

## The Dark Machines Anomaly Score Challenge

Based on arXiv: 2105.14027

https://github.com/bostdiek/DarkMachines-UnsupervisedChallenge

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The Dark Machines Anomaly Score Challenge: Benchmark Data and Model Independent Event Classification for the Large Hadron Collider

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https://arxiv.org/abs/2105.14027

Submitted to SciPost

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## **Challenge Justification and Goals**

- Goal is to perform model-agnostic searches
- Already examples of similar searches:
  - DØ Collaboration at Tevatron using SLEUTH
  - H1 Collaboration at HERA using 1-D signal detection algorithm
  - CDF Collaboration at Tevatron (using similar to above)
- Searching for localized excesses in events can be done by Machine Learning
  - We look at anomaly detection techniques
- Unlike LHC Olympics which looked at overdensities as signals in black box data
  - https://arxiv.org/abs/2101.08320

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## **Challenge Outline**

- Dataset of > 1 Billion SM Events (Les Houches: <a href="https://arxiv.org/pdf/2002.12220.pdf">https://arxiv.org/pdf/2002.12220.pdf</a>)
  - https://zenodo.org/record/3685861
- Hackathon Dataset: (https://zenodo.org/record/3961917)
  - 4 different channels (channels here defined as distinct datasets based on selection cuts)
  - 11 different BSM signals (19 total mass points)
  - 34 unique signal/channel combinations
- Train each method 4 times (once per channel) using SM
- Select ML methods which perform best to apply to blinded Secret Dataset: https://zenodo.org/record/4443151

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## **General Strategy**

#### Detection of "expected" signal events

#### Detection of "unexpected" anomalous events



Challenge object is an event-by-event anomaly score and we use this to define a signal region

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## **The Standard Model Datasets**

SM processes								
Physics process	Process ID	$\sigma$ (pb)	$N_{\rm tot} (N_{10{\rm fb}^{-1}})$					
$pp \rightarrow jj(+2j)$	njets	$19718_{H_T > 600 \text{GeV}}$	415331302 (197179140)					
$pp \rightarrow l^{\pm} \nu_l(+2j)$	w_jets	$10537_{H_T > 100 \text{GeV}}$	$135692164 \ (105366237)$					
$pp \rightarrow \gamma j(+2j)$	gam_jets	$7927_{H_T > 100 \text{GeV}}$	123709226 (79268824)					
$pp \rightarrow l^+l^-(+2j)$	z_jets	$3753_{H_T>100 \text{GeV}}$	60076409 (37529592)					
$pp \rightarrow t\bar{t}(+2j)$	ttbar	541	13590811 (5412187)					
$pp \rightarrow t + jets(+2j)$	$single_top$	130	7223883 (1297142)					
$pp \rightarrow \bar{t} + \text{jets}(+2j)$	$single_topbar$	112	7179922 (1116396)					
$pp \rightarrow W^+W^-(+2j)$	ww	82.1	17740278 (821354)					
$pp \rightarrow W^{\pm}t(+2j)$	wtop	57.8	5252172(577541)					
$pp \rightarrow W^{\pm} \bar{t}(+2j)$	wtopbar	57.8	4723206 (577541)					
$pp \rightarrow \gamma \gamma (+2j)$	2gam	47.1	17464818 (470656)					
$pp \rightarrow W^{\pm}\gamma(+2j)$	Wgam	45.1	18633683 (450672)					
$pp \rightarrow ZW^{\pm}(+2j)$	zw	31.6	13847321 (315781)					
$pp \rightarrow Z\gamma(+2j)$	Zgam	29.9	15909980 (299439)					
$pp \rightarrow ZZ(+2j)$	ZZ	9.91	7118820 (99092)					
$pp \rightarrow h(+2j)$	single_higgs	1.94	2596158 (19383)					
$pp \rightarrow t\bar{t}\gamma(+2j)$	ttbarGam	1.55	95217 (15471)					
$pp \rightarrow t\bar{t}Z$	ttbarZ	0.59	300000 (5874)					
$pp \rightarrow t\bar{t}h(+1j)$	ttbarHiggs	0.46	200476 (4568)					
$pp \rightarrow \gamma t(+2j)$	atop	0.39	2776166 (3947)					
$pp \rightarrow t\bar{t}W^{\pm}$	ttbarW	0.35	279365 (3495)					
$pp \rightarrow \gamma \bar{t}(+2j)$	atopbar	0.27	4770857 (2707)					
$pp \rightarrow Zt(+2j)$	ztop	0.26	3213475 (2554)					
$pp \rightarrow Z\bar{t}(+2j)$	ztopbar	0.15	2741276 (1524)					
$pp \rightarrow t\bar{t}t\bar{t}$	4top	0.0097	399999 (96)					
$pp \rightarrow t \bar{t} W^+ W^-$	ttbarWW	0.0085	150000 (85)					



Madgraph+Pythia+Delphes | jets, b-jets, electrons, muons, photons

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## **The Analysis Channels**

Channel 1: 214K SM Events

- $H_{T} \ge 600 \text{ GeV}$
- MET ≥ 200 GeV
- MET/H<sub>T</sub>  $\ge 0.2$
- At least 4 (b)-jets with  $p_T > 50 \text{ GeV}$
- At least 1 (b)-jets with  $p_T > 200 \text{ GeV}$

Channel 2b: 340K SM Events

- $H_T \ge 50 \text{ GeV}$
- MET  $\geq$  50 GeV
- At least 2  $\mu$ /e with  $p_T$  > 15 GeV

### Channel 2a: 20K SM Events

- MET  $\geq$  50 GeV
- At least 3  $\mu/e$  with  $p_{\scriptscriptstyle T}>$  15 GeV
- At least 1 (b)-jets with  $p_T > 200 \text{ GeV}$
- <u>Few training events, many ML</u> <u>methods struggle</u>

Channel 3: 8.5M SM Events

- $H_T \ge 600 \text{ GeV}$
- MET  $\geq$  100 GeV
- <u>Large dataset, timed out training on</u> <u>some methods</u>

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## **The Methods**

Abbreviation	Algorithm	Section	Hyperparameters	# Submitted
$\mathbf{SimpleAE}$	Autoencoders	4.1	Tab. 6	1
VAEs	Variational Autoencoders	4.2	Tab. <b>7</b>	140
DeepSetVAE	Deep Set Variational Autoencoders	4.3	Tab. 8	4
ConvVAE (NoF)	Convolutional Variational Autoen- coders	4.4	Tab. 9	1
Planar	ConvVAE+Planar Flows	4.5.1	Tab. 10	1
SNF	ConvVAE+Sylvester Normalizing Flows	4.5.2	Tab. 11	3
IAF	ConvVAE+Inverse Autoregressive Flows	4.5.3	Tab. 12	1
ConvF	ConvVAE+Convolutional Normal- izing Flows	4.5.4	Tab. 13	1
CNN	Convolutional $(\beta)$ VAE	4.6		2
KDE	Kernel Density Estimation	4.7	Tab. 14	36
Flow	Spline autoregressive flow	4.8	Tab. 15	2
Deep SVDD	Deep SVDD	4.9	Tab. 16 & 17	80
Combined (Deep SVDD & Flow)	Spline autoregressive flow with Deep SVDD	4.10		8
DAGMM	Deep Autoencoding Gaussian Mix- ture Model	4.11	Tab. 19	384
ALAD	Adversarial Anomaly Detection	4.12	Tab. 21	96
Latent	Anomaly Detection in the Latent Space	4.13	Tab. 22	288

- Top 9 and the last use some form of encoding decoding with a recon error anomaly score
- Planar, SNF, IAF, ConvF, Flow and Combined use some form of flow based likelihoods
- KDE, DAGMM and Latent use clustering or density estimation
- # submitted refers to number of methods of this type that were created

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## **Metrics for Results**

#### **Figures of Merit:**

- Area under the ROC curve (AUC)
- The signal efficiency at a background efficiency of 10<sup>-2</sup>
- The signal efficiency at a background efficiency of 10<sup>-3</sup>
- The signal efficiency at a background efficiency of 10<sup>-4</sup>



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## **Summary Results**

- Each method is a point on the boxand-whisker plot
- Each row is a BSM signal
- Some BSM easy for most methods
- Some BSM challenging for all methods
- Some BSM are easier than others to get a good anomaly score with

Each figure of merit has its own top methods, can we combine to form a single metric?



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## **Best Performing Methods**

 $10^{1}$ 

#### Compare Hackathon and Secret Data results Flow-Efficient\_Likelihood DAGMM\_0.001 ☆ Combined-AND-DeepSVDD-Flow Planar 1 • $10^{1}$ Combined-AVG-DeepSVDD-Flow VAE-dynamic-beta1-z13\_Radius $\nabla$ Flow-Efficient-No-E Likelihood ALAD\_bs5000\_F Combined-PROD-DeepSVDD-Flow $\triangleleft$ KDE \$ Combined-AND-VAE\_beta1\_z21-Flow ALAD\_bs5000\_L1 Combined-OR-DeepSVDD-Flow $ALAD_{bs5000}L2$ 0 Combined-OR-VAE\_beta1\_z21-Flow ALAD\_bs5000\_CH $10^{0}$ Combined-AVG-VAE\_beta1\_z21-Flow $\bigcirc$ 1 ALAD\_bs500\_L1 Combined-PROD-VAE\_beta1\_z21-Flow ÷ ALAD\_bs500\_CH DeepSetVAE\_weight\_10.0 SimpleAE ALAD\_bs500\_L2 DeepSetVAE\_weight\_1.0 ALAD\_bs500\_F ConvF 53 DAGMM\_0.01

Hackathon Data Median TI

 $10^{0}$ 

#### Methods with Median TI > 2 on both datasets

Secret Data Median TI

 $10^{-1}$ 

 $10^{-1}$ 

Model	Hackathon Data	Secret Data	
Combined-OR-DeepSVDD-Flow	6.30	19.02	
$DeepSetVAE\_weight\_1.0$	3.50	4.27	
$Combined-AVG-VAE\_beta1\_z21-Flow$	6.00	3.21	
$Combined-PROD-VAE\_beta1\_z21-Flow$	6.00	3.20	
$Combined-AND-VAE\_beta1\_z21-Flow$	7.00	2.98	
Combined-AVG-DeepSVDD-Flow	10.00	2.31	
Combined-AND-DeepSVDD-Flow	10.00	2.26	
DeepSetVAE_weight_10.0	3.75	2.03	

 TI: Total Improvement → maximum Significant Improvement over all background rejections over all channels

$$SI \equiv \frac{\epsilon_S}{\sqrt{\epsilon_B}}$$

- Apply the models to the same signals on the hackathon and secret datasets

- Each of the best performing models has some fixed target component (Deep SVDD, bVAE with b=1) and latent space seems to be important

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## Conclusion

- Model-agnostic searches
- Primarily use Variational Auto-Encoders
- Variety of channels and signals
- Best methods use some form of fixed target
- Anomaly Detection is hard: seems even the Median metric doesn't generalize well!
- https://twitter.com/dark\_machines?s=20
- https://darkmachines.org/



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# Backups

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## **Variational Autoencoder**

- Same structure as an Autoencoder (encoder, bottleneck, decoder) except the latent space is continuous by design
- Sampling can be done on latent vectors to produce a continuous set of outputs
- (Generally) Minimum Squared Error (MSE) + Kullback-Liebler Divergence used as error

$$(t_i - y_i)^2$$

$$\sum_{i=1}^{n} \sigma_i^2 + \mu_i^2 - \log(\sigma_i) - 1$$

**KL-Divergence** 

Typical MSE

14

Dense - 500  

$$\mu$$
Dense - 120  
 $\mu$ 
Dense - 30  
Dense - 30  
Dense - 120  
Dense - 120  
Dense - 500  
Output

Input

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## **Challenges with the VAE**

- Should the events be zero padded?
- Should we take a smaller number of objects?
- Which anomaly score to use:
  - Just one or the other of reconstruction or KL
  - Radius in the latent space
  - Beta parameters (and how to tweak them)



## **The BSM Physics**

BSM process	Channel 1	Channel 2a	Channel 2b	Channel 3
$Z' + { m monojet}$	×	×		×
Z'+W/Z				×
$Z' + { m single top}$	×			×
$Z'$ in lepton-violating $U(1)_{L_{\mu}-L_{\tau}}$		×	×	
R-SUSY stop-stop	×		×	×
<b>∦</b> -SUSY squark-squark	×			×
SUSY gluino-gluino	×	×	×	×
SUSY stop-stop	×			×
SUSY squark-squark	×			×
SUSY chargino-neutralino		×	×	
SUSY chargino-chargino			×	

Some processes have different mass spectra or decay modes: 19 signals, 34 Signal-Channel combinations

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## **Maximum Significant Improvement**

$$\sigma_{S} = \frac{S}{\sqrt{B}}$$

$$\sigma_{AD} = \frac{S'}{\sqrt{B'}}$$

$$= \frac{\epsilon_{S} S}{\sqrt{\epsilon_{B} B}}$$

$$= \frac{\epsilon_{S}}{\sqrt{\epsilon_{B}}} \sigma_{S}$$

 $\boldsymbol{\alpha}$ 

$$SI \equiv \frac{\epsilon_S}{\sqrt{\epsilon_B}}$$

Analysis of all models on all signals in the Dark Machines Unsupervised Challenge Hackathon Data



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## **Total Improvement Across Signals**

Total Improvement for models over all signals on Dark Machines Unsupervised Challenge Hackathon Data



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