Some Applications of Normalizing Flows to LHC and Gaia ML at GGI Workshop

David Shih September 12, 2022



LHC: Generative Modeling: CaloFlow



Detector simulation (GEANT4) and event generation (MG5, Pythia, Herwig, ...) are major — and growing — bottlenecks at LHC and other experiments

CERN-LHCC-2022-005















Surrogate model

(GAN, VAE, Normalizing Flow, ...) Learn underlying distribution of GEANT4 events





 10^{10} events

(GAN, VAE, Normalizing Flow, ...) Learn underlying distribution of GEANT4 events







 10^{10} events

(GAN, VAE, Normalizing Flow, ...) Learn underlying distribution of GEANT4 events

FAST and ACCURATE?





CaloFlow Krause & DS 2106.05285, 2110.11377

showers.



CaloGAN: Paganini, de Oliveira, Nachman [1705.02355, PRL; 1712.10321, PRD]

We showed that normalizing flows offer impressive performance gains over previous state of the art (GANs) in surrogate modeling of GEANT4 calorimeter



CaloFlow

Krause & DS 2106.05285, 2110.11377

- e^+ , γ , π^+ showers (100k each)
- incident E uniformly sampled 1-100 GeV



CaloGAN: Paganini, de Oliveira, Nachman [1705.02355, PRL; 1712.10321, PRD]

• goal: train generative model on the showers and learn $p(\vec{E}_{voxels} | E_{inc})$

CaloFlow Krause & DS 2106.05285

MAF with RQS transformations



Figure 5. Average shower shapes for e^+ . Columns are calorimeter layers 0 to 2, top row shows CALOFLOW, center row GEANT4, and bottom row CALOGAN



 10^{1}

10⁰

10-1

10-2

10-3

 10^{-4}

 10^{-5}

10-6



CaloFlow

Krause & DS 2106.05285

MAF with RQS transformations

AUC GEANT4 vs. CaloFlow GEANT4 vs. CaloGAN e^+ 1.000(0)0.847(8)0.660(6)1.000(0) γ π^+ 0.632(2)1.000(0)

First to ever pass the "ultimate classifier metric" test:

DNN binary classifier, generated vs reference samples

Perfect generative model $p_{gen}(x) = p_{ref}(x) = >$ classifier AUC=0.5





CaloFlow MAF with RQS transformations Krause & DS 2106.05285

Table 4. Generation time of a single calorimeter shower in ms. Times were obtained on a TITAN V GPU. GEANT4 needs 1772 ms per shower [8].

	Caloga	CALOFLOW	
batch size	batch size requested	100k requested	
10	455	2.2	835
100	45.5	0.3	96.1
1000	4.6	0.08	41.4
5000	1.0	0.07	36.2
10000	0.5	0.07	36.2

Main drawback of MAF: sampling is slow

Accurate, but not fast!

CaloFlow II IAF with RQS transformations Krause & DS 2110.11377

IAF cannot be trained with MLE loss.

Instead we developed a new teacher/student method to train it. Based on "Probability Density Distillation". van den Oord et al <u>1711.10433</u> Huang et al PMLR 2020

Idea: constrain IAF to be exact inverse of MAF, layer by layer and coupling by coupling

$$L = 0.5 \left(\underbrace{\text{MSE}(z, z') + \sum_{i} \text{MSE}(z^{(i)}, z'^{(i)}) + \sum_{i} \text{MSE}(p_{z}^{(i)}, p_{z}'^{(i)})}_{z\text{-loss}} \right) + 0.5 \left(\underbrace{\text{MSE}(x, x') + \sum_{i} \text{MSE}(x^{(i)}, x'^{(i)}) + \sum_{i} \text{MSE}(p_{x}^{(i)}, p_{x}'^{(i)})}_{x\text{-loss}} \right)$$



Training only involves fast directions of MAF and IAF



CaloFlow II IAF with RQS transformations Krause & DS 2110.11377

Similarly impressive accuracy

AUC / JSD		DNN		
		Geant4 vs.	Geant4 vs.	
		CALOFLOW V2 (student)	CALOFLOW V1 (teacher) [17]	
<i>e</i> +	unnormalized	$0.785(7) \ / \ 0.200(10)$	$0.847(8) \ / \ 0.345(12)$	
	normalized	$0.824(5) \ / \ 0.255(8)$	$0.869(2) \ / \ 0.376(4)$	
γ	unnormalized	$0.761(14) \ / \ 0.167(18)$	0.660(6) / 0.067(4)	
	normalized	0.761(4) / 0.159(6)	0.794(4) / 0.213(7)	
π^+	unnormalized	0.729(2) / 0.144(3)	$0.632(2) \ / \ 0.048(1)$	
	normalized	0.807(2) / 0.231(4)	0.751(4) / 0.148(4)	

And a factor of 500 faster, on par with GAN!

_	Table 4. Training and evaluation times of CALOFLOW and CALOGAN.								
		CALOFLOW		CALOGAN		G			
		v1 (teacher) $[17]$	v2 (student)						
	training	22+82 min	$+ 480 \min$	min 210 min					
	generation	time per shower							
	batch size			batch size req.	100k req.				
	10	$835 \mathrm{\ ms}$	$5.81 \mathrm{\ ms}$	$455 \mathrm{\ ms}$	$2.2 \mathrm{\ ms}$	1'			
	100	$96.1~\mathrm{ms}$	$0.60 \mathrm{\ ms}$	$45.5 \mathrm{\ ms}$	$0.3 \mathrm{\ ms}$	1'			
	1000	$41.4 \mathrm{\ ms}$	$0.12 \mathrm{\ ms}$	$4.6 \mathrm{ms}$	$0.08 \mathrm{\ ms}$	1'			
	10000	$36.2 \mathrm{ms}$	0.08 ms	$0.5 \mathrm{ms}$	0.07 ms	1			



CaloChallenge 2022

Fast Calorimeter Simulation Challenge 2022

View on GitHub

Welcome to the home of the first-ever Fast Calorimeter Simulation Challengel

The purpose of this challenge is to spur the development and benchmarking of fast and high-fidelity calorimeter shower generation using deep learning methods. Currently, generating calorimeter showers of interacting particles (electrons, photons, pions, ...) using GEANT4 is a major computational bottleneck at the LHC, and it is forecast to overwhelm the computing budget of the LHC experiments in the near future. Therefore there is an urgent need to develop GFANT4 emulators that are both fast. (computationally lightweight) and accurate. The LHC collaborations have been developing fast simulation methods for some time, and the hope of this challenge is to directly compare new deep learning approaches on common benchmarks. It is expected that participants will make use of cutting-edge techniques in generative modeling with deep learning, e.g. GANs. VAEs and normalizing flows.

This challenge is modeled after two previous, highly successful data challenges in HEP - the top tagging community challenge and the LHC Olympics 2020 anomaly detection challenge.

Datasets

The challenge offers three datasets, ranging in difficulty from "easy" to "medium" to "hard". The difficulty is set by the dimensionality of the calorimeter showers (the number layers and the number of voxels in each layer).

Each dataset has the same general format. The detector geometry consists of concentric cylinders with particles propagating along the z-axis. The detector is segmented along the z-axis into discrete layers. Each layer has bins along the radial direction and some of them have bins in the angle o. The number of layers and the number of bins in r and d is stored in the binning .xml files and will be read -out by the HighLevelFeatures class of helper functions. The coordinates $\Delta \phi$ and $\Delta \eta$ correspond to the x- and y axis of the cylindrical coordinates. The image below shows a 3d view of a geometry with 3 layers, with each layer having 3 bins in radial and 6 bins in angular direction. The right image shows the front view of the geometry, as seen along the z axis.



Ongoing data challenge for fast calorimeter simulation

Organizers: Giannelli, Kasieczka, Krause, Nachman, Salamani, **DS**, Zaborowska

3 datasets:

Tentative deadline: ML4Jets2022@Rutgers in November

https://calochallenge.github.io/homepage/

• "easy" — official ATLAS CaloSim (~ 10^2 voxels) • "medium" — GEANT4 example detector (~ 10^3 voxels) • "hard" — GEANT4 example detector (~ 10^4 voxels)



LHC: Anomaly Detection: ANODE and CATHODE

A Classic (Semi-)Model-Agnostic Search **1D Bump Hunt**

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!



Enhancing the Bump Hunt



primary resonant feature (m_{JJ})

Q: If the signal is localized in additional features, can we find it in a model-independent way?



additional features



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

<u>Claim</u>: the optimal model-agnostic discriminant would be (Neyman & Pearson)

"Idealized Anomaly Detector"



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

Proof:

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

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

"Idealized Anomaly Detector"





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"Idealized Anomaly Detector"

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









Cutting on $R(x) > R_c$ can greatly enhance the significance of the signal over the background.

Can combine with regular bump hunt in primary resonant feature m_{II} for data-driven background estimation.



Collins, Howe & Nachman 1805.02664,1902.02634

from <u>2109.00546</u>



Collins, Howe & Nachman 1805.02664,1902.02634

from <u>2109.00546</u>



Train a NN classifier on SR vs SB data, learn

 $R_{classifier}(x) \approx \frac{p_{data,SR}(x)}{p_{data,SB}(x)} = \frac{p_{data,SR}(x)}{p_{bg,SB}(x)}$

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Train a NN classifier on SR vs SB data, learn



If $p_{bg,SB}(x) = p_{bg,SR}(x)$ [i.e. features x are independent of *m* in the background] then the classifier gives the desired likelihood ratio.

$$R_{classifier}(x) \rightarrow \frac{p_{data,SR}(x)}{p_{bg,SR}(x)}$$





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"CWoLa Hunting"







Nachman & **DS** 2001.04990

from <u>2109.00546</u>





Nachman & **DS** 2001.04990

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Train two separate *normalizing flows (MAFs)* on SR and SB events to learn $p_{data}(x \mid m \in SR)$ and $p_{data}(x \mid m \in SB) = p_{bg}(x \mid m \in SB).$





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The SB MAF automatically interpolates into the SR, giving an estimate of $p_{bg}(x \mid m \in SR)$.





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Pros: robust against correlations!





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Construct likelihood ratio explicitly.

- Pros: robust against correlations!
- Cons: density estimation much harder than classification





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Idea: density estimation+classification

Hallin, Isaacson, Kasieczka, Krause, Nachman, Quadfasel, Schlaffer, DS & Sommerhalder 2109.00546

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Sample synthetic bg events from the interpolated SB MAF as in ANODE.





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from <u>2109.00</u>546





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"Classifying Anomalies THrough **Outer Density Estimation** (CATHODE)"







Summary of methods

from <u>2109.00546</u>



- <u>CWoLa Hunting</u>: classifier between SB and SR data
- <u>ANODE</u>: two conditional density estimators on SB and SR data; interpolate SB density estimator into SR
- <u>CATHODE</u>: single **conditional density estimator** on SB data; sample interpolated SB density estimator in SR; classifier between sampled events and data in SR



We compared the methods on a common toy dataset:

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



No explicit search at the LHC for this scenario!

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



Background: QCD dijets (1M events)

LHCO2020 R&D Dataset



 $m = m_{JJ}$

Benchmark signal strength:

SSR/BSR~0.6%, SSR/JBSR~2.2

Additional features



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



Signal Region





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

Signal Region





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

Signal Region

Initial significance was ~2.20 = a ~30 σ anomaly could be hiding in the data right now!



Gaia: Anomaly Detection: Via Machinae



Stellar streams are cold, tidally-stripped remnants of globular clusters and dwarf galaxies, orbiting our galaxy







Stellar streams are cold, tidally-stripped remnants of globular clusters and dwarf galaxies, orbiting our galaxy





Known Stellar Streams (candidates)





Stellar Streams and Dark Matter

They are very interesting objects of study for astrophysicists and particle physicists. In particular, they could be unique probes into dark matter substructure.







Properties of stellar streams



Streams are local overdensities in position, proper motion, and photometric space.



STREAMFINDER Malhan & Ibata 2018



STREAMFINDER is the current state of the art and has found many new stream candidates in the Gaia data.

They assume a particular form of the Galactic potential and isochrones, and integrate trial orbits to find statistically significant groups of stars consistent with a stream.





Via Machinae

DS, Buckley, Necib & Tamanas 2104.12789 and 2209.xxxxx



- \bullet

We were interested if a more model-independent search for stellar streams could be performed, one that didn't assume anything about the form of the Galactic potential or isochrones.

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











Since they are **cold**, the stars in the stream are fully localized in both proper motions.





Since they are **cold**, the stars in the stream are fully localized in both proper motions.

Can sideband in either one of the proper motions and use enhanced bump hunt methods to look for local overdensities!





- General idea: train enhanced bump hunt method with $m = \mu_{\alpha}$ (for example) and $x = (\mu_{\delta}, \alpha, \delta, G, B - R)$
 - ANODE in space:
 - DS, Buckley, Necib & Tamanas (2104.12789 and 2208.xxxx)
 - CWoLa in space: \bullet
 - Thanvantri, Pettee, Nachman, DS, Buckley, Collins ... (22xx.xxxx)
 - CATHODE in space:
 - Hallin, Krause, DS, Buckley, ... (22xx.xxxx)



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Example: GD-1

- GD-1 is one of the most prominent and well-studied cold stellar streams
 - ~2000 stars stretching across ~100° of the sky
 - Age ~10 Gyr, distance ~8 kpc
 - Discovered by Grillmair & Dionatos in SDSS data (2006)
 - Many subsequent studies with Gaia and other instruments





GD-1 with ANODE









10

5 15 L

20 E







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

All stars in a SR containing GD-1 $\mu_{\lambda} \in [-17, -11]$

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





So the method works!



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- How do we apply this to the entire sky?



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Exclude patches too close to the disk (too many stars) and overlapping with the LMC and SMC

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Sity .

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200 patches

- We ran this on the NERSC supercomputer at LBNL









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- What worked instead was to further subdivide SRs into slices by the orthogonal proper motion => "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 $\sim 10^5$ ROIs —> need an automated way to scan them for potential streams and a way to cut down on trials factor!
 - Hough transform for line finding => 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



We find 80 stream candidates with a 95% UL on fpr of 13%!

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







Results: known streams



We find essentially all of GD-1, plus possibly a slight extension

Results: known streams







1.0



We also find (and potentially extend) many other known streams



Results: known streams







We also find (and potentially extend) many other known streams







Results: new streams



-75°

Potentially many new streams (~50-60) discovered



Gaia: Density Estimation: Measuring Galactic Mass Density



Mass density from phase space density

Buckley, Lim, Putney & DS 2205.01129 Green et al 2011.04673, 2205.02244, Naik et al 2112.07657, An et al 2106.05981

- could also have other interesting applications
- Galaxy (or at least all the nearby ones) could be very powerful.
- In particular, we can directly infer the mass density $\rho(\vec{x})$ of the Galaxy from

• We also realized the same normalizing flows we trained on the sky for ViaMachinae

• Having access to the full 6D phase space density $p(\vec{x}, \vec{v})$ of all the stars in the

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



Mass density from phase space density

Buckley, Lim, Putney & **DS** <u>2205.01129</u> Green et al 2011.04673, 2205.02244, Naik et al 2112.07657, An et al 2106.05981

- Liouville theorem: phase space density is conserved
- Stars are well-approximated as collisionless, only interacting through longranged gravitational force
- So they must obey the collisionless Boltzmann equation:

$$\begin{bmatrix} \frac{\partial}{\partial t} + \overrightarrow{v} \cdot \frac{\partial}{\partial \overrightarrow{x}} + \overrightarrow{a}(\overrightarrow{x}) \cdot \frac{\partial}{\partial \overrightarrow{v}} \end{bmatrix} p$$
$$\overrightarrow{a}(\overrightarrow{x}) = -\frac{d\Phi(\overrightarrow{x})}{d\overrightarrow{x}} \quad \text{Acceleration}$$

 $\Phi(\vec{x})$ is the gravitational potential of the Galaxy (DM+stars+gas...)

- $p(\overrightarrow{x}, \overrightarrow{v}; t) = 0$
- ations



Mass density from phase space density

Buckley, Lim, Putney & **DS** <u>2205.01129</u> Green et al 2011.04673, 2205.02244, Naik et al 2112.07657, An et al 2106.05981

$$\left[\overrightarrow{v}\cdot\frac{\partial}{\partial\overrightarrow{x}}+\overrightarrow{a}(\overrightarrow{x})\cdot\frac{\partial}{\partial\overrightarrow{v}}\right]p(\overrightarrow{x},\overrightarrow{v})=0$$

- accelerations $\overrightarrow{a} = -\nabla \Phi$
- Taking another derivative gives us the mass density of the Galaxy!

$$4\pi G\rho = \nabla^2 \Phi = \nabla \cdot \overrightarrow{a}$$

• If the stars are also in dynamical equilibrium, then $\partial p/\partial t = 0$ and we get:

• Just from knowledge of $p(\vec{x}, \vec{v})$ and its derivatives we can determine the



More on determining the accelerations

Green & Ting 2011.04673, An et al 2106.06981, Naik et al 2112.07657, Buckley, Lim, Putney & DS 2205.01129

$$\left[\overrightarrow{v}\cdot\frac{\partial}{\partial\overrightarrow{x}}+\overrightarrow{a}(\overrightarrow{x})\cdot\frac{\partial}{\partial\overrightarrow{v}}\right]p(\overrightarrow{x},\overrightarrow{v})=0$$

- How can we solve for 3 acceleration functions $\vec{a}(\vec{x})$ with just a single equation?
- $\overrightarrow{a}(\overrightarrow{x})$, one for each choice of \overrightarrow{v}
- best-fit $\overrightarrow{a}(\overrightarrow{x})$

$$L(\overrightarrow{a}(\overrightarrow{x})) = \frac{1}{N} \sum_{\alpha=1}^{N} \left(\left[\overrightarrow{v}_{\alpha} \cdot \frac{\partial}{\partial \overrightarrow{x}} + \overrightarrow{a}(\overrightarrow{x}) \cdot \frac{\partial}{\partial \overrightarrow{v}} \right] p(\overrightarrow{x}, \overrightarrow{v}_{\alpha}) \right)^{2}$$

• $\vec{a}(\vec{x})$ doesn't depend on velocity! So this is actually an infinite number of equations for

We choose to perform least-squares minimization over a sample of velocities to determine





Proof-of-concept

Buckley, Lim, Putney & **DS** <u>2205.01129</u>

- Training data: state-of-the-art Nbody+hydro galaxy simulation from "Nbody shop" collaboration [https://b2share.eudat.eu/records/c9f232d8ac804785aad35004177a704e]
- Milky Way like Galaxy h277



- number of stars star particles 153,174 (<< size of Gaia 6D dataset)
- observer's location
 - [8.122, 0., 0.0208] kpc
- observing radius = 3.5 kpc
- simulation resolution: 0.173 kpc
- Using only kinematic information: position and velocity

Results: density estimation

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Results: accelerations

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Accelerations to within 5% accuracy!

We estimated uncertainties from:

- random training initialization
- finite training data statistics (bootstrap)
- measurement error



Results: mass density

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Mass density to within 10-20% accuracy!

We estimated uncertainties from:

- random training initialization
- finite training data statistics (bootstrap)
- measurement error





Comparison to existing measurements

 Existing measurements typically use Jean's equation (second moment of Boltzmann equation)

$$\overline{v_i v_j} \frac{\partial \nu(\vec{x})}{\partial x_i} + \nu(\vec{x}) \frac{\partial \overline{v_i v_j}}{\partial x_i} = -\nu(\vec{x}) \frac{\partial \overline{v_i v_j}}{\partial x_i} = -\nu(\vec{x$$

- Assume axisymmetry, reflection symmetry...
- Bin data and perform parametric fits to extract $\Phi(\vec{x})$
- Results can seem precise but might not be accurate (biased)



