Isolating Unisolated Upsilons with Anomaly Detection in CMS Open Data

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in collaboration with Rikab Gambhir, Benjamin Nachman, Jesse Thaler

AD4HEP Workshop

06/18/2025

The elephant in the room: is this novel?

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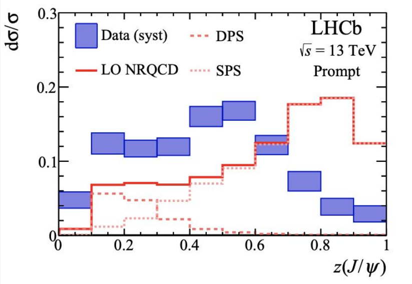
hep-ph/1701.05116



Studying quarkonia produced within jets probes the transition between perturbative and nonperturbative QCD

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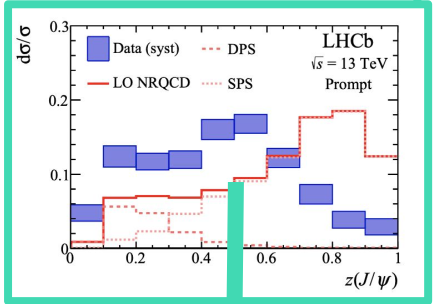

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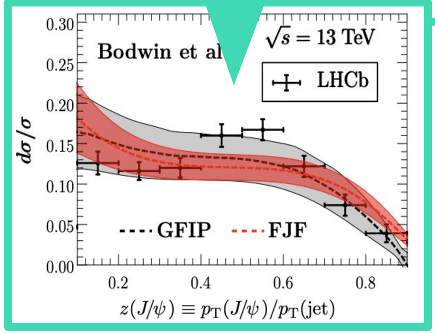

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Jet fragmentation functions are improved by comparing to observations J/Ψ's within jets

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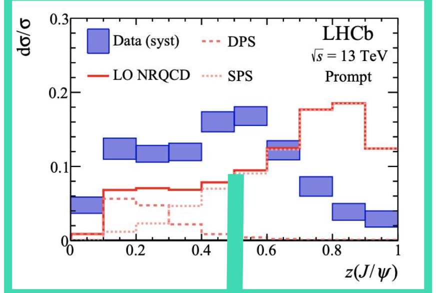

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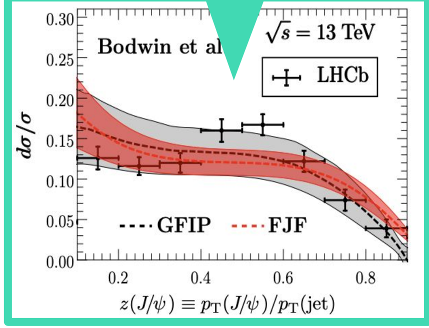
See Rikab's talk — we apply a new ML method!



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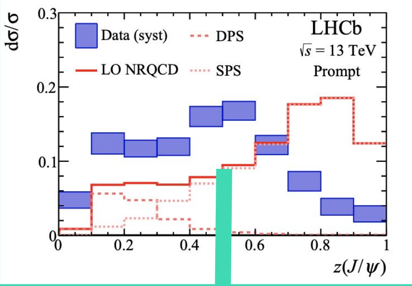

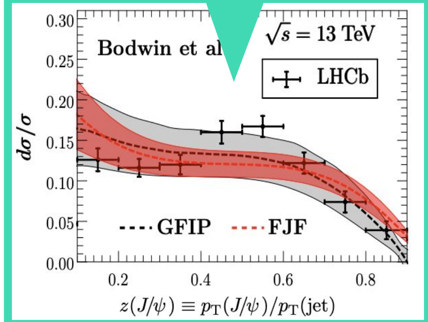

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Studying quarkonia produced within jets probes the transition between perturbative and nonperturbative QCD

Jet fragmentation functions are improved by comparing to observations J/Ψ's within jets

See Rikab's talk — we apply a new ML method!

Try it yourself!

This is the first application of anomaly detection to open collider data

Dataset and event selection

We pull our data from the DoubleMuon primary dataset, made available on the CERN Open Data Portal.

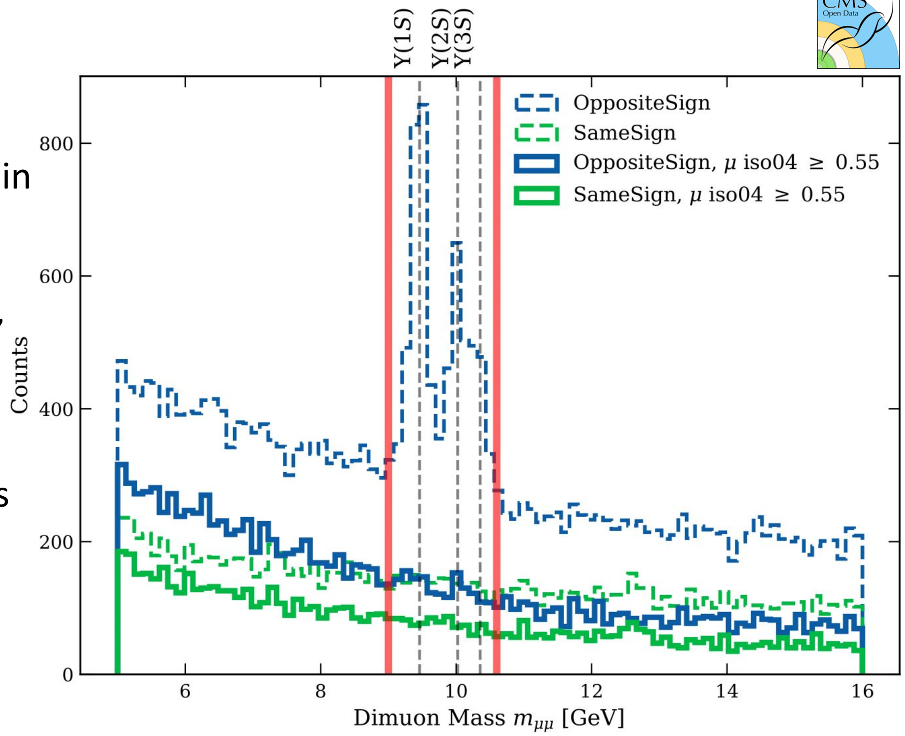
The dataset consists of μμ pairs produced during Run 2 in 2016 of the LHC at the CMS experiment, that

- pass the `HLT_TrkMu15_DoubleTrkMu5NoFiltersNoVtx` trigger,
- pass the p_T cuts 17 GeV, 8 GeV,
- pass the `TightID` criteria.

We further impose an **anti-isolation cut** to select for ϒ's produced in jets:

$$\mu \text{ iso04} = \sum_{\substack{\text{hadronic particles} \\ \text{within } \Delta R = 0.4}} \frac{p_{T\,\text{hadronic}}}{p_{T\,\mu}} \geq 0.55$$

We are left with ~12,000 dimuon events.



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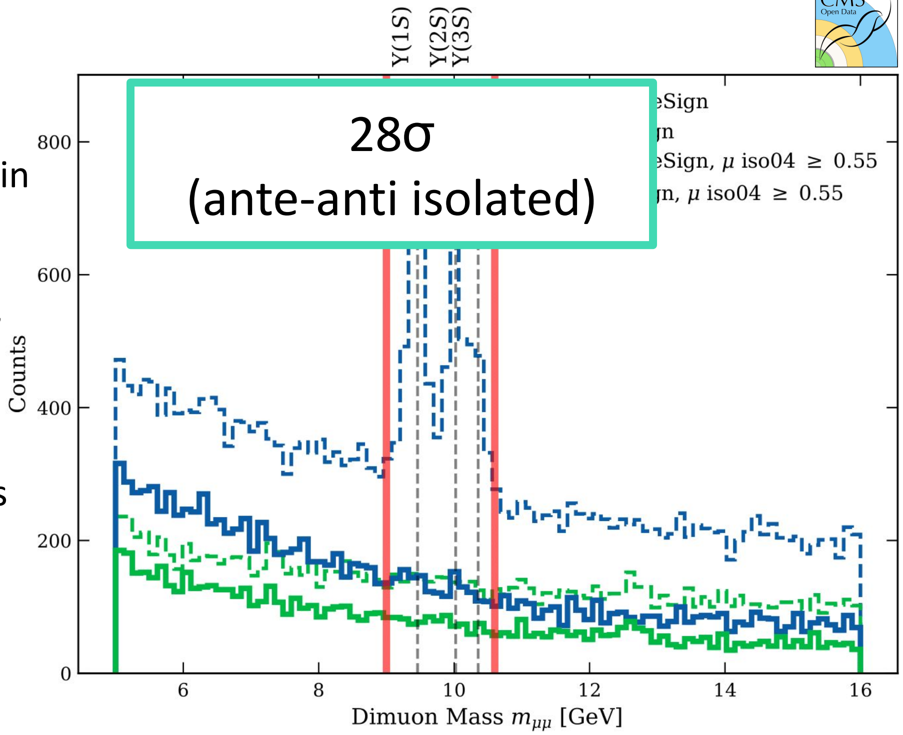

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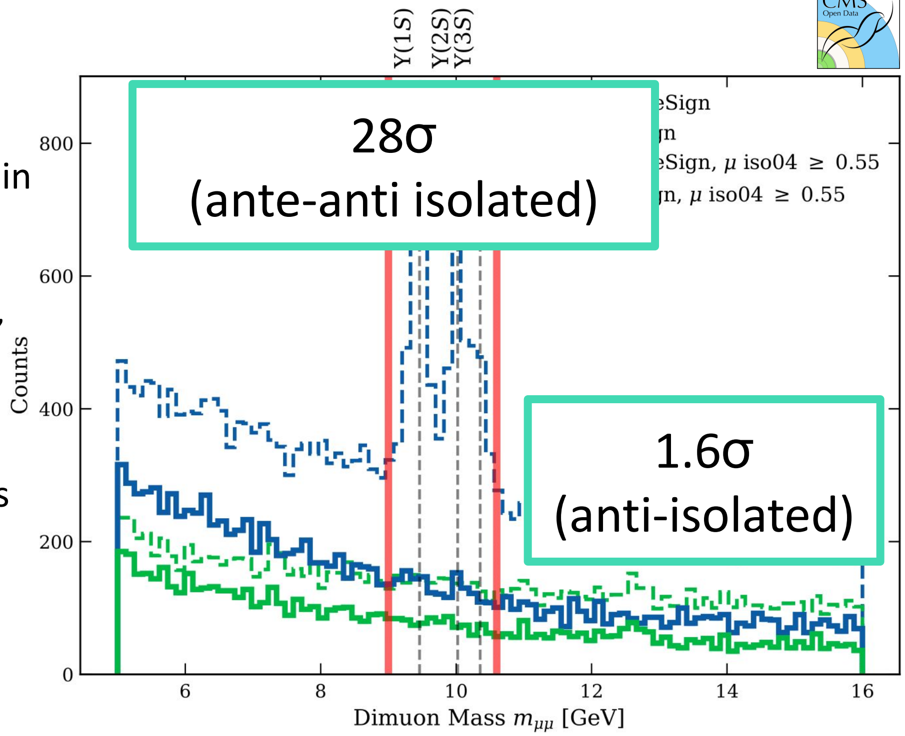
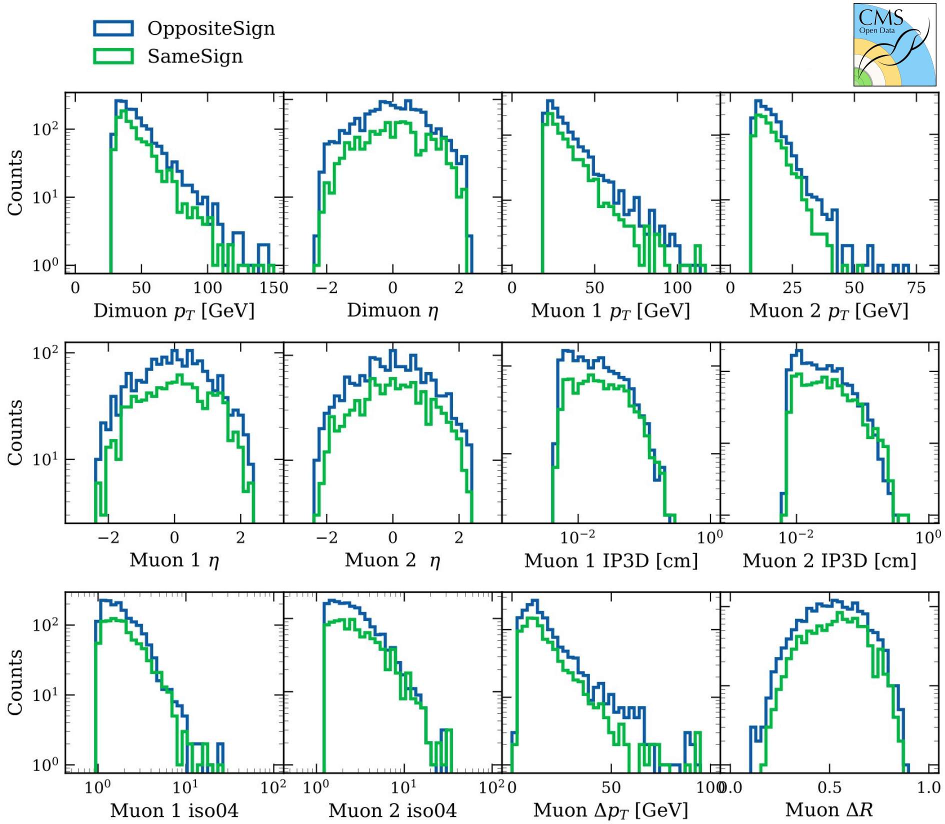


Auxiliary feature selection

We considered a large number of auxiliary observable sets, but one set worked particularly well*:

- ❖ Dimuon p_T
- ❖ Muon 1 3D impact parameter
- ❖ Muon 2 3D impact parameter

* e.g. no background sculpting, good signal elevation



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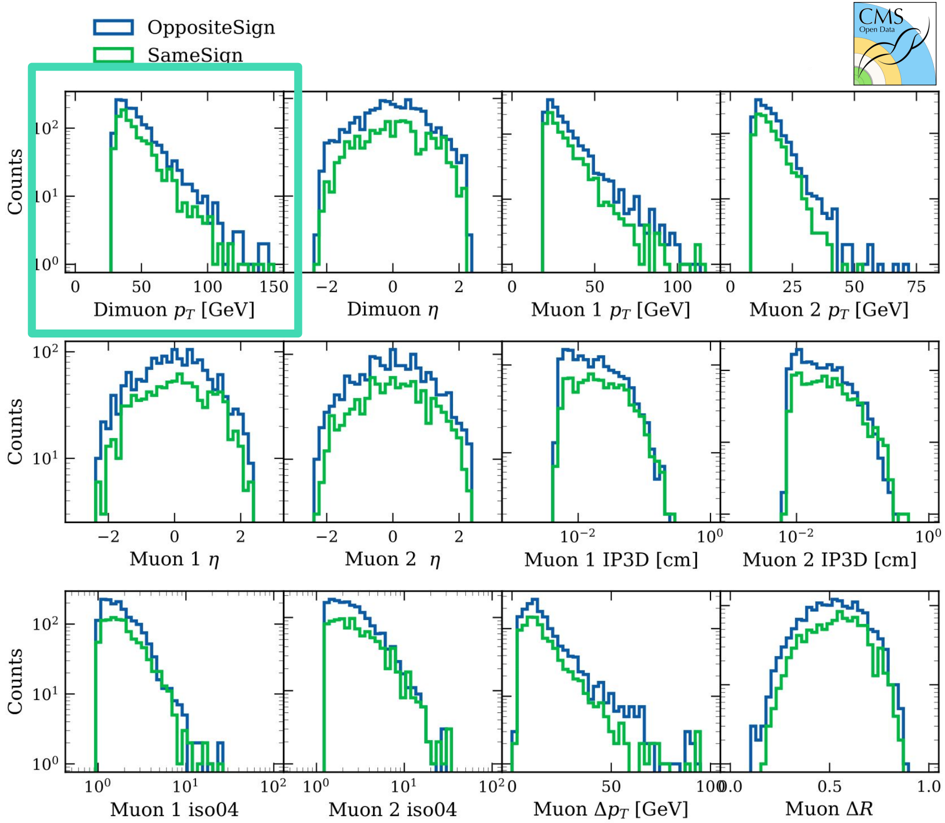

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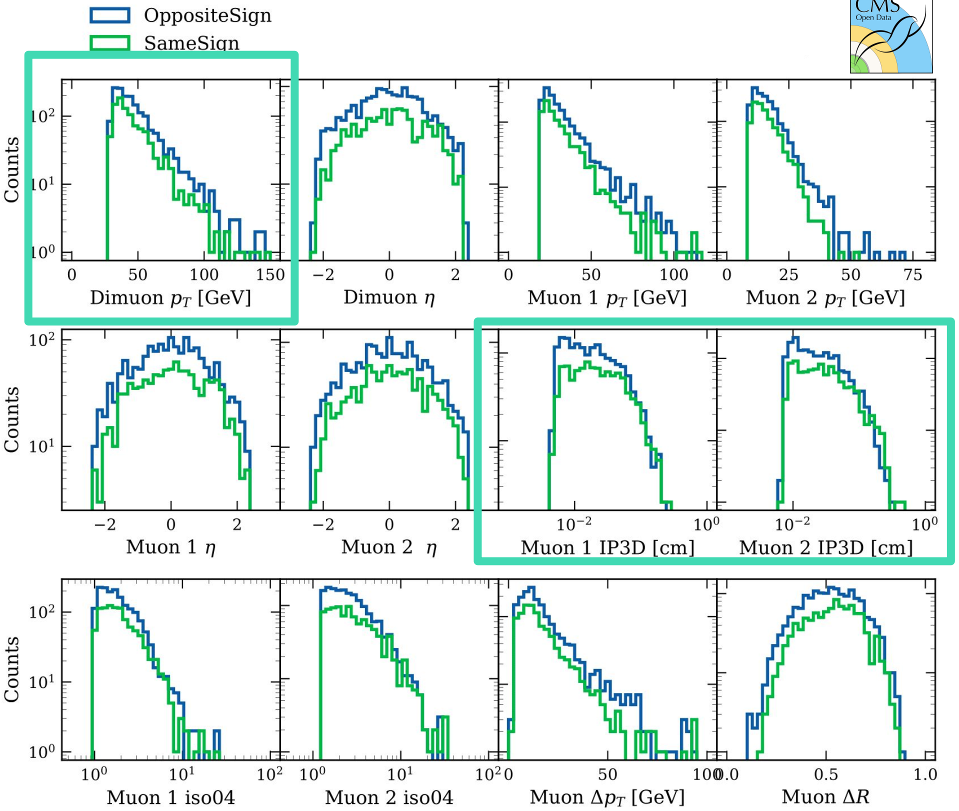

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Analysis procedure

- Use **CATHODE** to generate a set of background-like (i.e. non-Υ-like) samples
- Train Boosted Decision Trees to discriminate **CATHODE** samples from data. (i.e. Classification Without Labels, `hep-ph/1708.02949`). The classifiers learn:

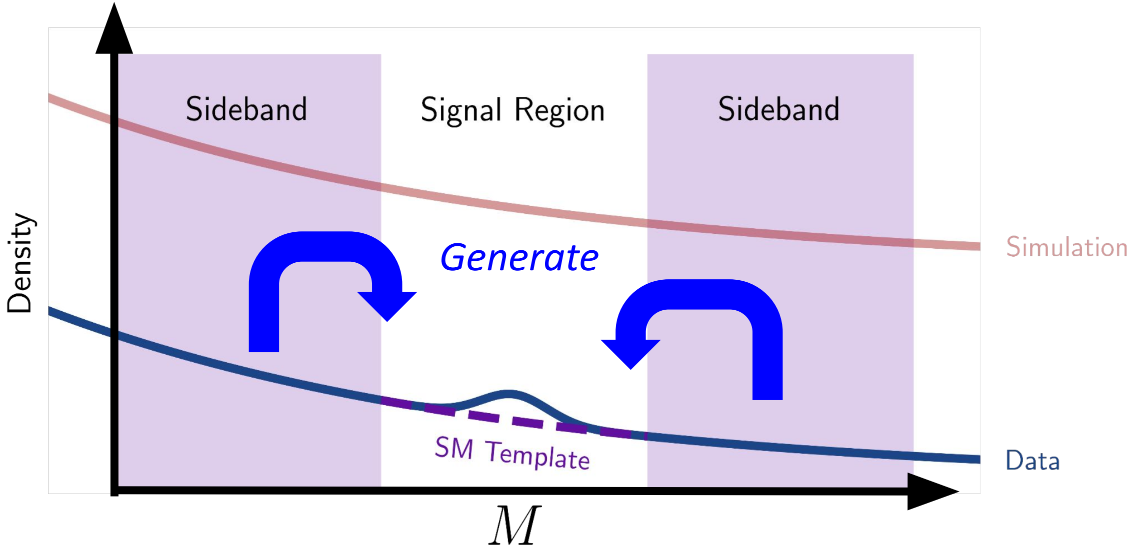
$$\boxed{C(x) = \frac{p_{\text{Data}}(x)}{p_{\text{Samples}}(x)} = \frac{\mu p_{\text{Signal}}(x) + (1-\mu) p_{\text{Background}}(x)}{p_{\text{Background}}(x)} = \mu \frac{p_{\text{Signal}}(x)}{p_{\text{Background}}(x)} + (1-\mu)}$$

  - ML test 1: cut on the BDT score
  - ML test 2: Rikab's talk
- Compare these ML tests to classical tests (i.e. cutting on the individual kinematic observables)

See backup slides for architecture details.

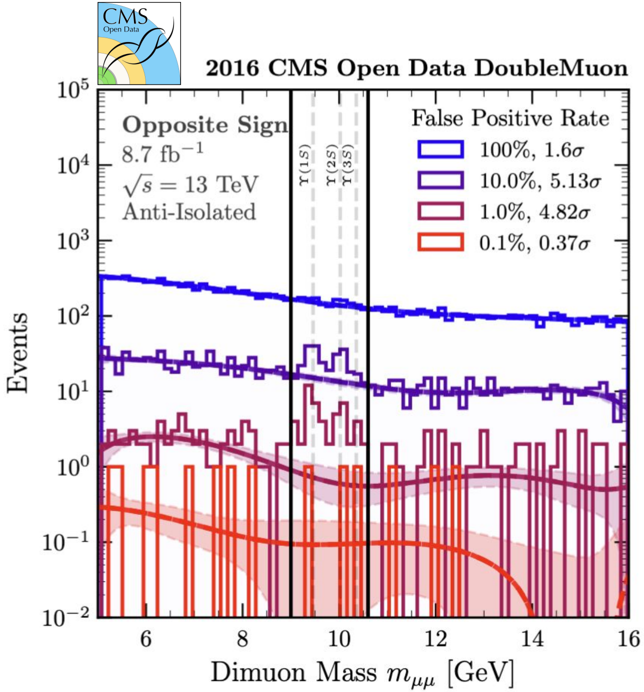
Generating background samples with CATHODE

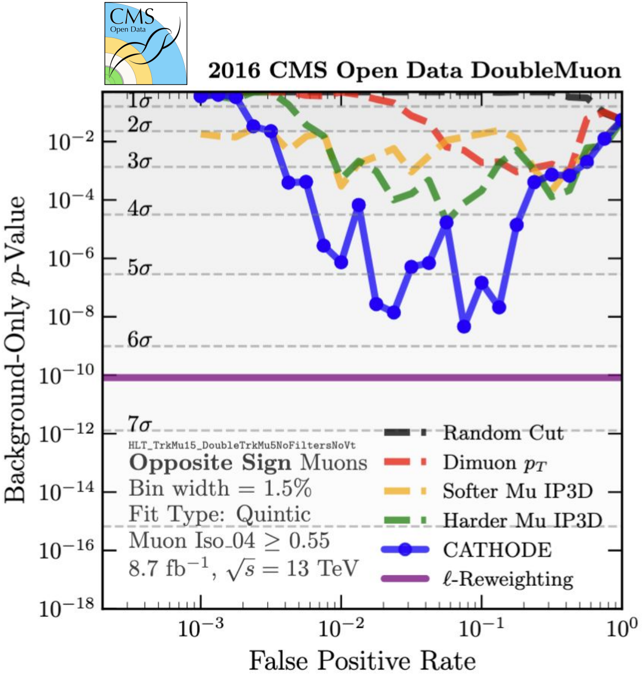
Classifying Anomalies THrough Outer Density Estimation
(hep-ph/2109.00546)



- ❖ A normalizing flow learns the **distribution** of **data** (i.e. the auxiliary observables) in sidebands, conditioned on the dimuon mass
- ❖ The flow is interpolated into the signal region to **generate** realistic background samples

Results: finding Υ's within jets





best classical test: 4.1σ

ML test 1: 5.7σ

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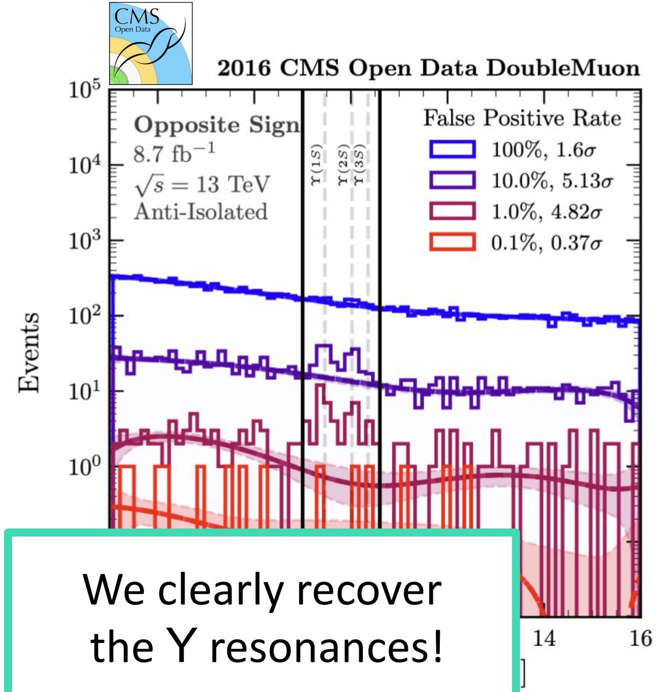
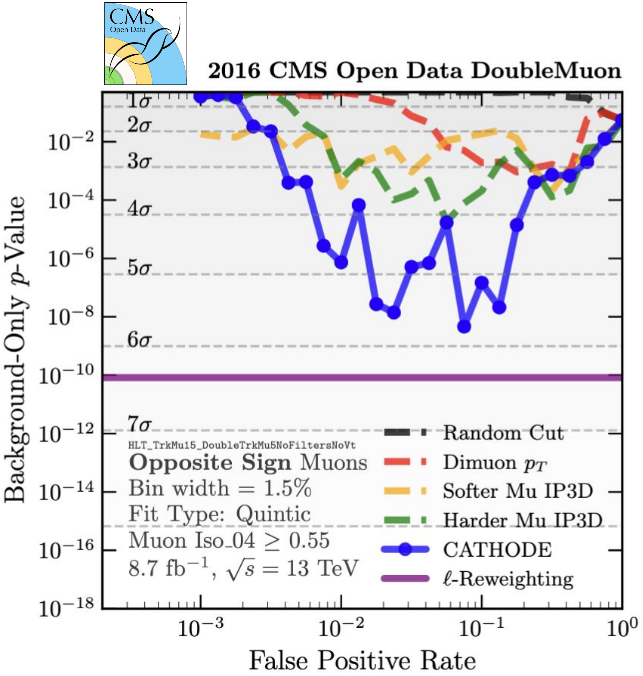


We clearly recover the Υ resonances!



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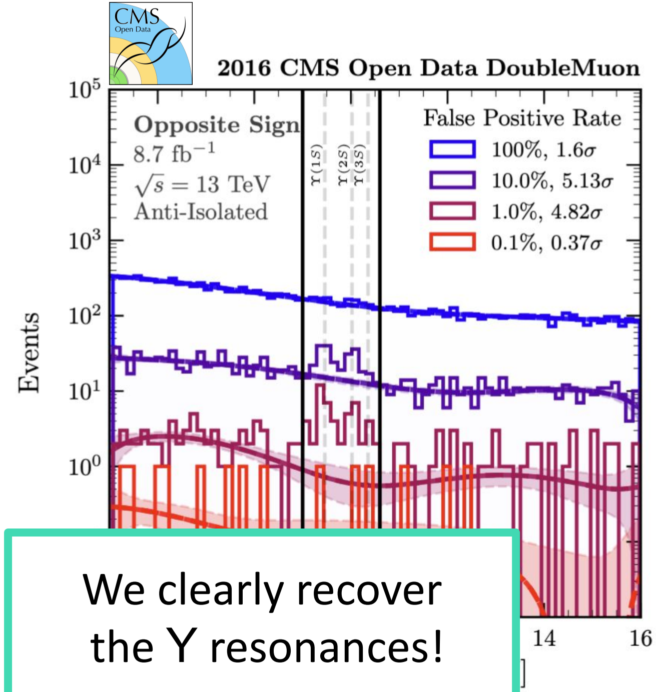

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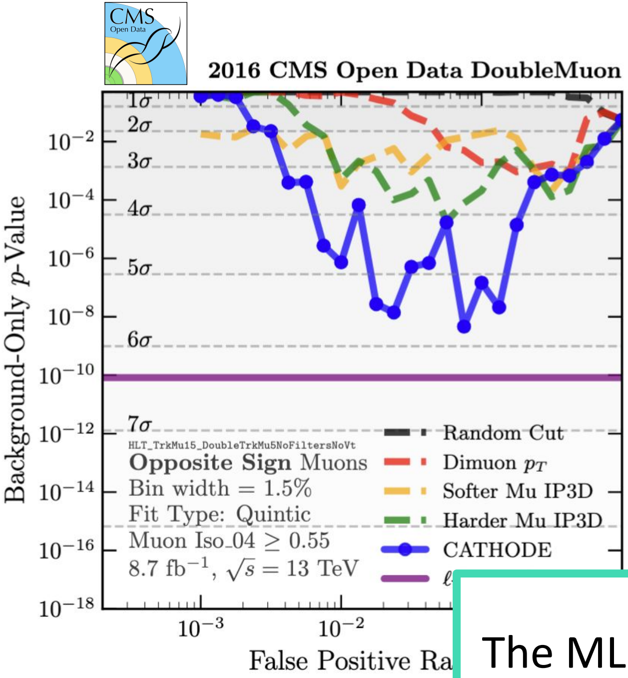

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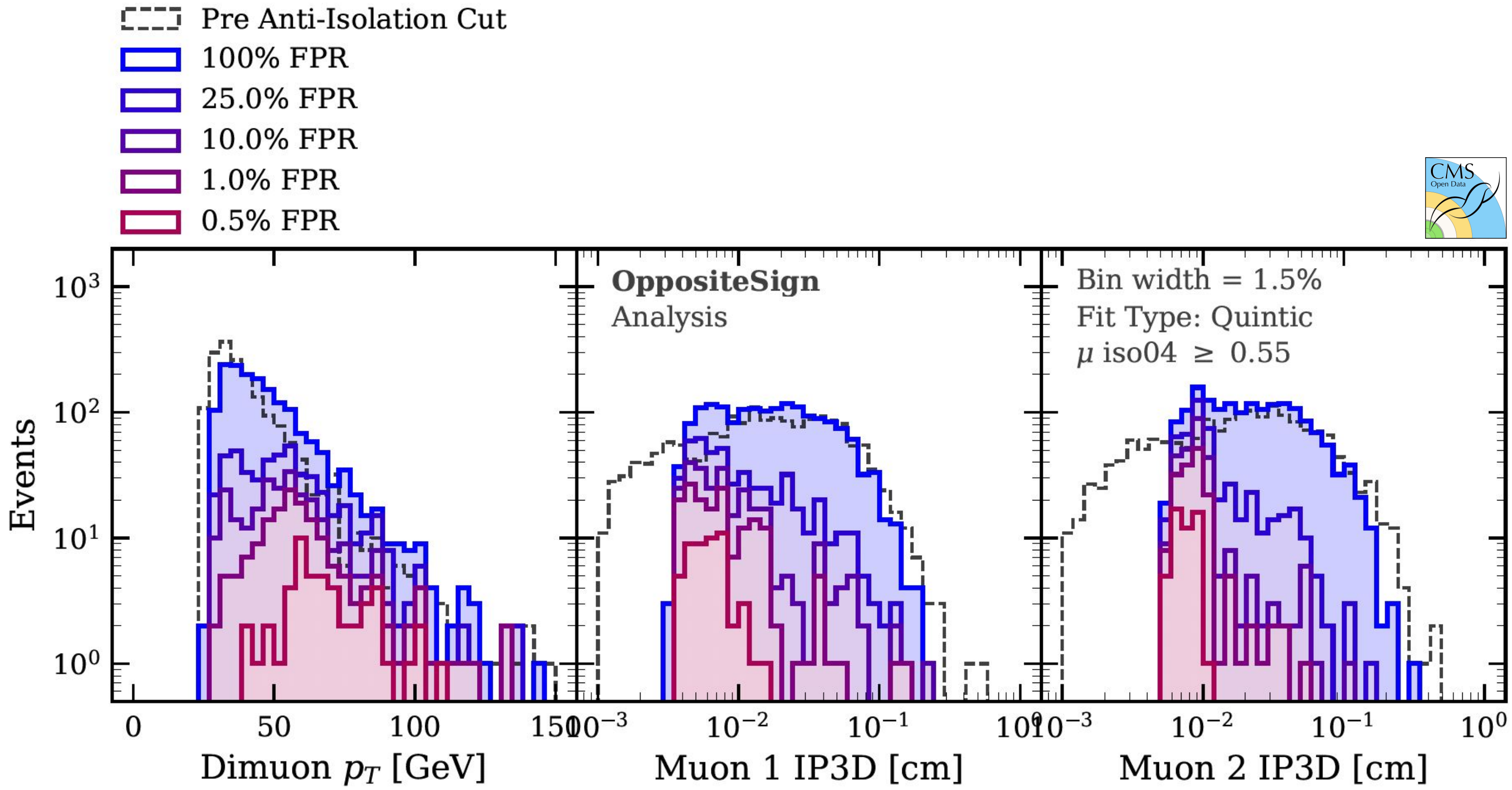
The ML test outperforms all of the classical tests!

The BDT learns genuine physical properties of ϒ's



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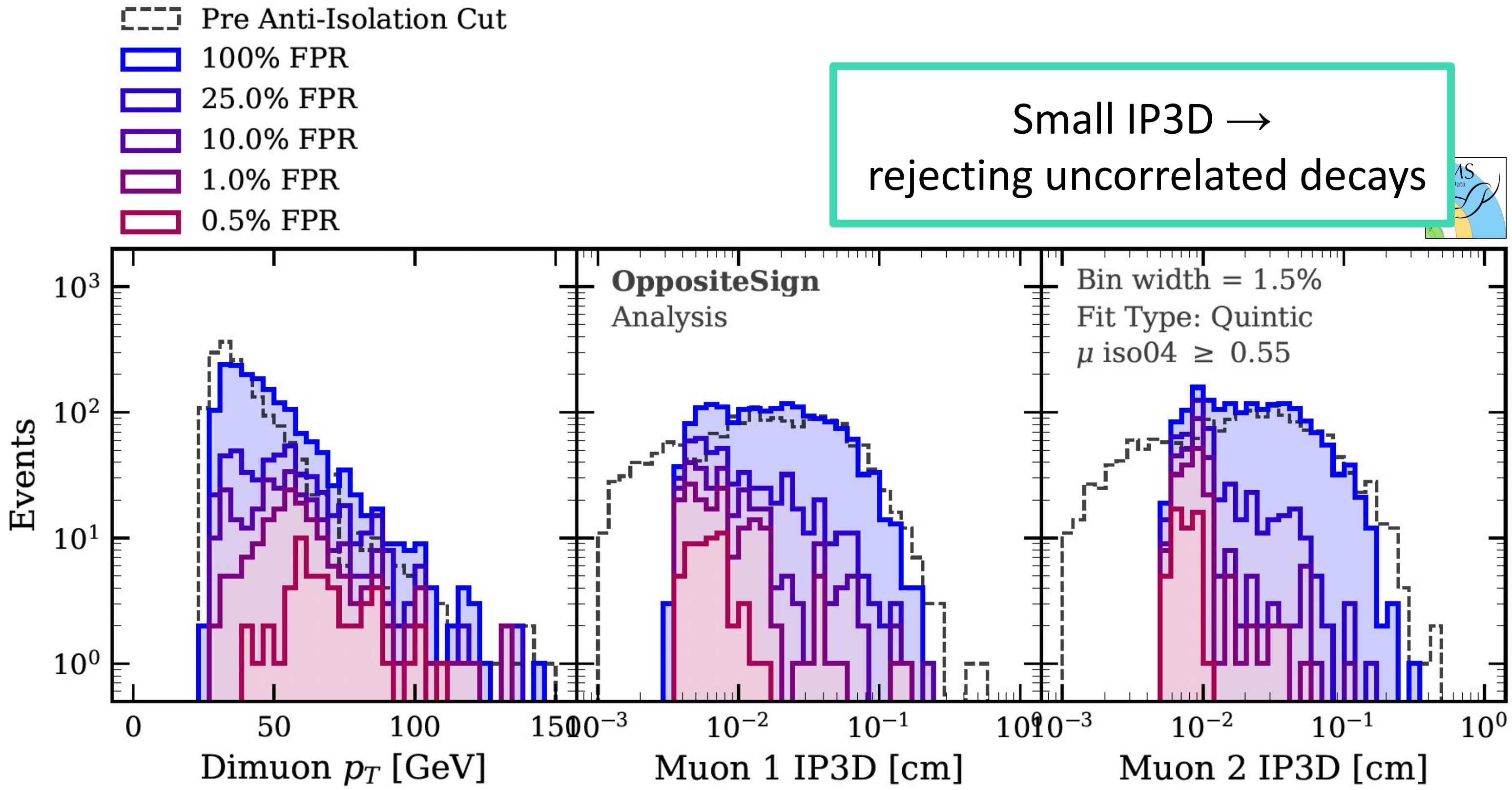
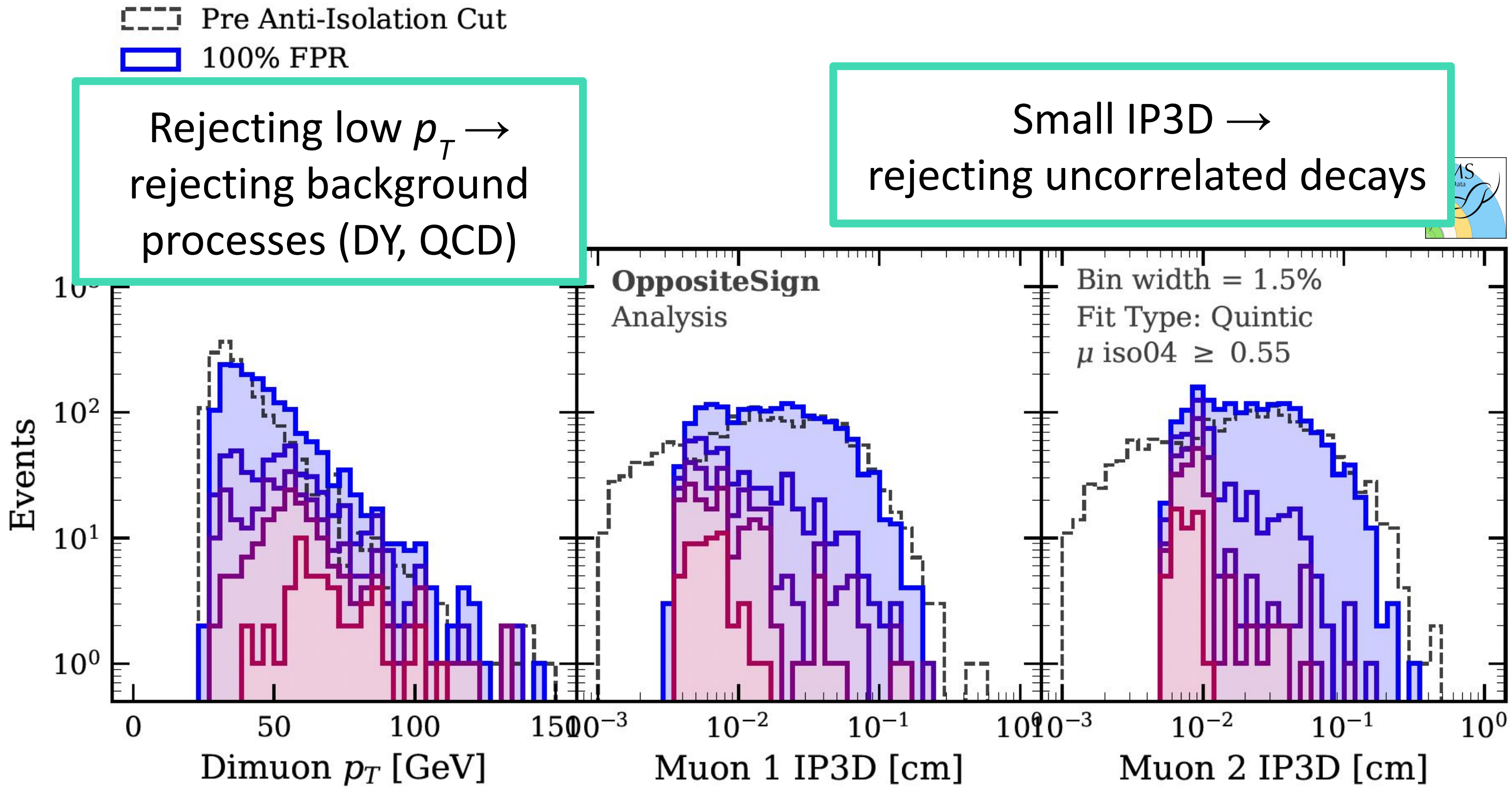


Small IP3D →
rejecting uncorrelated decays

The BDT learns genuine physical properties of Υ’s

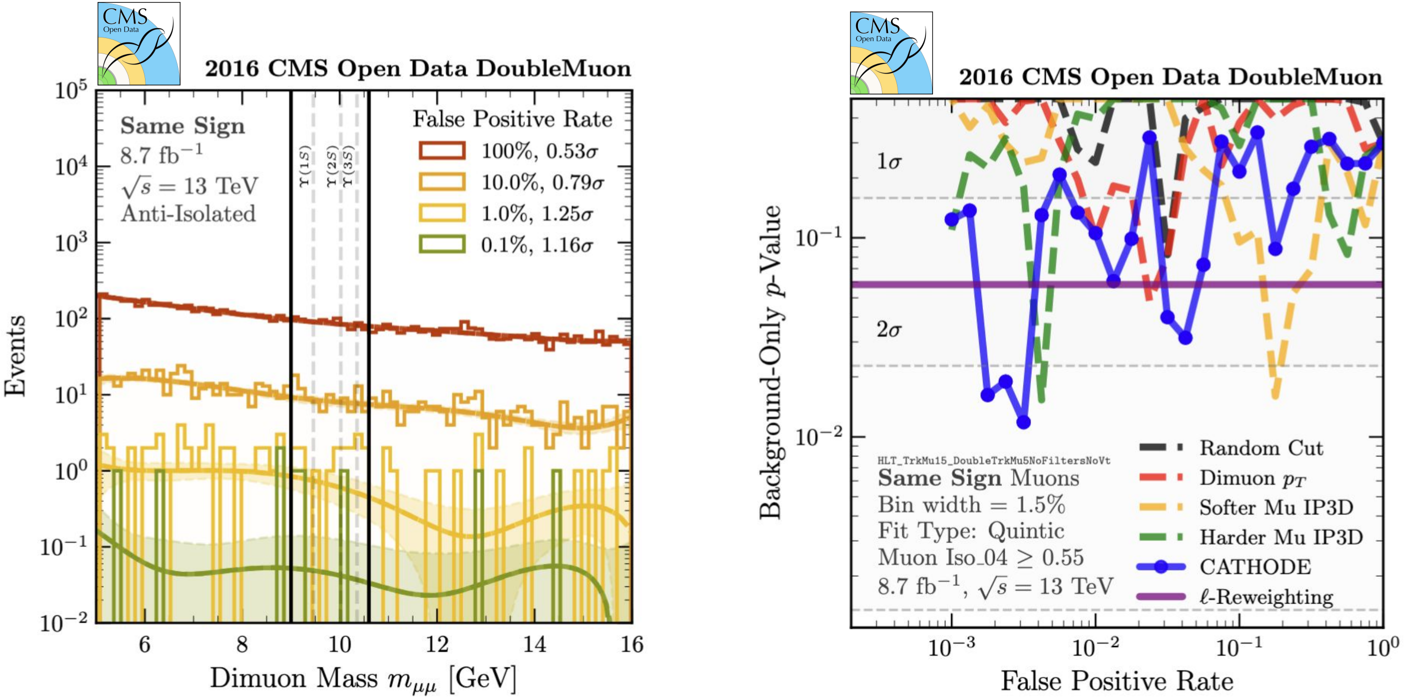
Rejecting low $p_T \longrightarrow$ rejecting background processes (DY, QCD)

Small IP3D $\longrightarrow$ rejecting uncorrelated decays



Validating the analysis

We rerun the entire analysis using same-sign dimuon pairs and find no evidence of sculpting



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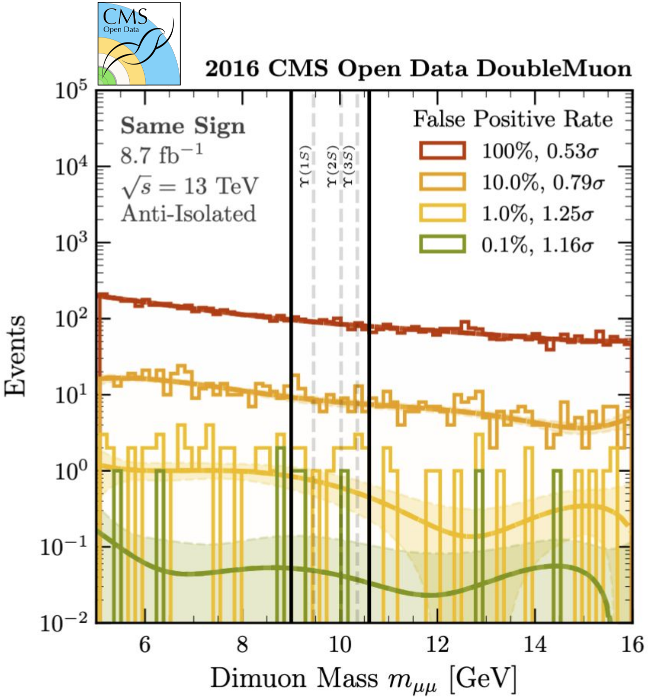
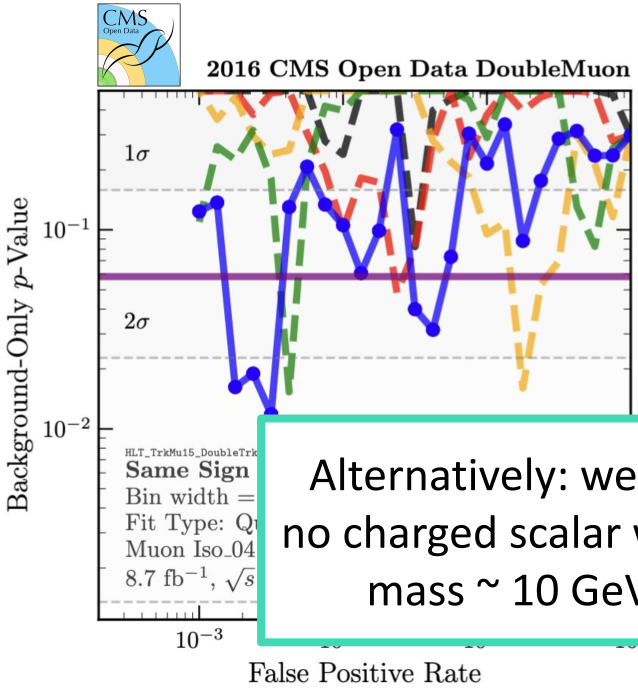
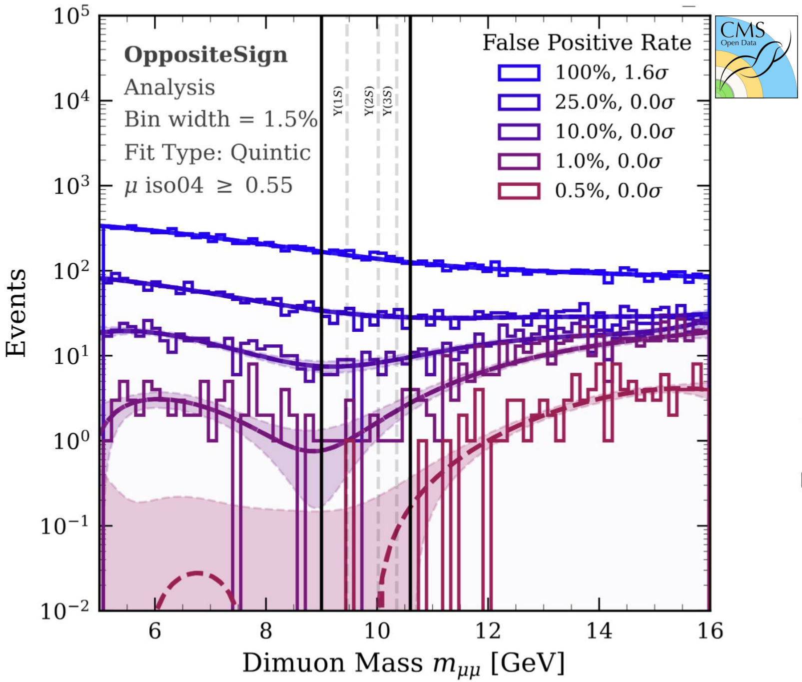


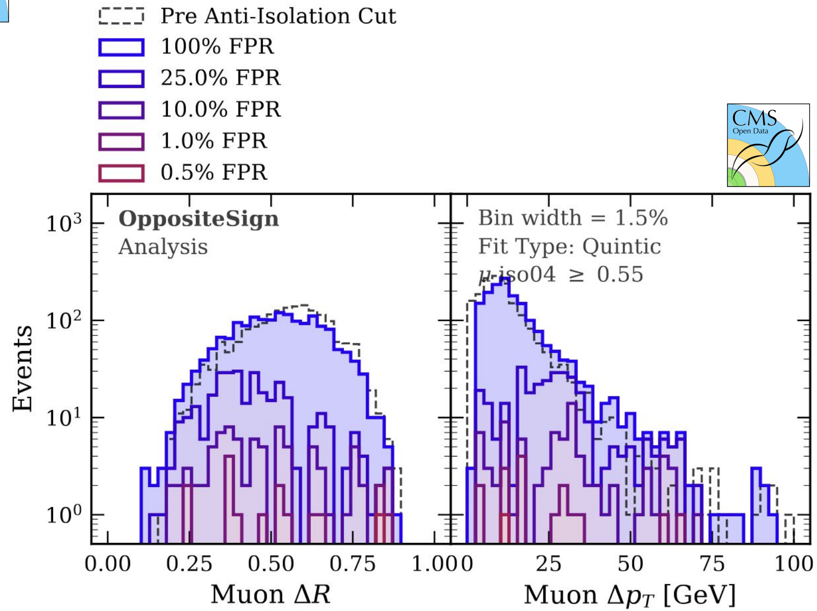


Alternatively: we find no charged scalar with a mass ~ 10 GeV!

Not all observables led to Υ discovery!

Many feature sets had significant background sculpting and / or did not elevate the Υ signal





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Conclusions

1. We carry our the first study of anti-isolated upsilons (Υ’s) produced within jets, which can probe the perturbative-nonperturbative QCD transition

2. (New ML method – wait until the next talk!)

3. We show that it is possible to use ML to find nontrivial signals in real collider data

Most importantly, this study highlights the work left to be done!

- Real data is messy and has irrelevant features.
- Background sculpting is a huge problem!

We encourage the community to test out new methods on our distilled Υ dataset $\longrightarrow$

GitHub

Data

CMS Open Data

Backup slides

Muon TightID

Plain-text description	Technical description	Comments
The candidate is reconstructed as a Global Muon	`recoMu.isGlobalMuon()`	
Particle-Flow muon id	`recoMu.isPFMuon()`	the exclusive effect of this requirement is very small, i.e. PFMuon is keeping almost all Tight Muons without this cut
χ^2/ndof of the global-muon track fit < 10	`recoMu.globalTrack()->normalizedChi2() < 10.`	To suppress hadronic punch-through and muons from decays in flight (see CMS AN 2008/098). This cut might need to be re-tuned due to the change to fully segment based global fit in 50X releases and later. It will need a retuning when muon APEs will be activated in the global track fit.
At least one muon chamber hit included in the global-muon track fit	`recoMu.globalTrack()->hitPattern().numberOfValidMuonHits() > 0`	To suppress hadronic punch-through and muons from decays in flight.
Muon segments in at least two muon stations This implies that the muon is also an arbitrated tracker muon, see SWGuideTrackerMuons	`recoMu.numberOfMatchedStations() > 1`	To suppress punch-through and accidental track-to-segment matches. Also makes selection consistent with the logic of the muon trigger, which requires segments in at least two muon stations to obtain a meaningful estimate of the muon p_T.
Its tracker track has transverse impact parameter d_{xy} < 2 mm w.r.t. the primary vertex	`fabs(recoMu.muonBestTrack()->dxy(vertex->position())) < 0.2` Or `dB() < 0.2` on `pat::Muon` [1]	To suppress cosmic muons and further suppress muons from decays in flight (see CMS AN 2008/098). The 2 mm cut preserves efficiency for muons from decays of b and c hadrons. It is a loose cut and can be tightened further with minimal loss of efficiency for prompt muons if background from cosmic muons is an issue. Another way to obtain a better cosmic-ray suppression is to complement the d_{xy} cut with a cut on the opening angle α or use a dedicated cosmic-id algorithm (see Section 7.1 of MUO-10-004). innerTrack() is also supported for dxy cut, as the performance of the two is very close.
The longitudinal distance of the tracker track wrt. the primary vertex is d_z < 5 mm	`fabs(recoMu.muonBestTrack()->dz(vertex->position())) < 0.5`	Loose cut to further suppress cosmic muons, muons from decays in flight and tracks from PU. innerTrack() is also supported for dz cut, as the performance of the two is very close.
Number of pixel hits > 0	`recoMu.innerTrack()->hitPattern().numberOfValidPixelHits() > 0`	To further suppress muons from decays in flight.
Cut on number of tracker layers with hits >5	`recoMu.innerTrack()->hitPattern().trackerLayersWithMeasurement() > 5`	To guarantee a good p_T measurement, for which some minimal number of measurement points in the tracker is needed. Also suppresses muons from decays in flight.

Network architectures and training specifications

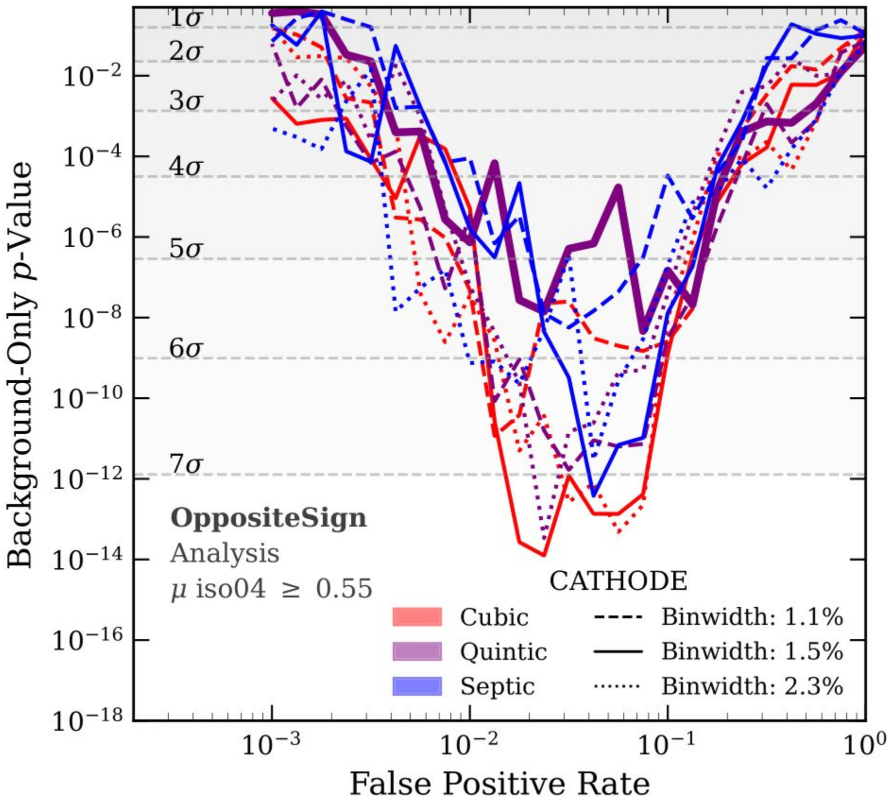
Normalizing flow architecture

- Masked Autoregressive Flow with Affine transformations
  - 1 layer of 6 MADE blocks each with 128 hidden features and each followed by a Reverse Permutation layer.
  - We use tanh activation functions and apply batch normalization after each epoch with momentum 1.
- The flow is trained for up to 1000 epochs with a learning rate of 7.5e-4 and weight decay of 1e-6. The network is evaluated at (i.e. sampled from) the epoch of lowest validation loss.
- To mitigate random model initialization and stochastic gradient descent fluctuations, we train an ensemble of five CATHODE models and draw SM proxy samples from each one (oversampling factor of 5).

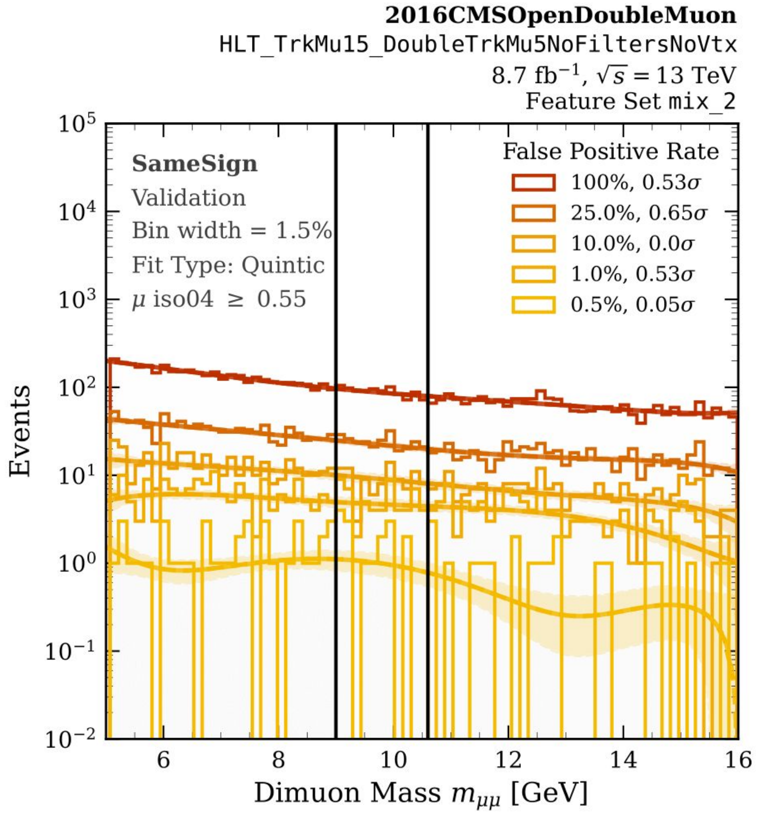
BDT architecture

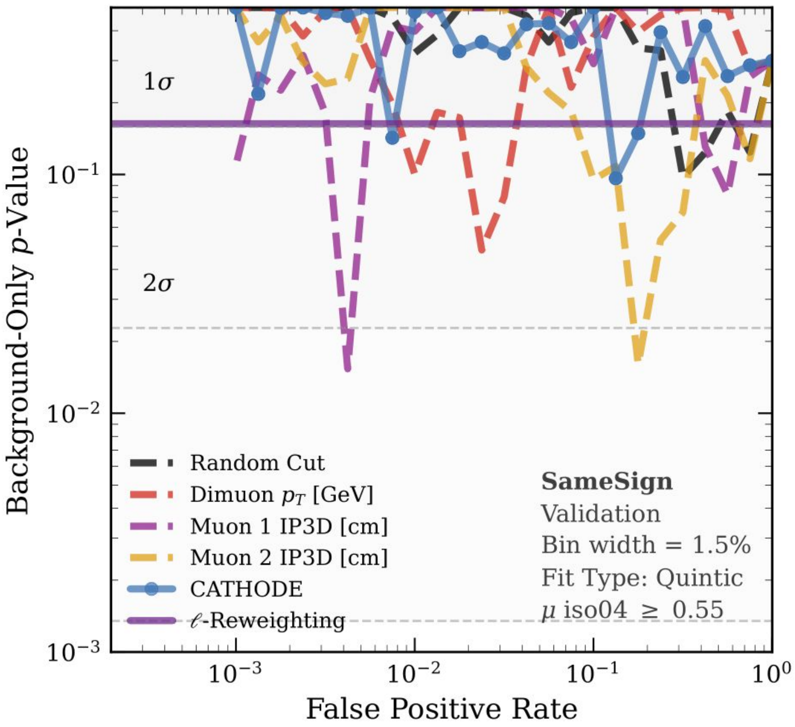
- Individual trees have a max depth of 3 and are trained on a random 70% subsample of the data.
- We train for up to 300 epochs with a learning rate of 1e-1, stopping when the validation loss does not decrease for 10 epochs. Trees are evaluated at the epoch of lowest validation loss.
- We ensemble over 100 BDT networks (which may contain an arbitrary number of trees depending on when the early stopping kicked in).

Systematic variations of binning and background fit

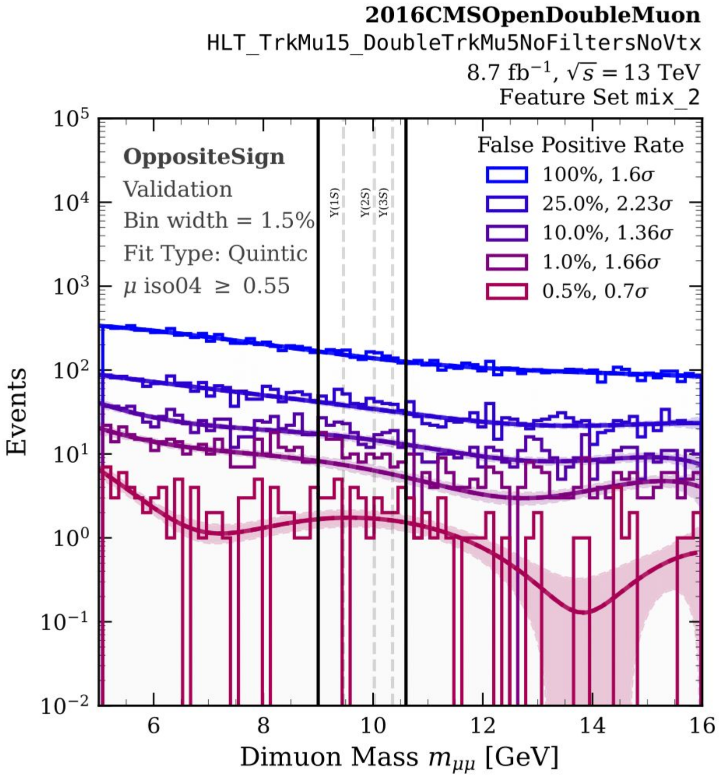


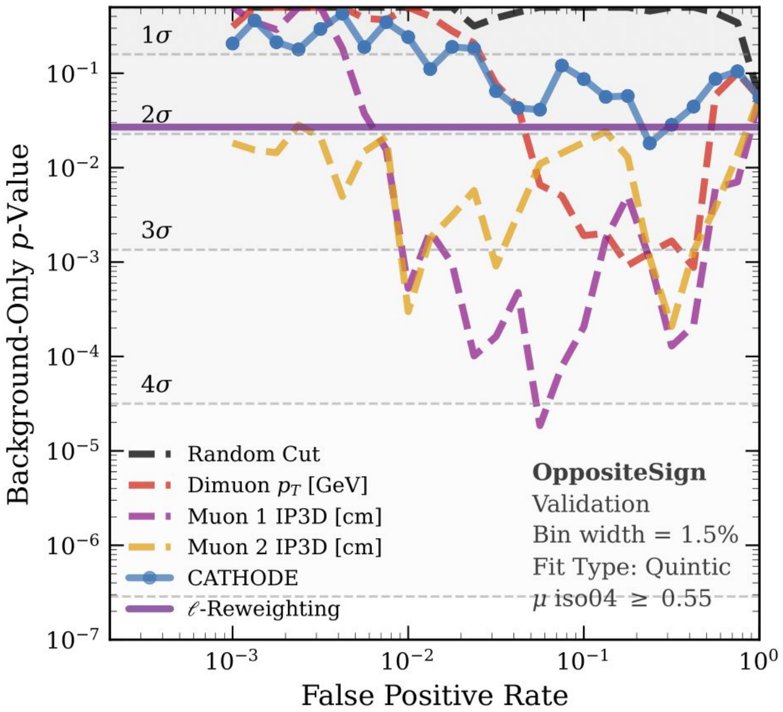
Validation: applying the OS BDT's to SS data



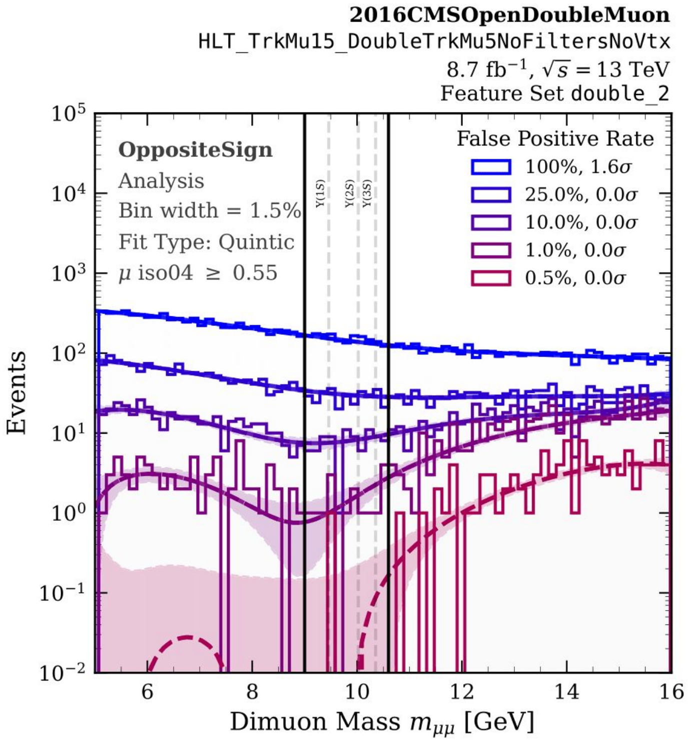


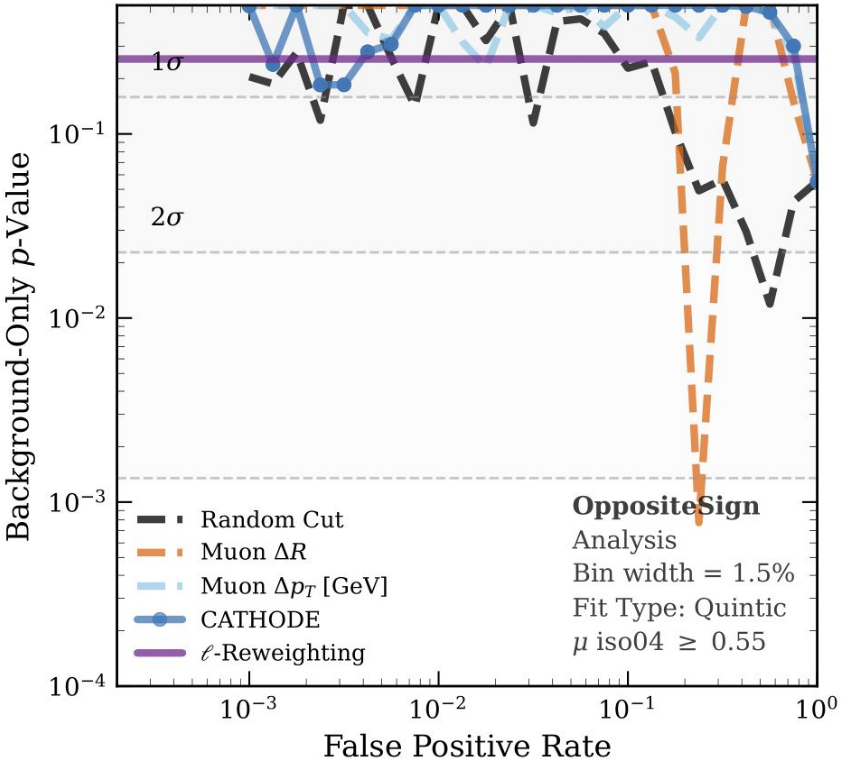
Validation: applying the SS BDT's to OS data



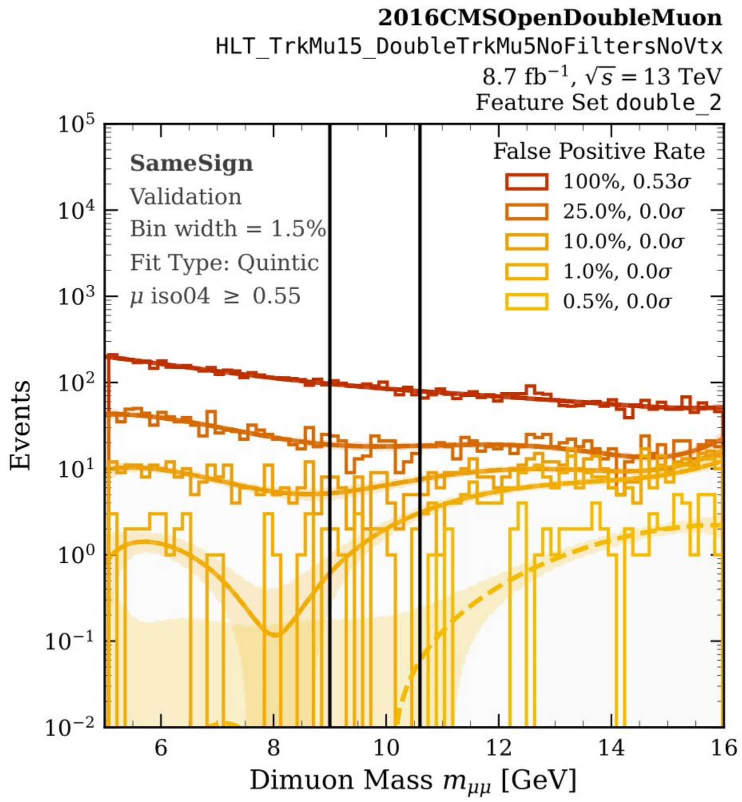


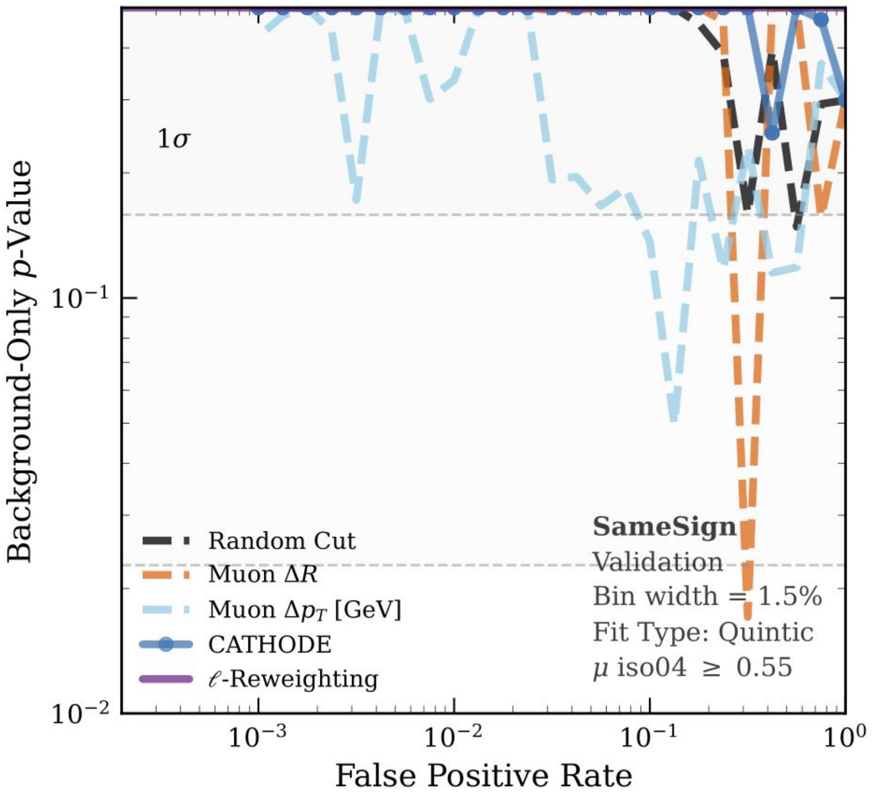
Alternative feature set: OS analysis



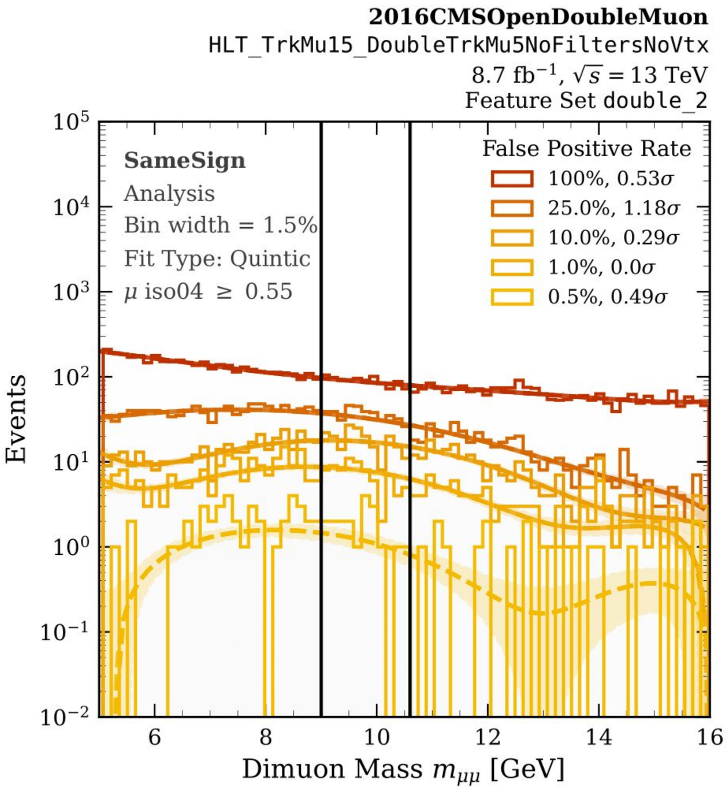


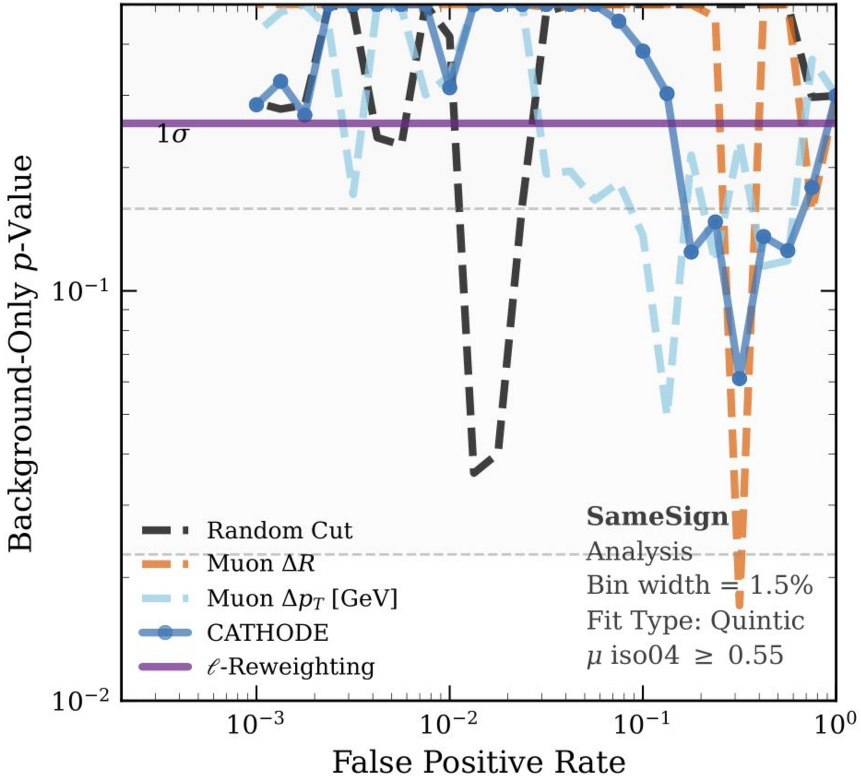
Alternative feature set: SS validation





Alternative feature set: SS analysis





Alternative feature set: OS validation