Unsupervised Anomaly Detection with CATHODE

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CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE

» Anomaly Search

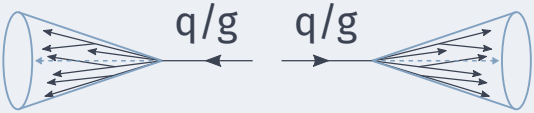
Majority of searches for new physics rely heavily on both signal and SM background models

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

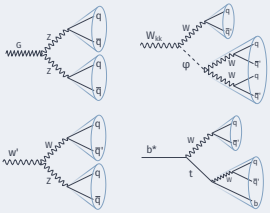
Test scenario:

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

Ultimately want to tell this:

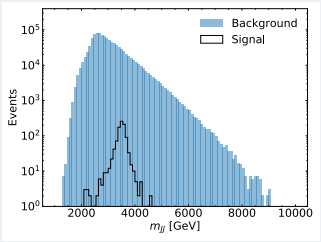


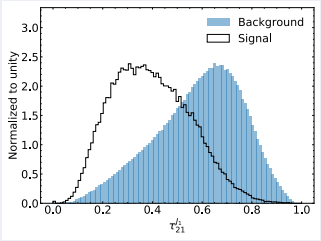
from any of these:



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
- $m_{W'} = 3.5\,\text{TeV}$, $m_Y = 500\,\text{GeV}$, $m_Z = 100\,\text{GeV}$
- 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}

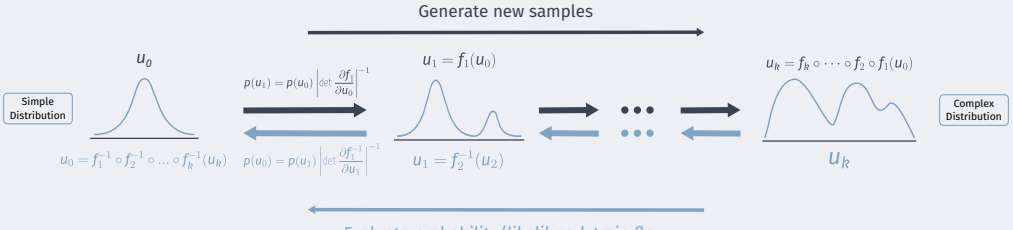
We need to take LR in SR:
→Interpolate $p_B(\boldsymbol{x}|\mathrm{SB})$ into SR
→Construct estimate of LR: $\frac{p_{S+B}(\boldsymbol{x}|SR)}{p_B(\boldsymbol{x}|SR)}$

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

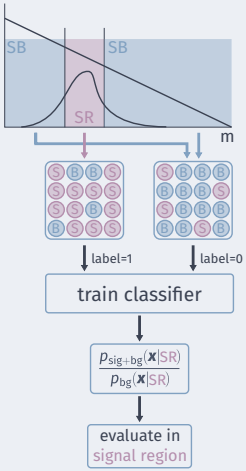
» Normalizing Flows

- 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)

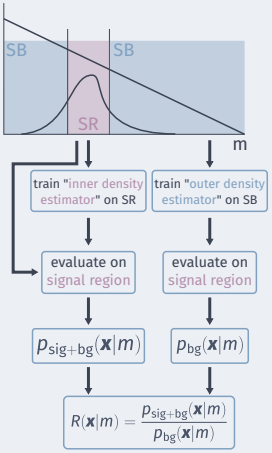


\+ Simple classification task

\+ Basic DNN architecture

\− Highly dependent on correlations between $\boldsymbol{x}$ and m
→Variables $\boldsymbol{x}$ need to be hand-picked

Anomaly Detection with Density Estimation (ANODE)



\+ Direct estimation of conditional densities

\+ Easy to interpolate p_{bg}

\+ Robust against correlations between $\boldsymbol{x}$ and m
→Arbitrary choice of $\boldsymbol{x}$

\− Computationally intense

\− Estimation of signal contribution difficult

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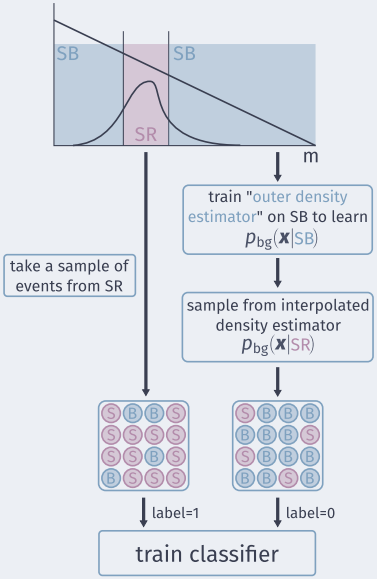
DOI:10.1103/PhysRevD.101.075042

CATHODE

Classifying Anomalies THrough Outer Density Estimation (CATHODE)

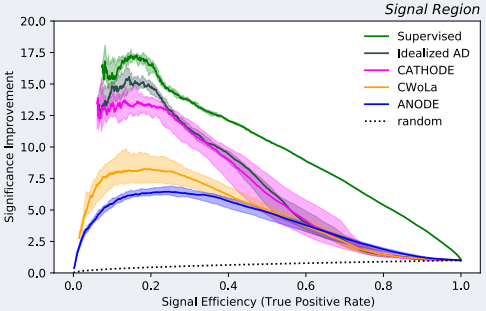
+ Only one density estimator needed
+ Due to interpolation: robust against correlations between $\boldsymbol{x}$ and m →Arbitrary choice of $\boldsymbol{x}$
+ Final tagger based on simple classification task
+ No density estimator for signal contribution needed
− Computationally intense



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

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



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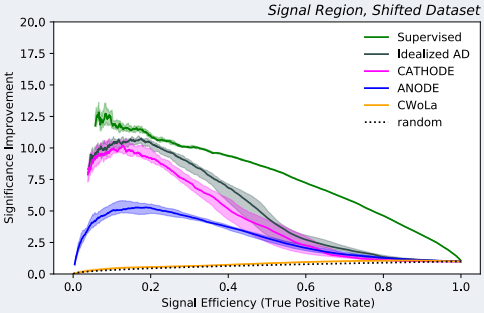
Robustness Against Correlations

- 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



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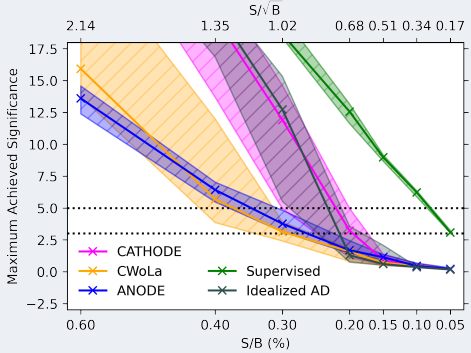
» Summary

- 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

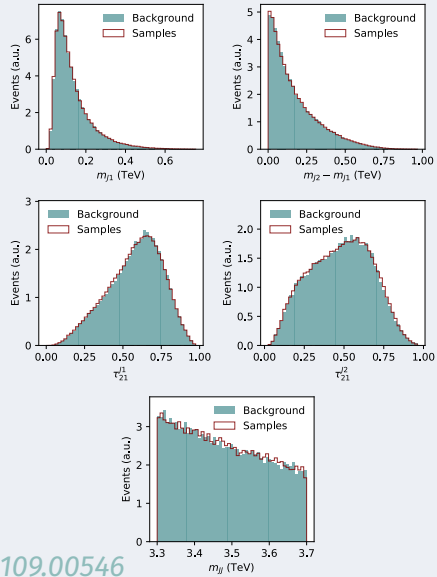
- Comparison for different amounts of signal injected
- CATHODE outperforms other AD methods significantly down to a S/B as low as 0.3%
- CATHODE achieves similar performance as idealized anomaly detector
- Below 0.2% S/B: even idealized AD cannot raise significance above 3σ
  →Too limited number of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



arxiv:2109.00546

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
  →Interpolation into SR
- We can oversample to produce more samples than we have in data
- Background densities are modelled well by flow



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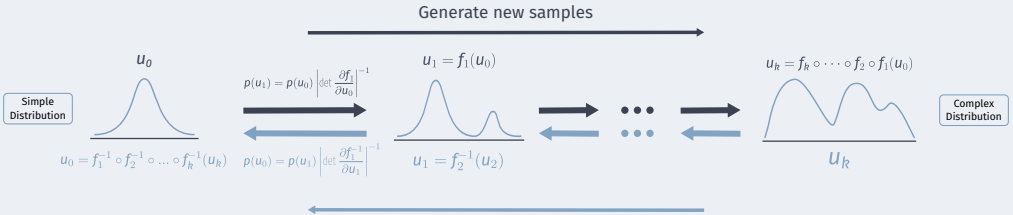
» Normalizing Flows

- Flows based on random variable transformation
- $f : U \to X;\ p(x) = p(u) \left| \frac{df(u)}{du} \right|^{-1}$
- Multivariate case: scale with Jacobian determinant
- Flow: repeat (invertible) transformation to get complex distributions

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

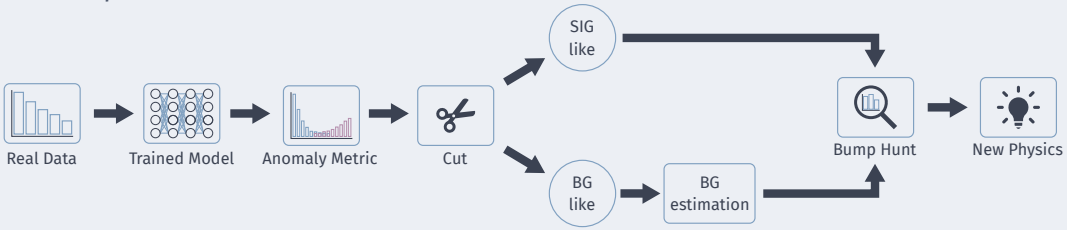


CASE (**C**MS **A**nomaly **SE**arch):
Explore different techniques, all involving **ML models trained directly on data!**

Currently investigated methods:

- (Variational) autoencoders
- Weak supervision (CWoLa hunting, Tag N' Train)
- Quasi-anomalous knowledge (QUAK)
- Density estimation & classification (CATHODE)

General procedure:



» Autoregressive Flows

Autoregressive property:

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

Conditional densities depend on trainable parameters:

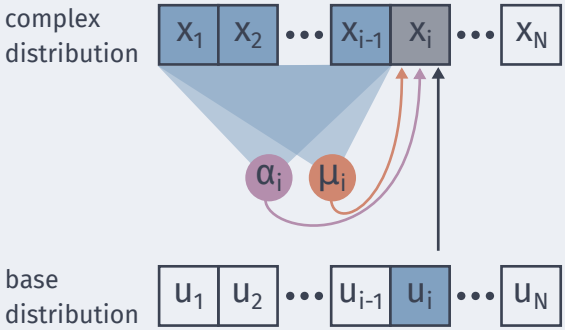
$p(x_i|x_{1:i-1}) = \mathcal{N}(x_i|\mu_i, (\exp \alpha_i)^2)$

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

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

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

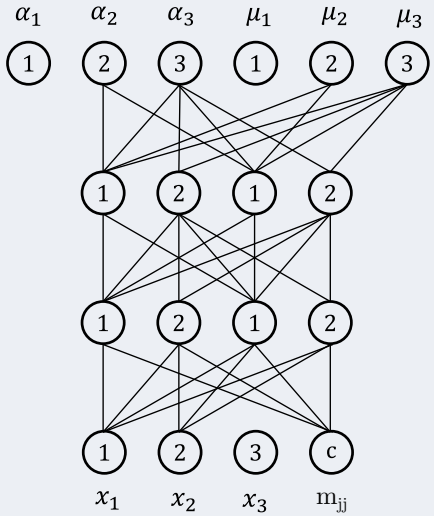
$x_i = f(u_i) = u_i \cdot \exp(\alpha_i) + \mu_i$



Autoregressive property →Jacobian is upper triangular

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

- DNN architecture to implement a single f_i in autoregressive flows (1502.03509)
- Compute α and μ in one forward pass
- Outputs α_j and μ_j only connected to inputs $\{x_1, ..., x_{j-1}\}$ →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