

Anomaly detection for new physics searches in dijet events at CMS

CMS-EXO-22-026

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Many open questions in cosmology and particle physics

Experiment-driven:

Dark Matter & Dark Energy

Matter-antimatter asymmetry

Theory-driven:

Hierarchy problems (weakness of gravity, fine tuning at level 10^{16})

Why 3 generations of fermions?

 \rightarrow New physics within LHC reach?

IT'S A UTTLE TOO

quantumdiaries.org

CMS established rich search program for new physics

Are we searching for the wrong signatures?

Maybe looking in the wrong spots or for the wrong models?

→ Need **safeguard** against missing signs of new physics

Are we searching for the wrong signatures?

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Re-formulate the question

"Does this event look like BSM theory XYZ?"

"Does this event look like the Standard Model?"

Outline

1. What are jets at CMS

2. Anomaly hunting

3. Expected performance

4. Actual look into data

Different particles \rightarrow different substructure

 \rightarrow Exploit substructure (e.g., N-subjettiness τ_{21} , grooming algorithms)

light jet

Anomalous jets

- **No assumption** on how exotic jets look like, but they could have:
	- long decay chains of SM resonances
	- completely exotic particles & weird radiation patterns
- Want our algorithm as model-independent as possible

Model independence:

1.) Not assuming specific signal model 2.) Not relying on imperfect background model (\rightarrow QCD Monte Carlo) either

→ Train directly on data!

Searching in dijet topology

- Target narrow resonance $A \rightarrow BC$, B & C decay hadronically
- Goal is to be sensitive to broad range of possible A,B,C
- Assumption: m_A >> m_B , m_C
	- \circ Results in highly boosted B, C
	- Decay products contained in large-radius jets
	- \rightarrow Anomalous large-radius jet on either side
- Select events with at least two AK8 jets $\rho_{\rm T}$ > 300 GeV, $|\eta|$ < 2.5
- Dijet invariant mass m_{ii} > 1455 GeV \circ Dictated by trigger turn-on
- $\Delta \eta_{ij}$ < 1.3 (to target *s*-channel resonance)

Developing and testing with a suite of BSM signals

Jet B substructure

Jet C

Outline

2. Anomaly hunting

Analysis Strategy

Increasing Model Dependence

Increasing Model Dependence

Autoencoder Fundamentals

- Train on non-anomalous examples, learns to reconstruct input
- Force information through a bottleneck
	- Focus on core features of normal examples

Autoencoder Fundamentals

Anomaly Score

- Train on non-anomalous examples, learns to reconstruct input
- Force information through a bottleneck
	- Focus on core features of normal examples
- \rightarrow Fails at reconstructing exotic examples

Variational Autoencoder (VAE)

● VAE encouraging (through additional loss term) latent space to be Gaussian

- Trained on jets from signal-depleted $\Delta\eta_{\rm{ii}}$ sideband $\Delta \eta_{\textrm{ii}}$ > 1.4
- Jet represented by 100 highest- p_{T} constituents: $\rho_{\sf x},\,\rho_{\sf y},\,\rho_{\sf z}$
- Constituents sorted by clustering sequence
	- More expressive in terms of substructure
- 100 x 3 matrix processed with 2D and 1D convolutional layers, bottleneck dimension = 12
- Anomaly metric: min(loss j1, loss j2)

Variational Autoencoder: Decorrelation from dijet mass

Variational Autoencoder: Decorrelation from dijet mass

Increasing Model Dependence

Weak Supervision Fundamentals

[JHEP 10 \(2017\) 174](https://arxiv.org/abs/1708.02949)

- Two mixed samples of signal and background events **with different purities**
- Train classifier on the two samples
	- Learns to distinguish signal vs background
	- Bias from also learning different background shapes if they are different
- Higher signal fraction \rightarrow better classifier performance

3 weakly supervised methods presented here \rightarrow Differ in how they construct the mixed samples

Weak Supervision #1: CWoLa

- **Assume** signal is a narrow resonance \rightarrow narrow peak, **choose** a mass window accordingly
	- \circ Signal-rich sample = events from window in m_{ii}
	- \circ Background-rich sample = events from sidebands
- Train a NN classifier on jets from signal-rich sample vs. background-rich sample
- \bullet Must ensure NN classifier does not learn m.
- \rightarrow Train separate classifiers for heavier and lighter jet*
	- \circ Allows to reweight jets in $p_{\rm T}^{\parallel}$ so that distributions are identical between two samples
	- Avoids learning m_{ii} through jet *p*_T
- \rightarrow Event anomaly score: max(score j1, score j2)

* modification w.r.t. original paper

Weak Supervision #2: Tag N' Train (TNT)

● Similar to CWoLa, but **enhance** signal purity of Mixed Sample 1 **with autoencoder** ○ Autoencoder: 2D CNN trained on jet images from jets in sideband

[Phys.Rev.D 106 \(2022\) 5, 055006](https://arxiv.org/abs/2109.00546) **Weak Supervision #3: CATHODE**

- Instead of using sidebands for Mixed Sample 2, **interpolate** their distributions into signal region \circ More robust to feature correlations with m_{ii}
- Train normalizing flows to learn **density** $p_{data}(x | m_{ii})$ of features *x* in sidebands, conditioned on *m*jj ○ Results in bijective, invertible map $f(x; m_{ii})$
	-
- **Interpolate** to get density in the signal window
- Draw samples in signal window to construct a **synthetic** background sample in SR → Mixed Sample 2
	- Proceed as usual (train classifier Mixed Sample 1 vs. Mixed Sample 2)

Weak Supervision: Training Quirks

- Weakly supervised methods assume signal window for training
	- \circ Fine if signal well within window, not fine if at the edge
	- Need to **slide window** and **repeat trainings** to cover full mass range
- Define two sets of bins, A and B
- Set B is shifted by half window w.r.t. Set A
- In total 12 signal regions, different trainings and event selection for each one 26

Increasing Model Dependence

Quasi Anomalous Knowledge (QUAK)

- **Hybrid** approach between model-independent and standard search
- Idea: encode prior knowledge of how a signal could look
- Train density estimator (normalizing flow) on colorful mix of simulated signals
- Train additional normalizing flow on background **simulation**
- Construct 2D space, select events with high background loss and low signal loss

QUAK: general vs. specific

Increasing Model Dependence

- Which signals to use for encoding prior knowledge?
	- general mixture of several signal models
	- specific using only model to be probed
- Can use QUAK to "interpolate" towards fully supervised approach

Input features

Nice complementarity

Checking the correlations

- Complementary architectures and input features reflected in low Pearson correlation among anomaly scores
- \bullet TNT and CWoLa most similar (in approach and thus in score) $\qquad \qquad _{31}$

Cut definition

Outline

3. Expected performance

- Injected $X \rightarrow YY'$ signal with 24 fb cross-section
- Quantifying performance on **simulated** mock dataset worth \sim 30 fb⁻¹
- Model background and signal with analytic functions
- Signal not visible by eye on top of background
Significance of excess: inclusive

Significance of excess: decent traditional cut

- Cut on N-subjettiness τ_{21} to enrich in 2-prong jets
- Sizeable improvement over inclusive search
- τ_{21} used in many searches

Significance of excess: decent traditional cut

- Cut on N-subjettiness τ_{21} to enrich in 2-prong jets
- Sizeable improvement over inclusive search
- τ_{21} used in many searches
- Cut on N-subjettiness τ_{32} to enrich in 3-prong jets gives worse sensitivity than inclusive search

Significance of an excess: TNT

- Prominent peak after cut on TNT anomaly metric
- At 18 fb: Improving from 3 sigma (for τ_{21}) to 7 sigma!

The full picture: a couple of observations

- Model specific QUAK performs best ○ used knowledge about the exact signal
- CATHODE-b worse than CATHODE
	- B tag score in normalizing flows has detrimental effect on signal without b quarks (acts as noise)
- VAE and CWoLa little or no improvement w.r.t. inclusive search

The full picture: a couple of observations

- CATHODE-b better than CATHODE for signals with b quarks (W' \rightarrow B'(bZ)t \rightarrow qqq qqq)
- VAE and CWoLa performing well on rich, broad jets

Outline

4. Actual look into data

Data spectra - no excess

- Reminder: for VAE, only 1 anomaly cut, totally independent of probed mass
- Six different A regions for weakly supervised models (B regions in Backup)
- \overline{a} No significant excess \overline{a} and \overline{a}

CMS Experiment at the LHC, CERN Data recorded: 2018-Sep-06 05:06:55.343296 GMT
Run / Event / LS: 322332 / 851591650 / 487

VAE says:

two anomalous jets

Data spectra - no excess

No significant excess for remaining methods either

Discovery sensitivity

- No excess observed \rightarrow Which injected cross section would have lead to $3\sigma/5\sigma$?
- All methods almost always better than inclusive / traditional search strategy
- For every benchmark, at least one method could claim discovery where inclusive strategy can only set upper limits

 $m(Y) = 170$ GeV, $m(B', R, H) = 400$ GeV

Model-dependent searches: setting limits

- Statistical inference gives upper limit on number of signal events still allowed in data, N_{UL}
	- \rightarrow Which cross section does this correspond to?

$$
N_{\text{sig}} = \sigma \times \mathcal{L} \times A \times \epsilon
$$

 \rightarrow Solve for σ . Done.

Model-dependent searches: setting limits

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Not the full story!

For weakly supervised methods, efficiency **depends** on number of signal events in data!

- Much signal present \rightarrow classifier learns well how to pick up on it \rightarrow high selection efficiency
- Low signal present \rightarrow classifier cannot learn it properly \rightarrow low selection efficiency

not constant

$$
N_{\rm sig}(\sigma) = \sigma \times \mathcal{L} \times A \times \mathcal{E}(\sigma)
$$

• Need to find σ such that $N_{\rm{sin}} = N_{\rm{UL}}$

$$
(N_{\text{sig}}(\sigma)) = \sigma \times \mathcal{L} \times A \times \epsilon(\sigma)
$$

- Inject different $#$ signal, retrain algorithms, measure efficiencies
	- Shaded band: syst. + stat. error
- Gives number of selected signal events

$$
N_{\text{sig}}(\sigma) = \sigma \times \mathcal{L} \times A \times \epsilon(\sigma)
$$

- Inject different $#$ signal, retrain algorithms, measure efficiencies ○ Shaded band: syst. + stat. error
- Gives number of selected signal events
- Find intersection with obs. / exp. event limits

Obs. & exp. limits on cross section!

Final limits

Several 3 TeV resonance scenarios ○ 5 TeV in Backup

- Large improvement over inclusive strategy
- Dominant uncertainty from substructure modelling for signal
- Dedicated W_{KK} search beats all anomaly detection methods (expected)

 $m(Y) = 170$ GeV, $m(B', R, H) = 400$ GeV

Summary

- For the first time: search with five different & complementary anomaly detection algorithms
- Cast a wide net to catch potential new heavy resonances A decaying into B, $C \rightarrow$ dijet final state
- Large sensitivity improvements over inclusive search or searches with generic traditional cuts
- No excess observed
- Check out CMS-EXO-22-026 & CMS-NOTE-2023-013
- Stay tuned for more

I've created a "Where's Waldo?" style image set at a high energy physics conference for you. Look closely among the scientists and researchers, amidst the posters and presentations, to find Waldo. Enjoy your search in this academically rich scene!

BACKUP

Want a starting point as clean as possible

- Jets inevitably not a perfect representation of the resonance decay
- Not everything in jet comes from particle at origin
	- Initial-state radiation, underlying event, pileup
- Measurement inaccuracies for constituents

Can give appearance of anomalous radiation patterns

Can reduce expressiveness of truly exotic features, pronginess, etc …

Jet energy mismeasurement

- Need to resolve products from up to 50 simultaneous collisions
	- Tracks: good pointing resolution
	- Neutrals: poor pointing resolution
- PUPPI algorithm discards neutral pileup particles by extrapolating from charged to neutrals
- Large improvement in jet resolution $+$ substructure

Grooming the jet with soft-drop algorithm

- Soft-drop algorithm to remove soft and wide-angle radiation
- Iteratively undo clustering and remove sub-jets that fail:
- Moves QCD Sudakov peak out of the way \rightarrow soft-dropped jet mass $m_{\rm SD}$ much more expressive

0

 ΔR_{12}

=

0.1

"

 \geq $(z_{\rm cut}$

 $\frac{\min(p_{T1}, p_{T2})}{\min(p_{T1}, p_{T2})}$

 $p_{T1} + p_{T2}$

CMS uses **Particle Flow** reconstruction:

- Aimed at reconstructing each individual particle
- "Follow" the path of a particle through the detector
- Match deposits between subdetectors
- For each particle combine subdetector information for best E/momentum measurement

Weak Supervision #2: Tag N' Train (TNT)

- **Train Mixed Sample 1 vs Mixed Sample 2**
- \rightarrow Anomaly score: score j1 $*$ score j2

Weak Supervision #3: CATHODE

QUAK Signal Prior

- Train 6 separate normalizing flows (six-layer autoregressive rational quadratic splines) on different signal samples
	- \circ Grouped by daughter masses (M80-M80), (M80-M170), (M80-M400), (M170-M170), (M170-M400), (M400-M400)
- Normalize each score so mean 0, std 1
- Combine 6 scores into single 'sig-like' score using L5 signed norm $(|s1|$ ^5+ $|s2|$ ^5+...)^ $($ ^{1/5})

Signal B Regions

What happens if no signal present?

- No sculpting
- No artificial excesses
- Checked for all methods
- Validated also on data in $\Delta\eta_{\text{ii}}$ sideband (2.0 < $\Delta \eta_{ii}$ < 2.5)

Signal extraction - bump hunt on dijet mass spectrum

● After anomaly selection, all methods share common statistical framework

- **•** Bump hunt performed on m_{ij} spectrum with 4 GeV bin size to emulate an unbinned fit (for plots, coarser binning is used)
- Background distribution modeled with standard dijet function

$$
\frac{dN}{dm_{jj}} = \frac{P_0(1-x)^{P_1}}{(x)^{P_2+P_3\log(x)+P_4\log^2(x)}}
$$

- Starting with P3, P4 = 0, but can be added if found they improve fit quality (Fisher's F-test)
- For signal use a double Crystal ball (from fits to MC); generic shape
- Fit quality: compute chi2/ndf \rightarrow p value > 0.05

Fit bias study

- Test for bias in functional form
- Generate toys according to alt. fit functions, fit & check bias in signal strength
- Perform for different signal regions / masses
- No significant bias seen

Global p value for weakly supervised methods

- Approximate each SR as fully indep. search \rightarrow trial factor of 12 for whole scan
- Within each signal region, use traditional methods (toys) to compute effective trial factor based on mass points scanned
- Global pval = (local pval) $*$ (SR trial factor) $*$ 12

Effect of Signal in Data on Limit Setting

- Presence of the **same signal already in the data** prior to injection for limit setting would lead to biased estimate of signal efficiency \rightarrow limits could undercover
- Tested in two MC studies
	- \circ One using the CATHODE method on a 5 TeV Y \rightarrow HH signal (low stats. regime)
	- \circ One using the TNT method on a 3 TeV X \rightarrow YY signal
- For each study, construct 100 mock datasets containing some signal
	- Run limit setting procedure on each dataset (assuming no signal)
	- Compare distribution of limits to true xsec to check coverage
- Excellent coverage observed for signal strengths giving up to 2sigma
- TNT sees some undercoverage (85%) for very large (3.6σ) signal
- In data no excesses larger than \sim 2.5 $\sigma \rightarrow$ these studies demonstrate we will have coverage

Mismatched signals?

- \bullet If signal already in the data (A) that is different from the one we are setting a limit on (B), that will affect results
- During injections, training will be performed with both A & B signal events
- Found that efficiency when training on A+B is the same or less than the efficiency when training on just A/just B
- Same or lower eff. \rightarrow same or more-conservative limits

Protocol if we see something

- Consult with detector experts to look at most anomalous events and exclude detector noise, etc.
- Look at features for most anomalous jets vs. standard jets
- Should be clear indication which feature(s) are triggering excess
- Can inform more targeted search with traditional methods / features
3 TeV limits

5 TeV limits

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 \sim

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 $\mathcal{R}^{\mathcal{L}}$

 \mathcal{N}

5 TeV limits

Systematic Uncertainties

- Effects on signal efficiency considered for:
	- Substructure modeling
	- Pileup
	- PDF uncertainties
	- B tagging
	- Jet energy scale & resolution
	- Renormalization / factorization scales

Substructure Modeling

- No correction factors for signals with >3 prongs can be derived with SM proxy
- Derive per-prong correction via Lund Plane Reweighting [\(CMS-DP-2023-046](https://cds.cern.ch/record/2866330/files/DP2023_046.pdf))
	- Derived on boosted W's, validated on boosted tops
	- Applicable to signals with any number of prongs
- Recluster large-radius jet with exclusive kt algorithm, recluster subjects with CA algorithm to get splittings,
- Sort splittings into Lund plane, divide Data/MC for per-splitting correction
- Per splitting \rightarrow per subjet \rightarrow per jet \rightarrow per event

