David Shih December 11, 2023

Intro to Unsupervised ML and Anomaly Detection

COFI Winter School 2023 Old San Juan, Puerto Rico

Outline

- 1. Motivation: new physics and the LHC
- 2. Model-agnostic new physics searches with modern ML
	- Outlier detection
	- Overdensities
- Astro

3. Common tools, cross-cutting domains: Anomaly Detection from LHC to

By now, there are countless searches for new physics at the LHC. Almost all cut-based, model-specific. No sign of new physics yet…

*Only a selection of the available mass limits on new states or
phenomena is shown. Many of the limits are based on simplified models, c.f. refs. for the assumptions made.

 10^{-1}

ATLAS Preliminary

ATLAS SUSY Searches* - 95% CL Lower Limits

Mass scale [TeV]

 $\overline{1}$

By now, there are countless searches for new physics at the LHC. Almost all cut-based, model-specific. No sign of new physics yet…

*Only a selection i phenomena is sl simplified model: 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 ΔM 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 ΔM , respectively, unless indicated otherwise.

ATLAS Preliminary

By now, there are countless searches for new physics at the LHC. Almost all cut-based, model-specific. No sign of new physics yet…

$ATLA$

Mo $\tilde{q}, \tilde{q} \rightarrow$ $\overline{\text{ge}}$ $\tilde{g}\tilde{g}, \tilde{g} \rightarrow$

The quantities ΔM and x represent the \imath sparticle and the LSP relative to $\Delta M,$ re

 $X_{3/3}X_{3/3}$ + tWtW

(Upper Cross Section Limit [fb])

Almost all cut-based, model-specific. No sign of new physics yet…

Model-agnostic NP searches?

TABLE I. Existing two-body exclusive final state resonance searches at $\sqrt{s} = 8$ TeV. The \varnothing symbol indicates no existing search at the LHC.

	ϵ		τ	\sim				$\,W\,$	Ζ	
ϵ	$\pm\mp 4 ,\pm\pm 5 $	$\pm\pm[5, 6]$ ' $\pm\mp$ 6,	$7\vert$	Ø	Ø	Ø	Ø	Ø	Ø	Ø
μ		$\pm\mp[4], \pm\pm[5]$	7	Ø	Ø	Ø	Ø	Ø	Ø	Ø
			[8]	Ø	Ø	Ø	$[9]$	Ø	Ø	Ø
					$[10]$ $[11-13]$	Ø	Ø	$\left\lceil 14\right\rceil$	[14]	Ø
					$\left[15\right]$	[16]	$\left\lceil 17\right\rceil$	$\left[18\right]$	$\left[18\right]$	Ø
						[16]	$\left\lceil 19\right\rceil$	Ø	Ø	Ø
$t\,$							$\left[20\right]$	$\left[21\right]$	Ø	Ø
$W \$								$[22 - 25]$	[23, 24, 26, 27]	$[28 - 30]$
Z									[23, 25, 31]	[28, 30, 32, 33]
h										$[34 - 37]$

TABLE II. Theory models motivating two-body final state resonance searches. Here *Z*⁰ and *W*⁰ denote additional *From Craig, Draper, Kong, Ng & Whiteson 1610.09392*

What if NP is not like any of the models we have searched for?

There are a lot of NP scenarios that are not covered by existing searches!

Model-agnostic NP searches?

Why aren't there more model-agnostic new physics searches?

Modern ML can help!

- *• model-specific ~ supervised ML*
- *• model-agnostic ~ less-than-supervised ML*
- *• unbinned analysis of high dimensional feature spaces (100s or 1000s of features)*
- *• (nearly) optimal classifiers*
- *• density estimation*

• generative modeling

• …

2. Model-agnostic NP searches with modern ML

Model-agnostic NP Searches @ LHC

The LHC Olympics 2020

A Community Challenge for Anomaly Detection in High Energy Physics

Gregor Kasieczka (ed),¹ Benjamin Nachman (ed),^{2,3} David Shih (ed),⁴ Oz Amram,⁵ Anders Andreassen, ⁶ Kees Benkendorfer, ^{2,7} Blaz Bortolato, ⁸ Gustaaf Brooijmans, ⁹ Florencia Canelli, 10 Jack H. Collins, 11 Biwei Dai, 12 Felipe F. De Freitas, 13 Barry M. Dillon,^{8,14} Ioan-Mihail Dinu,⁵ Zhongtian Dong,¹⁵ Julien Donini,¹⁶ Javier Duarte,¹⁷ D. A. Faroughy¹⁰ Julia Gonski, ⁹ Philip Harris, ¹⁸ Alan Kahn, ⁹ Jernej F. Kamenik, ^{8, 19} Charanjit K. Khosa, ^{20,30} Patrick Komiske, ²¹ Luc Le Pottier, ^{2,22} Pablo Martín-Ramiro,^{2,23} Andrej Matevc,^{8,19} Eric Metodiev,²¹ Vinicius Mikuni,¹⁰ Inês Ochoa,²⁴ Sang Eon Park,¹⁸ Maurizio Pierini,²⁵ Dylan Rankin,¹⁸ Veronica Sanz,20*,*²⁶ Nilai Sarda,²⁷ Uro˘s Seljak,2*,*3*,*¹² Aleks Smolkovic,⁸ George Stein,2*,*¹² Cristina Mantilla Suarez,⁵ Manuel Szewc,²⁸ Jesse Thaler,²¹ Steven Tsan,¹⁷ Silviu-Marian Udrescu,¹⁸ Louis Vaslin, 16 Jean-Roch Vlimant, 29 Daniel Williams, 9 Mikaeel Yunus 18

²*Physics Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA* <https://arxiv.org/abs/2101.08320> ³*Berkeley Institute for Data Science, University of California, Berkeley, CA 94720, USA*

T. Aarrestad*^a* M. van Beekveld*^b* M. Bona*^c* A. Boveia*^e* S. Caron*^d* J. Davies*^c* A. De Simone*f,g* C. Doglioni*^h* J. M. Duarte*ⁱ* A. Farbin*^j* H. Gupta*^k* L. Hendriks*^d* L. Heinrich*^a* J. Howarth*^l* P. Jawahar*m,a* A. Jueid*ⁿ* J. Lastow*^h* A. Leinweber*^o* J. Mamuzic*^p* E. Merényi*^q* A. Morandini*^r* P. Moskvitina*^d* C. Nellist*^d* J. Ngadiuba*s,t* B. Ostdiek*u,v* M. Pierini*^a* B. Ravina*^l* R. Ruiz de Austri*^p* S. Sekmen*^w* M. Touranakou^{x,a} M. Vaškevičiūte^l R. Vilalta^y J.-R. Vlimant^t R. Verheyen^z M. White^{*o*} E. Wulff^{*h*} E. Wallin^{*h*} K.A. Wozniak^{α, a} Z. Zhang^{*d*}

^gINFN, 34149 Trieste TS, Italy A lot of new ideas for model-agnostic searches!

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

^fSISSA, 34136 Trieste TS, Italy

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University of California San Diego, La Jolla, CA 92093, USA

` <https://arxiv.org/abs/2105.14027>

Proofs-of-concept are becoming actual LHC searches! signal regions. An iterative procedure is applied until \mathcal{L} Proots-ot-concept are becoming $t \sim t$ ensure that the pine that the fit t are uncorrelated. If the fit σ actual LHC searches!

wiodel-adnostic Ni $t \sim \frac{1}{\sqrt{2}}$, combined with the adjacent with the adjacent with the adjacent \sim searcnes w LHU region in the presence or absence of a true signal. First, the **Model-agnostic NP Searches @ LHC**

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Two modes of anomaly detection

a. Outlier detection ("point anomalies")

b. Overdensity detection ("group anomalies")

 $p_{bg}(x)$

Autoencoders Farina, Nakai & **DS** [1808.08992](https://arxiv.org/abs/1808.08992) Heimel et al [1808.08979](https://arxiv.org/abs/1808.08979) Cerri et al [1811.10276](https://arxiv.org/abs/1811.10276)

Data vs bg test statistic D'Agnolo et al [1806.02350](https://arxiv.org/abs/1806.02350),[1912.12155,](https://arxiv.org/abs/1912.12155) [2111.13633](https://arxiv.org/abs/2111.13633)

… Density estimation Caron, Hendriks, Verheyen [2106.10164](https://arxiv.org/abs/2106.10164)

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Enhanced bump hunts CWoLa Hunting [Collins, Howe & Nachman [1805.02664,](https://arxiv.org/abs/1805.02664) [1902.02634\]](https://arxiv.org/abs/1902.02634) ANODE [Nachman & **DS** [2001.04990\]](https://arxiv.org/abs/2001.04990) CATHODE [**DS+** Hallin et al [2109.00546,](https://arxiv.org/abs/2109.00546) [2210.14924\]](https://arxiv.org/abs/2210.14924) CURTAINS [Raine et al [2203.09470\]](https://arxiv.org/abs/2203.09470)

2a. Outlier detection *Entropy* **2021**, *23*, 1690 2 of 19

- Pros:
	- can be fully unsupervised views and the can be fully unsupervised goes beyond issues of estimation, approximation, or optimization errors [37]. We highlight
	- can potentially find very rare anomalies d density-based methods for an online continuous \mathbf{r}_i
- Cons:
	- "low p(x)" is coordinate dependent! An event can be anomalous or not depending on parametrization of features [Le Lan & Dinh [2012.03808](https://arxiv.org/abs/2012.03808%5D), DS+ Kasieczka et al [2209.06225\]](https://arxiv.org/abs/2209.06225) with current practices by building adversarial cases, even under strong distributional • Given the resulting tension between the use of these anomaly detection methods and their

low $p(x)$

Example: searching for NP with autoencoders

Farina, Nakai & **DS** 1808.08992; Heimel, Kasieczka, Plehn & Thompson 1808.08979; Cerri et al 1811.10276; and many more…

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An autoencoder maps an input into a "latent representation" and then representation, in the case of the case 6-dim, and then decoded. attempts to reconstruct the original input from it.

 $T_{\rm{ke}}$ Force and the concert on the second water that the patterns The encoding is lossy, so the reconstruction is not perfect.

Many real world applications of autoencoders, including anomaly detection, fraud detection, denoising, compression, generation, density estimation

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 $L =$ Loss function for autoencoder: $L = \frac{1}{N} \sum_{i=1}^{N} (x_i^{in} - x_i^{out})^2$ "reconstruction error"

12

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 $L =$ Loss function for autoencoder: $L = \sum (x_i^{in} - x_i^{out})^2$ "reconstruction error"

12

Then when the autoencoder encounters "anomalous" outlier events, its performance should be worse.

$$
= \frac{1}{N} \sum_{i=1}^N (x_i^{in} - x_i^{out})^2
$$

 $L =$ Loss function for autoencoder:

12

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Can use reconstruction error as an anomaly score!

"reconstruction error"

 $L =$ Loss function for autoencoder: $L = \frac{1}{2\pi} \sum (x_i^{in} - x_i^{out})^2$

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Then when the autoencoder encounters "anomalous" outlier events, its performance should be worse.

Can use reconstruction error as an anomaly score!

"reconstruction error"

Example: searching for NP with autoencoders

[See Maria's talk next for other ways to use (variational) autoencoders for anomaly detection]

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Challenges:

Challenges:

• Uncontrolled, not very sensitive, optimality not guaranteed — the AE will find what it finds...

Challenges:

• The AE can fail to detect outliers if they are "simpler" than the background

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- T. Weber MSc Thesis [G. Kasieczka]; Dillon et al 2104.08291; Finke et al 2104.09051

• Uncontrolled, not very sensitive, optimality not guaranteed — the AE will find what it finds...

Top jets (more complex) are identified as anomalous when AE trained on QCD jets (simpler)

But not vice versa

Normalized autoencoders $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ *Z✓* $\overline{}$

Yoon et al <u>2105.05735</u>, Dillon et al <u>2206.14225</u> 222 . We omit an explicit normalization of the energy by a temper-

Add additional normalization term to usual AE loss to further penalize outliers during training and model parameters over the model parameters of the model parameters of the model p

 $\mathbf{v} = -\ln \sigma n_o(\mathbf{v}) = F_o(\mathbf{v}) + \ln \sigma Z_o \implies \mathbf{v} = \mathbf{v}$ $\mathcal{L}(x) = -\log p_{\theta}(x) = E_{\theta}(x) + \log Z_{\theta} \implies \mathcal{L} = \langle$

Figure 3: Distribution of the energy or MSE after training on QCD jets (left) and on top jets (right). We show the energy for QCD jets (blue) and top jets (orange) in both cases.

$$
\Rightarrow \qquad \mathcal{L} = \left\langle E_{\theta}(x) + \log Z_{\theta} \right\rangle_{x \sim p_{\text{data}}}
$$

Now performance of AE is "symmetrical"!

- Tops are identified as anomalous when AE trained on QCD
- QCD are identified as anomalous when AE trained on Tops

• Background estimation with outlier anomaly detection

- Background estimation with outlier anomaly detection
	- Can combine with bump hunt at cost of model-independence Farina, Nakai & **DS** 1808.08992; Heimel, Kasieczka, Plehn & Thompson 1808.08979

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	- **• New idea: Double Decorrelated AE** Mikuni, Nachman & **DS** 2111.06417

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	- **• New idea: Double Decorrelated AE** Mikuni, Nachman & DS 2111.06417 <u>lous idea</u> . I
		- Train *two* autoencoders and force them to be statistically independent of one another $\frac{1}{2}$ and the comparing data to a reference sample $\frac{1}{2}$. However, $\frac{1}{2}$. Irain two autoencoders and force them to be statistically inde

Autoencoders: challenges

 α ^{*i*}(*DisCo*^{*i*} "DisCo Decorrelation" rameter, and DisCo is the distance correlation [82–85]. *Kasieczka & DS 2001.05310*

szekely et al U8U3.4101 et seq *Szekely et al 0803.4101 et seq*

$$
L[f_1, f_2, g_1, g_2] = \sum_i R_1(x_i)^2 + \sum_i R_i
$$

of one another
$$
+ \lambda \operatorname{DisCo}^2[R_1(X)],
$$

- Background estimation with outlier anomaly detection these conventional methods. By using two decorrelated \mathbf{B} autorencoders, we can trigger out of the can trigger on the can trigger on \mathbf{r}_i
- Can combine with bump hunt at cost of model-independence Farina, Nakai & **DS** 1808.08992; Heimel, Kasieczka, Plehn & Thompson 1808.08979 Farina, Nakal & DS T808.08992; Heimel, Kasleczka, Pienn & Thompson T808.08 e Can combine w anti-tagged events in a matter significant entity in a matter of the settimation of the settimation entity of the settimation of the settimation of the settimation entity \mathbf{D} fine counts *N*7*,*7(~
	- **• New idea: Double Decorrelated AE** Mikuni, Nachman & DS 2111.06417 <u>lous idea</u> . I lecorrelat
- Train *two* autoencoders and force them to be statistically independent of one another $\frac{1}{2}$ and the comparing data to a reference sample $\frac{1}{2}$. However, $\frac{1}{2}$. Irain two autoencoders and force them to be statistically inde the technique of the technique of decorrelations in the decorrelation and \sim Train two auto
- Use ABCD method for fully data-driven background estimation merical results with the ABCD me

Autoencoders: challenges ventional triggers are complemented by *support* triggers where *^Ri*(*x*)=(*fi*(*gi*(*x*)) *^x*)² rameter, and DisCo is the distance correlation [82–85].

Challenges: ground estimation of the first control provides the first control provides the first control provides the first
The first control provides the first control provides the first control provides the first control provides th

amples *x*, which are realizations of the random variable *X*. Given an autor and all consequence via Eq. 2, we can determine the can determined via Eq. 2, we can de-
2, 08992: Heimel Kasieczka, Plehn & Thompson 1808 08979 **c**) = P
c

ion with outlier anomaly detection

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its arguments are independent. The capital *SZEKEI y* et al. 0603.4101 et seq *Szekely et al 0803.4101 et seq*

Decorrelated AE

\n
$$
L[f_1, f_2, g_1, g_2] = \sum_i R_1(x_i)^2 + \sum_i R_i
$$
\n2111.06417

\nders and force them to be statistically independent of one another
$$
+ \lambda \text{DisCo}^2[R_1(X),
$$

$$
\sum_{i,j}^{\text{colicted}}(\vec{c}) = \frac{N_{>,<}(\vec{c})N_{<,>}(\vec{c})}{N_{<,<}(\vec{c})}
$$

Double Decorrelated AE

Mikuni, Nachman & **DS** 2111.06417

The method works!

First complete strategy for unsupervised, non-resonant anomaly detection are shown as independent entries.
Are shown as independent entries as independent entries as independent entries.

Can also be used online as an anomaly trigger

2b. Overdensity detection

• Pros:

- reparametrization invariant
- asymptotically optimal

- Requires more precise knowledge of background (reference) distribution).
Illirae mora nraciea knowladoa of hackoround of performance (as internet) distribution
- Performance suffers when signal is too rare

• Cons:

18 ticular does not have to learn the sharp increase in *p*data

sifier (as in CWoLa Hunting) to distinguish *p*data(*x|m*)

Classic Overdensity Search 1D Bump Hunt

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

Interpolate from **sidebands** into **signal region** (eg window in invariant mass), search for an excess.

Used in many discoveries!

x: *additional* features where NP could be localized

 $\vec{x} \in \mathbb{R}^d$

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x: *additional* features where NP could be localized

Learn model-agnostic **anomaly score** $R(x)$ from data

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Learn model-agnostic **anomaly score** $R(x)$ from data

Idealized Anomaly Detector

 $p_{data}(x)$ $p_{bg}(x)$

Claim: the optimal model-agnostic discriminant would be (Neyman & Pearson)

R(*x*) = *"Idealized Anomaly Detector"*

Idealized Anomaly Detector

Claim: the optimal model-agnostic discriminant would be (Neyman & Pearson)

"Idealized Anomaly Detector"

Proof:

$$
R(x) = \frac{p_{data}(x)}{p_{bg}(x)}
$$

$$
p_{data}(x) = \epsilon_{sig} p_{sig}(x) + (1 - \epsilon_{sig}) p_{bg}(x)
$$

$$
R(x) = (1 - \epsilon_{sig}) + \epsilon_{sig} \frac{p_{sig}(x)}{p_{bg}(x)}
$$

Idealized Anomaly Detector

Claim: the optimal model-agnostic discriminant would be (Neyman & Pearson)

"Idealized Anomaly Detector"

 $R(x)$ is monotonic with signal-to-background likelihood ratio *regardless of unknown, arbitrary signal strength and probability density*

Proof:

$$
R(x) = \frac{p_{data}(x)}{p_{bg}(x)}
$$

$$
p_{data}(x) = \epsilon_{sig} p_{sig}(x) + (1 - \epsilon_{sig}) p_{bg}(x)
$$

$$
R(x) = (1 - \epsilon_{sig}) + \epsilon_{sig} \frac{p_{sig}(x)}{p_{bg}(x)}
$$

Train a neural network to classify data vs MC simulation of the SM.

-
- If the NN classifier is optimal, its output should be (monotonic with)

 $p_{data}(x)$

 $p_{MC}(x)$

the data vs MC likelihood ratio (Neyman-Pearson).

 $R_{\text{classifyier}}(x) =$

-
- If the NN classifier is optimal, its output should be (monotonic with)
	- $p_{data}(x)$ $p_{MC}(x)$

 $R_{\text{classifyier}}(x) = \frac{P \text{ data}}{x}$ *componential inclusive contraction trick*"

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D'Agnolo et al 2111.13633

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This can work if simulations are reliable and their systematic uncertainties are well-understood.

D'Agnolo et al 2111.13633

- Train a neural network to classify data vs MC simulation of the SM.
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"The likelihood-ratio trick" $p_{data}(x)$ $p_{MC}(x)$

the data vs MC likelihood ratio (Neyman-Pearson).

 $R_{\text{classifyier}}(x) =$

This can work if simulations are reliable and their systematic uncertainties are well-understood.

Alternatively, can we get $p_{data}(x)$ and $p_{bg}(x)$ in a data-driven way?

Collins, Howe & Nachman 1805.02664,1902.02634

Collins, Howe & Nachman 1805.02664,1902.02634

Train a NN classifier on SR vs SB data, learn sifier (as in CWoLa Hunting) to distinguish *p*data(*x|m*)

 $N_{classifier}(X) \approx \frac{1}{N} = \frac{1}{N}$ $Pdata, SB(\lambda)$ $Pbg, SB(\lambda)$ $R_{classifier}(x) \approx$ $P_{data,SR}(x)$ $P_{data,SB}(x)$ = $P_{data,SR}(x)$ $p_{bg,SB}(x)$

Collins, Howe & Nachman 1805.02664,1902.02634

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If $p_{\text{max}}(x) = p_{\text{max}}(x)$ li.e. features x are in $\log_{10}D_{\rm X}$ and $\log_{10}N_{\rm X}$ and $\log_{10}N_{\rm X}$ of m in the background] then the classifier gives the desired likelihood ratio. If $p_{bg, SB}(x) = p_{bg, SR}(x)$ [i.e. features x are independent

$$
R_{\text{classifyier}}(x) \rightarrow \frac{P_{\text{data,SR}}(x)}{P_{\text{bg,SR}}(x)}
$$

Collins, Howe & Nachman 1805.02664,1902.02634

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$$
R_{\text{classifyier}}(x) \rightarrow \frac{P_{\text{data,SR}}(x)}{P_{\text{bg,SR}}(x)}
$$

"CWoLa Hunting" and actual data events in the actual data events

Nachman & **DS** 2001.04990

from [2109.00546](https://arxiv.org/abs/2109.00546)

Tight connection between *generative models* and *anomaly detection*!

Nachman & **DS** 2001.04990

Train two separate *pormalizing flows* on S sifier (as in case of the contract of the distinguish ρ in ρ ρ ρ) ρ events to learn $p_{data}(x | m \in SR)$ and $p_{data}(x | m \in SB) = p_{bg}(x | m \in SB).$ $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ (LHC) and $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ and $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ and $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ and $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ Train two separate *normalizing flows* on SR and SB

Nachman & **DS** 2001.04990

The SB NF automatically interpolates into the SR, ment characteristic characteristic that greatly surpasses both CWOLA and giving an estimate of $p_{bg}(x | m \in SR)$. sections. Cathode easily outperforms Anode because it

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Nachman & **DS** 2001.04990

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Train two separate *pormalizing flows* on S sifier (as in case of the contract of the distinguish ρ in ρ ρ ρ) ρ events to learn $p_{data}(x | m \in SR)$ and $p_{data}(x | m \in SB) = p_{bg}(x | m \in SB).$ $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ (LHC) and $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ and $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ and $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ and $\mathcal{L}_{\mathcal{L}_{\mathcal{L}}}$ Train two separate *normalizing flows* on SR and SB

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DS+ Hallin et al 2109.00546, 2210.14924

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from [2109.00546](https://arxiv.org/abs/2109.00546)

Consiguired the open line **TH** resurb bassilying Andrianes Through URA HUNTING IS CONSICTED STREAMS IN THE ACTUAL CONTROL IN THE ACTUAL CONTRACTOR IN THE ACTUAL CONTRACTOR IN TH the side of $\mathsf{CATHODE}$ ²⁹ sifier. Secondly, the features are slightly correlated with the features are slightly correlated with the feat
The features are slightly correlated with the features are slightly correlated with the features are slightly \mathcal{L} \mathcal{L} \mathcal{L} \mathcal{L} \mathcal{L} accifying $\mathbf{\Lambda}$ no background and of the synthetic samples. The synthetic samples \sim malies **TH**rough the background of the b "Classifying Anomalies THrough signal distribution in the SR (SR). For all the variation in the SR (SR). For all the variations were well as \leq **Outer Density Estimation** same classifier architecture. This consists of 3 hidden **(CATHODE)"**

Summary of methods

- CWoLa Hunting: **classifier** between SB and SR data
- **ANODE: two conditional density estimators** on shead SR data: internolate SR density from *p*bg(*x|m*) in the SR. SB and SR data; interpolate SB density estimator into SR
- Ω Ω Γ Ω <u>CATITODE</u>. Single Conditional density e on SB data; sample interpolated SB density estimator in SR; classifier between sampled sections. Cathode easily output in \overline{CD} does not have to directly learn *p*data in the SR, and in par-• CATHODE: single **conditional density estimator** events and data in SR
- ticular does not have to learn the sharp increase in *p*data • Many other approaches also proposed!
- CURTAINS: invertible NN for SB->SB interpolation [Raine et al *oversample* the outer density estimator, leading to more 2203.09470]
- Simulation assisted resonant anomaly detection: SALAD [Andreassen, Nachman & DS 2001.05001], SA-CWoLa [Benkendorfer et al [2009.02205\]](https://arxiv.org/abs/2009.02205%5D), FETA [Golling et al [2212.11285](https://arxiv.org/abs/2212.11285)]

We compared the methods on a common toy dataset:

27

Background: QCD dijets (1M events)

- Simulated with Pythia8 + Delphes
- pT(J1)>1.2 TeV trigger
- 4-vectors of every reconstructed particle in the event

LHC Olympics 2020 R&D dataset [[https://doi.org/10.5281/zenodo.2629072\]](https://doi.org/10.5281/zenodo.2629072)

No explicit search at the LHC for this scenario!

LHCO2020 R&D Dataset

Benchmark signal strength:

Benchmark signal strength:
S_{SR}/B_{SR}~0.6%, S_{SR}/√B_{SR}~2.2

Additional features

Significance improvement characteristic (SIC): $\epsilon_S / \sqrt{\epsilon_B}$

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GATHODE OUTPENOMIS GWOLA and ANODE and nearly saturates the idealized CATHODE outperforms CWoLa and ANODE and nearly saturates the idealized anomaly detector!

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 t_{in} : The solid lines are deduced from a median value of Ω fully independent trainings on the same training Ω validation and evaluation set. The uncertainty bands quantify the variance from retraining the NNs on the same, fixed dataset Initial significance was ~2.2σ

$-$ are defined such that they contain 68% of the runs around the median. => **a ~30σ anomaly could be hiding in the data right now!**

Current frontiers of resonant anomaly detection

Robustness

DS+ Buhmann et al 2310.06897 Das, Kasieczka & DS, 2311.nnnnn

3. Anomaly Detection from LHC to Astro

Searching for Stellar Streams in Gaia

- could be applied to **Gaia data** to search for **stellar streams**
	- *An example of power of ML to cut across domains!*

• We realized the same ML-enhanced bump hunt methods developed for LHC

Gaia satellite:

- Launched in 2013; ongoing
- Angular positions, proper motions, color and magnitude of over **1 billion stars** in our Galaxy
- Distances and radial velocities for a smaller subset of nearby stars

-
-
-
-
-
-

lux

840

850

Spectroscopic Radial Velocity = $-68.89 + -3.17$ km/s

860

870

→ GAIA'S HERTZSPRUNG-RUSSELL DIAGRAM

Total number of sources

Number of sources with full astrometry

Number of 5-parameter sources

Number of 6-parameter sources

Number of 2-parameter sources

Gaia-CRF sources

Sources with mean G magnitude

Sources with mean G_{BP}-band photometry

Sources with mean GRP-band photometry

Sources with radial velocities

Sources with mean G_{RVS}-band magnitudes

Sources with rotational velocities

Mean BP/RP spectra

Mean RVS spectra

Variable-source analysis

Total number of sources

Number of sources with full astrometry

Number of 5-para 1.5B stars with 5d information (a Number of 6-para positions, proper motions, para
Number of 2-parameter sources

Gaia-CRF sources

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Total number of sources

Number of sources with full astrometry

Number of 5-para $1.5B$ stars with 5d information (a Number of 6-para positions, proper motions, parallax Number of 2-parameter sources

(much smaller subset of nearby Gaia-CRF sources Sources with mean G

with "well-measured" parallax

Sources with mean G_{BP}-band photometry

Sources with mean G_{RP}-band photometry

Sources with radial velocities

Sources with mean G_{RVS}-band magnitudes

Sources with rotational velocities

Mean BP/RP spectra

Mean RVS spectra

Variable-source analysis

Stellar Streams

Stellar streams are the very old remnants of tidally disrupted globular clusters and dwarf galaxies.

Unique probes into the formation history and gravitational potential of the Galaxy, and into dark matter substructure.

Collection of stars moving together along a common orbit — concentrated spatially and in velocity.

Stellar Streams

Unique probes into the formation history and gravitational potential of the Galaxy, and into dark matter substructure.

Bonaca et al. (2014)

Stellar Streams

photometry, reveal two significant gaps located at 1 ̊ 20 and 1 ̊ 40, and dubbed G-20 and G-20 and G-20 and G-
There is a 1 state of 1 and G-20 and G-20 and G-20 and G-40, respectively. The respectively. The respectively.

is a long, thin spur extending for the G-40 gap. (Bottom) An idealized model of GD-1, whose program and GD-1, whose program \sim

decade dynamical evidence of a dark halo substructure 3014) and substructure 3014

the Galaxy, and into dark matte -5

Known Stellar Streams of the Milky Way

[\[DS, Buckley, Necib '23\]](https://arxiv.org/abs/2303.01529) [\[DS, Buckley, Necib, Tamanas '21\]](https://arxiv.org/abs/2104.12789)

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• Streams are local overdensities in multiple features — ideal for **enhanced bump hunt methods**!

[\[DS, Buckley, Necib '23\]](https://arxiv.org/abs/2303.01529) [\[DS, Buckley, Necib, Tamanas '21\]](https://arxiv.org/abs/2104.12789)

-
- Choose either proper motion coordinate as resonant feature

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- Use ANODE method to learn anomaly score with remaining five features motion distribution (with observations in red, model solutions in blue, and the full DR2 sample in grey), and the colour-magnitude motion distribution (with observations in red, model solutions in blue, and the full DR2 sample in grey), and the colour-magnitude motion distribution (with observations in red, model solutions in blue, and the full DR2 sample in grey), and the colour-magnitude

[\[DS, Buckley, Necib '23\]](https://arxiv.org/abs/2303.01529) [\[DS, Buckley, Necib, Tamanas '21\]](https://arxiv.org/abs/2104.12789)

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All stars in a patch of the sky containing (part of) GD-1 (ra,dec)=(148.6,24.2)

Core method — illustrated with GD-1 Stream

40

[\[DS, Buckley, Necib, Tamanas '21](https://arxiv.org/abs/2104.12789)]

Fully data driven, simulation independent!

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Stars in SR after cut on *R*(*x*) obtained from ANODE

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[\[DS, Buckley, Necib, Tamanas '21](https://arxiv.org/abs/2104.12789)]

patch centered on (U*,* X) = (148*.*6*,* 24*.*2). (Note the streaking in angular position due to non-uniform coverage in *Gaia* DR2.) Bottom row: As above, with stars identified by PWB18 as likely GD-1 stars shown in red, along with an example search region `_ 2 [17*,* 11] mas/yr in proper motion. in the `_ 2 [17*,* 11] mas/yr SR of our example patch centered on (U*,* X) = (148*.*6*,* 24*.*2). Bottom row: As the upper row, applying the ' *>* 'cut cut on **The method works!**

Fully data driven, simulation independent!

All stars in a patch of the sky containing (part of) GD-1 (ra,dec)=(148.6,24.2)

Stars in SR after cut on *R*(*x*) obtained from ANODE

Core method — illustrated with GD-1 Stream

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[\[DS, Buckley, Necib, Tamanas '21](https://arxiv.org/abs/2104.12789)]

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Need to train ANODE ~12,000 times to cover the entire sky!! Each training takes O(10h)

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Need to train ANODE ~12,000 times to cover the entire sky!!

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- **Each training takes O(10h)** We ran this on the NERSC supercomputer at LBNL

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ANODE on Gaia data

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- We found a defining a single threshold on R(x) across all SRs was insufficient to find other known streams besides GD-1.
- What worked instead was to further subdivide SRs into slices by the orthogonal proper motion \Rightarrow "ROIs"
- In each ROI, take the 100 highest R stars
- Increases the sensitivity to real streams, but at the cost of a bigger look elsewhere effect.

Building streams from fragments

- We end up with \sim 10⁵ ROIs \rightarrow need an automated way to scan them for potential streams and a way to cut down on trials factor!
	- Hough transform for line finding \Rightarrow significance
	- Cluster together ROIs from independent runs of ANODE => build stream fragments in each patch and cut down on LEE
	- Cluster together significant stream fragments in different patches to build full stream candidate

Galaxia false positive rate

mock catalog (bottom) in Galactic coordinates using Aito↵ produced a projection. The Galactic center is in the middle and Galactic center is in the middle and Galactic c 300 appelidates with a OEO/ III en **We find 100 stream candidates with a 95% UL on fpr of 11%!** 44

To quantify our false positive rate, we ran our full method on a semi-realistic Gaia mock catalog called Galaxia (Rybizki et al 2018) which does not have stellar streams i aldiog called galaxia (nybizki et d Since the Gaia photometric bands span a broad wave-

Results: known streams

We confirm 6 previously discovered stream candidates

Others are either too wide, or have too few stars

Results: known streams

We also recover fragments of the Sagittarius Stream, despite it generally being much too wide for our narrow stream search

New stream candidates from Gaia DR2

[\[DS, Buckley, Necib 2303.01529\]](https://arxiv.org/abs/2303.01529)

Applied to Gaia DR2: many (~ 80-90) new streams potentially discovered!

3. Bonus: unsupervised ML for measuring DM density with Gaia data

- interesting applications
- the nearby ones) carries a wealth of information about Galactic dynamics.
- In particular, we can directly infer the mass density $\rho(\vec{x})$ of the Galaxy from

• We realized that training density estimators on the Gaia dataset could have other

• The full 6D phase space density $p(\vec{x},\vec{v})$ of all the stars in the Galaxy (or at least all

knowledge of $p(\vec{x},\vec{\nu})$, and from that the mass density $\rho_{DM}(\vec{x})$ of the dark matter.

Mapping the local density of DM in 3d Buckley, Lim, Putney & **DS** [2205.01129,](https://arxiv.org/abs/2205.01129) [2305.13358](https://arxiv.org/abs/2305.13358) Green et al 2011.04673, 2205.02244, Naik et al 2112.07657, An et al 2106.05981

Local dark matter density

Knowing the local dark matter density $\rho_{DM}(x)$ is very important for many reasons:

Could potentially resolve the presence of dark matter substructure

formation and nature of dark matter

• Baryons+DM source the galactic potential $\Phi(x)$. Gravitational tracers (stars) drawn from $p(\vec{x}, \vec{v}, t)$ accelerate in response to $\Phi(x)$.

$$
\frac{dp}{dt} = \left[\frac{\partial}{\partial t} + \vec{v} \cdot \frac{\partial}{\partial \vec{x}} + \vec{a}(\vec{x}) \cdot \frac{\partial}{\partial \vec{v}}\right] p = 0 \qquad \vec{a}(\vec{x}) = -\nabla \Phi(\vec{x})
$$

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$$

- Over many dynamic timescales, $p(\vec{x}, \vec{v}, t)$ equilibrates $\rightarrow p(\vec{x}, \vec{v})$
- ∂ $\partial \vec{v}$ $p = 0$ $\vec{a}(\vec{x}) = -\nabla \Phi(\vec{x})$

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$$

- Over many dynamic timescales, $p(\vec{x}, \vec{v}, t)$ equilibrates $\rightarrow p(\vec{x}, \vec{v})$
- We can use a snapshot of $p(\vec{x},\vec{v})$ today to infer the acceleration field $\vec{a}(\vec{x})$

 ∂ $\partial \vec{v}$ $p = 0$ $\vec{a}(\vec{x}) = -\nabla \Phi(\vec{x})$

From phase space density to mass density

Buckley, Lim, Putney & **DS** [2205.01129,](https://arxiv.org/abs/2205.01129) [2305.13358](https://arxiv.org/abs/2305.13358) Green et al 2011.04673, 2205.02244, Naik et al 2112.07657, An et al 2106.05981

Comparison with previous approaches

- Existing measurements typically use **Jean's equation** (second moment of Boltzmann equation) or **rotation curves**
- **They make many assumptions** (axisymmetry, reflection symmetry, simple parametric models…) and **bin the data**
- Results can seem precise but might not be accurate (biased)

From de Salas & Widmark [2012.11477](https://arxiv.org/abs/2012.11477) 53

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Our approach using normalizing flows is model-free, does not assume symmetries, and is unbinned

First ever fully 3d measurement of dark matter density in the solar neighborhood

From de Salas & Widmark [2012.11477](https://arxiv.org/abs/2012.11477) 53

- After validating our method with a realistic hydrodynamical cosmological simulation, we applied it to Gaia DR3.
- Selected stars in Gaia DR3 within 4 kpc with
	- full 6d features
	- brightness cut to ensure completeness
- dominated by **"red clump" stars** which are supposed to be a good equilibrium tracer population => **5.8M stars**

From proof-of-concept to real data Buckley, Lim, Putney & **DS** [2205.01129](https://arxiv.org/abs/2205.01129), [2305.13358](https://arxiv.org/abs/2305.13358)

Results: density estimation

Results: accelerations

Symmetries to ~10% level:

- north-south
- azimuthal (phi)

=> Expected from dynamical equilibrium

	Gaia EDR3 $[56]$	This work
$a_x \left(10^{-10} \text{m/s}^2\right)$	-2.32 ± 0.16	-1.94 ± 0.22
$a_y(10^{-10} \text{m/s}^2)$	0.04 ± 0.16	0.08 ± 0.08
$a_z(10^{-10} \text{m/s}^2)$	-0.14 ± 0.19	-0.06 ± 0.08
$ \vec{a} $ (10 ⁻¹⁰ m/s ²)	2.32 ± 0.16	1.94 ± 0.22

TABLE I: Galactic acceleration at the Solar location \vec{a}_{\odot} in Cartesian coordinates, calculated by averaging the solution to the Boltzmann equation within a 100 pc sphere centered on the Sun. We list for comparison the acceleration at the Solar location obtained from $Gaia$ DR3 quasar measurements $[56]$.

Results: mass density

Result is consistent with nonzero, spherically symmetric DM density!

Error bars include:

• MAF training variance • Gaia measurement error • Finite training statistics

Results: mass density

Our result: $\rho_{DM}(r_{\odot}) = 0.47 \pm 0.05 \text{ GeV/cm}^3$

Excellent agreement with previous measurements, with hopefully more realistic error bars

Results: mass density

Lim, Putney, Buckley & **DS** 2305.13358

Radial profile broadly consistent with recent NFW fits

Summary and Outlook

• While countless searches for new physics have been performed at the LHC, nearly

• This represents a **huge opportunity** for a new paradigm of model-agnostic search

• Motivated in part by community data challenges (LHCO2020, DarkMachines, ADC2022), theorists, experimentalists (and others!) have developed many new and

- all of them are highly model-specific.
- strategies.
- exciting model-agnostic methods using the tools of modern ML.
-
- cutting power of ML tools!

• Some of these ideas are beginning to be ported over to ATLAS and CMS and implemented as actual analyses on real data, but much work remains to be done!

• Methods are also being ported over to the Astro domain — highlights the cross-

Thanks for your attention!