Classifying Anomalies THrough Outer Density Estimation (CATHODE)

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QUANTUM UNIVERSE

» Anomaly Search

Majority of searches for new physics rely heavily on both signal and SM background models

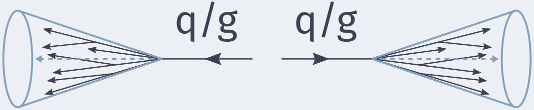
Impossible to cover all models/phase space regions with a dedicated search
→Need **model-independent** searches

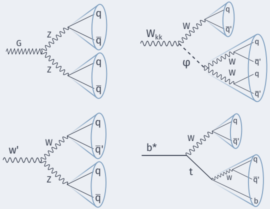
Test scenario:

→Dijet anomaly search **X→YZ**, Y & Z decaying hadronically
→Look for **resonant** new physics with **anomalous jet substructure**

from any of these:

Ultimately want to tell this:

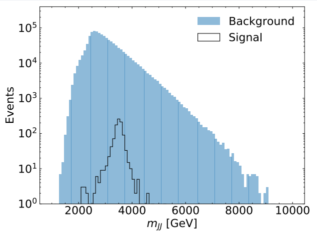


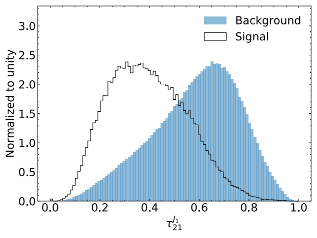


» Anomaly Search

Benchmark Dataset

- Benchmark: LHC Olympics 2020 challenge R&D dataset (*arxiv:2101.08320*)
- Background: 1M simulated QCD multijet events
- Signal: 100k W'→YZ events where Y→qq and Z→qq
- $m_{W'} = 3.5$ TeV, $m_Y = 500$ GeV, $m_Z = 100$ GeV
- Input: 4 variables
  - Lower jet mass m_{j1}
  - mass difference $\Delta m_{1,2}$
  - Jet subjettiness ratios $\tau_{21,j1}$ and $\tau_{21,j2}$





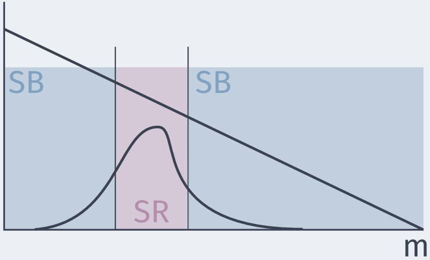
arXiv:2001.04990

Given distributions of signal $p_S(\boldsymbol{x})$ and background $p_B(\boldsymbol{x})$ in some set of variables $\boldsymbol{x}$,
Neyman-Pearson-Lemma:
→best test based on likelihood ratio

Problem: Signal is buried under large amount of background
→We can't estimate $p_S(\boldsymbol{x})$ directly

The best we can do: Estimate $p_{S+B}(\boldsymbol{x}|\mathrm{SR})$ in "Signal Region" and $p_B(\boldsymbol{x}|\mathrm{SB})$ from region without signal ("Sidebands")
→Conditional variable containing resonance: m_{jj}

We need to take LR in SR:
→Interpolate $p_B(\boldsymbol{x}|\mathrm{SB})$ into SR
→Construct estimate of LR: $\frac{p_{S+B}(\boldsymbol{x}|SR)}{p_B(\boldsymbol{x}|SR)}$

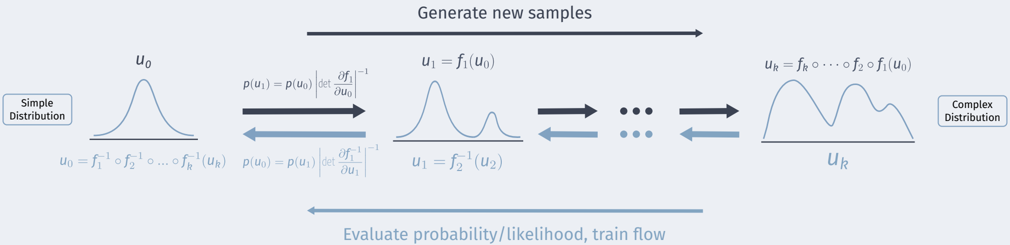


Get estimate of LR using:
→**classification**
→**density estimation**
(Normalizing Flows)

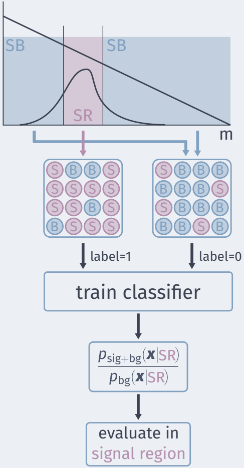
» Normalizing Flows

- Flows based on random variable transformation
- $f : U \to X;\; p(x) = p(u)\left|\frac{df(u)}{du}\right|^{-1}$
- Learn invertible mapping f from latent variables $\boldsymbol{u}$ to data $\boldsymbol{x}$
- Flow: stack many invertible transformations f_i: $f = f_k \circ \ldots \circ f_2 \circ f_1$

$$p(\boldsymbol{x}) = p(f^{-1}(\boldsymbol{x}))\prod_i \left|\det\left(\frac{\partial f_i^{-1}}{\partial \boldsymbol{x}}\right)\right| = p(\boldsymbol{u})\prod_i \left|\det\left(\frac{\partial f_i}{\partial \boldsymbol{u}}\right)\right|^{-1}$$



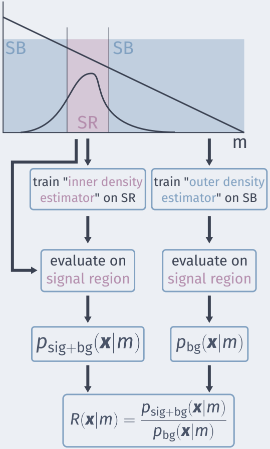
Classification Without Labels (CWoLa)



+ Simple classification task
+ Basic DNN architecture
− Highly dependent on correlations between $\boldsymbol{x}$ and m
$\rightarrow$Variables $\boldsymbol{x}$ need to be hand-picked

DOI:10.1007/JHEP10(2017)174

Anomaly Detection with Density Estimation (ANODE)



+ Direct estimation of conditional densities
+ Easy to interpolate p_{bg}
+ Robust against correlations between $\boldsymbol{x}$ and m
$\rightarrow$Arbitrary choice of $\boldsymbol{x}$
− Computationally intense
− Estimation of signal contribution difficult

DOI:10.1103/PhysRevD.101.075042

Classifying Anomalies THrough Outer Density Estimation (CATHODE)

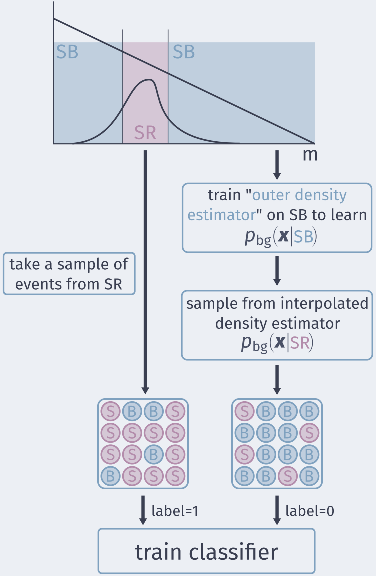
\+ Only one density estimator needed

\+ Due to interpolation: robust against correlations between $\boldsymbol{x}$ and m
$\rightarrow$Arbitrary choice of $\boldsymbol{x}$

\+ Final tagger based on simple classification task

\+ No density estimator for signal contribution needed

– Computationally intense

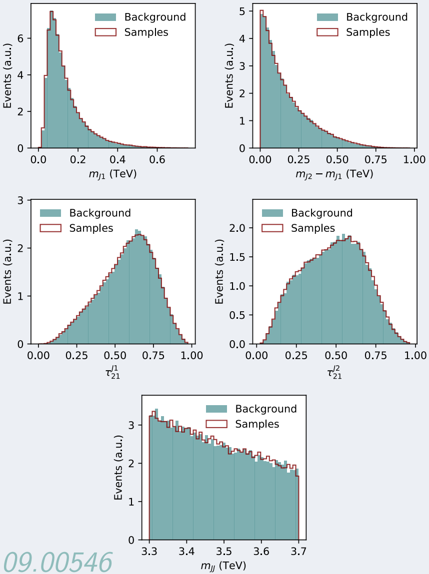


arxiv:2109.00546

» CATHODE

Training & Sampling

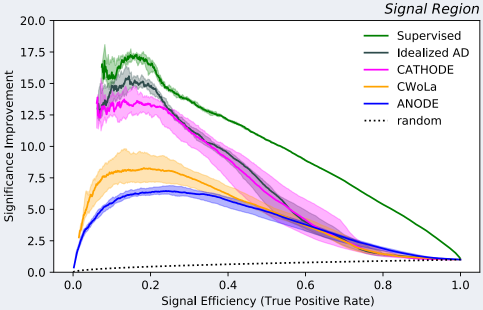
- Flow trained for 100 epochs
- Model ensembling: pick 10 epochs with lowest validation loss
- Draw m_{jj} values from a KDE in signal region
- Use these values as conditional and sample from density estimator
  $\rightarrow$Interpolation into SR
- We can oversample to produce more samples than we have in data
- Background densities are modelled well by flow



arxiv:2109.00546

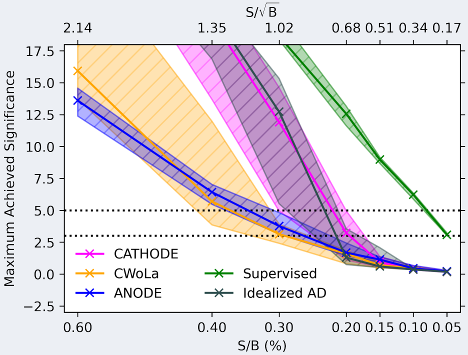
- Most important performance measure: **significance improvement characteristic (SIC)**
- "Supervised" training using signal/background labels →overall upper performance limit
- "Idealized AD": distinguish actual sample vs. background-only sample from signal region →upper limit for unsupervised anomaly search
- CATHODE shows highest SIC amongst non-idealized anomaly taggers
- Performance reaches idealized AD limit
- Significance improvement about factor 14

$$\mathrm{SIC} = \frac{\left.\frac{S}{\sqrt{B}}\right|_{\mathrm{cut}}}{\left.\frac{S}{\sqrt{B}}\right|_{\mathrm{no\ cut}}} = \frac{\mathrm{TPR}}{\sqrt{\mathrm{FPR}}}$$



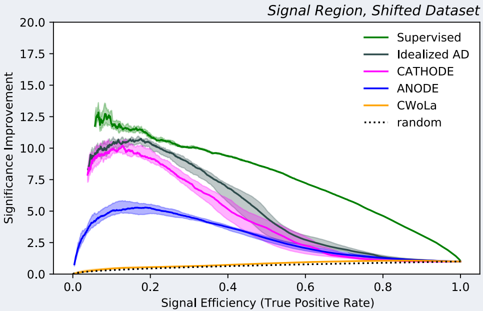
arxiv:2109.00546

* Comparison for different amounts of signal injected
* CATHODE outperforms other AD methods significantly down to a S/B as low as 0.3%
* CATHODE achieves similar performance as idealized anomaly detector
* Below 0.2% S/B: even idealized AD cannot raise significance above 3σ
  $\rightarrow$Too limited number of data points in the signal region



arxiv:2109.00546

* Study impact of correlations between $\boldsymbol{x}$ and m_{jj}
* Introduce artificial correlations
* Add 10% of corresponding m_{jj} value to m_{j1} and $\Delta m_{1,2}$
* All methods suffer performance →"Smearing" of variables
* CWoLa performance completely breaks down
* CATHODE retains good performance, similar to idealized AD



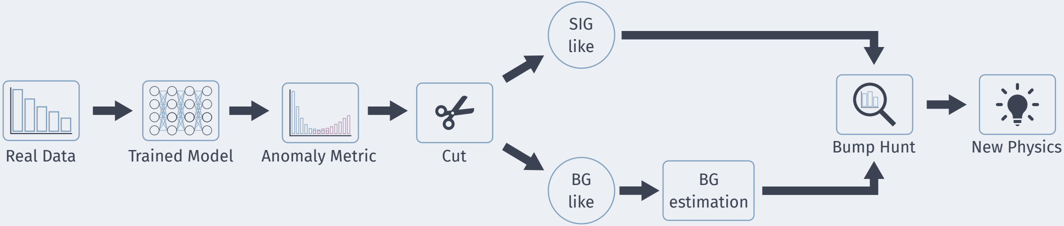
arxiv:2109.00546

» Summary

* Investigation of dijet resonances with anomalous jet substructure using normalizing flow–based density estimation & classification
* Introduction of new method: CATHODE that combines the advantages of purely density estimation–based (ANODE) and classification-based (CWoLa) approaches
* CATHODE outperforms all other non-idealized anomaly detectors
* Performance similar to idealized anomaly detector
* Robust against correlations between features $\boldsymbol{x}$ and conditional variable m_{jj}
* Future studies
    * Other datasets/topologies
    * Study sensitivity for different types of anomalies (e.g. very broad resonances)
    * Studies using more (low-level) features

BACKUP

General procedure:



» Autoregressive Flows

Autoregressive property:

$p(x) = \prod_i p(x_i|x_{1:i-1})$

Conditional densities depend on trainable parameters:

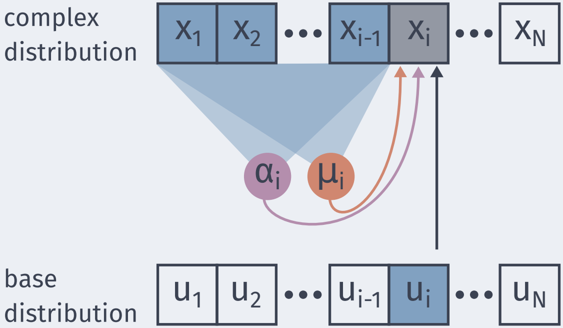
$p(x_i|x_{1:i-1}) = \mathcal{N}(x_i|\mu_i, (\exp\alpha_i)^2)$

$\mu_i = f_{\mu_i}(x_{1:i-1})$

$\alpha_i = f_{\alpha_i}(x_{1:i-1})$

$\rightarrow$Earlier variables must not depend on later variables
$\rightarrow$Solution: stack transformations into a normalizing flow, change ordering of the x_i after each transformation

$x_i = f(u_i) = u_i \cdot \exp(\alpha_i) + \mu_i$

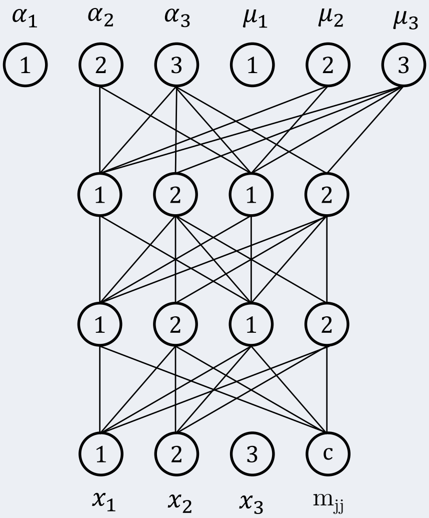


Autoregressive property $\rightarrow$Jacobian is upper triangular

$$\left|\det\left(\frac{\partial f}{\partial \boldsymbol{u}}\right)\right| = \exp\left(\sum_i \alpha_i\right)$$

» Masked Autoencoder for Distribution Estimation (MADE)

- DNN architecture to implement a single f_i in autoregressive flows (1502.03509)
- Compute $\boldsymbol{\alpha}$ and $\boldsymbol{\mu}$ in one forward pass
- Outputs α_j and μ_j only connected to inputs $\{x_1, \ldots, x_{j-1}\}$ $\rightarrow$autoregressive property
- No connection dropped for conditional input m_{jj}



* Stack MADE networks to build "Masked Autoregressive Flow" (MAF)
* Learn tranformation $\boldsymbol{u} = f^{-1}(\boldsymbol{x})$ from input features $\boldsymbol{x}$ to $\boldsymbol{u} \sim \mathcal{N}(0, \mathbb{I})$
* Compute $p(\boldsymbol{x})$ with normalizing flow from $p(\boldsymbol{u})$
* Minimize NLL loss $\mathcal{L} = -log(p(\boldsymbol{x}))$
* Architecture used for both density estimators