

IMPERIAL

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 10¹⁶)

Why 3 generations of fermions?

 \rightarrow New physics within LHC reach?

IT'S A UTTLE TOO HOT FOR 125 GeV...

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?



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

→ Need safeguard against missing signs of new physics

Re-formulate the question



"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



light jet

Different particles \rightarrow different substructure

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

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:

 Not assuming specific signal model
 Not relying on imperfect background model (→ QCD Monte Carlo) either

 \rightarrow 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: $m_A >> m_B, m_C$
 - Results in highly boosted B, C
 - Decay products contained in large-radius jets
 - → Anomalous large-radius jet on either side
- Select events with at least two AK8 jets \circ $p_{T} > 300$ GeV, $|\eta| < 2.5$
- Dijet invariant mass m_{jj} > 1455 GeV
 Dictated by trigger turn-on
- $\Delta \eta_{jj} < 1.3$ (to target *s*-channel resonance)



Developing and testing with a suite of BSM signals



Jet C

Jet B substructure

		1 prong	2 prong	3 prong	4 prong	5 prong	6 prong	
	1 prong		Q* → qW m _{Q*} = [2,3,5] TeV m _W = [25,80,170,400] GeV					
substructure	2 prong		$\begin{array}{c} \textbf{X} \rightarrow \textbf{YY'} \\ m_X = [2,3,5] \ \text{TeV} \\ m_Y = [25,80,170,400] \ \text{GeV} \\ m_{Y'} = [25,80,170,400] \ \text{GeV} \end{array}$		W_{KK} → RW → WWW $m_{WKK} = [2,3,5]$ TeV $m_R = [170,400]$ GeV	Search	prober	
	3 prong			W' → tB' $m_{W'} = [2,3,5] \text{ TeV}$ $m_{B'} = [25,80,170,400] \text{ GeV}$			signals unexp	ora
	4 prong	Expect sensitivity to many additional kinds of signals!			$\begin{array}{l} \textbf{X} \rightarrow \textbf{YH} \rightarrow \textbf{WWWW} \\ m_X = [2,3,5] \ \text{TeV} \\ m_Y = [170,400] \ \text{GeV} \\ m_H = [170,400] \ \text{GeV} \end{array}$			
	5 prong					Z' → T'T' → tZtZ m _{Z'} = [2,3,5] TeV m _{T'} = [400] GeV		
	6 prong						$\label{eq:main_state} \begin{array}{l} \textbf{Y} \rightarrow \textbf{HH} \rightarrow \textbf{tttt} \\ m_{Y} = [2,3,5] \; \text{TeV} \\ m_{H} = [400] \; \text{GeV} \end{array}$	

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1. Characterizing jets at CMS

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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 $\Delta \eta_{jj}$ sideband $\circ \Delta \eta_{ij} > 1.4$
- Jet represented by 100 highest- p_{T} constituents: p_{x} , p_{y} , p_{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

- 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 → 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
 - Signal-rich sample = events from window in m_{ii}
 - Background-rich sample = events from sidebands
- Train a NN classifier on jets from signal-rich sample vs. background-rich sample
- Must ensure NN classifier does not learn m_{ii}
- \rightarrow Train separate classifiers for heavier and lighter jet*
 - Allows to reweight jets in p_{T} 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



Weak Supervision #3: CATHODE

- Instead of using sidebands for Mixed Sample 2, interpolate their distributions into signal region
 More robust to feature correlations with m_a
- Train normalizing flows to learn **density** p_{data}(x | m_{jj}) of features x in sidebands, conditioned on m_{jj}
 Results in bijective, invertible map f(x;m_{ij})
- Interpolate to get density in the signal window
- Draw samples in signal window to construct a **synthetic** background sample in SR \rightarrow 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
 - 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

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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



targets events

Checking the correlations



- Complementary architectures and input features reflected in low Pearson correlation among anomaly scores
- TNT and CWoLa most similar (in approach and thus in score)



Cut definition

VAE	CWoLa	TNT	CATHODE	QUAK
Single event selection for all masses	Selection changes for each SR	same as CWoLa	Selection changes for each SR	Selection changes for each mass hypothesis
10% most anomalous events	Cut determined on sidebands Chosen such that eff == 1% for low m_{jj} , eff == 5% for high m_{jj}		Cut determined in SR Chosen such that eff == 1%	Iteratively select least-populated bins in sideband QUAK space, until decent population in SR

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- Injected $X \rightarrow YY'$ signal with 24 fb cross-section
- Quantifying performance on simulated mock dataset worth ~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

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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)
- No significant excess



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, $N_{\rm UL}$
 - \rightarrow Which cross section does this correspond to?

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

 \rightarrow Solve for σ . Done.

Model-dependent searches: setting limits

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

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

 \rightarrow Solve for σ . Done.

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 → classifier cannot learn it properly
 → low selection efficiency

not constant

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

• Need to find σ such that $N_{sig} = N_{UL}$



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

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



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

- 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

 \rightarrow 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 → 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. <u>Look</u> <u>closely</u> 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

Removing particles from pileup



- 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

0.1

 $>(z_{cut})$

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

 $p_{T1} + p_{T2}$

 ΔR_{12}



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
 - 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 $\Delta \eta_{jj}$ sideband (2.0 < $\Delta \eta_{ij}$ < 2.5)

Signal extraction - bump hunt on dijet mass spectrum

• After anomaly selection, all methods share common statistical framework

- Bump hunt performed on m_{jj} 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 → limits could undercover
- Tested in two MC studies
 - One using the CATHODE method on a 5 TeV Y \rightarrow HH signal (low stats. regime)
- 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 ~2.5 σ \rightarrow these studies demonstrate we will have coverage

Mismatched signals?

- 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

Signal Model	Daughter Masses (GeV)	Method	Exp. (Obs.) Limit (fb)	Improvement wrt
(3 TeV)	-		-	Inclusive
Q* ightarrow qW'	25	CWoLa Hunting	61.1 (30.1)	0.3
Q* ightarrow qW'	80	CATHODE	50.0 (95.2)	0.4
Q* ightarrow qW'	170	VAE-QR	52.5 (37.5)	0.4
Q* ightarrow qW'	400	CWoLa Hunting	45.8 (24.3)	0.5
$X \rightarrow YY' \rightarrow 4q$	25/25	CATHODE	8.0 (9.9)	0.9
$X \rightarrow YY' \rightarrow 4q$	25/80	CATHODE	7.6 (13.2)	0.9
$X \rightarrow YY' \rightarrow 4q$	25/170	CATHODE	10.3 (18.4)	0.7
$X \rightarrow YY' \rightarrow 4q$	25/400	VAE-QR	13.6 (12.5)	0.6
$X \to Y Y' \to 4 q$	80/80	CATHODE	4.2 (8.0)	1.6
$X \rightarrow YY' \rightarrow 4q$	80/170	CATHODE	5.7 (11.4)	1.2
$X \rightarrow YY' \rightarrow 4q$	80/400	CATHODE	6.0 (7.3)	1.2
$X \rightarrow YY' \rightarrow 4q$	170/170	CATHODE	3.7 (6.8)	1.9
$X \to Y Y' \to 4 q$	170/400	VAE-QR	4.4 (4.0)	1.7
$X \rightarrow YY' \rightarrow 4q$	400/400	VAE-QR	2.1 (1.9)	4.2
$W' \rightarrow B't \rightarrow bZt$	25	TNT	25.2 (17.4)	1.5
$W' \to B't \to bZt$	80	TNT	22.3 (14.6)	1.5
$W' \to B' t \to b Z t$	170	TNT	12.2 (7.3)	2.1
$W' \to B' t \to b Z t$	400	VAE-QR	15.2 (11.4)	1.8
$W_{KK} \rightarrow RW \rightarrow 3W$	170	TNT	25.1 (20.1)	1.4
$W_{KK} \rightarrow RW \rightarrow 3W$	400	CWoLa Hunting	23.8 (25.0)	1.5
$Z' \to T'T' \to tZtZ$	400	QUAK	28.3 (13.9)	2.7
$Y \to HH \to 4t$	400	QUAK	7.7 (3.7)	3.5

5 TeV limits

-

Signal Model	Daughter Masses (GeV)	Method	Exp. (Obs.) Limit (fb)	Improvement wrt
(5 lev)				Inclusive
$\mathrm{Q*} ightarrow \mathrm{qW'}$	25	QUAK	3.5 (3.1)	0.7
$\mathrm{Q*} ightarrow \mathrm{qW'}$	80	QUAK	3.2 (2.8)	0.8
${ m Q}* ightarrow { m q}{ m W}'$	170	QUAK	3.3 (3.6)	0.8
${ m Q}* ightarrow { m q}{ m W}'$	400	QUAK	3.9 (9.9)	0.7
$X \rightarrow YY' \rightarrow 4q$	25/25	QUAK	1.7 (1.6)	0.5
$X \rightarrow YY' \rightarrow 4q$	25/80	QUAK	1.3 (1.3)	0.7
$X \rightarrow YY' \rightarrow 4q$	25/170	QUAK	1.1 (1.1)	0.8
$X \rightarrow YY' \rightarrow 4q$	25/400	VAE-QR	1.0 (3.4)	0.9
$X \rightarrow YY' \rightarrow 4q$	80/80	TNT	1.1 (1.2)	0.8
$X \rightarrow YY' \rightarrow 4q$	80/170	QUAK	0.9 (1.0)	0.9
$X \rightarrow YY' \rightarrow 4q$	80/400	VAE-QR	0.9 (3.0)	0.9
$X \rightarrow YY' \rightarrow 4q$	170/170	CATHODE	0.7 (0.7)	1.2
$X \rightarrow YY' \rightarrow 4q$	170/400	VAE-QR	0.7 (2.3)	1.2
$X \rightarrow YY' \rightarrow 4q$	400/400	VAE-QR	0.4 (1.1)	2.3
W' ightarrow B't ightarrow b Zt	25	TNT	4.4 (6.2)	1.3
W' ightarrow B't ightarrow bZt	80	TNT	3.9 (5.7)	1.4
W' ightarrow B't ightarrow bZt	170	TNT	2.8 (3.5)	1.6
W' ightarrow B't ightarrow bZt	400	TNT	2.7 (3.8)	1.6
$W_{KK} \rightarrow RW \rightarrow 3W$	170	TNT	6.1 (7.2)	0.8
$W_{KK} \rightarrow RW \rightarrow 3W$	400	VAE-QR	5.4 (18.6)	0.9
$Y \rightarrow HH \rightarrow 4t$	400	TNT	1.5 (2.3)	2.5

N 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 (<u>CMS-DP-2023-046</u>)
 - 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



