# Anomaly Detection for BSM Using AI/ML

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- 1. Light Dark Matter Detection
- 2. Anomaly Detection using Generative Models
- 3. Precision Measurements using Deep Learning with Uncertainty Quantification

# **Light Dark Matter Detection**

# **Light Dark Matter**

- keV-GeV mass range
- Interacts with SM matter via new particle
- Vector portal: U(1) gauge boson coupling to electric charge
- Dark photon A' of mass m<sub>A'</sub> couples to SM with coupling constant ε; decays to LDM of mass m<sub>γ</sub> with dark coupling α<sub>D</sub>



 $\mathcal{L}_{LDM} \sim g_D A'_{\mu} J^{\mu}_{\chi} + \varepsilon e A'_{\mu} J^{\mu}_{EM} + [...]$  $y \equiv \frac{g_D^2 \epsilon^2 e^2}{4\pi} \left(\frac{m_{\chi}}{m_{A'}}\right)^4 \sim \langle \sigma v \rangle_{relic} m_{\chi}^2$ 

# **BDX Experiment**

- Beam dump experiment at Jefferson Lab Hall A
- Planned running in 2026-29
- A' produced in the beam dump would decay to LDM particles  $\chi$



X

 $\chi$ 

A

# Mini-BDX

- Pilot version of BDX Experiment
- Collected 6 months of data in 2019-20
- Detector consists of two layers of 22 PbWO<sub>4</sub> calorimeters each surrounded by two active veto layers
- Main sources of background: beam neutrinos + cosmics
- N<sub>EOT</sub> = 1.54e21
- Yields: 3623 beam on/3822 beam off events



# Setting Upper Limits on Signal

**Define Likelihood Model:**  $\mathcal{L} = \prod \left[ P(n_{on}^{j}; \mu_{c}^{j} + \mu_{\nu}^{j} + \alpha^{j} \cdot S) \cdot P(n_{off}^{j}; \mu_{c}^{j} \cdot \tau) \right]$ 

- S = number of singal
- μ<sub>c</sub>,μ<sub>v</sub>=cosmogenic/neutrino background yield
- $\tau = T_{off}/T_{on}$

Perform one sided hypothesis test to determine upper limit on S, S<sup>up</sup>

$$y = \epsilon^2 \alpha_D \left(\frac{m_{\chi}}{m_{A'}}\right)^4 = \epsilon_0^2 \sqrt{\frac{S^{UP}}{S}} \alpha_D \left(\frac{m_{\chi}}{m_{A'}}\right)^4 \qquad \qquad \epsilon^2 = \epsilon_0^2 \sqrt{\frac{S^{UP}}{S}},$$

Can we improve sensitivity by cutting on feature variables? Can do rectangular cuts but can machine learning perform better?

# XGBoost

- Gradient Boosted Decision Trees (BDTs)
  - combine multiple decision trees sequentially
  - trees in successive iterations are trained to correct the errors of the previous ones
  - minimizes loss along the gradient of the loss wrt the predictions
- Highly effective for classification and regression tasks
- XGBoost is an open-source library that uses gradient boosting
- Want to use BDT to discriminate dark matter signal from background (cosmics and neutrinos)



# **Input Features and Parameters**

- 1. Total energy deposited in the detector
- 2. Shower direction
- 3. Fraction of energy outside the seed (i.e. outside the highest energy crystal)
- 4. x-y position of the seed
- 5. Multiplicity (number of crystals above the threshold)

| Parameter            | Value           |  |
|----------------------|-----------------|--|
| Learning rate $\eta$ | 0.1             |  |
| Max tree depth       | 10              |  |
| Subsample ratio      | 0.8             |  |
| Number of trees      | 100             |  |
| Learning objective   | binary:logistic |  |



### Experimental reach improved by BDT cut



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# **Generative Models for Anomaly Detection**

# Flux + Mutability

- A conditional generative approach to One-Class Classification (OCC) and Anomaly Detection (AD)
- Can we use deep learning to separate two classes more efficiently than rectangular cuts?
- While remaining agnostic towards the unknown class?

t-SNE representation of N-dimensional objects



# Flux + Mutability: Architecture



- A. Inference Object fed through cAE
  - a. Features  $\otimes$  Kinematics
  - b. Features  $\otimes$  Residuals (x' x)
- B. Continuous Conditional Generation
  - a. Pre-fit KDE Objects in kinematic bins
  - b. Map inference kinematics to KDE object
  - c. Sample new Gaussian vectors from restricted domain
  - d. Gaussian Vectors & Inference Kinematics
  - e. Conditionally generate reference population via cMAF
- C. Compare inference object to **reference population** via Hierarchical clustering and quantile cuts

# **HDBSCAN** and Quantile Cuts



- Augment the inference particle into the reference cluster space
  - Two notions of membership: density-based & distance-based
- Combine the two PMFs and extract a probability of membership (P<sub>in</sub>)
- Define Outlier Score as complementary probability P<sub>out</sub> = 1 P<sub>in</sub>
- Extract reference population outlier score corresponding to a desired quantile

# Case 1: y/n Separation at GlueX (OCC)

- High confidence on one class
- Isolate highly active area of BCAL
- Reconstructed energy and z-position as kinematic conditions
- Simulated showers of photons (inference) and neutrons (reference)
- Strict preselection cuts
- Deploy fiducial cuts to extract only neutron showers which highly resemble photons
- 14 input features comprising of detector response variables
- 1.8M training events



### OCC: γ/n Separation at GlueX



# Case 2: BSM Dijet Separation at LHC (AD)

- Consider QCD dijet events as reference
- Isolate  $Z' \rightarrow t\bar{t}$  dijets as unknown
- Publicly available datasets generated via MADGRAPH and Pythia8 using the DELPHES framework for fast detector simulation
- Require leading jet transverse momenta 450 GeV <  $p_T$  < 800 GeV and sub-leading jet  $p_T$  > 200 GeV
- Consider leading jet  $\dot{p}_{\tau}$  as single kinematic condition
- 15 input features
  - Remaining 4 vector properties of the leading jet and n-subjettiness variables
  - Sub-leading jet 4 vector and n-subjettiness variables
- 600k training events/100k testing events

# Case 2: BSM Dijet Separation at LHC (AD)





- 15 input features
  - Remaining 4 vector properties of the leading jet and n-subjettiness variables
  - Sub-leading jet 4 vector and n-subjettiness variables
- Generated distributions of QCD dijets from the cMA match the original and reconstructed distributions to a high degree
- QCD and BSM dijets occupy the same region in phase space

# Anomaly Detection: BSM Dijet Separation at LHC



|     | F+M           | Fraser et al. | Cheng et al. |
|-----|---------------|---------------|--------------|
| AUC | 0.891 ± 0.005 | 0.87          | 0.89         |

# **DNN with Uncertainty Quantification for DIS**

## **Deep Inelastic Scattering**

DIS is governed by the 4-momentum squared of the exchange boson  $Q^2$ , the inelasticity *y*, and the Bjorken scaling variable *x* 



Are related to the center-of-mass energy s via the relation  $Q^2$ =sxy

$$s = (k+P)^2$$
,  $Q^2 = -q^2$ ,  $y = \frac{q \cdot P}{k \cdot P}$ , and  $x = Q^2/(sy)$ .

### **DIS Kinematic Reconstruction Methods**

- Conservation of momentum and energy overconstrain the DIS kinematics and leads to a freedom to calculate x, Q<sup>2</sup>, y from measured quantities
- Each method has advantages and disadvantages, and no single approach is optimal over the entire phase space. Each method exhibits different sensitivity to QED radiative effects

| Method name                | Observables                 | y  | $Q^2$                                 | $x \cdot E_p$                                      |
|----------------------------|-----------------------------|--|---------------------------------------|--|
| Electron $(e)$             | $[E_0, E, \theta]$          | $1 - \frac{\Sigma_e}{2E_0}$  | $\frac{E^2 \sin^2 \theta}{1-y}$       | $\frac{E(1+\cos\theta)}{2y}$                       |
| Double angle (DA) $[6, 7]$ | $[E_0, \theta, \gamma]$     | $\frac{\tan\frac{\gamma}{2}}{\tan\frac{\gamma}{2}+\tan\frac{\theta}{2}}$ | $4E_0^2\cot^2\frac{\theta}{2}(1-y)$   | $\frac{Q^2}{4E_0y}$                                |
| Hadron $(h, JB)$ [4]       | $[E_0, \Sigma, \gamma]$     | $\frac{\Sigma}{2E_0}$  | $\frac{T^2}{1-y}$                     | $\frac{Q^2}{2\Sigma}$                              |
| ISigma (I $\Sigma$ ) [9]   | $[E, \theta, \Sigma]$       | $\frac{\Sigma}{\Sigma + \Sigma_e}$                                       | $\frac{E^2 \sin^2 \theta}{1-y}$       | $\frac{E(1+\cos\theta)}{2y}$                       |
| IDA [7]                    | $^{[E,\theta,\gamma]}$      | $y_{\mathrm{DA}}$  | $\frac{E^2 \sin^2 \theta}{1-y}$       | $\frac{E(1\!+\!\cos\theta)}{2y}$                   |
| $E_0 E \Sigma$             | $[E_0, E, \Sigma]$          | $y_h$  | $4E_0E - 4E_0^2(1-y)$                 | $\frac{Q^2}{2\Sigma}$                              |
| $E_0 \theta \Sigma$        | $[E_0, \theta, \Sigma]$     | $y_h$  | $4E_0^2 \cot^2 \frac{\theta}{2}(1-y)$ | $\frac{Q^2}{2\Sigma}$                              |
| $\theta \Sigma \gamma$ [8] | $_{[\theta,\Sigma,\gamma]}$ | $y_{\mathrm{DA}}$  | $\frac{T^2}{1-y}$                     | $\frac{Q^2}{2\Sigma}$                              |
| Double energy $(A4)$ [7]   | $[E_0, E, E_h]$             | $\frac{E-E_0}{(xE_p)-E_0}$   | $4E_0y(xE_p)$                         | $E + E_h - E_0$                                    |
| $E\Sigma T$                | $[E, \Sigma, T]$            | $\frac{\Sigma}{\Sigma + E \pm \sqrt{E^2 + T^2}}$                         | $\frac{T^2}{1-y}$                     | $\frac{Q^2}{2\Sigma}$                              |
| $E_0 ET$                   | $[E_0, E, T]$               | $\tfrac{2E_0-E\mp\sqrt{E^2-T^2}}{2E_0}$                                  | $\frac{T^2}{1-y}$                     | $\frac{Q^2}{4E_0y}$                                |
| Sigma ( $\Sigma$ ) [9]     | $[E_0, E, \Sigma, \theta]$  | $y_{I\Sigma}$  | $Q_{1\Sigma}^2$                       | $\frac{Q^2}{4E_0y}$                                |
| $e$ Sigma $(e\Sigma)$ [9]  | $[E_0, E, \Sigma, \theta]$  | $\frac{2E_0\Sigma}{(\Sigma+\Sigma_e)^2}$                                 | $2E_0E(1+\cos\theta)$                 | $\frac{E(1+\cos\theta)(\Sigma+\Sigma_e)}{2\Sigma}$ |

**Table 1.** Summary of basic reconstruction methods that employ only three out of five quantities:  $E_0$  (electron-beam energy), E and  $\theta$  (scattered electron energy and polar angle),  $\Sigma$  and  $\gamma$  (lon-gitudinal energy-momentum balance,  $\Sigma = \sum_{\text{HFS}} (E_i - p_{z,i})$ , and the inclusive angle of the HFS). Alternatively, the A4 method makes use of the HFS total energy  $E_h$ . Shorthand notations are used

### **Kinematical Reconstruction with Deep Neural Networks**

- DNN shows improved kinematical reconstruction of DIS variables over standard reconstruction techniques for H1 and ATHENA data
- Exploited full kinematical information and accounting for the presence of QED radiation
- Did not consider event-level uncertainty quantification





# **Event-Level Uncertainty Quantification (ELUQuant)**

#### Total loss function is the sum of components

 $\mathcal{L}_{Tot.} = \mathcal{L}_{Reg.} + \alpha \mathcal{L}_{Phys.} + \beta \mathcal{L}_{MNF.}$ 

#### Learn the posterior over the weights

 $\begin{aligned} \mathcal{L}_{MNF.} &= -KL(q(\mathbf{W}) \| p(\mathbf{W})) \\ &= \mathbb{E}_{q(\mathbf{W}, \mathbf{z}_T)}[-KL(q(\mathbf{W} | \mathbf{z}_{T_f}) \| p(\mathbf{W})) + \log r(\mathbf{z}_{T_f} | \mathbf{W}) - \log q(\mathbf{z}_{T_f})] \end{aligned}$ 

Access epistemic (systematic) uncertainty through sampling MNF layers

### Learn the regression transformation

 $\mathcal{L}_{Reg.} = \frac{1}{N} \sum_{i} \sum_{j} \frac{1}{2} (e^{-\mathbf{s}_j} \|\mathbf{v}_j - \hat{\mathbf{v}}_j\|^2 + \mathbf{s}_j), \ \mathbf{s}_j = \log \sigma_j^2$ epistemic
Access aleatoric (statistical) uncertainty as a function of regressed output

#### **Constrain the physics**

$$\mathcal{L}_{Phys.} = \frac{1}{N} \sum_{i} \log \hat{Q}_i^2 - (\log s_i + \log \hat{x}_i + \log \hat{y}_i)$$



C. Fanelli, and J. Giroux. Machine Learning: Science and Technology 5.1 (2024): 015017.

# Input Features of ELUQuant

Define variables to characterize the strength of FSR/ISR :

$$\mathcal{D}_{T}^{bal} = 1 - \frac{p_{T.e}}{T} = 1 - \frac{\Sigma_e \tan \frac{\gamma}{2}}{\Sigma \tan \frac{\theta}{2}}$$

$$p_z^{bal} = 1 - rac{\Sigma_e + \Sigma}{2E_0}$$

5 additional features to indicate QED radiation:

- The energy, η, and Δφ of the reconstructed photon that is closest to the electron beam direction, with Δφ wrt scattered electron
- Sum of ECAL energy within a cone ΔR < 0.4 around the scattered electron divided by the scattered electron track momentum</li>
- Number of ECAL clusters within a cone ΔR < 0.4 around the scattered electron</li>

And 8 additional features:

- Scattered electron p<sub>Te</sub>, p<sub>ze</sub>, E
- HFS 4-vector quantities T, p<sub>z h</sub>, E<sub>h</sub>
- Δφ between the scattered electron and the HFS momentum vector
- The difference  $\Sigma_{e} \Sigma$

| Dataset | Training Events   | Validation Events | Testing Events    | Size on Disk |
|---------|-------------------|-------------------|-------------------|--------------|
| H1      | $8.7 \times 10^6$ | $1.9 \times 10^6$ | $1.9 \times 10^6$ | 8 GB         |

Arratia, M., Britzger, D., Long, O., & Nachman, B. (2022). Nucl. Instrum. Meth. A, 1025, 166160.

# **ELUQuant Performance Similar to DNN**



- Reconstruction of NC DIS kinematics from H1 comparable to DNN, both are superior to traditional methods
- Total aleatoric+epistemic uncertainties from ELUQuant comparable to RMS from DNN
   Distributions broader at
  - lower y, larger uncertainty

# Leveraging the Event-Level Information



- The ability to remove events with large event-level uncertainty allows us to improve the ratio to truth
- Can be exploited for anomaly detection

# Precision Measurement of $\sin^2\theta_{W}$

- Deviations from the SM prediction of the running of the weak mixing angle would be evidence of BSM
- Currently in progress: measuring sin<sup>2</sup>θ<sub>W</sub> at EIC kinematics using kinematics reconstructed with ELUQuant



Boughezal et al. (2022) Phys. Rev. D 106, 016006



# Summary

- Gradient Boosted Decision Trees with XGBoost demonstrate improved dark matter signal discrimination for BDX-MINI
- Flux + Mutability uses generative models in an unsupervised way to identify anomalies with respect to a reference class
- Event-level uncertainty quantification and kinematical reconstruction using BNN can allow for anomaly detection
- Thank you!



# Input Features for GlueX OCC

• Layer  $\mathbf{M}_{-}\mathbf{E} = \sum_{i}^{N} E_{i}$ 

 $M \in \{1,2,3,4\}$  is the layer number and  $E_i$  is the energy of the  $i^{th}$  reconstructed point in the layer.

- Layer Mby SumLayers\_ $\mathbf{E} = \frac{1}{E_{total}} \sum_{i}^{N} E_i$  $M \in \{1, 2, 3, 4\}$  is the layer number and  $E_i$  is the energy of the *i*<sup>th</sup> reconstructed point in the layer.
- Z Width =  $\sqrt{\frac{1}{E_{total}} \sum_{i}^{N} E_i (\Delta z_i)^2}$ ,  $\Delta z_i = (z_i + T_z) S_z$  $E_i$  and  $z_i$  are the energy and z position of the *i*<sup>th</sup> point in the shower.
- **R** Width =  $\sqrt{\frac{1}{E_{total}}\sum_{i}^{N}E_{i}(\Delta r_{i})^{2}}$ ,  $\Delta r_{i} = (R r_{i})$  $E_{i}$  and  $r_{i}$  are energy and radial position of the *i*<sup>th</sup> point.
- **T** Width =  $\sqrt{\frac{1}{E_{total}}\sum_{i}^{N}E_{i}(\Delta t_{i})^{2}}$ ,  $\Delta t_{i} = t_{i} S_{t}$  $E_{i}$  and  $t_{i}$  are the energy and timing information of the *i*<sup>th</sup> point.
- $\theta$  Width =  $\sqrt{\frac{1}{E_{total}}\sum_{i}^{N}E_{i}(\Delta\theta_{i})^{2}}$ ,  $\Delta\theta_{i} = \theta_{i} S_{\theta}$  $E_{i}$  and  $\theta_{i}$  are the energy and polar angle (from the target center) of the  $i^{th}$  point.
- $\phi$  Width =  $\sqrt{\frac{1}{E_{total}}\sum_{i}^{N}E_{i}(\Delta\phi_{i})^{2}}$ ,  $\Delta\phi_{i} = \phi_{i} S_{\phi}$  $E_{i}$  and  $\phi_{i}$  are the energy and azimuthal angle of the *i*<sup>th</sup> point.
- z Entry = (S<sub>z</sub> T<sub>z</sub>) <sup>R</sup>/<sub>S<sub>r</sub></sub> + T<sub>z</sub> The position at which the particle hits the inner radius of the BCAL.



Figure C2: **Photon and neutrons distributions:** Photon and neutron distributions. Original and scaled neutron distributions are also shown for comparison.

# **ELUQuant Computing Performance**

|   | Training Parameter              | value                 |  |
|---|---------------------------------|-----------------------|--|
|   | Max Epochs                      | 100                   |  |
|   | Batch Size                      | 1024                  |  |
|   | Decay Steps                     | 50                    |  |
|   | Decay Factor $(\gamma)$         | 0.1                   |  |
|   | Physics Loss Scale $(\alpha)$   | 1.0                   |  |
|   | KL Scale $(\beta)$              | 0.01                  |  |
|   | Training GPU Memory             | $\sim 1 \mathrm{GB}$  |  |
|   | Network memory on local storage | $\sim 7 \mathrm{MB}$  |  |
|   | Trainable parameters            | $611,\!247$           |  |
|   | Wall Time                       | $\sim 1 \text{ Day}$  |  |
| - |                                 |                       |  |
| _ | Inference Parameter             | value                 |  |
|   | Number of Samples (N)           | 10k                   |  |
|   | Batch Size                      | 100                   |  |
|   | Inference GPU Memory            | $\sim 24 \mathrm{GB}$ |  |
|   | Inference Time per Event        | $\sim 20ms$           |  |

ELUQuant at inference showed an impressive rate of 10,000 samples/event within a 20 milliseconds on an RTX 3090.