# Machine Learning in the Search for New Fundamental Physics

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#### CLUSTER OF EXCELLENCE

#### QUANTUM UNIVERSE





CDCS







Bundesministerium für Bildung und Forschung

CENTER FOR DATA AND COMPUTING

Partnership of Universität Hamburg and DESY

## Motivation

#### Why are neutrinos massive?

 Theoretical and experimental reasons to expect new physics beyond the Standard Model



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- Theoretical and experimental reasons to expect new physics beyond the Standard Model
- However, so far only negative results in searches



Selection of observed limits at 95% C.L. (theory uncertainties are not included). Probe **up to** the quoted mass limit for light LSPs unless stated otherwise. The quantities  $\Delta M$  and x represent the absolute mass difference between the primary sparticle and the LSP, and the difference between the intermediate sparticle and the LSP relative to  $\Delta M$ , respectively, unless indicated otherwise.

# Motivation

- Theoretical and experimental reasons to expect new physics beyond the Standard Model
- However, so far only negative results in searches
- Make sure that we do not miss potential discoveries at the LHC: Use machine learning to improve existing approaches and to inspire new ideas



## Outline

#### **REVIEWS**

#### Machine learning in the search for new fundamental physics

Georgia Karagiorgi 1<sup>1</sup><sup>1</sup>, Gregor Kasieczka<sup>2</sup>, Scott Kravitz <sup>3</sup>, Benjamin Nachman <sup>3,4</sup> and David Shih

Abstract | Compelling experimental evidence suggests the existence of new physics beyond the well-established and tested standard model of particle physics. Various current and upcoming experiments are searching for signatures of new physics. Despite the variety of approaches and theoretical models tested in these experiments, what they all have in common is the very large volume of complex data that they produce. This data challenge calls for powerful statistical methods. Machine learning has been in use in high-energy particle physics for well over a decade, but the rise of deep learning in the early 2010s has yielded a gualitative shift in terms of the scope and ambition of research. These modern machine learning developments are the focus of the present Review, which discusses methods and applications for new physics searches in the context of terrestrial high-energy physics experiments, including the Large Hadron Collider, rare event searches and neutrino experiments.

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For several decades, the standard model (SM) of particle physics has provided a clear theoretical guide for analysing large amounts of data in many dimensions to experiments, resulting in an extensive search proto find subtle patterns. Multivariate analysis has been gramme that culminated with the discovery of the Higgs commonplace in HEP for decades (for example, the boson<sup>1,2</sup>. Although the SM is now complete, there are TMVA 'toolkit')8, but the latest tools will qualitatively key experimental observations that compel the comextend the sensitivity to 'hypervariate analysis' whereby munity to expand the search efforts for new particles the entire phase space of available experimental inforand forces of nature beyond the SM (BSM). For exammation can be analysed holistically. These new tools ple, the existence of dark matter (DM) and dark energy also allow for new analysis strategies independent of is well established<sup>3</sup>, as are the mass of neutrinos<sup>4,5</sup> and the dimensionality (density estimation, variable-length the baryon–antibaryon asymmetry in the Universe<sup>6</sup> inputs and so on) yet none of these observations are explained by the SM. In tandem with the growing data volume, a related Additionally, 'aesthetic' problems plague the SM, includchallenge is the increasing need for efficient (in terms ing the unexplained weak-scale mass of the Higgs boson,

of computational time, power and resource utilization) the existence of three generations of fermions, and the and accurate data processing for high-throughput appliminuteness of the neutron dipole moment7. Current and cations. Efforts to that end include the development near-future high-energy physics (HEP) experiments and acceleration of deep learning-based processing have the potential to shed light on all of these fundaalgorithms on power-efficient hardware platforms? In addition to the growing data challenge, there is also

tens of thousands of tunable parameters) are well suited

ratory, or by observing interactions of new particles with the compounding challenge of simulating expectations for what experiments may observe. HEP experiments rely heavily on simulations for all aspects of research, from siderable data challenges. New particle interactions are experimental design all the way to data analysis. Built on a thorough understanding of the SM and the fundamental laws of nature, these simulations are extremely comprehensive and sophisticated, but they are still only an approximation to nature. It is therefore often necessary to combine simulations with information directly from data to improve simulation accuracy. The corresponding modern ML, with deep neural networks (NNs) and ML models must be robust against inaccuracies and be other advanced tools that contain (much) more than able to integrate uncertainties

NATURE REVIEWS | PHYSICS

mental challenges by creating new particles in the labo-

This great potential for discovery comes with con-

expected to be rare, and their signature could be only

subtly different from the SM. This means that researchers

must collect and sift through an immense amount of

complex data to isolate potential BSM physics. Machine

learning (ML) offers a powerful solution to this chal-

lenge. Deep learning techniques (used here to mean

normal matter or with other new particles.

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Despite the same title, this talk will be more focused on LHC physics and on recent work than our review (2112.03769)

- Improve existing approaches:
  - Better **performance** for new physics taggers
  - Increase stability
- New ideas:
  - Build model independent searches

See Danilo's excellent talk from <u>Monday</u> for a big picture view of computing challenges in the future

# Improving Performance



### Enter: Deep Learning



#### Improvement of factor 2-3 over shallow ML (and more over non-ML methods) in benchmark classification task



- Example application: hadronic top quark decays
- 1.2M simulated top quark and background events
- Either four-momenta of individual particles or high-level features
- Great test-bed to compare different data representations
  - (and, of course, useful for new physics searches)

 Basic motivation: Use physicists' knowledge about data as an implicit (or explicit bias) to help networks train faster / achieve better performance



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- Either by phrasing physics problems so that outside-solutions can be used ...



locality and translation invariance.

GK, Plehn, et al, 1701.08784; Macaluso, Shih, 1803.00107; ...

- Basic motivation: Use physicists' knowledge about data as an implicit (or explicit bias) to help networks train faster / achieve better performance
- Either by phrasing physics problems so that outside-solutions can be used ...
- ...or by constructing networks layers based
  on physical symmetries



Learn combinations of particles and suitable rest frames

GK, Plehn, et al, 1707.08966; Erdmann et al 1812.09722; Bogatskiy et al 2006.04780; ...

- Basic motivation: Use physicists' knowledge about data as an implicit (or explicit bias) to help networks train faster / achieve better performance
- Either by phrasing physics problems so that outside-solutions can be used ...
- ...or by constructing networks layers based on physical symmetries
- **Graphs** are a general + powerful framework that captures relevant properties for particle tagging
  - e.g. best performance of ParticleNet in original top tagging comparison
  - versatile and well suited





Henrion et al ML4PS 2017; Qu, Gouskos 1902.08570; Shalom, Battaglia, Valiant 2007.13681 (review)

### In practice



Both ATLAS and CMS confirm performance of graph-based (ParticleNet) approach on realistic simulations



# Use of object tagging

- Top tagging (+other heavy resonances, flavour, tau,...): standard model particles
  - Still important for BSM searches





CMS B2G-20-011 (just an example; majority of searches uses flavour/resonance tagging as ingredient)

# **Tagging other particles**

- Top tagging (+other heavy resonances, flavour, tau,...): standard model particles
  - Still important for BSM searches
  - Relatively easy calibration (signal & background samples in data exist)

For new physics: background calibration possible, larger uncertainty on signal



Example for domain adaptation

# **Tagging other particles**

- Top tagging (+other heavy resonances, flavour, tau,...): standard model particles
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For new physics: background calibration possible, larger uncertainty on signal

 Can assume all properties (mass,..)
 For new physics: Parametrised networks or decorrelation

Add term to loss function to decrease correlation with specific observable (e.g. invariant mass)

GK, Shih 2001.05310; Louppe, Kagan, Cranmer 1611.01046; Shimmin et al 1703.03507; Bradshaw et al 1908.08959; Dolen et al 1603.00027; Kitouni et al 2010.09745, ...



# **Estimating Backgrounds**

- Can take decorrelation further.
- For new physics searches, need to
  - Find two variables that:
  - Isolate a possible signal &
  - Are independent (and can be used for ABCD background estimation)
- Can phrase this directly as training task, again using DisCo



$$N_A = \frac{N_B N_C}{N_D}$$

$$\mathcal{L}[f,g] = \mathcal{L}_{\text{classifier}}[f(X),y] + \mathcal{L}_{\text{classifier}}[g(X),y] + \lambda \operatorname{dCorr}_{y=0}^{2}[f(X),g(X)]$$

GK et al 2007.14400; See also Mikuni, Nachman, Shih for decorrelating autoencoders: 2111.06417

# Back to Performance



# Attention is all you need

- In ParticleNet, data-space geometry defines neighbourhood in graph; aggregation over all neighbours
- Attention allows the network to learn which parts of the input are truly relevant

	Accuracy	AUC	Rej <sub>50%</sub>	Rej <sub>30%</sub>
P-CNN	0.930	0.9803	$201 \pm 4$	$759 \pm 24$
PFN		0.9819	$247 \pm 3$	$888 \pm 17$
ParticleNet	0.940	0.9858	$397\pm7$	$1615\pm93$
JEDI-net (w/ $\sum O$ )	0.930	0.9807		774.6
PCT	0.940	0.9855	$392\pm7$	$1533 \pm 101$
LGN	0.929	0.964		$435\pm95$
rPCN		0.9845	$364\pm9$	$1642\pm93$
LorentzNet	0.942	0.9868	$498 \pm 18$	$2195 \pm 173$
ParT	0.940	0.9858	$413\pm16$	$1602\pm81$
ParticleNet-f.t.	0.942	0.9866	$487\pm9$	$1771\pm80$
ParT-f.t.	0.944	0.9877	$691 \pm 15$	$2766 \pm 130$





Performance comparison on landscape dataset

Vaswani et al 1706.03762; Qu, Li, Qian 2202.03772; Mikuni, Canelli 2001.05311; ...

## Attention is all you need

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- Attention allows the network to learn which parts of the input are truly relevant
- Attention is data-hungry, transfer-learning helps! (Motivation for foundation models?)
- So far, observed trend: Higher physics performance comes at the cost of higher algorithm complexity & compute cost

	Accuracy	# params	FLOPs
PFN	0.772	86.1 k	4.62 M
P-CNN	0.809	354 k	15.5 M
ParticleNet	0.844	370 k	540 M
ParT	0.861	2.14 M	340 M
ParT (plain)	0.849	2.13 M	260 M

(plain: standard multi-head-attention vs particlemulti-head-attention)

Vaswani et al 1706.03762; Qu, Li, Qian 2202.03772; Mikuni, Canelli 2001.05311; Gong et al 2201.08187 for a combination of transformers and attention;

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- So far, observed trend: Higher physics performance comes at the cost of higher algorithm complexity & compute cost
- Is this the only way?

Vaswani et al 1706.03762; Qu, Li, Qian 2202.03772; Mikuni, Canelli 2001.05311; Gong et al 2201.08187 for a combination of transformers and attention

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# Looking for optimal feature set

- Energy Flow Polyonomials (EFPs) form a basis of jet substructure
- Depending on order considered, too many (e.g 7k) to efficiently train NN (many features work if there is structure, not so much for EFPs)
- Solution: Iterative feature selection, again based on DisCo



Das, GK, Shih, to be published; Faucett, Thaler, Whiteson, 2010.11998

# Looking for optimal feature set

- Energy Flow Polyonomials (EFPs) form a basis of jet substructure
- Depending on order considered, too many (e.g 7k) to efficiently train NN (many features work if there is structure, not so much for EFPs)
- Solution: Iterative feature selection, <sup>2</sup> again based on DisCo
- Same top tag performance as simple graph network but only O(10) inputs; factor 50 less parameters
- Also helps interpretability, calibration
- Useful for new physics searches?



Das, GK, Shih, to be published; Faucett, Thaler, Whiteson, 2010.11998

# Model Independent Searches



# **Anomaly Searches**

- Orthogonal strategy to model specific searches:
  - Discover new physics with making minimal assumptions
- Less sensitive to one specific model, broader coverage

#### **ML-assisted global comparison**

- Systematically compare simulation to recorded data, look for differences
- Con: Rely on imperfect simulation, maximally background model dependent
- Pro: Sensitive to all types of anomalies

#### Resonant anomaly detection / Enhanced bump hunts

- Estimate background in-situ from data
- Con: Need to make assumptions about signal shape
- Pro: Data-driven on background model

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#### Resonant anomaly detection / Enhanced bump hunts

- Estimate background in-situ from data
- Con: Need to make assumptions about signal shape
- Pro: Data-driven on background model
- Will focus on these for rest of the talk
- See <u>Andrea tomorrow</u> for an alternative view







Need to find a feature in which signal is resonant and background smooth.

No assumptions in other features.

Further generalisation as open issue.



No worry, will come back to HOW this is done is a moment



# ...so HOW to construct the anomaly score?

### Autoencoders



application: ATLAS-CONF-2022-045; ...

### Autoencoders





representatic Latent space

$$\mathcal{L}(x) = ||x - g_{\theta}(f_{\phi}(x))||_{2}$$
$$a(x) = \mathcal{L}(x)$$

- Upside: Powerful, conceptually simple, useful for trigger?
- Downside: Complexity bias



Weber MSc Thesis Hamburg 2019, Finke et al 2104.09051,...

## Autoencoders





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- Downside: Complexity bias (Overcome e.g. by normalised auto encoders)
   Ill-defined density under coordinate change



5.0

**Random Variable** 

7.5

10.0 12.5

#### Classifier

# CWoLa



- A classifier (i.e. a neural network) trained to distinguish two mixed samples learns to distinguish the components
- But needs S/B from same underlying distribution (e.g uncorrelated) between mixed samples 1 and 2 (does not hold in general)

$$L_{M_1/M_2} = \frac{p_{M_1}}{p_{M_2}} = \frac{f_1 \, p_S + (1 - f_1) \, p_B}{f_2 \, p_S + (1 - f_2) \, p_B} = \frac{f_1 \, L_{S/B} + (1 - f_1)}{f_2 \, L_{S/B} + (1 - f_2)}$$

Metodiev, Nachman, Thaler, 1708.02949; Howe, Nachman 1805.02664

# CATHODE



- 1) Train a generative model p(x|m) on auxiliary features in SB
- 2) Sample from p(x|m) in SR. Designate as p<sub>bg,est</sub>.



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- 3) Train binary classifer between p<sub>data</sub> and p<sub>bg,est.</sub>

Hallin, Isaacson, GK, et al 2109.00546; Nachman, 39 Shih 2001.04990; Raine et al 2203.09470

## CATHODE



- 1) Train a generative model p(x|m) on auxiliary features in SB
- 2) Sample from p(x|m) in SR. Designate as pbg,est.
- 3) Train binary classifer between p<sub>data</sub> and p<sub>bg,est.</sub>
- 4) Evaluate score, use in enhanced bump hunt

Hallin, Isaacson, GK, et al 2109.00546; Nachman, 40 Shih 2001.04990; Raine et al 2203.09470

# La(tent) CATHODE



- If R(x) is only calculated in signal region, it's extrapolation behaviour is not well-defined
- Potential problem for bump-hunt if it shapes distributions



Hallin, GK, et al, coming soon

## L-aCAT-HODE



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- Can overcome by training the classifier in latent space instead



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## LaCATHODE



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#### Closing

# Closing

- Machine learning aids new physics searches by improving existing approaches and opening up new techniques
  - Convergence of architectures share foundation models?
  - Understanding and dealing with correlations
  - Generative models as in-situ background estimators
- Rapid pace of innovation, still no end in sight



#### Thank you!

#### **Bonus Material**

#### **Online Learning**

# **Emphemeral Learning**

- CMS/ATLAS triggers:
  - Only able to store a subset (<1 in 10.000) of events
- Possible (wild) alternative:
  - Train a generative model online during data taking

No compression

Compress per event

Many numbers per event

Small set of numbers per **event** 

 $p(x \mid \theta)$ 

Compress entire dataset

Small set of numbers per **dataset** 

- Fixed size, independent of training data amount
- Radically different format from usual way of storing data, but might open up new approaches

## OnlineFlows



Schematic of proposed approach.

Focus on HLT, more technical challenges for use in hardware Trigger.

Main problem: How to make training work if each event is only available for short time?

### **Proof of concept**



## **Proof of concept**



Use LHCO dataset, train on high-level features on a mixture of background (99%) and signal (1%).

> Train classifier to distinguish a signal region and sideband (CWoLA appaorach)

Compare procedure directly carried out on data with output of flow.

2202.0937

#### **On Anomaly Detection**

# **Types of anomalies**

- Outliers/Point anomalies: Datapoints far away from regular distribution
- Examples:
  - Detector malfunctions
  - Background-free search
- Group anomlies: Individual examples not interesting, but signal is an overdensity with respect to background
- Examples:
  - Resonance searches
  - Transient signals in time series



## Assumptions

# **Rarity:** Pr(anomaly) « Pr(normal) **Overlap:**

max  $x p(x|anomaly)/p (x|normal) < \infty$  **Resonance:**  $Pr(|m - m0| > \delta|anomaly) \approx 0$  for some feature *m* (often a mass) and fixed *m*0,  $\delta$ 

**Smoothness:** p(x|m, normal) varies slowly with m so that one can use data with  $|m - m0| > \delta$  to estimate p(x|m, normal) for  $|m - m0| < \delta$ 



# Introducing: LHC Olympics

- Encourage development and comparison of modelagnostic search strategies
  - Focus on group anomalies, data-driven searches
  - Use for a convenient overview of space of techniques
  - Complementary to 2105.14027
- Provide a complete package, balance details vs accessiblity
- Datasets:
  - One R&D dataset for algorithm development
  - Three black box datasets (BB1-BB3)
    - Unblinded over time
- Timeline:
  - Spring 2019: Release R&D dataset (link)
  - Autumn 2019: Release BB datasets (link)
  - January 2020: Winter Olympics as part of ML4Jets, unblinding of BB1 (link)
  - July 2020: (Virtual) Summer Olympics, unblinding of BB2 and BB3 (<u>link</u>)
  - LHC Olympics paper (<u>https://arxiv.org/abs/</u> 2101.08320) public



https://lhco2020.github.io/homepage/



- Relatively simple signal
  - Known to differ in previously mentioned features from background distribution
- Unrealistically high S/B





X

m=500 GeV $_q$ 

Q



• 1): Choose one feature (m) in which to search for resonances



- 1): Choose one feature (m) in which to search for resonances
- 2): Use m divide spectrum into non-overlapping regions. Designate one as signal region (SR), others as sidebands (SB). Repeat the following for all choices of SR



 3) Train a generative model p(x|m) on auxiliary features in SB (used MAF, other choices including GAN/VAE possible as well)



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- 4) Sample from p(x|m) in SR. Designate as p<sub>bg,est</sub>.
- 5) Train binary classifer between p<sub>data</sub> and p<sub>bg,est.</sub> (mixed sample classifer)
- 6) Cut on high classifier scores to enrich sample with anomalies (and perform statistical analysis)

# Comments on anomaly detection

• As CATHODE approximates a likelihood ratio, it should be robust compared to methods that only use p<sub>Background</sub> (e.g. autoencoders)



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- As CATHODE approximates a likelihood ratio, it should be robust compared to methods that only use p<sub>Background</sub> (e.g. autoencoders)
- However, still can be sensitive to choice of input features



MSc thesis work of P. Prangchaikul

# Comments on anomaly detection

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- However, still can be sensitive to choice of input features
- Need also consider
  - Shaping of distributions under tigher anomaly detection cuts
  - Cost of signal-injection in training on data
  - How to efficiently estimate / compare / communicate sensitive regions of different anomaly detection algorithms
  - Make data-based anomaly detection more flexible

# Challenge datasets

- All contain total of 1M examples; might contain signal; no labels provided during 'content' phase (labels available no)
- All used different simulation parameters for background (to avoid unrealistic exploits)





 Situation seems better for density ratio based techniques (CWola, ANODE, CATHODE,..)

Per Neyman-Pearson: Likelihood-ratio is  
optimal test statistic  
Unfortunatly, 
$$p(x|anomaly)$$
 is not available $L_{S/B} = \frac{p(x|anomaly)}{p(x|normal)}$ Build data/background ratio: $L_{D/B} = \frac{p(x)}{p(x|normal)}$ Approximate background density using  
control measurement (e.g. sideband) $L_{D/B} \approx \frac{p(x)}{\tilde{p}(x|normal)}$ Expand $p(x) = f_{normal} p(x|normal) + f_{anomaly} p(x|anomaly)$ And insert: $L_{D/B} \approx f_{normal} + f_{anomaly} \frac{p(x|anomaly)}{\tilde{p}(x|normal)}$ 

• However...