Anomaly Detection Mini-Review

David Shih

May 24, 2021

Pheno 2021
Where is the new physics??

Despite thousands of searches for new physics at the LHC, nothing but limits and null results so far.

What if new physics is hiding in the data but we haven’t looked in the right places yet?
The most common approach

Model specific searches

Most NP searches at the LHC are heavily optimized with specific signals in mind (SUSY, extra dimensions, …)

ATLAS jets+MET 2010.14293

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<th>BDT-GGd1</th>
<th>BDT-GGd2</th>
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<td>$N_j$</td>
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<td>$\geq 4$</td>
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<td>$\Delta \phi(j_{1,2,3}, p_T^{miss})_{\text{min}}$</td>
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<td>$m_{\text{eff}}/m_{\text{eff}}(N_j)$</td>
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<td>$&gt; 0.2$</td>
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<td>$m_{\text{eff}}$ [GeV]</td>
<td>$&gt; 1400$</td>
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<td>$&gt; 800$</td>
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<td>BDT score</td>
<td>$&gt; 0.97$</td>
<td>$&gt; 0.94$</td>
<td>$&gt; 0.94$</td>
<td>$&gt; 0.87$</td>
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<td>$\Delta m(\tilde{g}, \tilde{\chi}^0_1)$ [GeV]</td>
<td>1600–1900</td>
<td>1000–1400</td>
<td>600–1000</td>
<td>200–600</td>
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Kinematic cuts (or BDTs) optimized using simulations of signal AND background.
The most common approach

Model specific searches

Most NP searches at the LHC are heavily optimized with specific signals in mind (SUSY, extra dimensions, …)

Kinematic cuts (or BDTs) optimized using simulations of signal AND background.

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<td>( m_{eff} ) (GeV)</td>
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<td>( \Delta m(g, \tilde{g}) )</td>
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Of course, we should continue to perform these model-specific searches, because NP could always be right around the corner…

**But we probably can’t cover every possible model this way…**
No explicit search at the LHC for this scenario!

Could be hiding in the dijet resonance search at >5sigma significance!!
General approaches to anomaly detection

Outlier detection

- Look for events where $p_{bg}(x) \ll 1$
- Can find rare signals, can be fully model independent (or at least, may not require very precise background model)
- Uncontrolled, no optimality guarantee — new physics may not be an outlier!

Group anomaly detection

- Look for over-densities in data over background expectation
- **Optimal discriminant:**

\[
R(x) = \frac{p_{\text{data}}(x)}{p_{bg}(x)}
\]

- Generally requires more assumptions on signal and background model — either data driven (eg sideband interpolation, ABCD method) or from simulation
Existing model-independent searches
“the bump hunt”

Idea: assume signal is localized in some feature (usually invariant mass) while background is smooth.

Interpolate from sidebands into signal region, search for an excess.

![Graph showing CMS data with S/(S+B) weighted sum and B component subtracted.](image)
Existing model-independent searches
“the bump hunt”

Idea: assume signal is localized in some feature (usually invariant mass) while background is smooth.

Interpolate from sidebands into signal region, search for an excess.

Classic method, used in many discoveries.
Existing model-independent searches
“the general search”

Idea: divide the phase space up into thousands of bins, compare data to SM simulation in each one

See also proposals by D’Agnolo, Wulzer et al (1806.02350, 1912.12155): train DNN on full phase space to distinguish data from background
Existing model-independent searches
“the general search”

Idea: divide the phase space up into thousands of bins, compare data to SM simulation in each one

Truly signal model independent, but still highly (background) simulation dependent

See also proposals by D’Agnolo, Wulzer et al (1806.02350, 1912.12155): train DNN on full phase space to distinguish data from background
New paradigms for model-agnostic searches

Can advances in machine learning open up new avenues for model-independent searches?

Figure 1. A graphical representation of searches for new particles in terms of the background and signal model dependence for achieving signal sensitivity (a) and background specificity (b). The Model Unspecific Search for New Physics (MUSiC) [??] and General Search [??] strategies are from CMS and ATLAS, respectively. LDA stands for Latent Dirichlet Allocation [??], ANODE detection with Density Estimation (ANODE) is the method presented in this paper, CWoLa stands for Classification Without Labels [??] and SALAD stands for Simulation Assisted Likelihood-free Anomaly Detection [??]. Direct density estimation is a form of side-banding where the multidimensional feature space density is learned conditional on the resonant feature (see Sec. ??).
New paradigms for model-agnostic searches

Can advances in machine learning open up new avenues for model-independent searches?

from Nachman & DS 2001.04990

Many new ideas recently!
Many new approaches inspired by the
LHC Olympics 2020 Data Challenge
[G. Kasieczka, B. Nachman & DS, organizers]

It consisted of three “black boxes” of simulated data (bg dominated!):
https://doi.org/10.5281/zenodo.3547721

- 1 million events each
- 4-vectors of every reconstructed particle (all hadronic) in the event
- Particle ID, charge, etc not included
- Single R=1 jet trigger pT>1.2 TeV

The goal of the challenge was for participants to analyze each box and

1. Decide whether or not it contains new physics
2. Characterize the new physics, if it’s there
LHC Olympics 2020: R&D Dataset

https://doi.org/10.5281/zenodo.2629072

Prior to the challenge, we also released a labeled R&D dataset consisting of 1M QCD dijet events and 100k signal events

Unofficial theme of LHCO2020: “enhancing the bump hunt”
Many new approaches inspired by the LHC Olympics 2020 Data Challenge

- 9 groups submitted results on box 1
- 5 groups submitted results on boxes 2 and 3
- (A number of additional groups could not finish the challenge in time but got results on the R&D dataset, or on the black boxes after unblinding)
- Two workshops:
  - “Winter Olympics” — special session of the ML4Jets conference, January 2020, NYU [box 1 opened]
  - “Summer Olympics” — virtual anomaly detection mini-workshop, July 2020, “Hamburg” [boxes 2 & 3 opened]

arxiv: 2101.08320
Many new approaches inspired by the LHC Olympics 2020 Data Challenge

Individual Approaches

3 Unsupervised
3.1 Anomalous Jet Identification via Variational Recurrent Neural Network
3.2 Anomaly Detection with Density Estimation
3.3 BuHuLaSpa: Bump Hunting in Latent Space
3.4 GAN-AE and BumpHunter
3.5 Gaussianizing Iterative Slicing (GIS): Unsupervised In-distribution Anomaly Detection through Conditional Density Estimation
3.6 Latent Dirichlet Allocation
3.7 Particle Graph Autoencoders
3.8 Regularized Likelihoods
3.9 UCluster: Unsupervised Clustering

4 Weakly Supervised
4.1 CWoLa Hunting
4.2 CWoLa and Autoencoders: Comparing Weak- and Unsupervised methods for Resonant Anomaly Detection
4.3 Tag N' Train
4.4 Simulation Assisted Likelihood-free Anomaly Detection
4.5 Simulation-Assisted Decorrelation for Resonant Anomaly Detection

5 (Semi)-Supervised
5.1 Deep Ensemble Anomaly Detection
5.2 Factorized Topic Modeling
5.3 QUAK: Quasi-Anomalous Knowledge for Anomaly Detection
5.4 Simple Supervised learning with LSTM layers

6 Discussion
6.1 Overall Results
6.2 Overall Lessons Learned

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Many new approaches inspired by the LHC Olympics 2020 Data Challenge

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arxiv: 2101.08320
Unsupervised Anomaly Detection

**General idea:** train ML algorithm directly on (background-dominated) data to identify outliers [events with low $p_{bg}(x)$]

**Example:** Autoencoders

Train lossy ML algorithm to map data to itself through a compressed latent space.

Rare anomalies should be poorly reconstructed

Heimel, Kasieczka, Plehn & Thompson 1808.08979
Farina, Nakai & DS 1808.08992
and many, many more!
Several successful LHCO2020 approaches were based on AEs.

VRNN, Kahn et al 2105.09274

Unsupervised Anomaly Detection

BuHuLaSpa
Bortolato et al 2103.06595

Particle Graph Autoencoders, Tsan et al
Weakly-supervised Anomaly Detection

**General idea:** Train ML algorithm to compare two datasets with different levels of signal, identify events with high \( \frac{p_{\text{data}}(x)}{p_{\text{bg}}(x)} \)

**Example:** "CwoLa Hunting" [Collins, Howe & Nachman 1805.02664]

Train a binary classifier on additional features \( x = m_{jj}, m_{j2}, \tau_{21}(j_1), \tau_{21}(j_2), \ldots \) to distinguish between signal region and sideband events.

If additional features are uncorrelated with \( m_{jj} \) in the background, should learn \( \frac{p_{\text{data}}(x)}{p_{\text{bg}}(x)} \) [Neyman-Pearson lemma]

\( Z' \rightarrow XY \) (boosted), \( X \rightarrow ? \), \( Y \rightarrow ? \)
Weakly-supervised Anomaly Detection

Another example: Simulation Assisted Likelihood-free Anomaly Detection (SALAD) [Andreassen, Nachman & DS 2001.05001]

Try to leverage simulated backgrounds for learning $p_{\text{data}}(x)/p_{\text{bg}}(x)$:

- reweight bg sim to look like data in sideband region using DCTR method
  [Andreassen & Nachman 1907.08209]
- interpolate into SR
- train classifier on data vs bg.
Between weak and un-supervised

ANOMaly detection with Density Estimation (ANODE): [Nachman & DS 2001.04990]

Use unsupervised approach to learn the likelihood ratio:

- Train density estimator to directly learn $p_{SR}(x)$ and $p_{SB}(x)$
- Interpolate latter in mJJ to obtain $p_{bg}(x)$ in the SR
- Construct likelihood ratio $R(x)=p_{data}(x)/p_{bg}(x)$ explicitly
Between weak and un-supervised

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Figure 4. Scatter plot of $R(x|m)$ versus $\log p_{background}(x)$ across the test set in the SR. Background events are shown (as a two-dimensional histogram) in grayscale and individual signal events are shown in red.

Figure 5. Left: Histogram of $R(x|m)$ evaluated on the test set; Right: the integrated number of events that survive a threshold on $R(x|m)$. The two distributions are scaled to represent the rates for 500,000 total background events and 500 total signal events, as introduced in Sec. 4.

A different regularization procedure was used in Ref. [32, 33] based on the validation loss and k-folding. The averaging here is expected to serve a similar purpose.

Figure 6. Distributions of $m_{J1}$ (left) and $m_{J2} \neq m_{J1}$ (right) in the signal region after applying a threshold requirement on $R(x|m)$.

Figure 7. Receiver Operating Characteristic (ROC) curve (left) and Significance Improvement Characteristic (SIC) curve (right).

The performance of ANODE is comparable to CWoLa hunting in Fig. 7, which does slightly better at higher signal efficiencies and much better at lower signal efficiencies. This may be a reflection of the fact that CWoLa makes use of supervised learning and directly approaches the likelihood ratio, while ANODE is unsupervised and attempts to learn both the numerator and denominator of the likelihood ratio. With this dataset, ANODE is able to enhance the signal significance by about a factor of 7 and would therefore be able to achieve a local significance above $5\sigma$ given that the starting value of $S/\sigma$ is 1.6.
Between weak and un-supervised

ANOMaly detection with Density Estimation (ANODE):
[Nachman & DS 2001.04990]

Use unsupervised approach to learn the likelihood ratio:

- Train density estimator to directly learn $p_{SR}(x)$ and $p_{SB}(x)$
- Interpolate latter in mJJ to obtain $p_{bg}(x)$ in the SR
- Construct likelihood ratio $R(x) = \frac{p_{data}(x)}{p_{bg}(x)}$ explicitly

Can enhance the significance of the bump hunt by a factor of up to 7!

$1.5\sigma$ (dijet bump hunt) => $10\sigma$ (ANODE+bump hunt)
(Semi)Supervised Anomaly Detection

**General idea:** train ML algorithm on signal and background simulation, apply to data to find “signal-like” events

**Example:** Quasi Anomalous Knowledge (QUAK)  
[Park, Rankin, Udrescu, Yunus, Harris 2011.03550]

Train separate autoencoders on signal models and background model.

Look for events in data with high background loss and low signal loss.
Summary and Outlook

- Advances in machine learning are opening up new and exciting avenues for model independent new physics searches at the LHC.

- The LHC Olympics 2020 provided a very useful testing ground for the development and common benchmarking of new approaches.

- Much work remains to be done in order to port these ideas over to ATLAS and CMS and implement them as actual analyses on real data.

- We need more ideas for model-independent searches at the LHC. This is just the beginning!
Q: Why is there no model independent search group???
A vision for the future…

Future Organization of Physics Analysis Groups at the LHC??

B physics

SM

Measurement Groups

Top

Higgs

Unsupervised

Weakly Supervised

(Semi) Supervised

Model Agnostic?

Supporting organizations

Search Groups

Exotics/Exotica

SUSY

B2G / HDBS

Statistics forum

ML forum

from G. Kasieczka, B. Nachman, DS (eds), et al 2101.08320
Thanks for your attention!
LHC Olympics 2020: R&D Dataset

Resonant feature

\[ m = m_{Z'} = m_{JJ} \]

Benchmark signal strength:

- \( S = 500 \)
- \( B = 500,000 \)
- \( B_{SR} = 61,000 \)

- \( S/B_{SR} \approx 6 \times 10^{-3} \)
- \( S/\sqrt{B_{SR}} \approx 1.5 \)
LHC Olympics 2020: R&D Dataset

Additional features: $\mathbf{x} = (m_{J_1}, m_{J_2}, \tau_{21}^{J_1}, \tau_{21}^{J_2})$
Box 1

Signal: 834 events

Z'→XY; X,Y→qq
(same topology as R&D dataset)

mZ' = 3823 GeV

mX = 732 GeV

mY = 378 GeV
results of unblinding the first black box. Shown are the predicted resonance mass (top left), the number of signal events (top right), the mass of the first daughter particle (bottom left), and the mass of the second daughter particle (bottom right). Horizontal bars indicate the uncertainty (only if provided by the submitting groups). In a smaller panel the pull (answer-true)/uncertainty is given. Descriptions of the tested models are provided in the text.

For Black Box 3 a resonance decaying to hadrons and invisible particles (PCA), a resonance with a mass between 5.4 and 6.4 TeV (LDA), at 3.1 TeV (embedding clustering), and between 5 and 5.5 TeV (QUAK) was reported. No signal was observed by one approach (VRNN). The true injected resonance with a mass of 4.2 TeV and two competing decay modes was not detected by any approach.

After unveiling the black boxes, further submissions and improvements to the anomaly detectors were made. The VRNN and BuHuLaSpa (Sec. 3.3) approaches now report an enhancement at an invariant mass below 4 TeV for black box 1, while no signal is observed for the other two black boxes. With deep ensemble anomaly detection (Sec. 5.1) a resonance at 3.5 TeV is seen for the first black box and for Latent Dirichlet Allocation a resonance not incompatible with 3.8 TeV is observed. Another new submission was Particle Graph Autoencoders (Sec. 3.7) which detected a resonance at 3.9 TeV for the first black box. Finally, a resonance at 3.5 TeV was seen using CWoLa hunting (Sec. 4.1). For Black Box 2 and three, no additional observations of a signal were reported after unblinding.

6.2 Overall Lessons Learned

This large and diverse number of submissions on the blinded and unblinded datasets is very encouraging. Even better, the resonance in the first black box was successfully detected – 89 –
Two approaches clearly stood out:
Conditional density estimation for anomaly detection
George Stein, Uros Seljak, Biwei Dai, He Jia

Two approaches clearly stood out:

Used the ANODE method with a novel density estimator!
Two approaches clearly stood out:

- ResNet + BDT
- PCA
- LSTM
- High-level features AE
- Tag N Train
- Density Estimation (GIS)
- VRNN
- Latent Dirichlet Allocation
- Human NN

Results of unblinding the first black box. Shown are the predicted resonance mass (top left), the number of signal events (top right), the mass of the first daughter particle (bottom left), and the mass of the second daughter particle (bottom right). Horizontal bars indicate the uncertainty (only if provided by the submitting groups). In a smaller panel the pull (answer-true)/uncertainty is given. Descriptions of the tested models are provided in the text.

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Used a combination of autoencoders and CWoLa hunting

Tag N’ Train

Oz Amram & Cristina Mantilla Suarez (Johns Hopkins)
Box 2

No signal! QCD background only.

4 of the 5 submissions found false positives...

Clearly a matter of concern / area of future improvement for anomaly detection approaches!
Box 3

Two decay modes of X resonance. Need to combine to reach discovery significance.

No jet substructure.

No approach succeeded in finding the signal.
Example of a new approach inspired by LHCO2020.
(See Ben’s talk for additional new approaches!)

Use **neural density estimation** to directly learn the conditional probability densities from the data

\[
P(x|\text{data}; \ m_{JJ} \in SR) \quad \quad P(x|\text{data}; \ m_{JJ} \notin SR) = P(x|bg; \ m_{JJ} \notin SR)
\]

\[
P(x|bg; \ m_{JJ} \in SR)
\]

Construct the likelihood ratio:

\[
R(x) = \frac{P(x|\text{data}; \ m_{JJ} \in SR)}{P(x|bg; \ m_{JJ} \in SR)}
\]
5.2 Background Estimation

This section explores the possibility of using the estimate of $p_{\text{background}}(x|m)$ to directly determine the background efficiency in the SR after a requirement on $R > R_c$. Figure 8 presents a comparison between integration methods (direct integration and importance sampling) described in Sec. 3.2 and the true background yields. Qualitatively, both methods are able to characterize the yield across several orders of magnitude in background efficiency. However, both methods diverge from the truth in the extreme tails of the $R$ distribution. The right plot of Fig. 8 offers a quantitative comparison between methods. For efficiencies down to about $10^{-3}$, both methods are accurate within about 25%. The direct integration method has a smaller bias of about 10%. This is consistent with Fig. 5, for which the standard deviation is between 10-20%.

5.3 Performance on a Dataset with Correlated Features

The results presented in the previous sections have established that ANODE is able to identify the signal and estimate the corresponding SM backgrounds introduced in Sec. 4. One fortuitous aspect of the chosen features $x$ introduced in Sec. 4 is that they are all relatively independent of $m_{jj}$. This is illustrated in Fig. 9, using the SR and neighboring sideband regions. As a result of this independence, the CWoLa method is able to find the signal and presumably the ANODE interpolation from SB to SR is easier than if there was a strong dependence.

The purpose of this section is to study the sensitivity of the ANODE and CWoLa hunting methods to correlations in the features $x$ with $m_{jj}$. Based on the assumptions of the two methods, it is expected that with strong correlations, CWoLa hunting will fail to find the signal while ANODE should still be able to identify the presence of signal in the SR as well.

Novel aspect of ANODE: can estimate backgrounds directly with $P(x|\text{bg}; m \in \text{SR})$
ANODE: Results on LHCO R&D Dataset
Ben Nachman & DS 2001.04990

Can also consider performance on a feature set which is not independent of m. We introduced artificial correlations just as proof of concept:

\[ m_{J,2} \rightarrow m_{J,2} + c m_{JJ} \]

ANODE is robust while CWoLa completely fails!