ATLAS EXPERIMENT

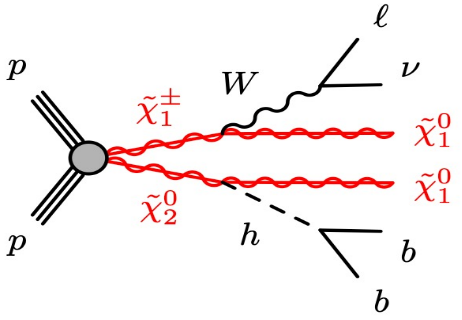
Use of advanced ML techniques in Searches for direct production of Supersymmetric electroweakinos in Wh1Lbb final states

Joe Carmignani
Flash Talk

From Graph Neural Networks to Explainable AI: comprehending and trusting Machine Learning algorithms
20 Sep 2023, 12:00 → 22 Sep 2023, 16:00 Europe/London

UNIVERSITY OF LIVERPOOL

Motivation



❖ Targeting direct EWK production of chargino-neutralino pairs and chargino pairs, decaying into LSP via on-shell Higgs bosons.

❖ LSPs (Lightest SUSY Particles), specifically the lightest neutralino $\tilde{\chi}_1^0$ and its decay mechanisms, as predicted by **Supersymmetry models,** could explain the observed discrepancy in the g-2 measurement with respect to the SM predictions and itself plays an important role as a Dark Matter candidate

❖ Typical HEP case-study:

1. Extract small signal of interest from large SM background
2. Subtle/complex differences in variable correlations distinguish signal from background
3. Complex numerical instance data, well-defined categories (underlying physics processes, 5 in our case)
   →This is the classic use-case for ML classification.
4. Build ML discriminator (**XGBoost)** to distinguish backgrounds from SUSY signals, trained on simulated Monte Carlo (split in 80:20 for training:validation) samples and use classifier output score as a discriminant variable for hypothesis testing

ML approach/challenge

- Training uses MC samples for both train and test sets (split in 80:20 for training:validation)
  - Before training, the modelling of the input variables are verified by comparing the input variable distributions of the SM backgrounds with data and comparing the linear correlations
  - Signal category includes samples with

$$m_{\tilde{\chi}_2^0/\tilde{\chi}^\pm} - m_{\tilde{\chi}_1^0} <= 200\text{GeV}$$

The **impact on the discovery potential** arises from:

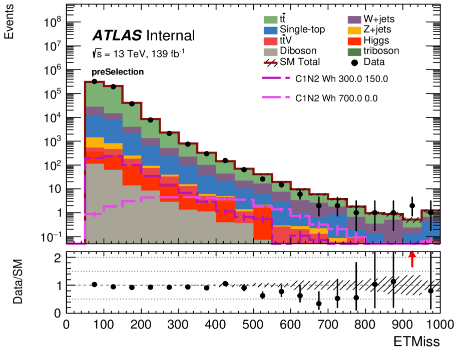
(1) limited statistics of simulated samples used for BDT training and impact on event classification process discrimination
(2) Similarity of Sig Scores to Background which impacts the final acceptance (see backup)
(3) systematic uncertainties on the modelling of the backgrounds which distort the training outcomes (see backup slides)

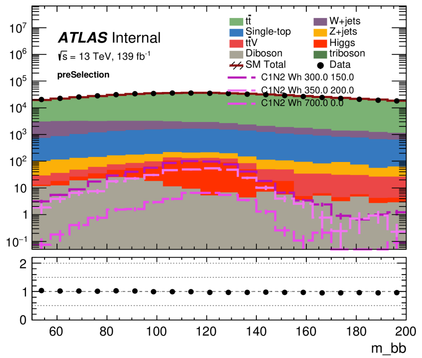
ML variable inputs
Object-level variables:
p_T^l, η^l, ϕ^l $p_T^{b_1}, \eta^{b_1}, \phi^{b_1}$ $p_T^{b_2}, \eta^{b_2}, \phi^{b_2}$ $p_T^{j_3}, \eta^{j_3}, \phi^{j_3}$ $b^{b_1}_{quantile}, b^{b_2}_{quantile}$ $b^{j_1}_{quantile}, b^{j_2}_{quantile}, b^{j_3}_{quantile}$
Event-level variables:
m_{bb} m_{CT} m_{T} $E_{\mathrm{T}}^{\mathrm{miss}}$ $\phi(E_{\mathrm{T}}^{\mathrm{miss}})$ a_{MT2} $E_{\mathrm{T}}^{\mathrm{miss}}$ Sig. [29] n_{Jets} $\Delta R_{b_1,b_2}$ m_{b1l} m_{b2l} $\Delta R_{l,b_1}$ $\Delta R_{l,b_2}$

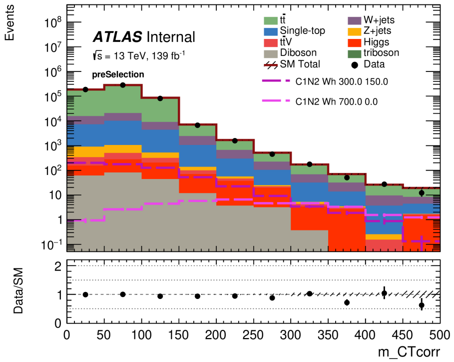
Kinematic Variables

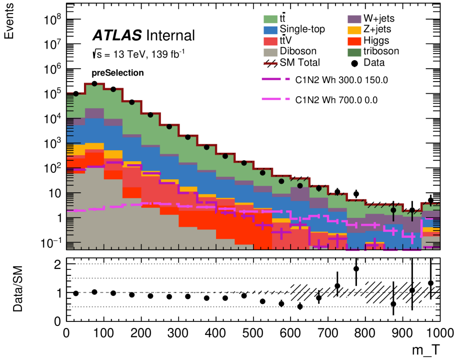
Background variables are broad identifying functions and not detector-based signatures of particle interactions

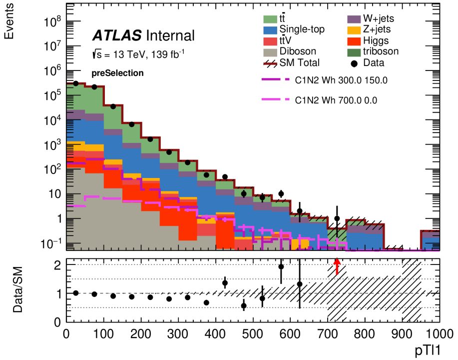
- Kinematic distributions are correlated
- Need a specialized treatment of Sig/Bkg overlap
- Powerful decorrelators and highly descriptive discriminants are needed even before treating systematics →





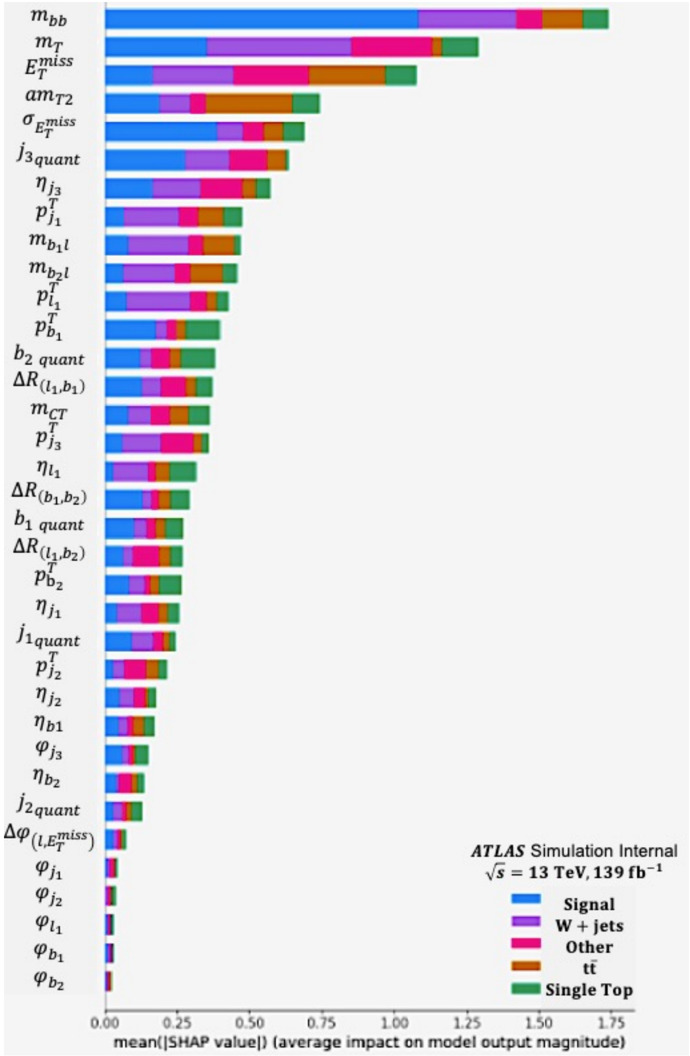






Signal region optimisation

- Problems only **partly mitigated** so far:
  - Better understanding of the distribution of most influential variables with SHAP (It evaluates the change in each output score when a feature is considered vs not considered)
  - Better Understanding of statistics in samples (systematics studies in backup slides)
  - The signal region is defined at high signal score. Note: the background scores are irrelevant as ***the 1 vs all training method*** makes them irrelevant in the instance where we are targeting signals.



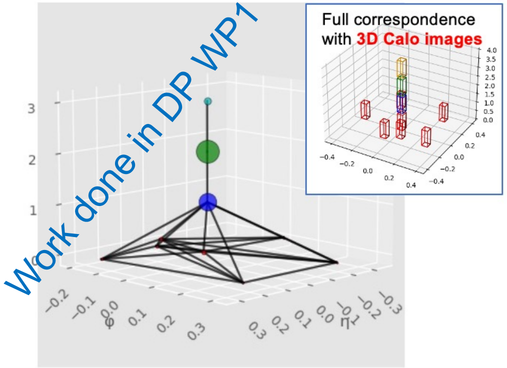
GNN-based Upgrade???

- Trusting **the ML outcome**:
  → Dependence on a given observable, minimize correlations ☑
  → Dependence on large systematics in the model ☑
  → Biasing of identified events: what features do these events have and are they what we expect ?
  → Can we discriminate and understand a structure in latent space?

(More complex than other projects with object –based analyses) →

- **Potential Transformer-based analysis Upgrade:**
  → Does a GNN learn different features with respect to a BDT
  If so, what can we gain by building such models ?
  → Can we take our variables and structure them efficiently from cloud to Graph-based format ?
  → Can a parametrization with Generative Adversarial Networks serve the purpose of reducing dependence on detailed modelling ?
  → Can we generate an inverted structure in latent space to better understand variable shapes, systematics and correlations ?

➨ How does a signal look like?



➨ How does the NN understands true positive (signal), true negative or false positive ?

T1.2: HEP1-DARK

Paper accepted by JHEP: https://arxiv.org/abs/2206.12181

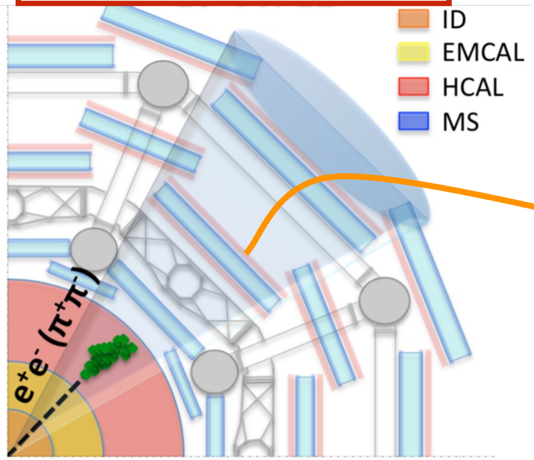
Search for “dark” photons, light particles belonging to a new hidden sector not yet discovered because too feebly interacting with ordinary matter:

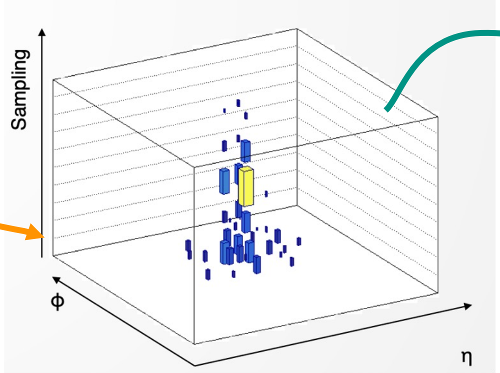
- In this case, signal leaves different signature in the detector wrt background
  - signal signature is effectively an unknown – study of systematics on the signal is non-trivial
- ML discriminator (3D-CNN) uses image classification trained to distinguish background processes from signal mapping clusters of hadrons (jets) in 3D coordinates

T1.2	**HEP1-DARK** (M1-M24; responsible: **6**; involved: 6): Use Dynamic Graph CNN to exploit multi-dimensional inputs and capabilities of describing irregular geometries. Compare results to those obtained merging of CNN approaches with graphs. Implement and evaluate xAI algorithms (see T1.3). Analyse Run2 data, prepare tools for Run3. **Staff:** PI, postdoc in M7-M24, un-costed UoL co-investigator (Dr C. Sebastiani) and PhD student. **Role of the participants:** data analysis, tools preparation, paper editors.

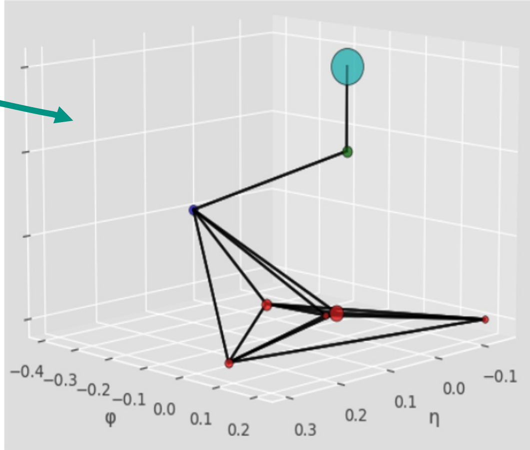
In the ATLAS data-analysis:
Build a map of jet energy deposits in ATLAS detector from: calorimeter cell positions (eta, phi, sampling layer) and energy

The ATLAS detector orthogonal view





PAM Talk



TauJETGraphs: 74 Variables (54+20)

Objects

```
"detann",
"dphinn",
"pt",
"jetpt",
"layer",
"detaECal",
"dphiECal",
"deta",
"dphi",
"CENTER_LAMBDA",
"DELTA_THETA",
"EM1CoreFrac",
"ENG_FRAC_CORE",
"ENG_FRAC_EM",
"ENG_FRAC_MAX",
"FIRST_ETA",
"LATERAL",
"LONGITUDINAL",
"NHitsInEM1",
"NPosECells_EM1",
"NPosECells_EM2",
"NPosECells_PS",
"SECOND_ENG_DENS",
"SECOND_R",
"charge",
"chiSquared",
"d0SigTJVA",
"d0TJVA",
"energy_EM1",
"energy_EM2",
"energyfrac_EM2",
"firstEtaWRTClusterPosition_EM1",
"firstEtaWRTClusterPosition_EM2",
"nCellsInEta","nDoF",
"nInnermostPixelHits",
"nPhotons",
"nPixelHits",
"nSCTHits",
"pi0BDT",
"pt1",
"pt3",
"pt5",
"ptSubRatio",
"secondEtaWRTClusterPosition_EM1",
"secondEtaWRTClusterPosition_EM2",
"z0sinthetaSigTJVA",
"z0sinthetaTJVA",
```

- These are the total node-level attributes 54 in total now
- All normalized on the mean and a 1 sigma Std

Jets

```
"jet_eta",
"jet_phi",
"nTracksTotal",
"nTracksFiltered",
"centFrac",
"EMPOverTrkSysP",
"innerTrkAvgDist",
"ptRatioEflowApprox",
"dRmax",
"trFlightPathSig",
"mEflowApprox",
"SumPtTrkFrac",
"absipSigLeadTrk",
"massTrkSys",
"etOverPtLeadTrk",
"ptIntermediateAxis",
"etaJetSeed",
"phiJetSeed",
"jet_pt",
"ptJetSeed",
```

Additional

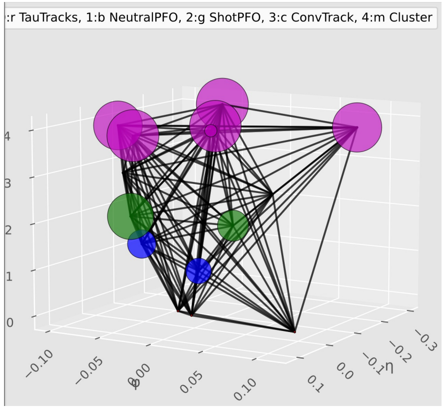
```
##newly added variables##
#########################
"chargedScoreRNN",
"isolationScoreRNN",
"conversionScoreRNN",
"fakeScoreRNN",
##ClusterVars
"e",
"SECOND_LAMBDA",
```

- All 54 available variables are there now; however, the nodes are **Homogeneous**. Objects do have common variables and counted once.
- 20 Global variables as they appear
- We want to stress the relevance of cluster variables influence further and quantify the overall effect with **newNtuples**

- Global variables are normalized, added now and used in the training just as July's Talk but with 2 added: "jet_phi" and "phiJetSeed"
- Tracks, PFOs are all taken with their specific variables as used in DeepSet and RNN with/without Clusters depending on model (to be stated later)

TauJETGraphs: Data and NN Structure

- Nodes with their attributes (74 variables) are constructed in hierarchy per object from (Dict of Dicts) in HDF5 files
- Edges are added later to connect all nodes in same and across layers to build a 3D graph (Eta, Phi, layer)



Objects are represented in node **colors**:

Red for layer 0 (TauTracks)

Blue for layer 1 (NeutralPFOs)

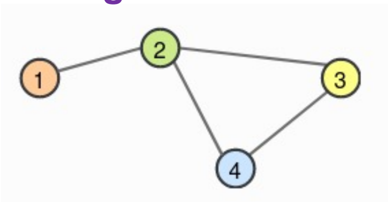
Green for layer 2 (ShotPFOs)

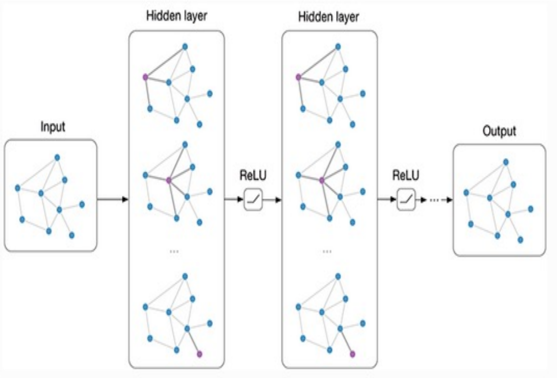
Cyan for layer 3 (ConvTracks)

Magenta for layer 4 (Clusters)

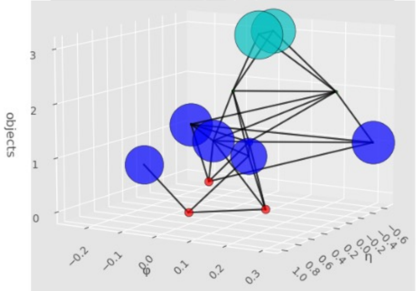
pT can also be represented and visualised in node **"size" as seen on top right**

3D visualization
Homogeneous Nodes





TauJETGraphs NN Model Pipeline



BatchNorm Layer

ARMA Conv Layers

Global Pooling Layers

FC Linear Layer

Output score

Summary and Prospects

- **Potential Expansion**: The concept of the BDT discriminant can be extended to Graph Neural Networks (GNNs), which may offer benefits such as improved sensitivity to New Physics signals (with unknown Signatures), more efficient feature extraction from complex data, and the ability to capture subtle dependencies in parameter space.

- **Hoped-for Benefits of GNNs**:

  - **Complex Data Handling**: GNNs can efficiently process complex event data with varying topologies.

  - **Incorporating Context**: GNNs can capture contextual information from parameter space, improving signal-background discrimination, overcoming statistical and systematics limitations, and amplifying acceptance.

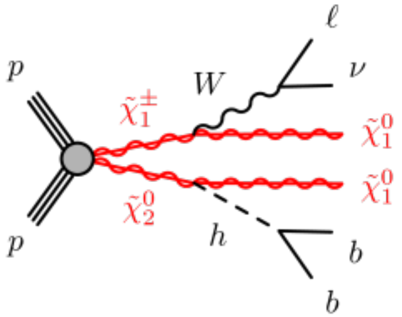
Finally, this analysis showcases the utility of ML techniques like BDT and offers a complex case-study to investigate potential benefits of applying Graph Neural Networks to particle physics research, aiming for improved sensitivity and data analysis capabilities in searches for New and Beyond Standard Model Physics.

Backup Slides

Scope and samples

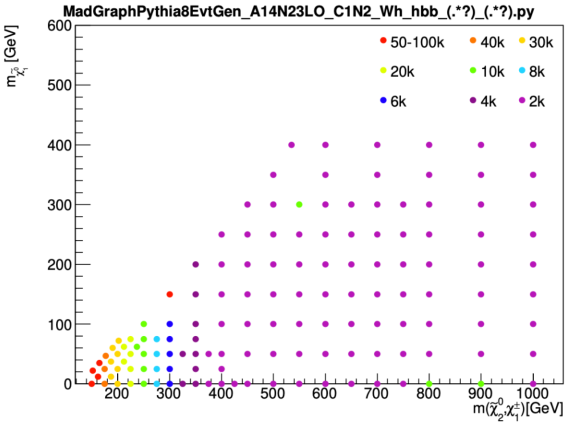
- Targeting **full Run 2 data** of **139 fb^{-1}**.

C1N2-Wh 1lbb



- **Targets compressed scenarios** with low MET using **ML method** (XGBoost).
- Latest result with 139 fb^{-1}:
  Eur. Phys. J. C 80 (2020) 691
  All hadronic analysis latest published

- **Signal samples with p4172**
  - generated using **aMC@NLO + Pythia 8**.
  - Cross sections at **NLO+NLL**.
  - produced using **full or fast simulation depending on their mass splitting**.



- **Background samples with p4172**
  - using full detector simulation.

Process	MC generator
W+jets	Sherpa 2.2.1
*** Z+jets	Sherpa 2.2.1
Diboson	Sherpa 2.2.1, 2.2.2
ttbar	Powheg + Pythia 8
Single top	Powheg + Pythia 8
Multiboson	Sherpa 2.2.1
V+H	Powheg + Pythia 8
tt+H	Powheg + Pythia 8
tt+V	aMC@NLO + Pythia 8

- **Data samples with p4173**.
- All samples are **SUSY5 derivation**.
- n-tuples production produced with **AB 21.2.148** and updated CP recommendation.

Object definitions – ML Specs

Electrons

- **Combi-basline**:
  - $p_T > 4.5$ GeV
  - $|\eta| < 2.47$
  - LooseAndBLayerLLH
  - $\Delta z_0 \sin\theta < 0.5$ mm
- **Baseline**:
  - $p_T > 7$ GeV
- **Signal**:
  - FCLoose
  - FCHighPtCaloOnly if $p_T > 75$ GeV
  - TightLLH
  - $d_0/\sigma_{d0} < 5$

Muons

- **Combi-baseline**:
  - $p_T > 3$ GeV
  - $|\eta| < 2.7$
  - Medium
  - $\Delta z_0 \sin\theta < 0.5$ mm
- **Baseline**:
  - $p_T > 6$ GeV
  - $|\eta| < 2.5$
- **Signal**:
  - Loose_VarRad
  - TightTrackOnly_VarRad if $p_T > 75$ GeV
  - $d_0/\sigma_{d0} < 3$
  - Bad muon veto

PFlow Jets

- Anti-k_t algorithm (R = 0.4)
- $p_T > 30$ GeV
- $|\eta| < 2.8$
- JVT tight WP for $p_T < 120$ GeV and $|\eta| < 2.5$

B-tagging

- DL1r @ Pseudo-Continuous 77% WP.

Large-R jets (not relevant for Wh)

- Anti-k_t algorithm (R = 1.0)
- Trimmed with $f_{cut} = 0.05$ and $R_{sub} = 0.2$
- $p_T > 200$ GeV; $|\eta| < 2.0$
- **W/Z-tagging**: 3-var, 50% WP

MET

- baseline objects + TST.
- Tight WP.

- **Overlap removal procedure** applied to **baseline objects** and relied on **SUSY background forum recommendation**.
- **Combination requirements** on **number of combi-baseline leptons** applied.

Triggers

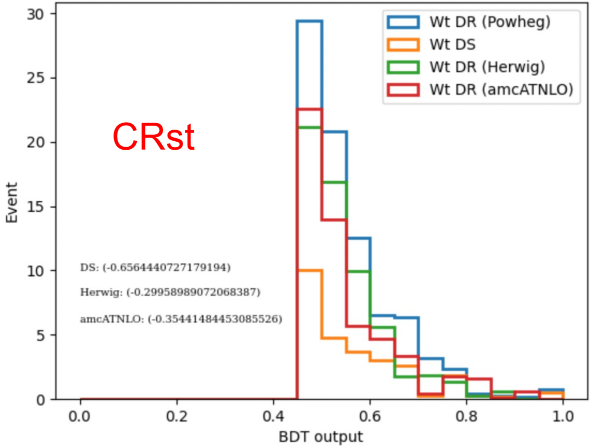
- Using **Single-lepton trigger**
  - logical OR combination of multiple single electron and single muon triggers.

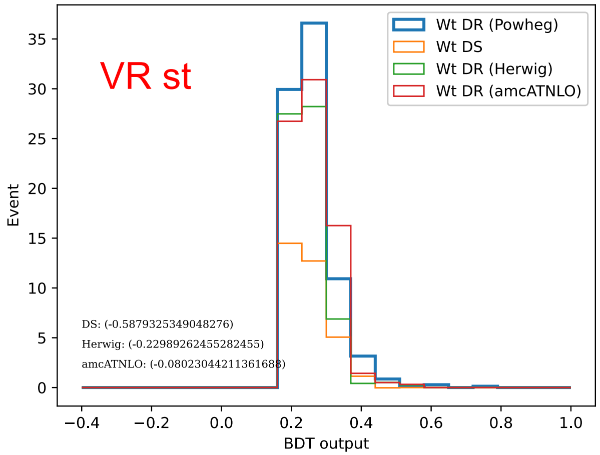
Trigger	Trigger name	Year	HLT cut [GeV]	Offline cut [GeV]
single electron trigger	HLT_e24_lhmedium_L1EM20VH	2015	24	25
	HLT_e60_lhmedium	2015	60	61
	HLT_e120_lhloose	2015	120	121
	HLT_e26_lhtight_nod0_ivarloose	2016-2018	26	27
	HLT_e60_lhmedium_nod0	2016-2018	60	61
	HLT_e140_lhloose_nod0	2016-2018	140	141
single muon trigger	HLT_mu20_iloose_L1MU15	2015	20	21
	HLT_mu26_ivarmedium	2016-2018	26	27.3
	HLT_mu50	2015-2018	50	52.5

- Single lepton triggers preferred to MET triggers as compressed region might lead to softer MET (while leptons are NOT soft as coming from a real W)
- Lepton pT requirements according to increased trigger thresholds over the years going from 25 (21) GeV to 27 (27.3) GeV for electron (muon) events

Systematic uncertainties: tt / Wt interference

- As in many other analyses before this one, the predictions of the MC samples generated with the diagram-subtraction scheme (DS) are found VERY different from nominal
- Yields, uncertainties and TF uncertainties in CR Single Top and SRs compared to unc from herwig (second largest in SRs)
- Validation region yields also clearly indicate that DS predictions are 2.5 times less than nominal





	CRST	SR1	SR2	SR3	SR4	Integrated
Nominal	84.82	3.24	2.62	1.86	0.87	8.59
DS	29.14	0.10	0.80	0.00	0.32	1.21
Herwig	59.41	2.91	2.85	2.02	1.33	9.11

Uncertainty on yield

	CRST	SR1	SR2	SR3	SR4	Integrated
DS	-65.64%	-97.02%	-69.41%	-100.00%	-63.61%	-85.88%
Herwig	-29.96%	-10.21%	8.74%	8.42%	53.63%	6.05%

TFs

	CRST	SR1	SR2	SR3	SR4	Integrated
Nominal		0.03821	0.03088	0.02197	0.01021	0.10127
DS	-	0.00331	0.02750	0.00000	0.01082	0.04163
Herwig	-	0.04898	0.04795	0.03400	0.02240	0.15333

TF uncertainty

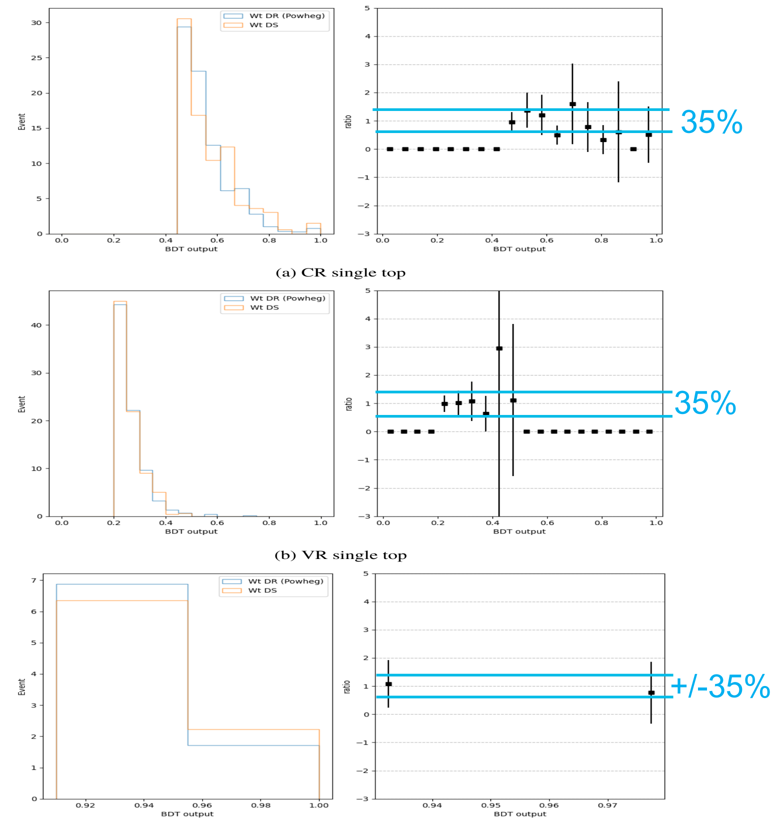
	CRST	SR1	SR2	SR3	SR4	Integrated
DS	-	-91.33%	-10.96%	-100.00%	5.94%	-58.89%
Herwig	-	28.20%	55.26%	54.80%	119.34%	51.41%

Additional test and adoption of 35%

- It was suggested to normalize the DS yields to the DR (nominal) and consider as uncertainty the residual shape uncertainty
- A good solution in principle – however the issue is that DS predictions in Signal regions are practically 0 hence there is not much to be normalized there:
  - Very few raw events pass the selection

	SR1	SR2	SR3	SR4	Integrated
Nominal	3.24	2.62	1.86	0.87	8.59
DS	0.10	0.80	0.00	0.32	1.21

- Solution:
  - Add manually an uncertainty consistent with previous studies with WWbb truth samples:
    - **35% for SR closer to the present selection**
    - **Shape uncertainty from normalized ratio lower where there is stats: conservative**



(a) CR single top

(b) VR single top

(c) SR inclusive.

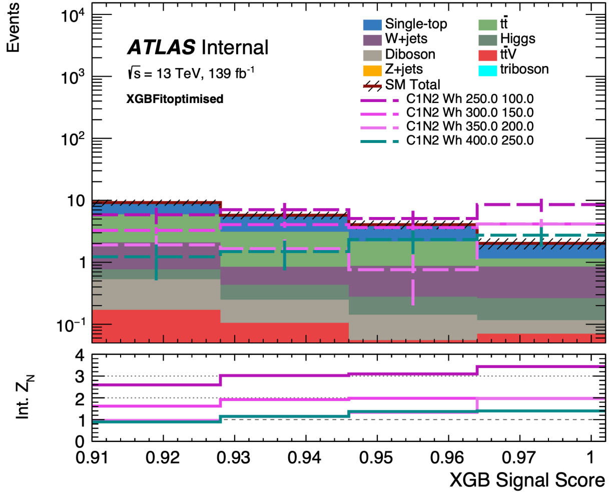
Signal region definition

- From pre-selection to SR:

$(1)\sigma_{E_T^{miss}}$ significance raised to 8

$(2)m_{bb}$ in the range 90-140 GeV

- Inclusive signal region: **Score [0.91-1], split then in 4 bins**



Exclusion regions – multibin fit using 4 bins

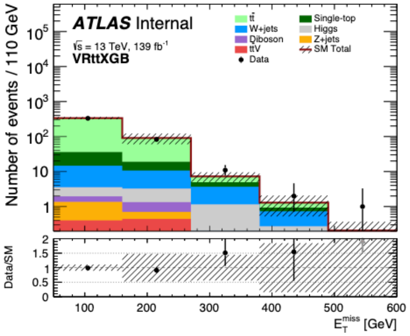
w_{Sig}	4 bins $\in [0.91, 0.928, 0.946, 0.964, 1]$

yields	SR_Inclusive	Bin0 [0.91,0.928]	Bin 1 [0.928,0.946]	Bin 2 [0.946,0.964]	Bin 3 [0.964, 1]
MC exp. SM+Signal events	30.95 ± 3.96	11.67 ± 2.77	8.15 ± 2.72	6.89 ± 2.09	4.26 ± 1.41
MC exp. SM events	20.92 ± 3.51	9.15 ± 1.84	5.72 ± 2.04	4.05 ± 1.14	2.01 ± 0.84
MC exp. Z events	0.08 ± 0.04	$0.04^{+0.07}_{-0.04}$	$0.04^{+0.08}_{-0.04}$	$0.00^{+0.02}_{-0.00}$	$0.02^{+0.07}_{-0.02}$
MC exp. W events	2.91 ± 1.09	1.32 ± 0.84	$0.41^{+0.51}_{-0.41}$	0.60 ± 0.24	0.59 ± 0.19
MC exp. ttbar events	7.68 ± 2.11	3.83 ± 1.63	2.26 ± 1.88	1.29 ± 0.86	$0.30^{+0.55}_{-0.30}$
MC exp. st events	8.59 ± 2.18	3.24 ± 1.31	2.62 ± 1.03	1.86 ± 0.77	0.87 ± 0.70
MC exp. diboson events	0.64 ± 0.21	0.36 ± 0.20	0.14 ± 0.11	$0.09^{+0.12}_{-0.09}$	0.05 ± 0.04
MC exp. Higgs events	0.71 ± 0.27	$0.24^{+0.29}_{-0.24}$	0.18 ± 0.05	0.14 ± 0.02	0.15 ± 0.03
MC exp. ttV events	0.32 ± 0.08	0.13 ± 0.07	$0.06^{+0.10}_{-0.06}$	0.08 ± 0.07	0.05 ± 0.02
MC exp. C1N2_Wh_450.0_250.0 events	10.03 ± 1.83	2.51 ± 2.07	2.43 ± 1.79	2.84 ± 1.49	2.25 ± 1.13
Other signal yields (stat only)					
MC exp. C1N2_Wh_250.0_100.0 events	26.53 ± 3.78	5.85 ± 1.72	7.06 ± 2.00	5.08 ± 1.71	8.54 ± 2.10
MC exp. C1N2_Wh_300.0_150.0 events	15.13 ± 0.85	3.28 ± 0.39	4.06 ± 0.45	3.64 ± 0.41	4.16 ± 0.45
MC exp. C1N2_Wh_350.0_200.0 events	8.27 ± 1.73	1.91 ± 0.79	1.66 ± 0.68	0.76 ± 0.56	4.14 ± 1.27
MC exp. C1N2_Wh_400.0_250.0 events	6.36 ± 1.16	1.75 ± 0.56	0.83 ± 0.37	1.57 ± 0.51	2.22 ± 0.80

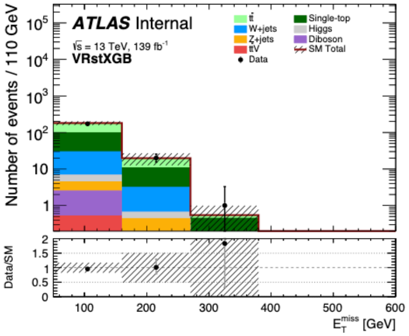
Discovery regions:

- SR d1 [w_{sig}>0.91]
- SR d2 [w_{sig}>0.928]
- SR d3 [w_{sig}>0.946]
- SR d4 [w_{sig}>0.964]

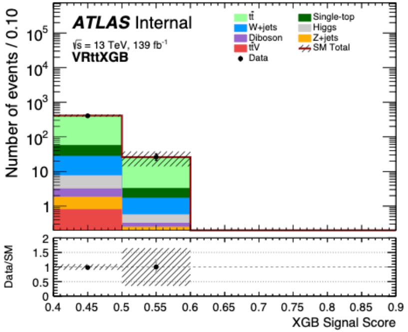
Systematic Uncertainties

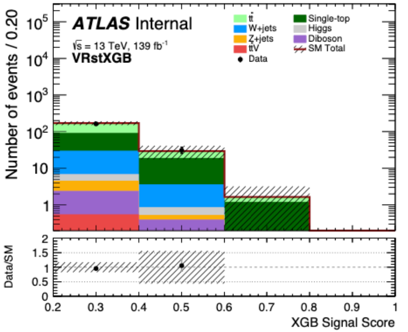


(a)



(b)





C1C1-Wh model	SRXGB Bin 1 [0.91, 0.928)	SRXGB Bin 2 [0.928, 0.948)	SRXGB Bin 3 [0.948, 0.964)	SRXGB Bin 4 [0.964, 1]
Total background expectation	9.41	5.73	4.15	2.15
Total background systematic	±2.13 [22.65%]	±2.03 [35.41%]	±1.39 [33.62%]	±0.73 [34.14%]
Theoretical systematic uncertainties				
$t\bar{t}$	±1.08 [11.5%]	±0.71 [12.3%]	±0.52 [12.4%]	±0.10 [4.7%]
Single top	±1.17 [12.4%]	±0.91 [15.8%]	±0.91 [21.9%]	±0.37 [17.4%]
W+jets	±0.17 [1.8%]	±0.14 [2.4%]	±0.12 [2.7%]	±0.04 [1.7%]
Other backgrounds	±0.14 [1.7%]	±0.13 [1.8%]	0.13 [3.0%]	0.1 [3.2%]
MC statistical uncertainties				
MC statistics	±1.04 [11.0%]	±0.79 [13.9%]	±0.66 [16.0%]	±0.41 [18.8%]
Uncertainties in the background normalisation				
Normalisation of dominant backgrounds	±1.26 [13.4%]	±0.89 [15.6%]	±0.51 [12.3%]	±0.19 [8.7%]
Experimental systematic uncertainties				
Jet energy resolution	±1.11 [11.7%]	±1.15 [20.1%]	±0.57 [13.8%]	±0.41 [19.2%]
Jet energy scale	±0.52 [5.5%]	±0.31 [5.3%]	±0.33 [8.0%]	±0.07 [3.0%]
b-tagging	±0.12 [1.4%]	±0.75 [13.1%]	±0.05 [1.5%]	±0.06 [2.7%]
Pile-up/JVT	±0.43 [4.5%]	±0.49 [8.6%]	±0.29 [7.2%]	±0.09 [4.3%]
Lepton and $E_{\mathrm{T}}^{\mathrm{miss}}$ uncertainties	±0.05 [0.6%]	±0.36 [4.6%]	±0.14 [3.4%]	±0.12 [3.7%]

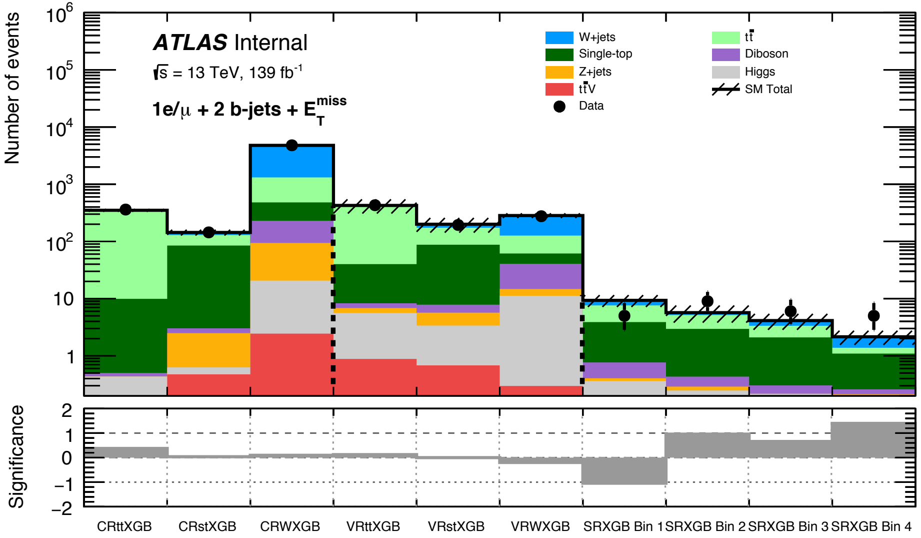
- VR plots in Good agreement within uncertainties (bands are large where stat is low)

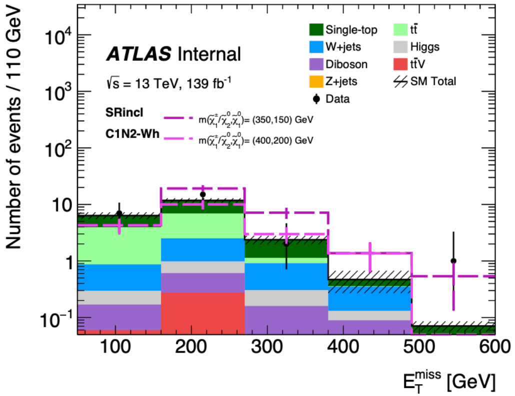
Huge effort spent to make systematics coherent with EWK, with the only exception of a conservative 35% uncertainties on the Wt interference term (see back-up for details)

Analysis Summary

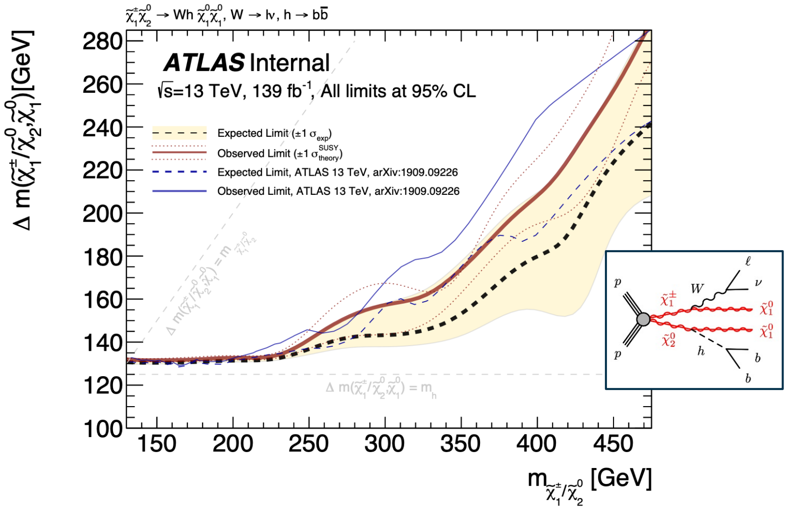
C1N2_Wh:

- Targeting full Run 2 data of 139 fb^{-1}.
- Final state: exactly one isolated lepton (e^- or μ), 2b-jets and large missing transverse momentum.
- Final states with small mass-splitting ($m_{\tilde{\chi}_1^{\pm}/\tilde{\chi}_2^0} = m_h$)
- Two b-tagged jets identify the Higgs
- **BDT multi-classifier scores identify orthogonally the 4 bins of Signal Regions in the complex compressed phase-space of C1N2**



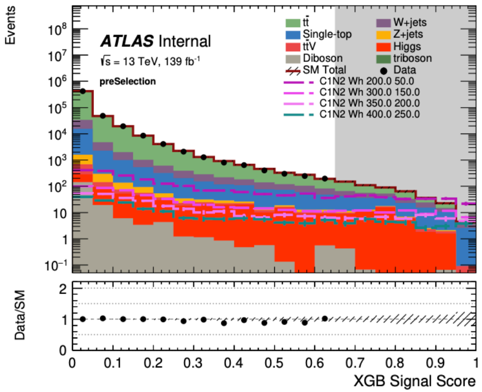


Overall yields agree with SM predictions. Interpreted in simplified SUSY signal models

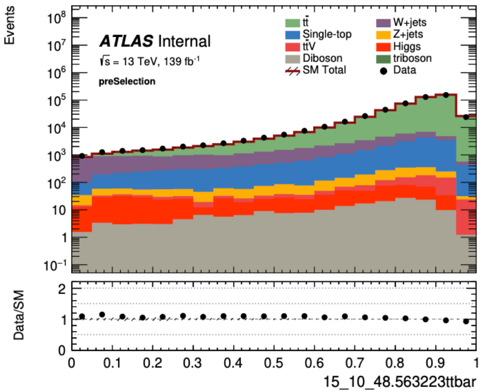


➢ *<u>BDT-based C1N2_Wh</u>* search for LSP exceeds previous constraints by up to 40 GeV in the range of **200 − 260 GeV** and **280 − 470 GeV** in $\tilde{\chi}_1^{\pm}/\tilde{\chi}_2^0$ mass.

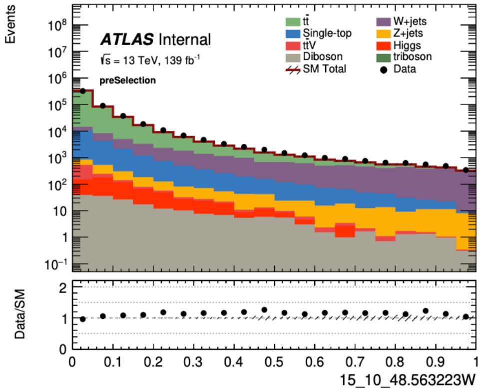
BDT scores Sig/Bkg



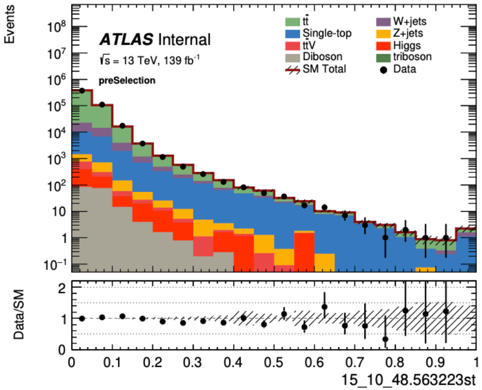
(a) Signal score



(b) $t\bar{t}$ score



(c) W+jets score



(d) Single-top score