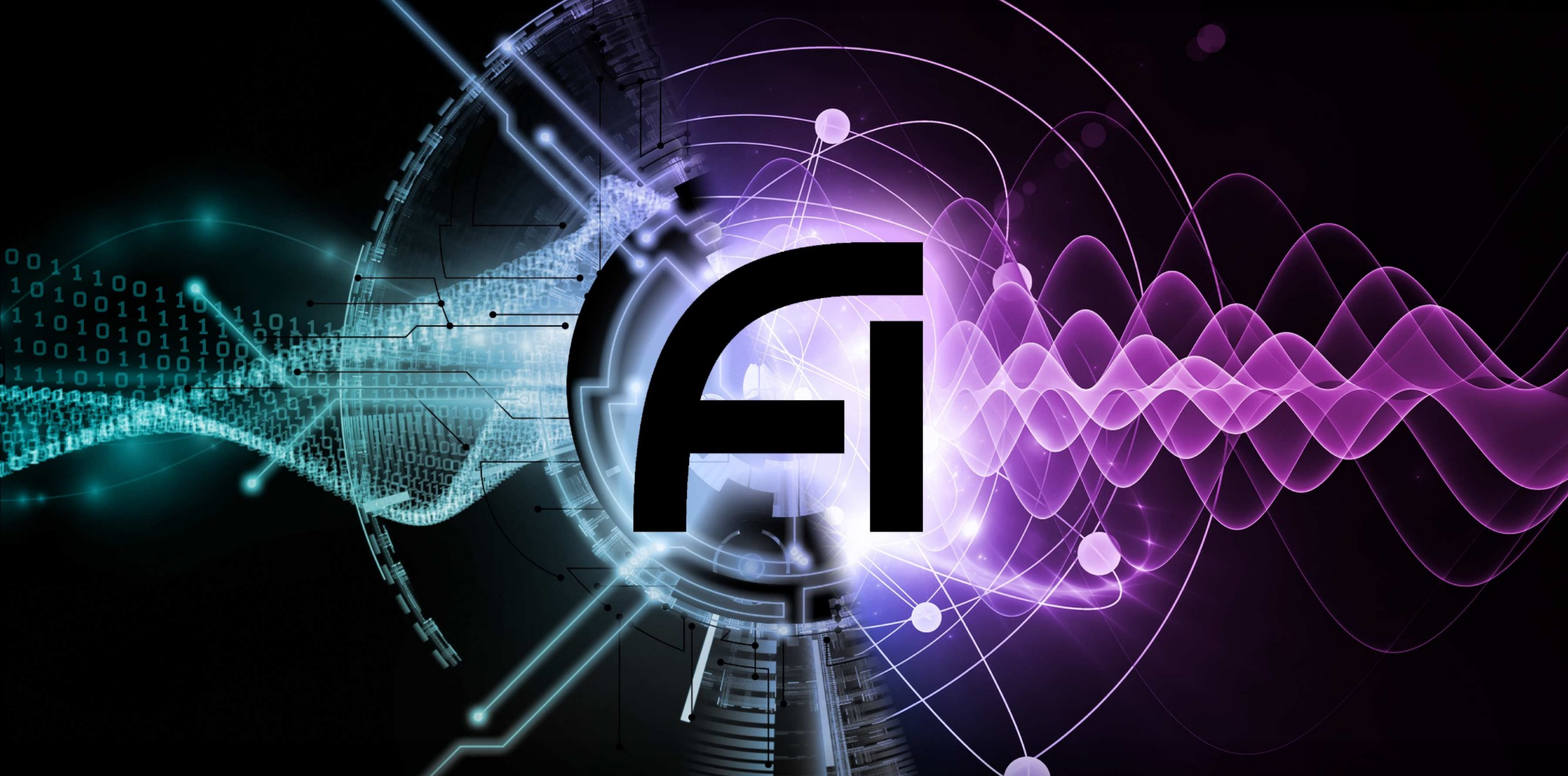
Machine Learning in Collider Physics

Jesse Thaler

Snowmass Energy Frontier Workshop — March 29, 2022

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI /aɪ-faɪ/ iaifi.org)



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

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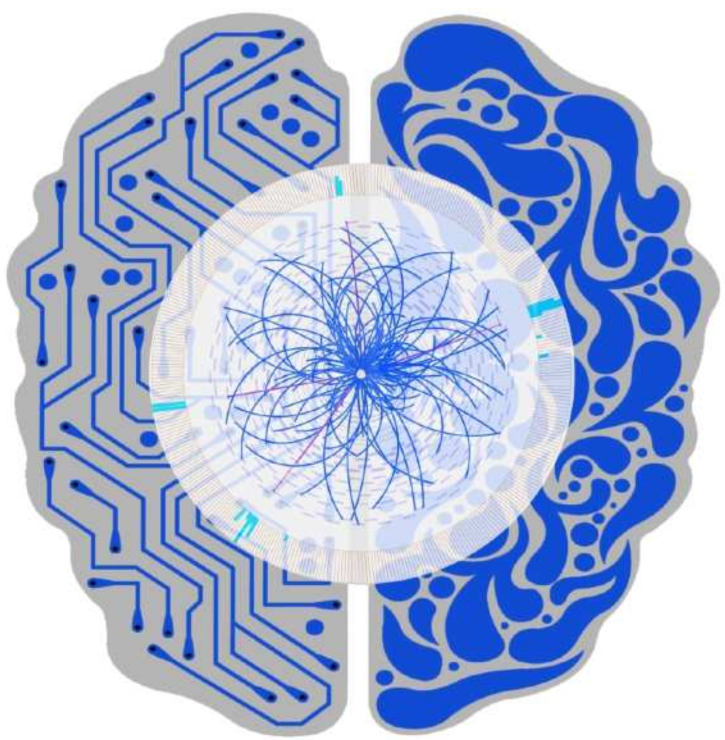

Infuse physics intelligence into artificial intelligence

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

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

Pushing the Frontiers of Collider Physics

$$\sigma_{\text{obs}} \simeq \frac{1}{2E_{\text{CM}}^2} \sum_{n=2}^{\infty} \int d\Phi_n \, |\mathcal{M}_{AB\to 12\ldots n}|^2 \, f_{\text{obs}}(\Phi_n)$$

cross section — phase space — amplitude — observable

Opportunity to rethink every ingredient in this formula

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cross section phase space amplitude observable

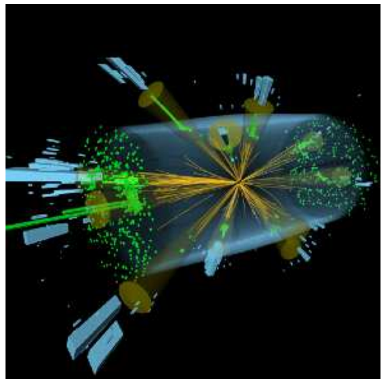
Opportunity to rethink every ingredient in this formula

Opportunity to leverage new frameworks to advance our understanding of (B)SM physics

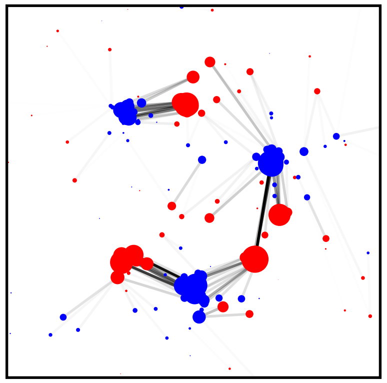
This Talk: Machine Learning
Moult's Talk: Conformal Physics

Battel's Talk:
(Un-)Naturalness

My (Evolving) Perspective



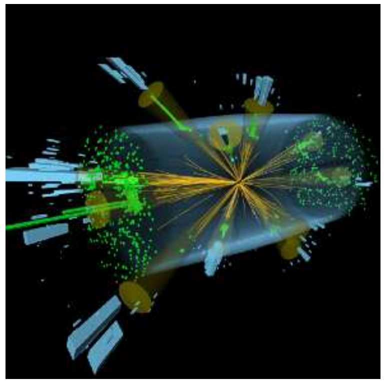
Collider physics (theory and experiment) has been irreversibly impacted by the rise of deep learning



The buzz is around "AI", but we should leverage analysis strategies from various areas of mathematics, statistics, and computer science

We have an opportunity to translate aspects of collider physics into a computational language

In the spirit of Snowmass, looking forward to *your* ideas and perspectives!



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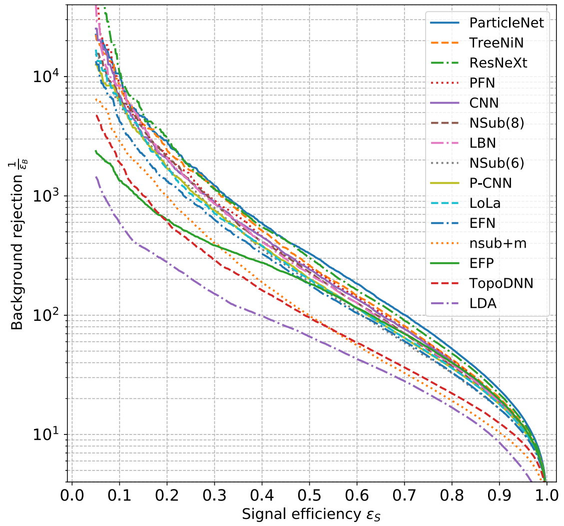
Cue the TF07 Deep Learning Montage!

Apologies: citations are representative, not exhaustive!

[see HEPML-LivingReview for extensive bibliography]

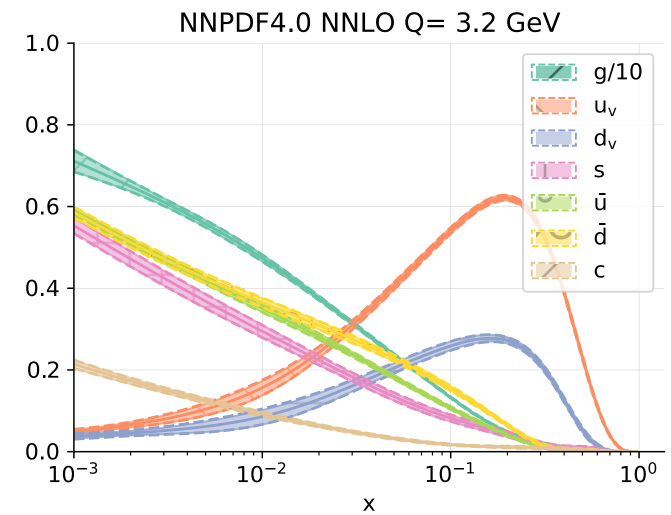
Deep Learning for Colliders (TF07)

Jet Classification



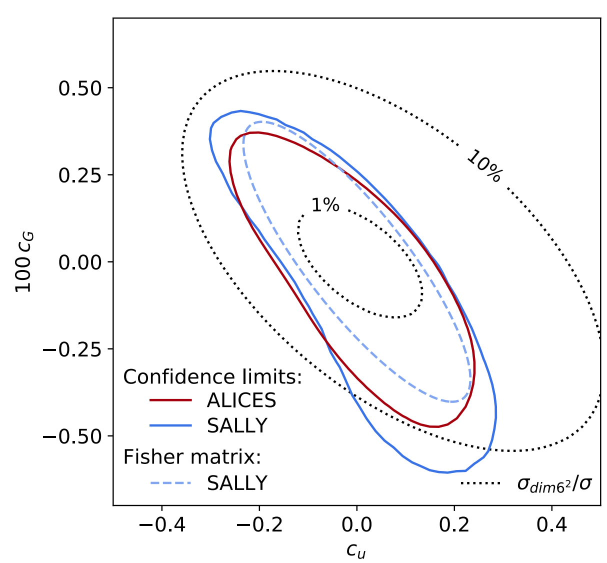
[e.g. Kasieczka, Plehn, et al., SciPost 2019]

Parton Distribution Functions



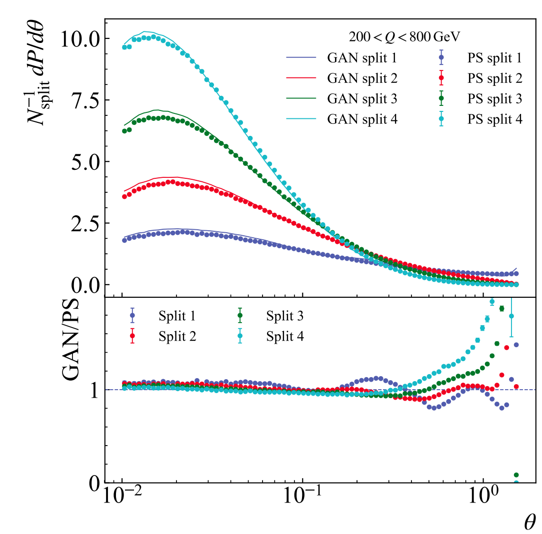
[e.g. NNPDF Collaboration, JHEP 2022]

Parameter Inference



[e.g. Brehmer, Kling, Espejo, Cranmer, CSBS 2020]

Parton Shower Modeling/Tuning



[e.g. Lai, Neill, Płoskoń, Ringer, arXiv 2020;
see also Andreassen, Feige, Frye, Schwartz, EPJC 2019]

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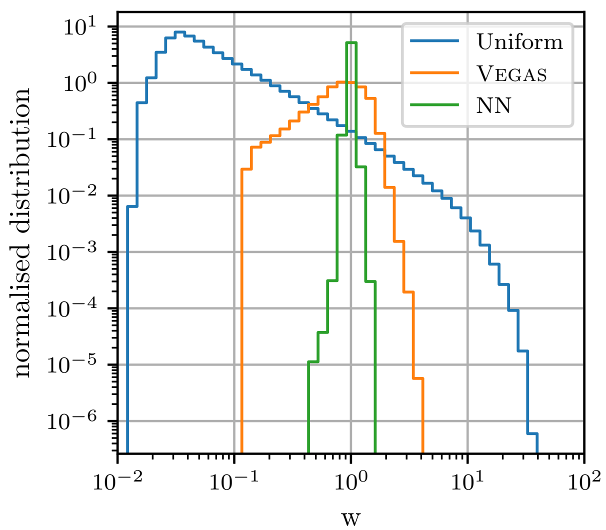
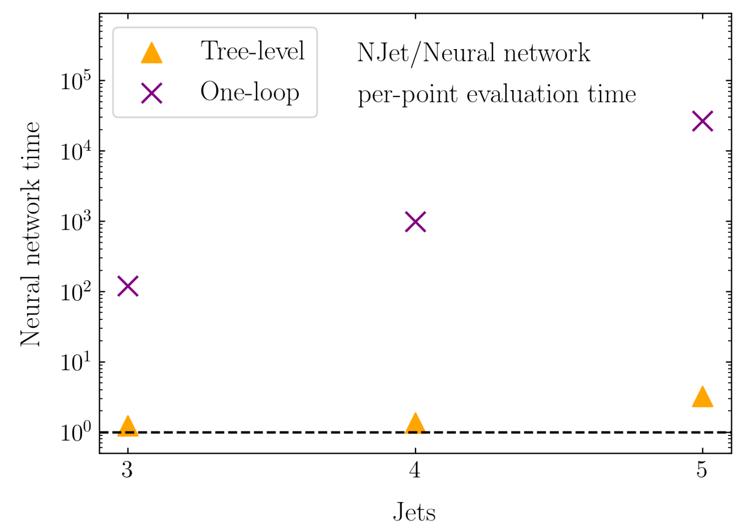
More Deep Learning for Colliders (TF07)

Phase Space Integration



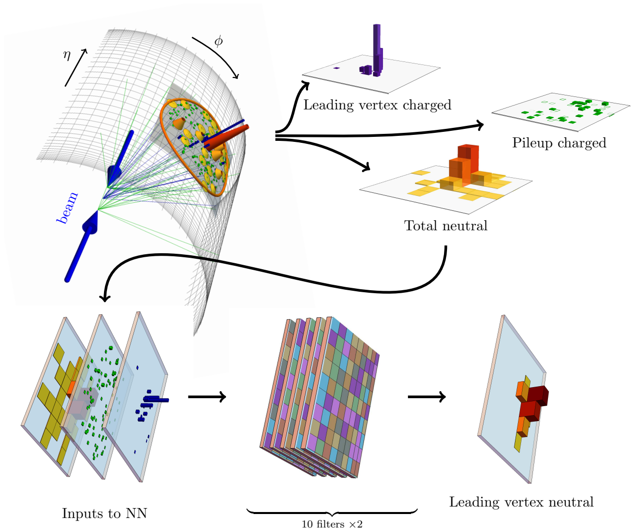
[e.g. Bothmann, Janßen, Knobbe, Schmale, Schumann, SciPost 2020; see also Gao, Höche, Isaacson, Krause, Schulz, PRD 2020]

Amplitude Approximations



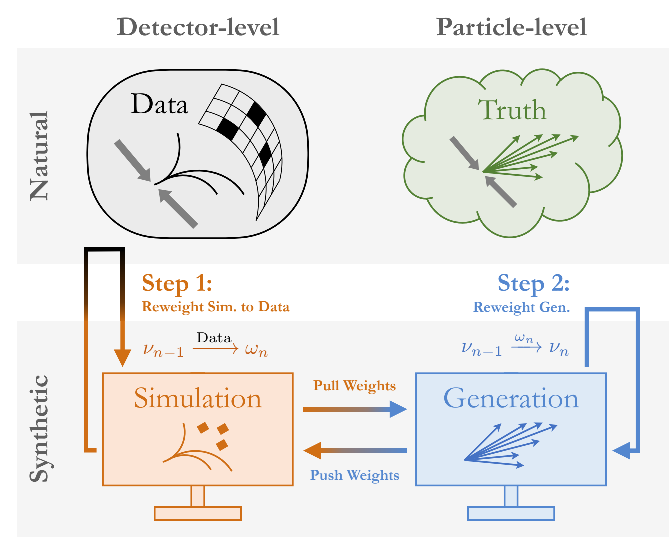
[e.g. Badger, Bullock, JHEP 2020]

Pileup Mitigation



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

Deconvolution/Unfolding



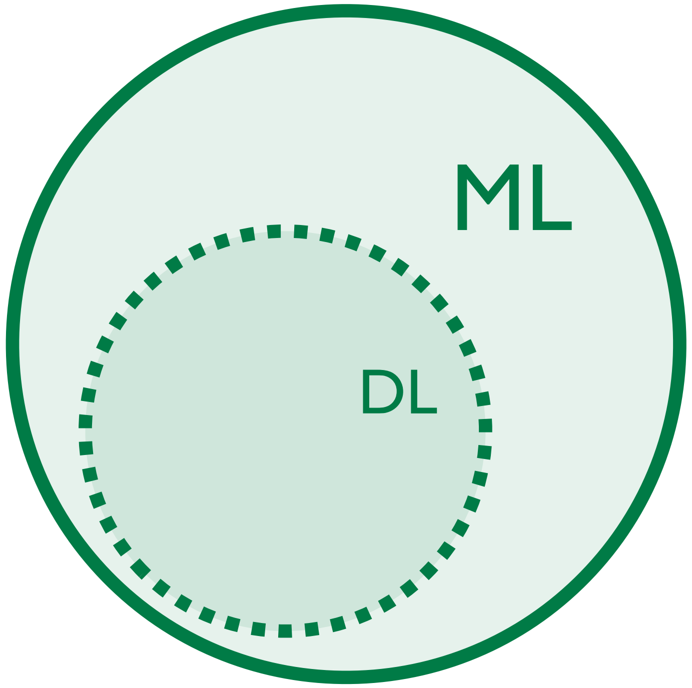
[e.g. Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020; see also Bellagente, Butter, Kasieczka, Plehn, Rousselot, Winterhalder, Ardizzone, Köthe, SciPost 2020]

. . .

"Ok, but what is the machine learning?"

Hmm, I'd like to move away from anthropomorphizing algorithms…

Space of Analysis Strategies



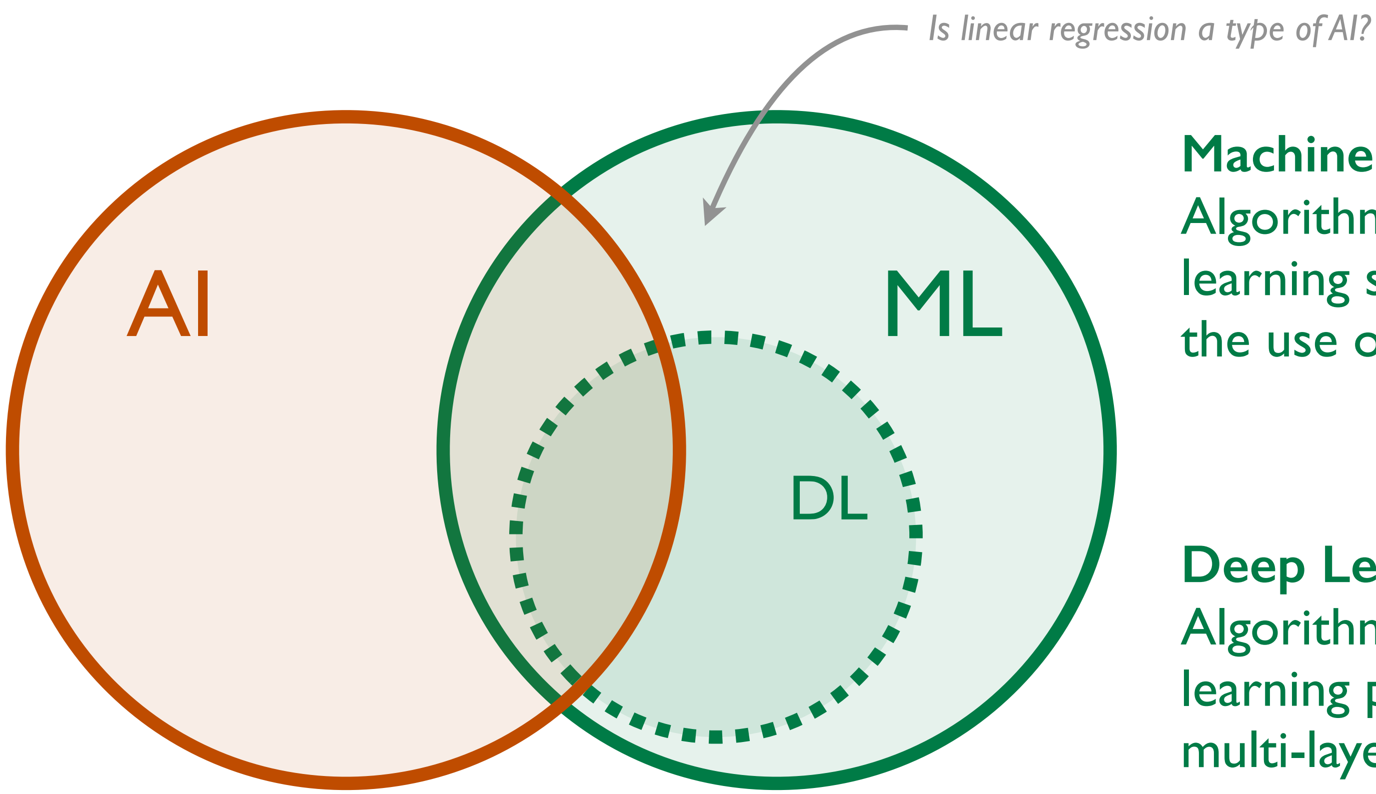
Machine Learning:
Algorithms based on learning solutions through the use of data

Deep Learning:
Algorithms based on learning parameters of multi-layer neural networks

In most cases, the machine is learning an approximate solution to a well-specified optimization problem

Space of Analysis Strategies

Artificial Intelligence:
Algorithms to perform tasks that are typically associated with intelligent beings



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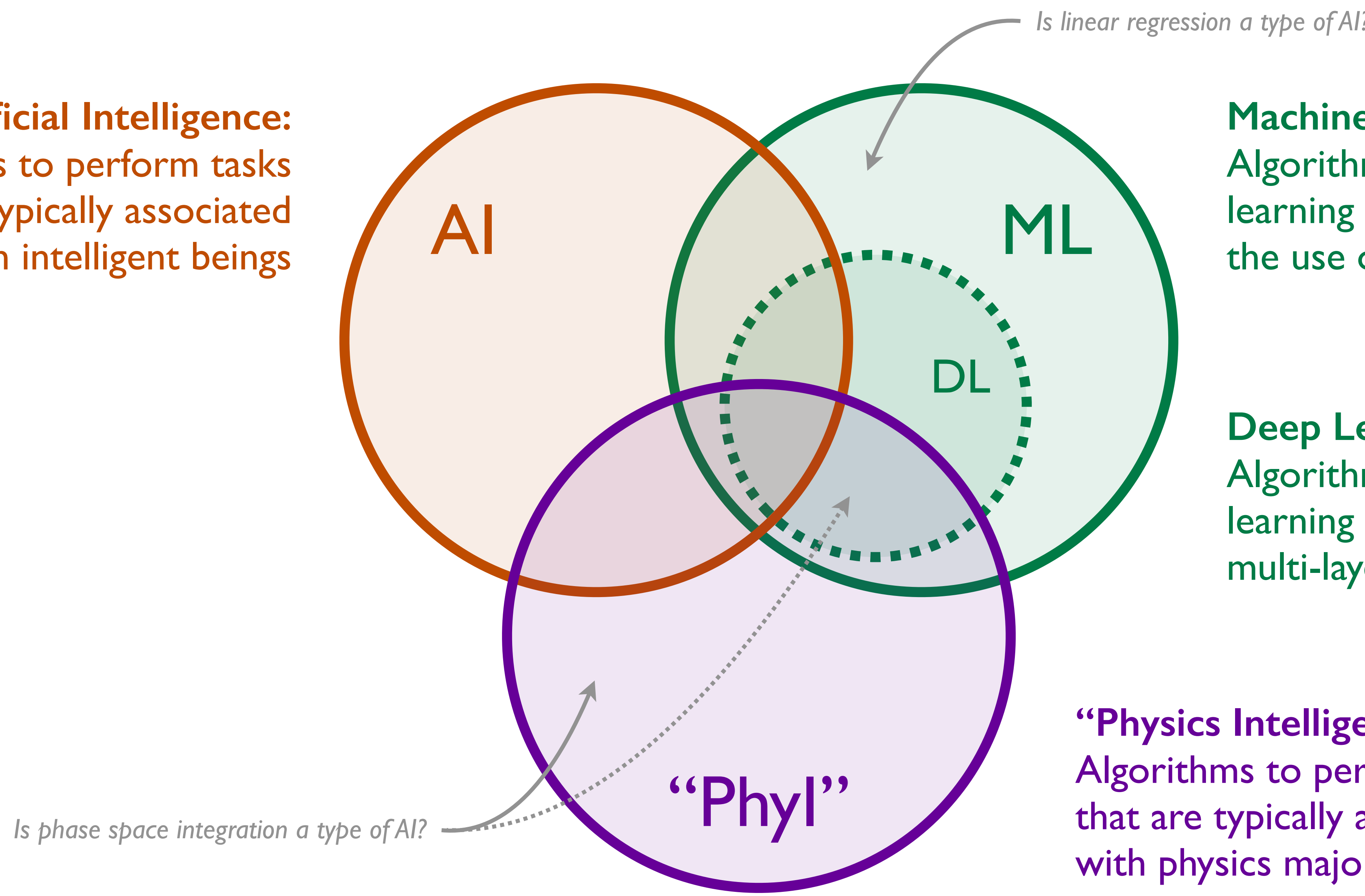

Machine Learning:
Algorithms based on learning solutions through the use of data

Deep Learning:
Algorithms based on learning parameters of multi-layer neural networks

"Physics Intelligence":
Algorithms to perform tasks that are typically associated with physics majors/PhDs

In most cases, the machine is learning an approximate solution to a well-specified optimization problem

Progress made not just because of
increased computational power and large datasets…

…but also because we have understood the
structure of the underlying problems

And the structure of many HEP problems are optimization tasks; more discussion in backup

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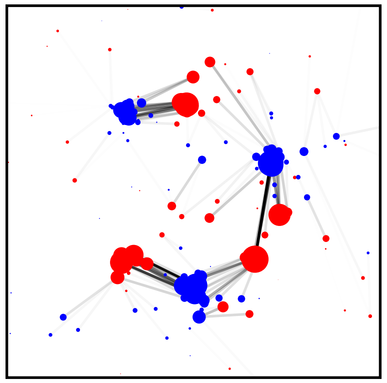

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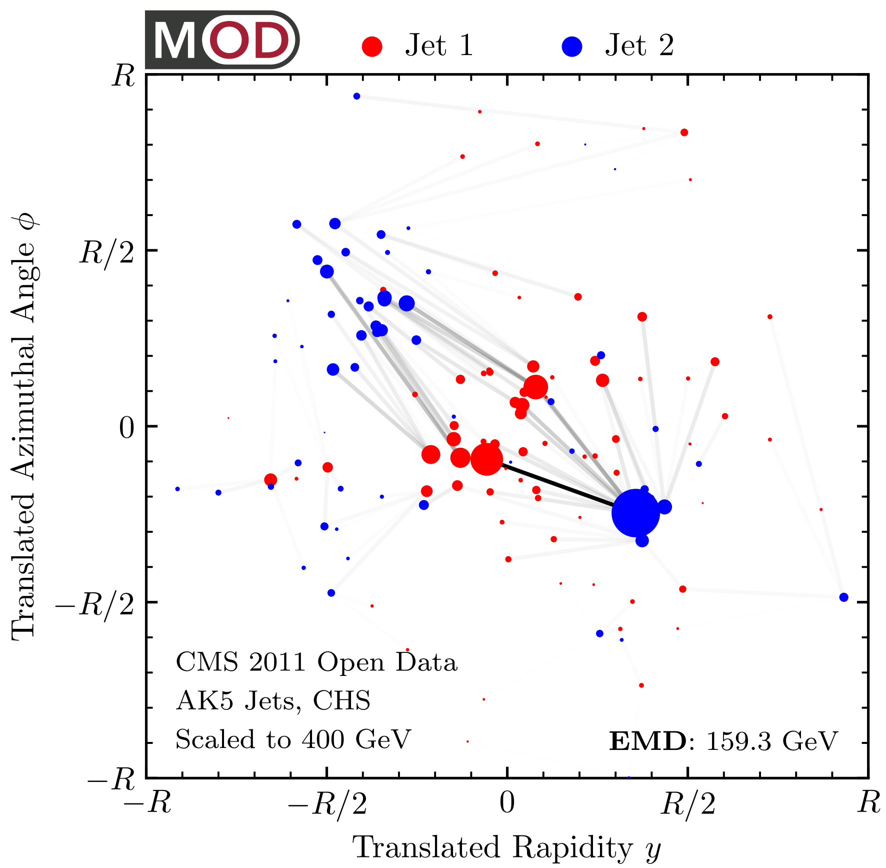
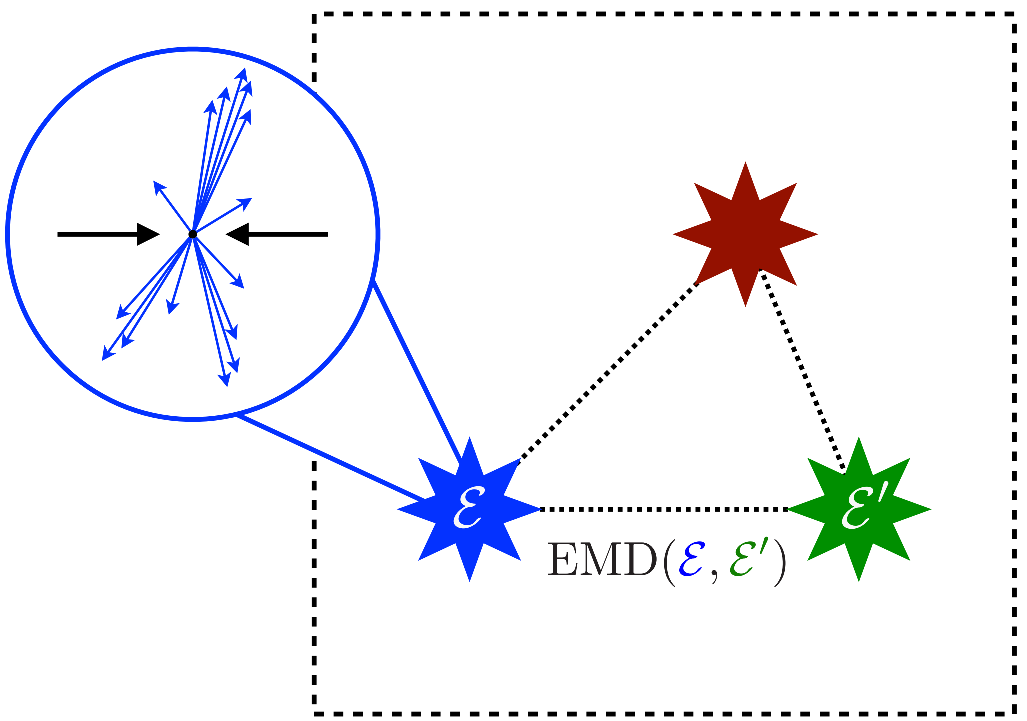
Optimal Transport for Collider Geometry

Energy Mover's Distance ⇒ Metric Space of Collider Events





New insights into high-energy physics facilitated by advances in mathematics, statistics, and computer science

[Komiske, Metodiev, JDT, PRL 2019; code at Komiske, Metodiev, JDT, energyflow.network; open data study in Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]
[based on Peleg, Werman, Rom, IEEE 1989; Rubner, Tomasi, Guibas, ICCV 1998, ICJV 2000; Pele, Werman, ECCV 2008; Pele Taskar, GSI 2013]
[flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, EPJC 2021; linearized and unbalanced transport in Cai, Cheng, Craig, Craig, PRD 2020, arXiv 2021]

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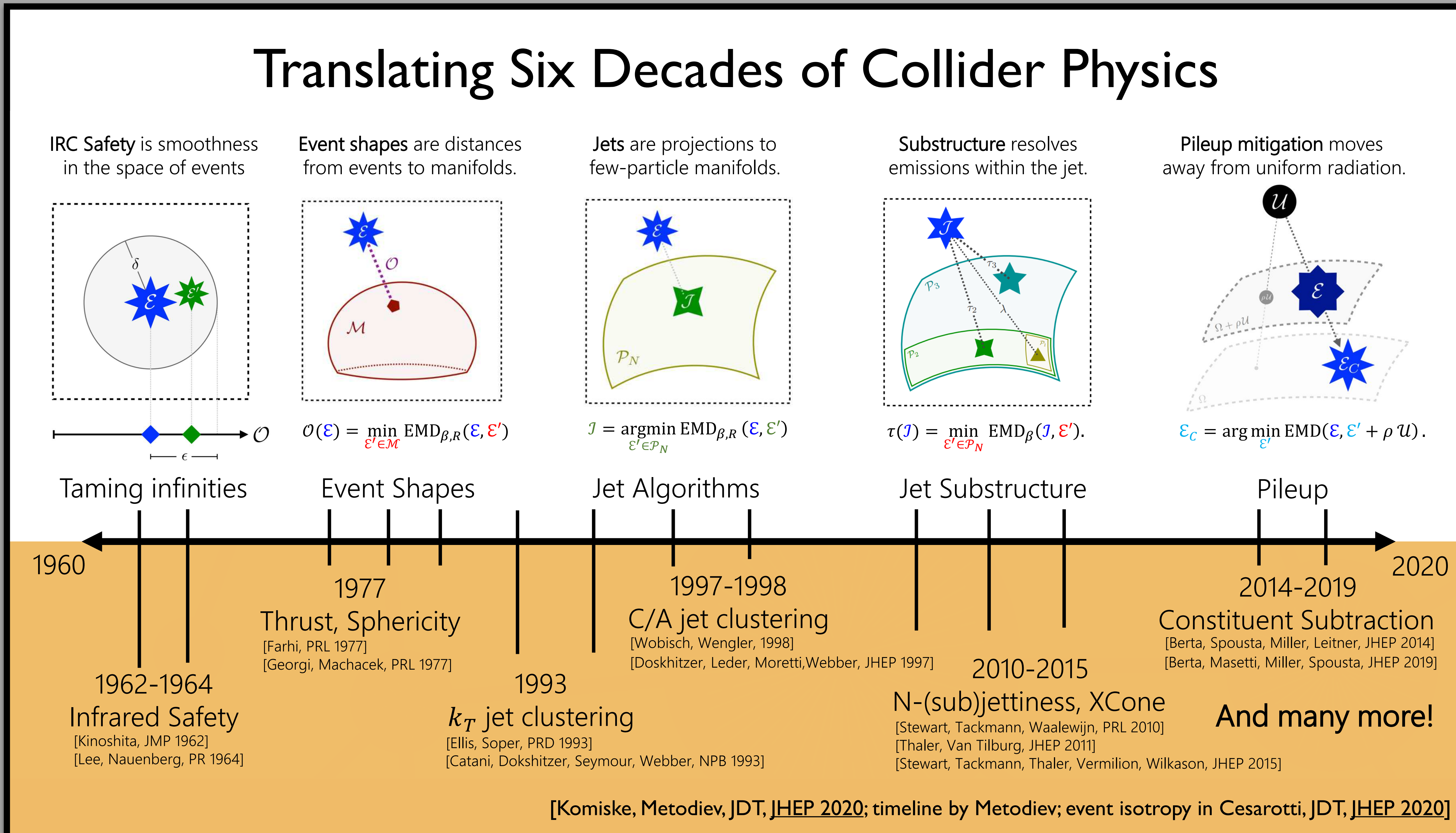

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The New York Times
By Dennis Overbye
Nov. 23, 2020

Can a Computer Devise a Theory of Everything?


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I loathe this question

Overhyping deep learning, which is just one of many computational strategies relevant for the physical sciences

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Can a Computer Devise a Theory of Everything?

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Overhyping deep learning, which is just one of many computational strategies relevant for the physical sciences

I love this question

Reframes the scientific process and raises questions about what aspects of reductionist logic could be automated

ML for BSM Physics?

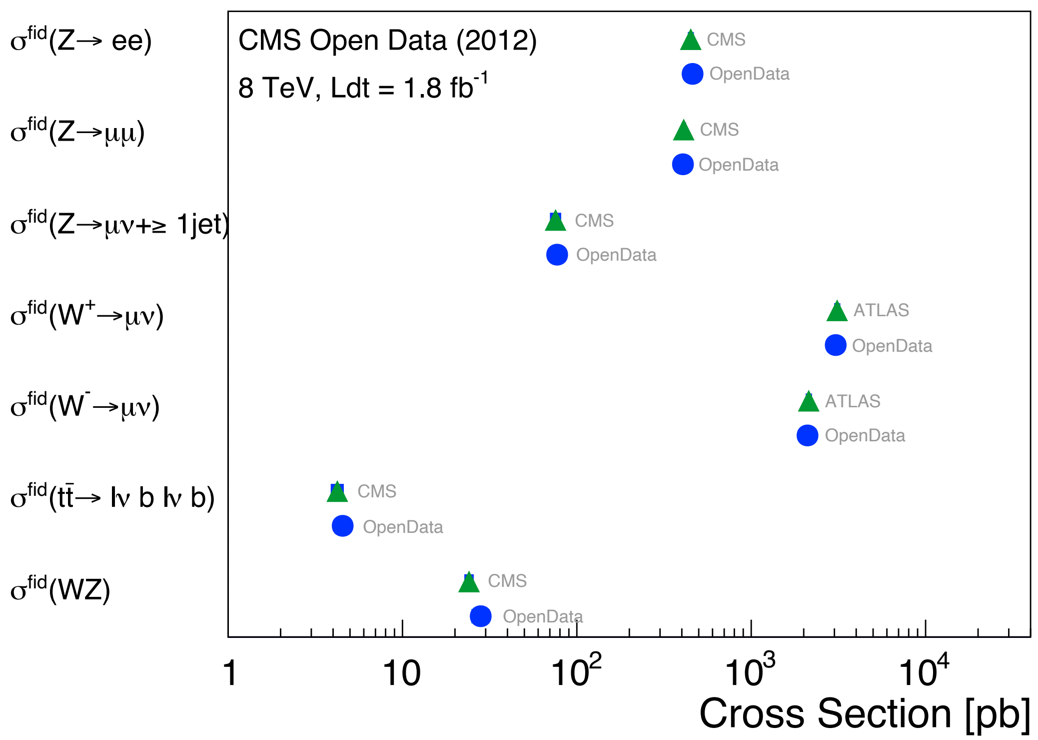
E.g. Anomaly Detection

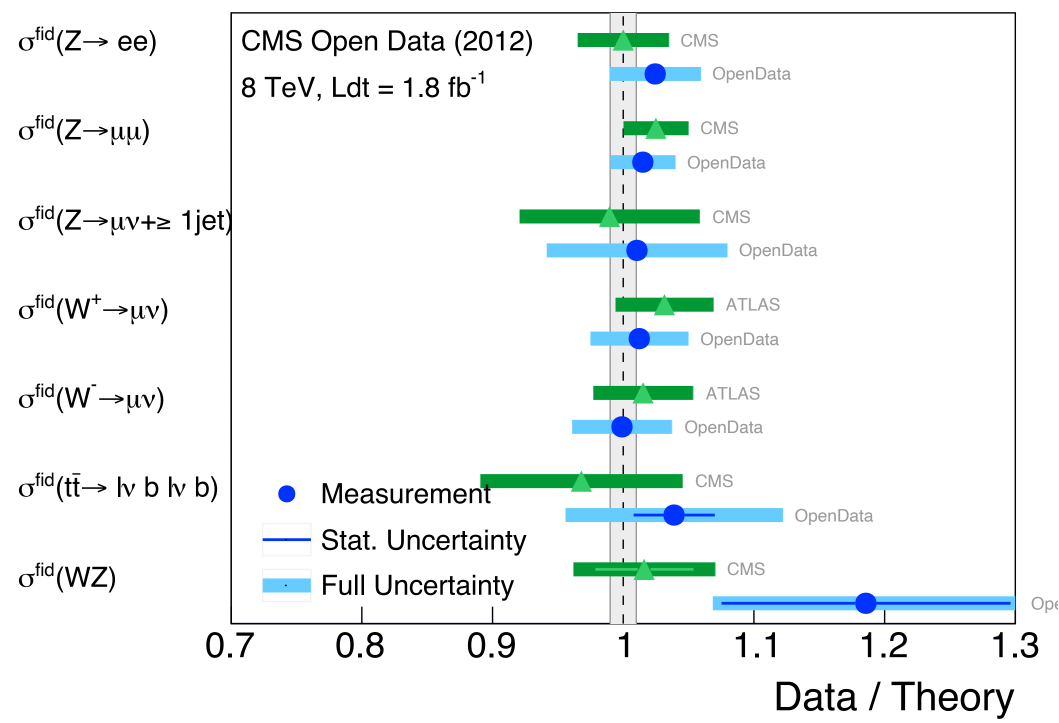
[image from LHC Olympics 2022; see Kasieczka, Nachman, Shih et al., RPP 2021]

What aspects of BSM phenomenology could be streamlined, systematized, and automated?

ML for SM Physics?

E.g. Open Data / Uncertainty Quantification

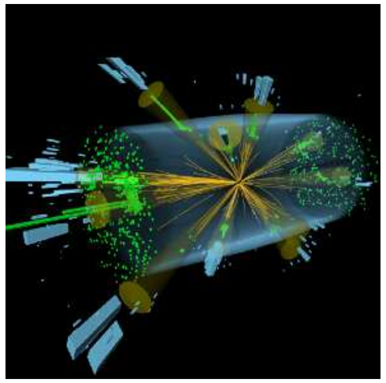




[plots from Apyan, Cuozzo, Klute, Saito, Schott, Sintayehu, JINST 2020]

Can we more tightly integrate theory and experiment to future-proof analyses?

Machine Learning in Collider Physics



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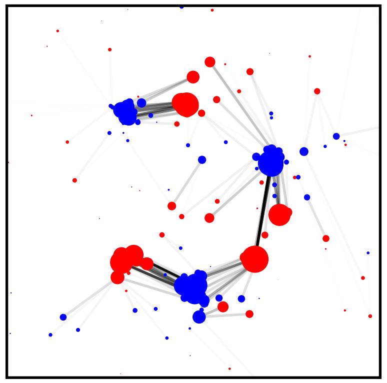

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Backup Slides

E.g. Likelihood Ratio Trick

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. 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, JDT, PRD 2021]

E.g. Likelihood Ratio Trick

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. 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, JDT, PRD 2021]

Machine Learning Ingredients

Many HEP theory tasks can phrased as ML optimization

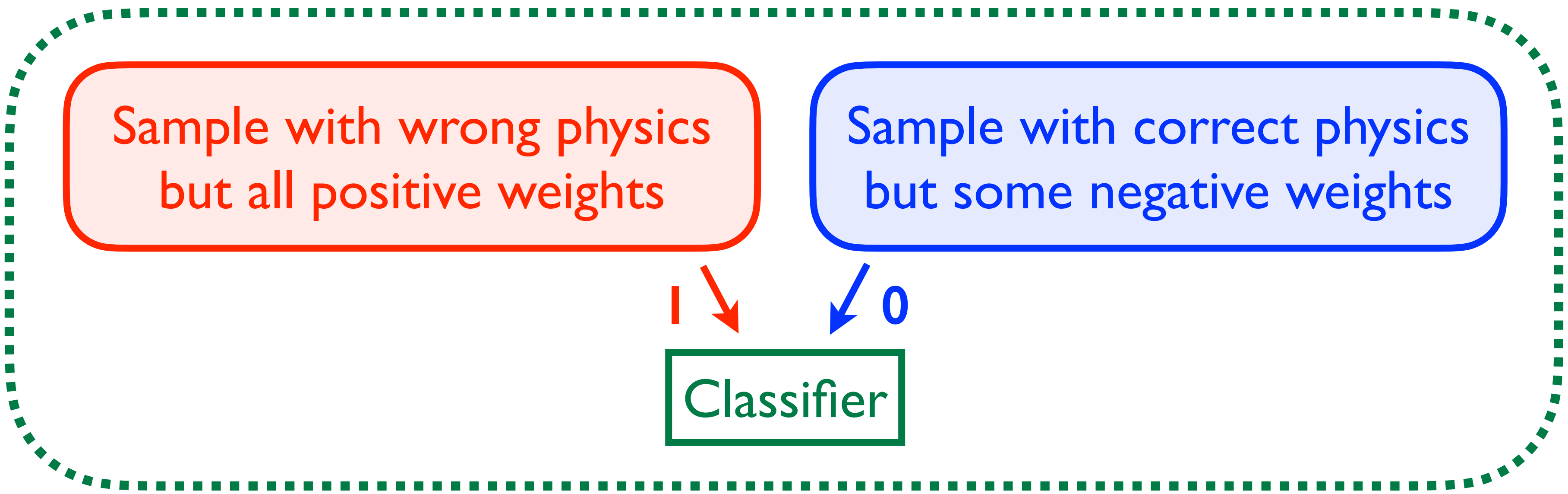
Well-Specified Loss — *E.g. classification, regression, generation, …*
With implicit or explicit regularization

Reliable Training Data — *Real or synthetic, fixed or dynamic*
Labeled, partially labeled, or unlabeled

Learnable Function — *Linear/logit function, neural network,*
normalizing flow, other parametrized form, …

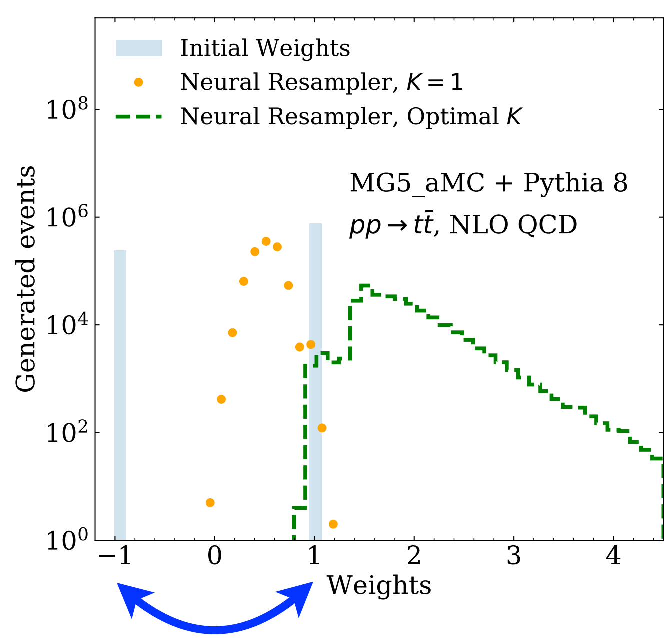
Physics input essential for robust usage of these tools,
but interdisciplinary training also valuable

E.g. Neural Resampling for MC Beyond LO

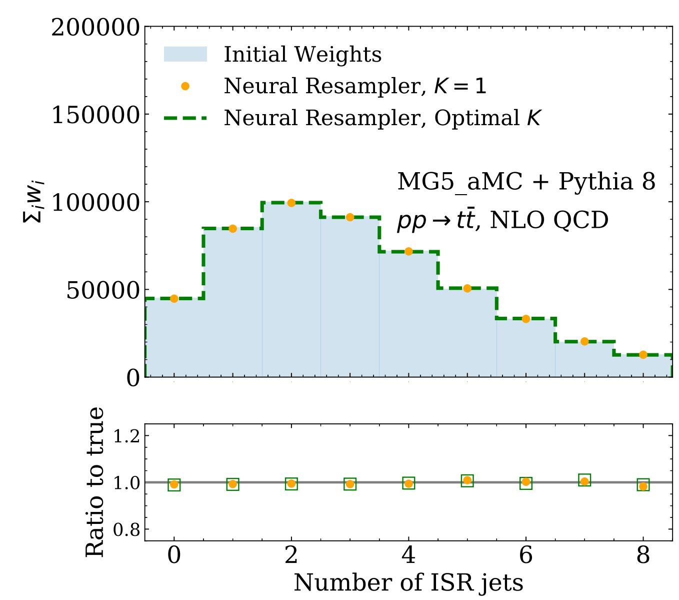


$\Rightarrow w(x)$

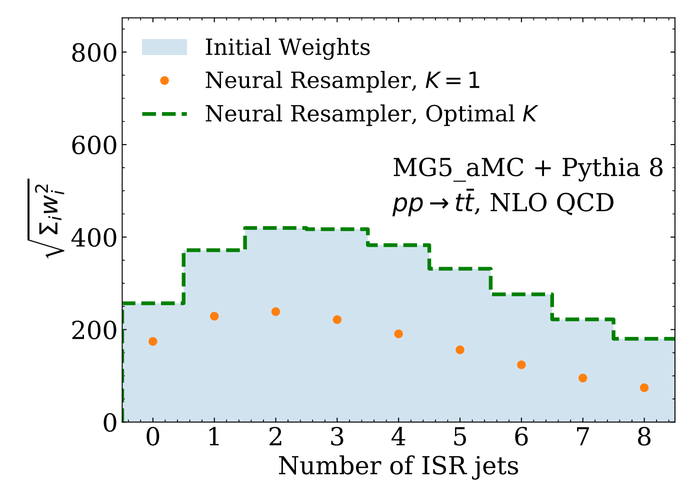
MC@NLO: large weight cancellations



Reweighting recovers desired distribution



Resampling recovers desired uncertainties



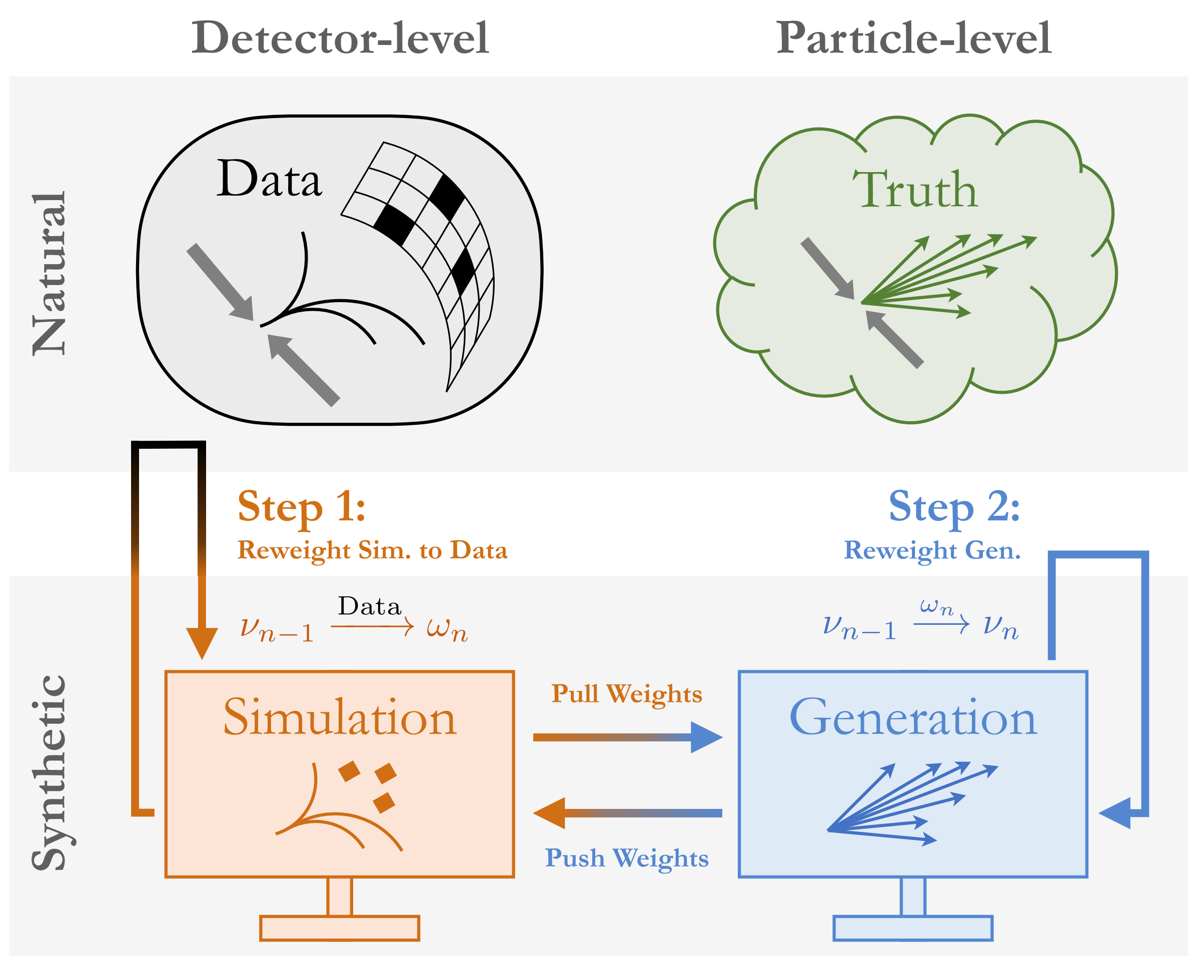
Using custom ML strategy

[Nachman, JDT, PRD 2020; inspired by Andersen, Gutschow, Maier, Prestel, EPJC 2020]

E.g. Detector Unfolding

OmniFold

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

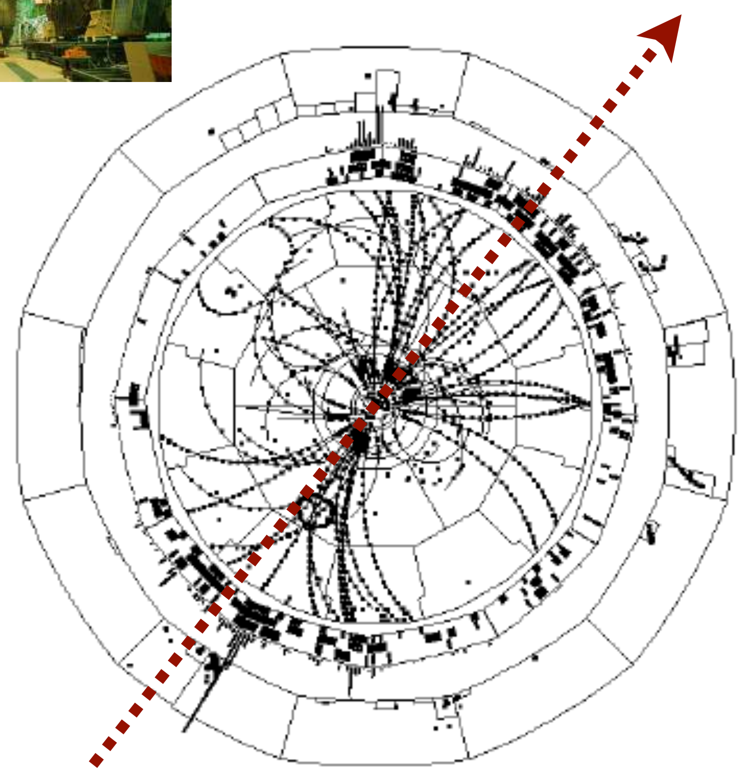


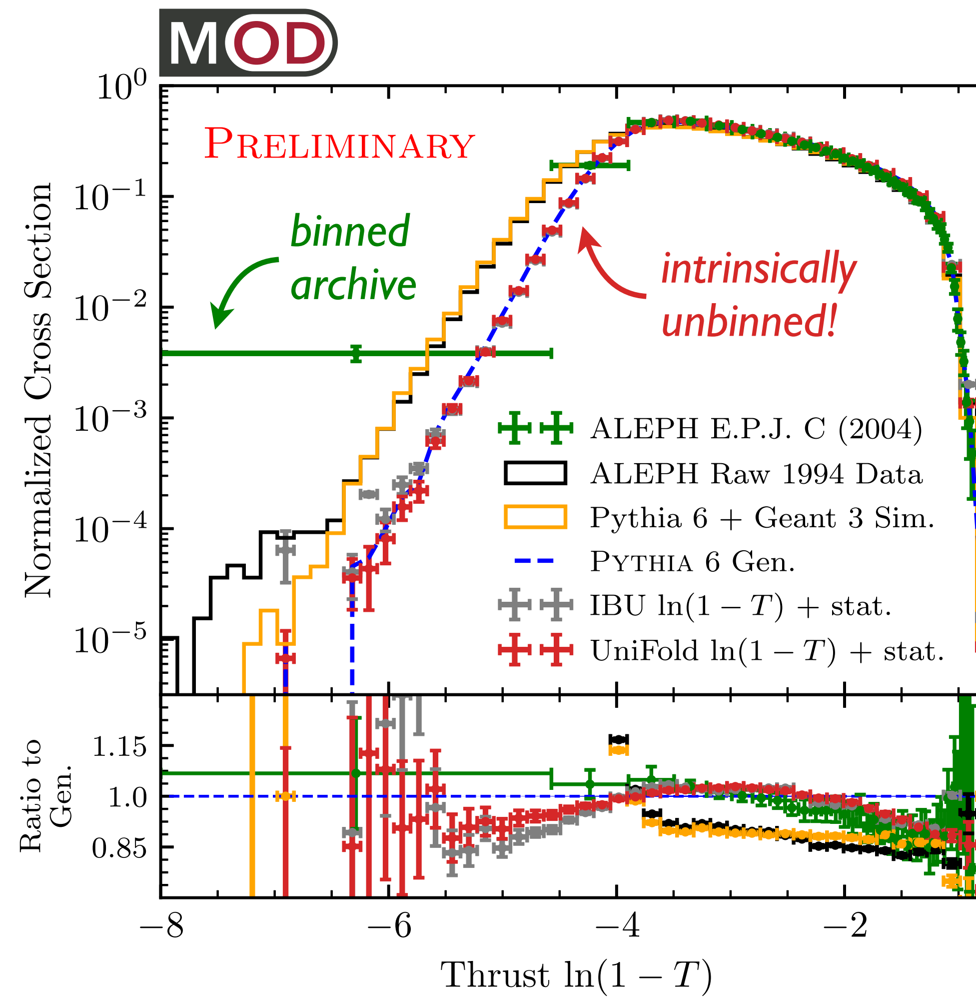
Use ML to compute reweighting factors

[Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020; + Suresh, ICLR SimDL 2021;
Komiske, McCormack, Nachman, PRD 2021; see unfolding comparison in Petr Baron, arXiv 2021]
[see alternative in Bellagente, Butter, Kasieczka, Plehn, Rousselot, Winterhalder, Ardizzone, Köthe, SciPost 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; H1, DIS2021]

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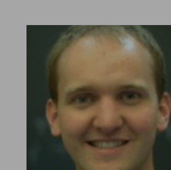
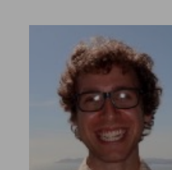
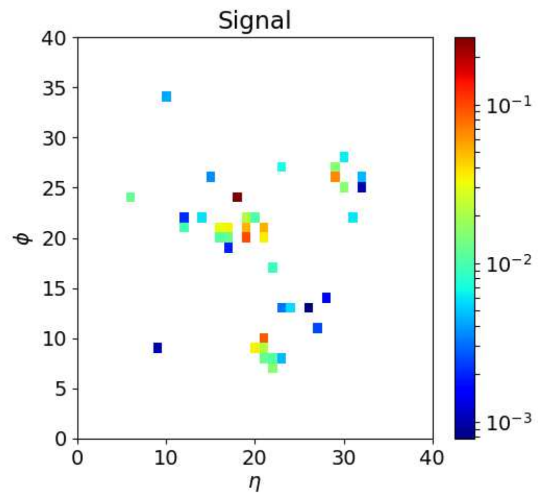




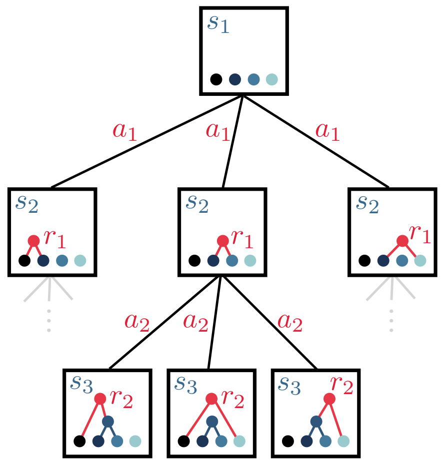
Theoretical Priors ⇒ Network Architectures

Pixelized Calorimetry



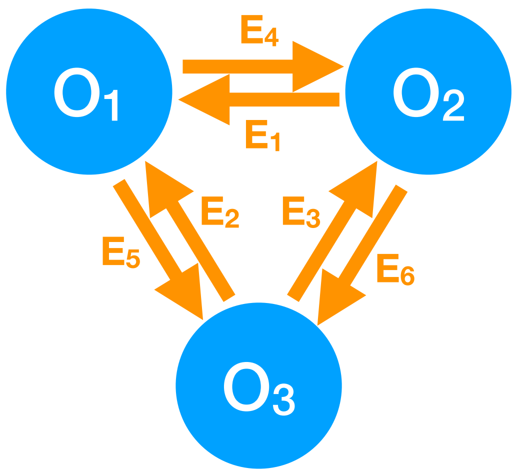
[review in Kagan, arXiv 2020]

Hierarchical Showers



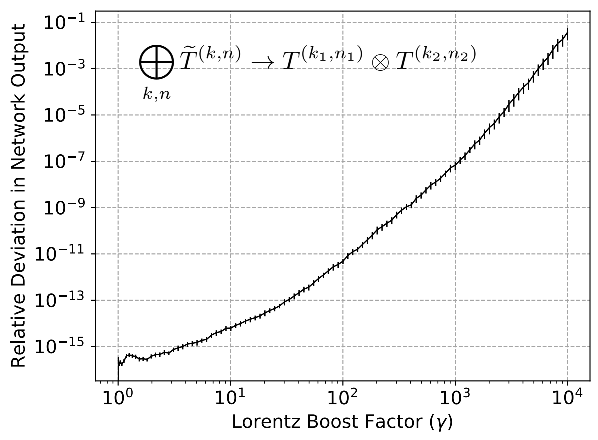
[e.g. Brehmer, Macaluso, Pappadopulo, Cranmer, NeurIPS 2020]

Pairwise Interactions



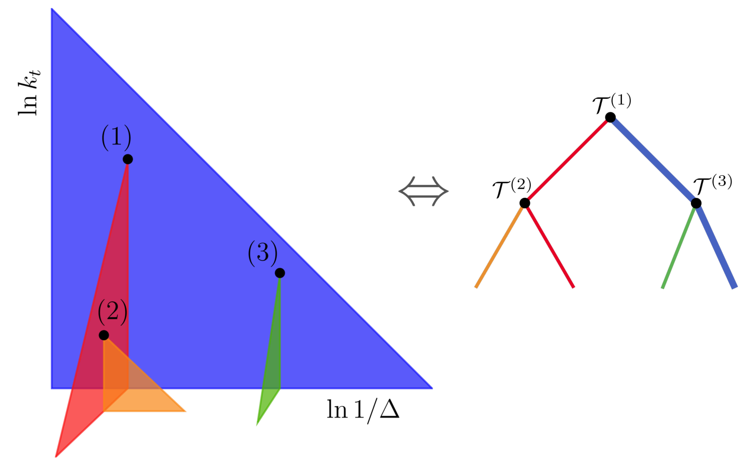
[e.g. Moreno, Cerri, Duarte, Newman, Nguyen, Periwal, Pierini, Serikova, Spiropulu, Vlimant, EPJC 2020]

Lorentz Equivariance



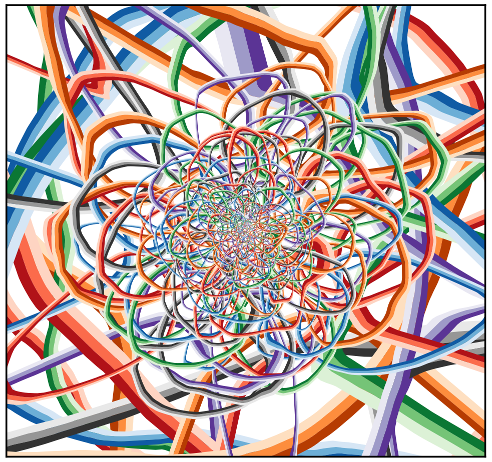
[e.g. Bogatskiy, Anderson, Offermann, Roussi, Miller, Kondor, arXiv 2020]

Lund Plane Emissions



[e.g. Dreyer, Qu, JHEP 2021]

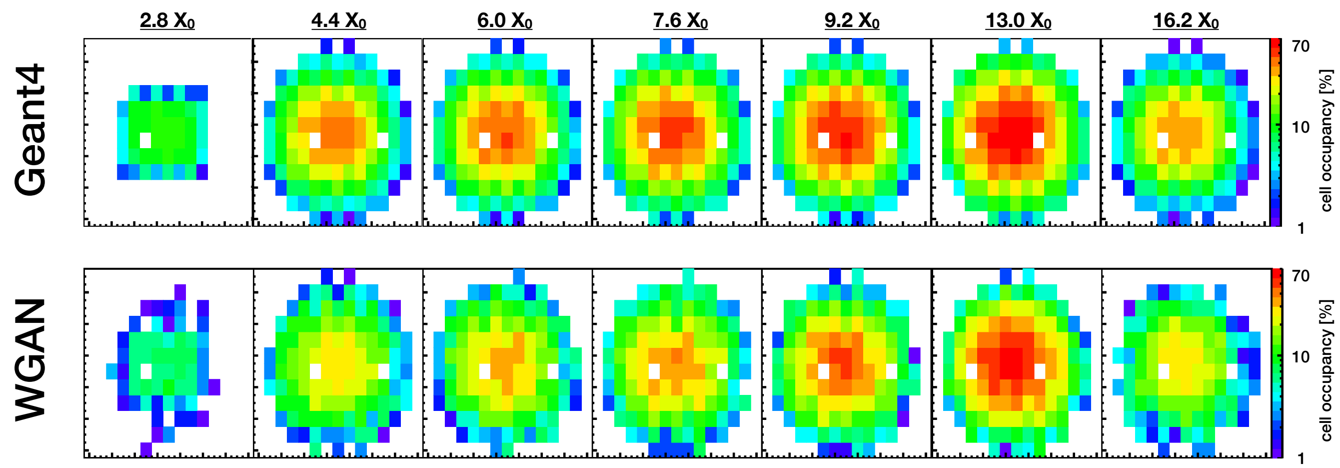
Infrared and Collinear Safety



[e.g. Komiske, Metodiev, JDT, JHEP 2019; see also Dolan, Ore, PRD 2021; Konar, Ngairangbam, Spannowsky, JHEP 2022]

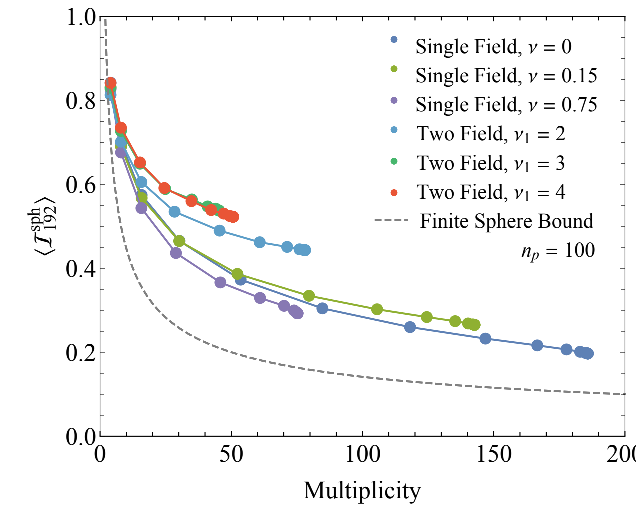
Wasserstein Elsewhere in HEP

Generative Modeling



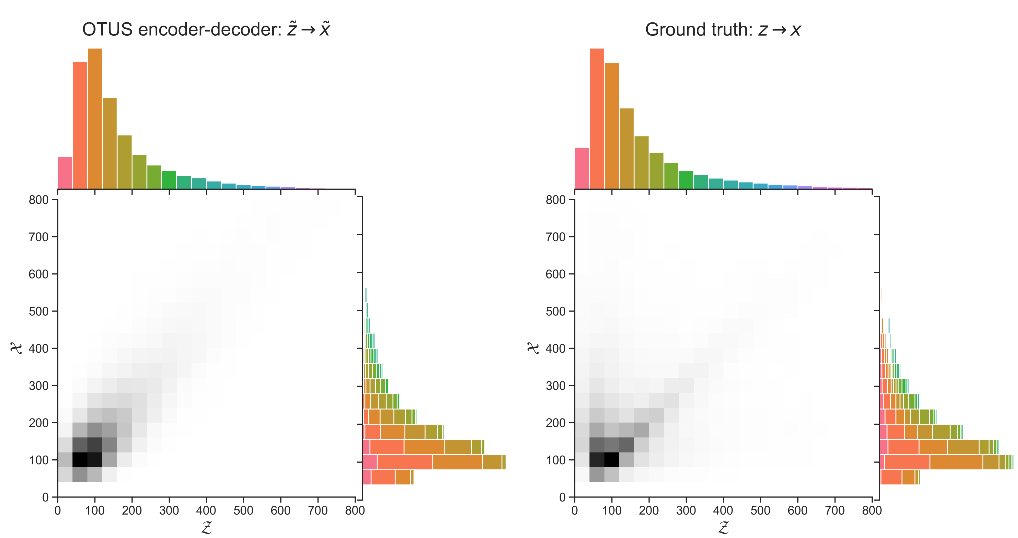
[Erdmann, Geiger, Glombitza, Schmidt, CSBS 2018; Erdmann, Glombitza, Quast, CSBS 2019; Chekalina, Orlova, Ratnikov, Ulyanov, Ustyuzhanin, Zakharov, CHEP 2018]

BSM Characterization



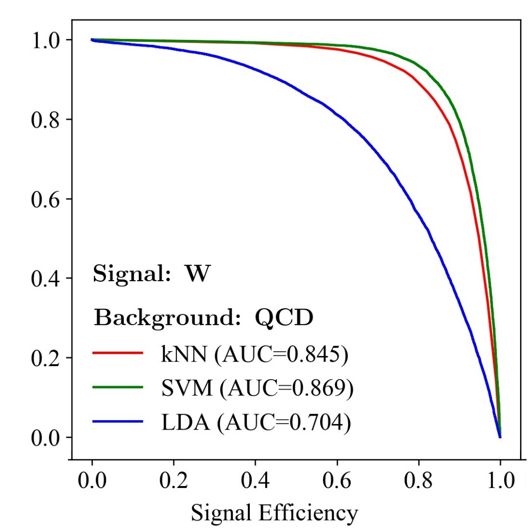
[Cesarotti, Reece, Strassler, JHEP 2021, arXiv 2020]

Estimated Simulation/Unfolding



[Howard, Mandt, Whiteson, Yang, arXiv 2021]

Jet Classification

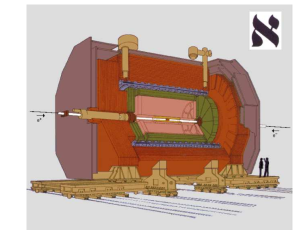


[Cai, Cheng, Craig, Craig, PRD 2020]

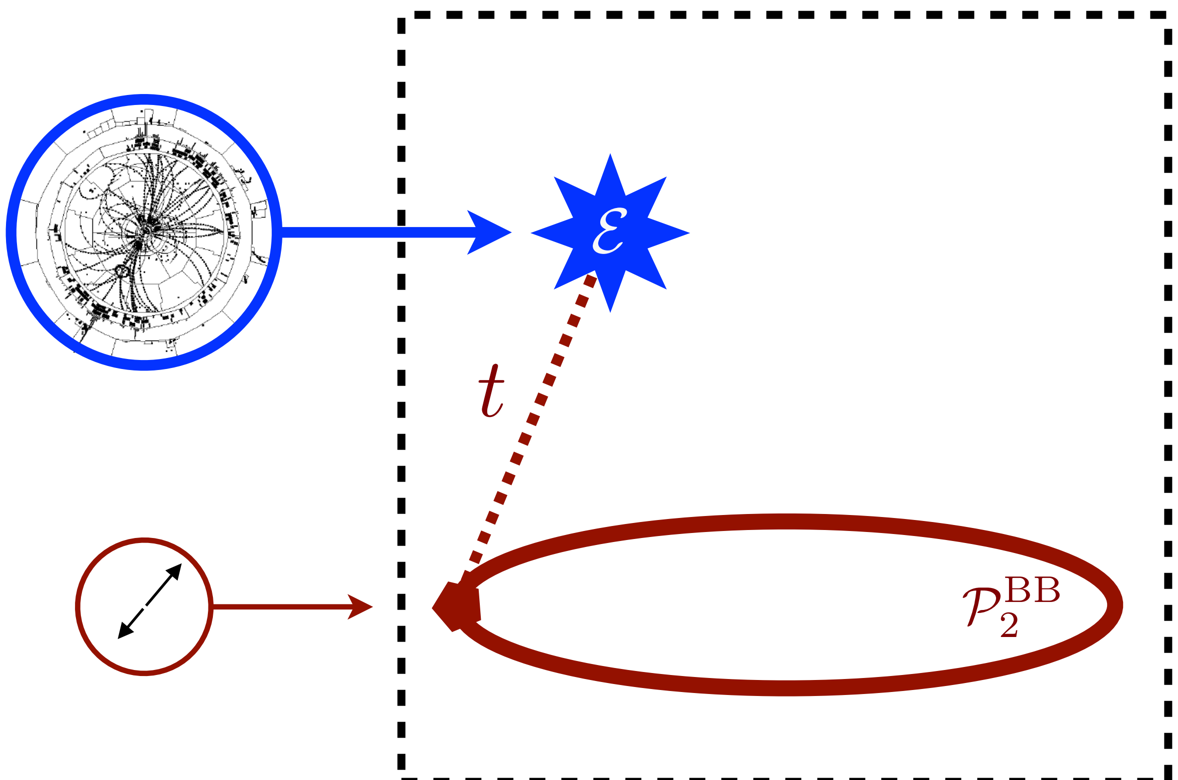
...

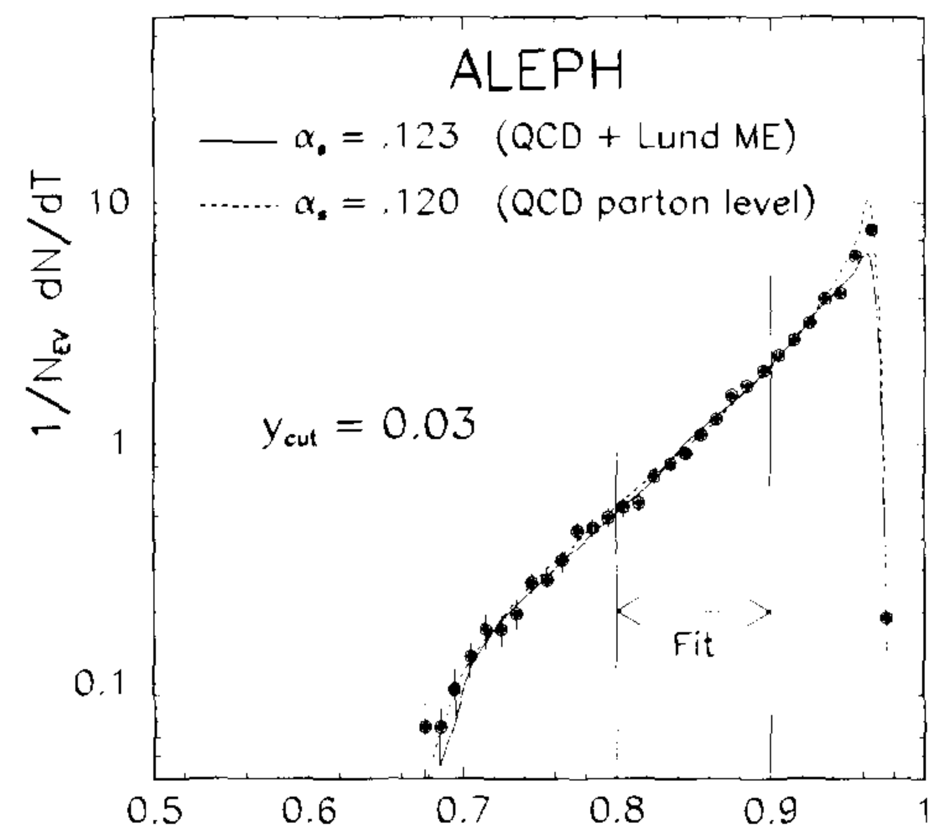
E.g. Thrust

How dijet-like is an event?



$$t(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_2^{\mathrm{BB}}} \mathrm{EMD}_2(\mathcal{E}, \mathcal{E}')$$

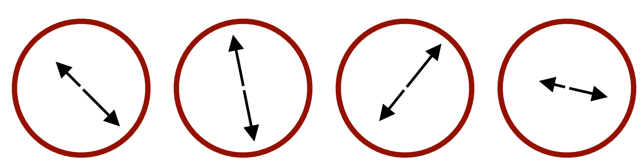




$$1 - \frac{t}{2E_{\mathrm{CM}}}$$

All Back-to-Back Two Particle Configurations

$$\mathcal{P}_2^{\mathrm{BB}} = \left\{ \quad \cdots \right\}$$



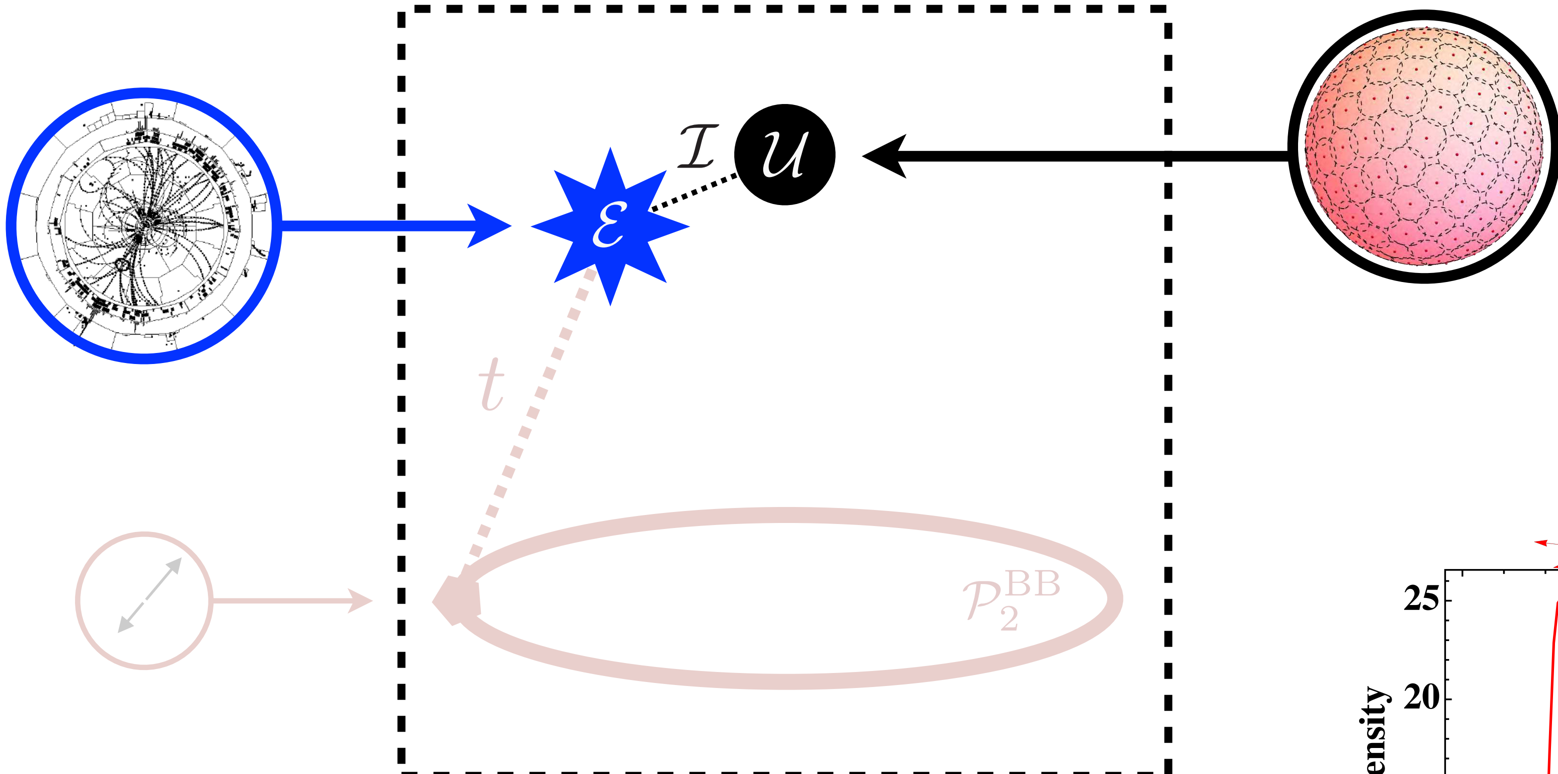
(using β=2 EMD variant)

cf. $T(\mathcal{E}) = \max_{\hat{n}} \frac{\sum_i |\vec{p}_i \cdot \hat{n}|}{\sum_j |\vec{p}_j|}$

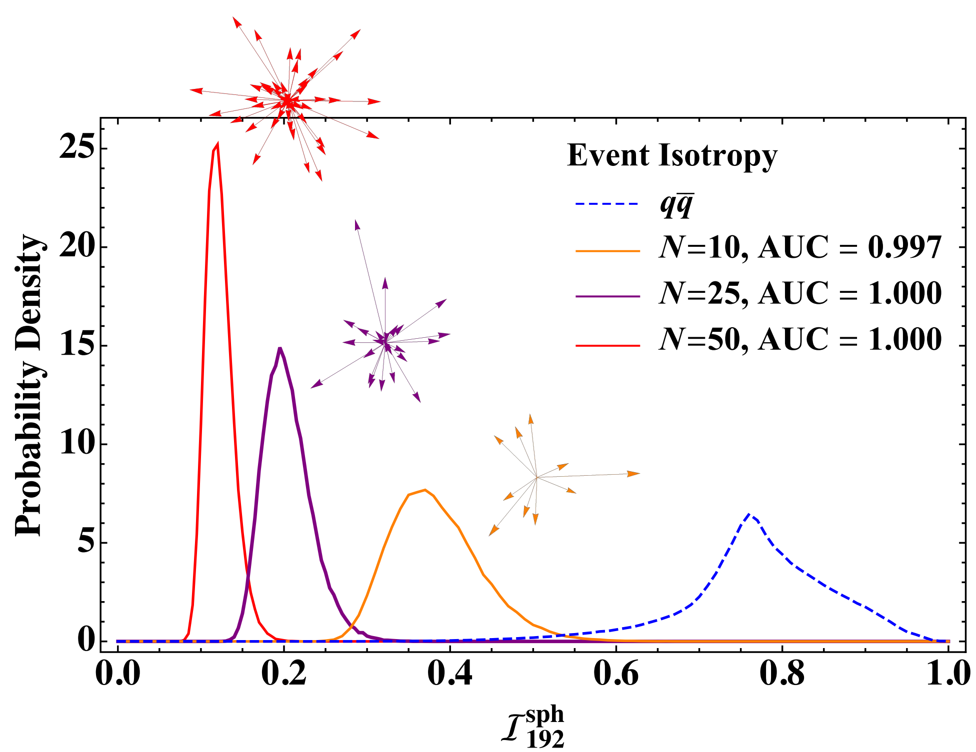
[Komiske, Metodiev, JDT, JHEP 2020]
[Brandt, Peyrou, Sosnowski, Wroblewski, PL 1964; Farhi, PRL 1977; ALEPH, PLB 1991]

New! Event Isotropy

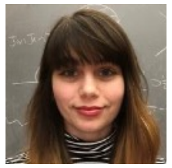
How isotropic is an event?



$$\mathcal{I}(\mathcal{E}) = \mathrm{EMD}(\mathcal{E}, \mathcal{U})$$

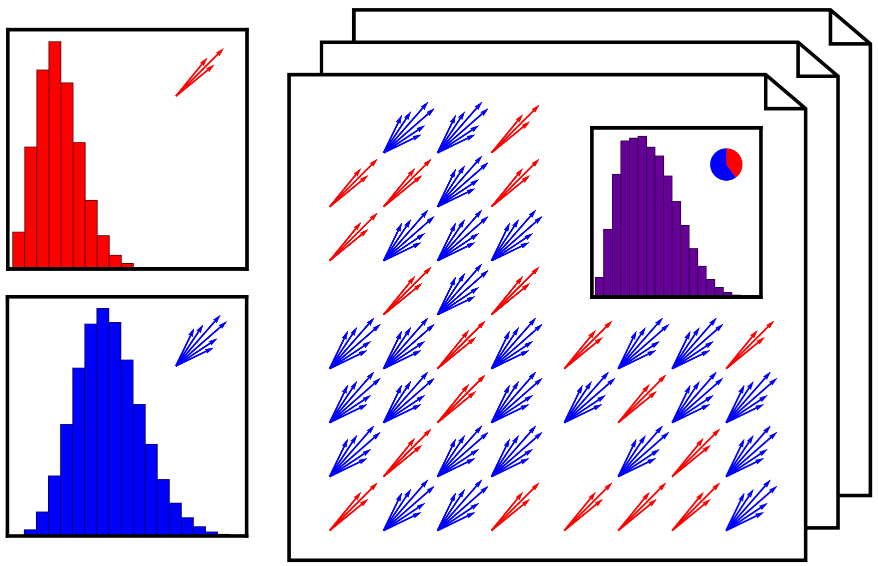


[Cesarotti, JDT, JHEP 2020;
see also Cesarotti, Reece, Strassler, JHEP 2021]



Other Examples from My Group's Research

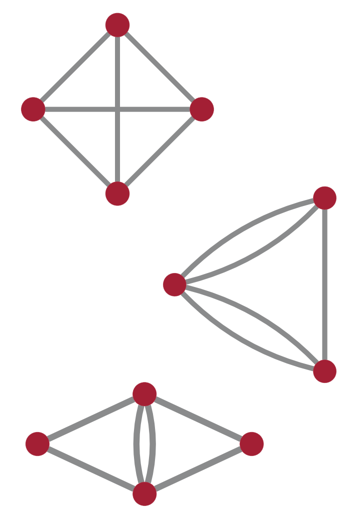
Quark/Gluon Definitions
via Blind Source Separation



[Komiske, Metodiev, JDT, JHEP 2018;
Brewer, JDT, Turner; PRD 2021]

Kinematic Decomposition
via Graph Theory

	Leafless Multigraphs	
	Connected	All
Edges d	A307317	A307316
1	0	0
2	1	1
3	2	2
4	4	5
5	9	11
6	26	34
7	68	87
8	217	279
9	**718**	**897**
10	**2 553**	**3 129**
11	**9 574**	**11 458**
12	**38 005**	**44 576**
13	**157 306**	**181 071**
14	**679 682**	**770 237**
15	**3 047 699**	**3 407 332**
16	**14 150 278**	**15 641 159**



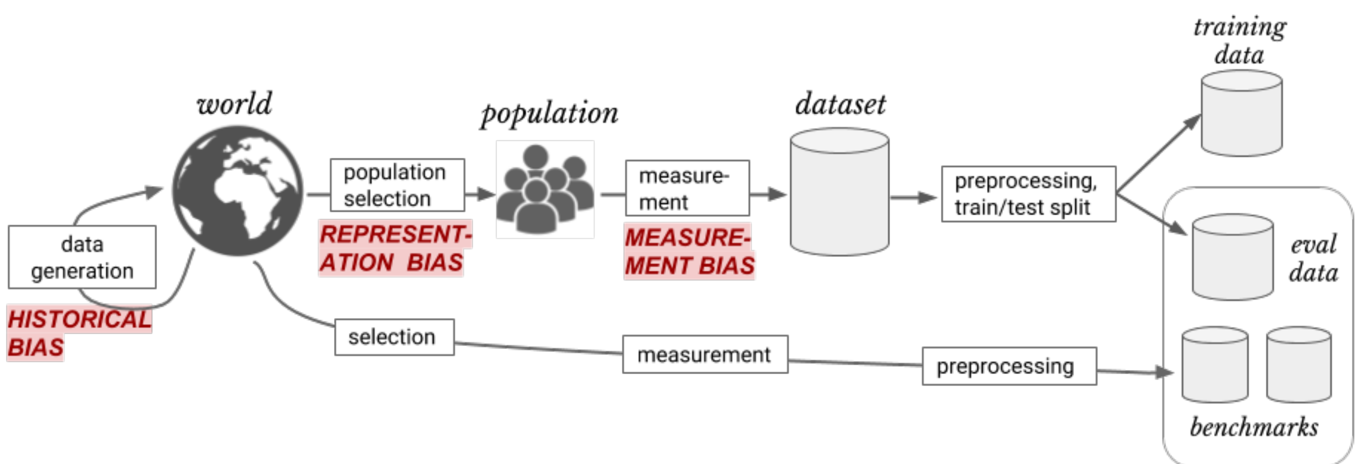
[Komiske, Metodiev, JDT,
JHEP 2018, PRD 2020]

New insights into high-energy physics facilitated by advances in mathematics, statistics, and computer science

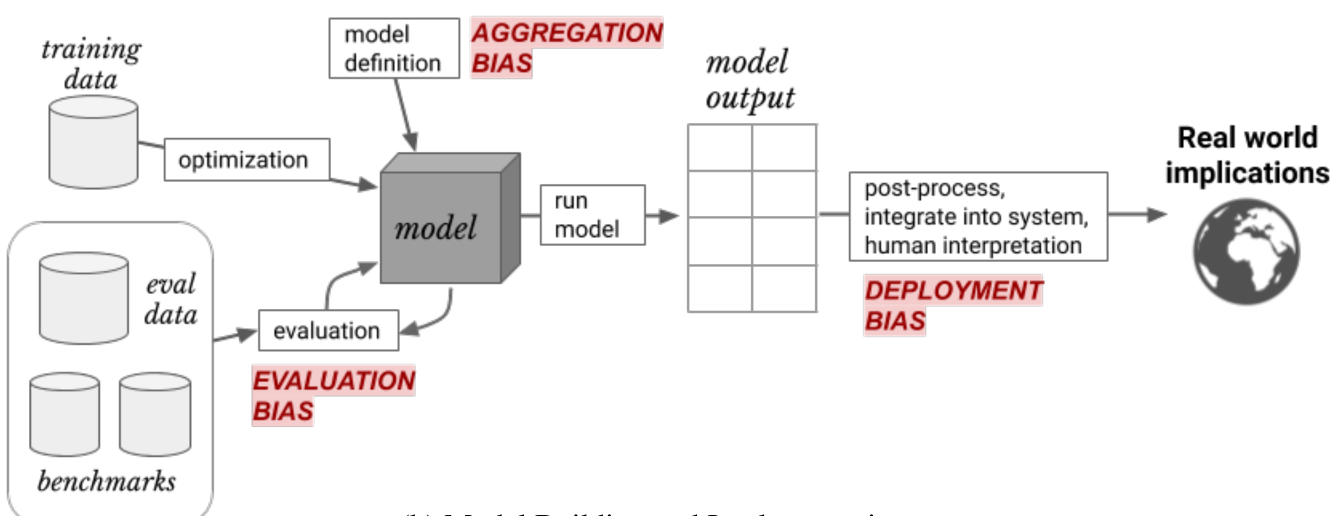
(and vice versa!)

Reasons to be Wary

“A Framework for Understanding Unintended Consequences of Machine Learning”



(a) Data Generation



(b) Model Building and Implementation

1. **Historical bias** arises when there is a misalignment between world as it is and the values or objectives to be encoded and propagated in a model. It is a normative concern with the state of the world, and exists even given perfect sampling and feature selection.
2. **Representation bias** arises while defining and sampling a development population. It occurs when the development population under-represents, and subsequently fails to generalize well, for some part of the use population.
3. **Measurement Bias** arises when choosing and measuring features and labels to use; these are often proxies for the desired quantities. The chosen set of features and labels may leave out important factors or introduce group- or input-dependent noise that leads to differential performance.
4. **Aggregation bias** arises during model construction, when distinct populations are inappropriately combined. In many applications, the population of interest is heterogeneous and a single model is unlikely to suit all subgroups.
5. **Evaluation bias** occurs during model iteration and evaluation. It can arise when the testing or external benchmark populations do not equally represent the various parts of the use population. Evaluation bias can also arise from the use of performance metrics that are not appropriate for the way in which the model will be used.
6. **Deployment Bias** occurs after model deployment, when a system is used or interpreted in inapppropriate ways.

For HEP, “bias” ≈ “systematic uncertainty”

[h/t David Kaiser, MIT SERC; Suresh, Guttag, arXiv 2019]