Implementation of full and simplified likelihoods in CheckMATE

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Abstract

Multibin searches in Checkmate

1 Introduction

2 Technical implementation

In this section, we introduce the methods of implementation the simplified and full likelihoods in CheckMATEand user switches for controlling their execution.

2.1 ATLAS

The functionality of combining signal regions for recasting in ATLAS searches can be implemented using either the full likelihood model [1] or following a simplified approach detailed in Ref. [2]. Table 1 lists the ATLAS analyses with likelihood functionality implemented in CheckMATE. The simplified likelihood method requires background rates and uncertainties that were already available in the implemented searches. The full likelihood requires an appropriate file in the JSON format and these file were released by ATLAS for 7 searches already implemented in CheckMATE. For the searches atlas_2004_14060, atlas_2006_05880, atlas_2111_08372 and atlas_2202_07953 the full model files are not available but using the published data one can still perform simplified model fitting in multibin signal regions.

The full likelihoods statistical models are encoded in the JSON files by the ATLAS collaboration. The information provided includes the number of background events for all signal and control regions and for each major background category separately. This results in a large number of nuisance parameters and the complexity of the procedure makes the hypothesis testing very CPU-expensive. Additionally, on the recasting side, in order to fully exploit the method one should also implement CRs, which was not a standard approach in CheckMATE. Currently, just one search atlas_2010_14293 has a full implementation of all CRs. In other searches it is assumed that the contribution of signal to CRs is negligible. This assumption is not obviously fulfilled in all imaginable new physics models.

On the technical side, after the usual evaluation of events within CheckMATE, a JSON patchset is created which encapsulates signal contributions to SRs (and CRs if applicable). The patchset is then combined with the background-only input from ATLAS. This is further evaluated using the package pyhf [3–5], which is a Python implementation of the HistFactory specification for binned statistical models [6, 7]. The signal strength μ is the parameter of interest. Depending on the user choices output can contain information about expected and observed upper limit on μ, with 2-σ bounds, along with observed and expected CL_s for $\mu = 1$. The default method of calculation is by using the asymptotic calculator, see [3].

By default the above calculation will be executed using the Spey program [8]. Spey is a cross-platform Python-based package that allows for a statistical inference of hypotheses using different likelihood prescriptions.[♮1] In our setup it gives a somewhat better control over the calculation than the above mentioned CheckMATE-pyhf interface, but nevertheless the calculation is still performed in pyhf framework. The main motivation, however, for using Spey was a possibility of combining different searches (also across experiments), which is planned in the next release of CheckMATE. In any case. a direct evaluation using pyhf and by-passing Spey also remains available.

Since the evaluation of full likelihoods is normally time consuming it is not practical for large scans of the parameter space. Therefore the alternative approach to likelihood evaluation relies on the concept of simplified likelihood [2]. In this case the background model is approximated with the total SM background rate obtained in the background-only fit in the full model. A single nuisance

[♮1] Installation of Spey is straightforward: `pip install spey`. Please refer to the Spey online documentation for more details [9].

Name	Description	#SR	N_{bin}	Full	Ref.
`atlas_1908_03122`	Search for bottom squarks in final states with Higgs bosons, b-jets and E_T^{miss}	2	7	✓	[10]
`atlas_1908_08215`	Search for electroweak production of charginos and sleptons in final states with 2 leptons and E_T^{miss}	1	52	✓	[11]
`atlas_1911_06660`	Search for direct stau production in events with two hadronic taus	1	2	✓	[12]
`atlas_1911_12606`	Search for electroweak production of supersymmetric particles with compressed mass spectra	2	76	✓	[13]
`atlas_2004_14060`	Search for stops in hadronic final states with E_T^{miss}	3	14	✗	[14]
`atlas_2006_05880`	Search for top squarks in events with a Higgs or Z boson	3	23	✗	[15]
`atlas_2010_14293`	Search for squarks and gluinos in final states with jets and E_T^{miss}	3	60	✓	[16]
`atlas_2101_01629`	Search for squarks and gluinos in final states with one isolated lepton, jets, and E_T^{miss}	1	26	✓	[17]
`atlas_2106_01676`	Search for chargino–neutralino production in final states with 3 leptons and E_T^{miss}	2	72	✓	[18]
`atlas_2111_08372`	Search for associated production of a Z boson with an invisibly decaying Higgs boson or dark matter candidates	1	22	✗	[19]

Table 1: List of implemented ATLAS analyses which have likelihood-based signal regions (all searches at $\sqrt{s} = 13$ TeV and $\mathcal{L} = 139$ fb^{-1}).

parameter correlated over all bins and representing post-fit background uncertainty is constrained by unit normal distribution. The evaluation is also performed using the `pyhf` package.

2.2 CMS

The simplified likelihood framework was defined in Ref. [20]. This assumes correlation between background contributions that can be modelled using the multivariate Gaussian distribution:

$$\mathcal{L}_S(\mu, \boldsymbol{\theta}) = \prod_{i=1}^{N} \frac{(\mu \cdot s_i + b_i + \theta_i)^{n_i} e^{-(\mu \cdot s_i + b_i + \theta_i)}}{n_i!} \cdot \exp\left(-\frac{1}{2}\boldsymbol{\theta}^T \mathbf{V}^{-1} \boldsymbol{\theta}\right) \tag{1}$$

where the product runs over all bins and μ is the signal strength (and the Parameter of Interest - POI), n_i the observed number of events, s_i an expected number of signal events, b_i an expected number of background events, θ_i a background nuisance parameter and $\mathbf{V}$ the covariance matrix. It is implemented using the covariance matrices provided by the CMS Collaboration which are included in the `CheckMATE` distribution in the JSON format. Evaluation of the above model is performed using the `Spey` package and the `default_pdf.correlated_background` PDF.

2.3 `CheckMATE` parameters

`CheckMATE` provides several switches and parameters to control details of statistical evaluation. These are summarized in Tab. 3. The switches are divided into two groups: one providing a control of what statistical tests are performed and the other to control different modes of calculation. By default no statistical evaluation is performed. For the sake of speed and stability one switch, `scan`, provides a quick and reliable way of obtaining `Allowed/Excluded` result but with limited additional information. Generally the available statistics include CL_s tests and calculation of upper

Name	Description	N_{bin}	Ref.
cms_1908_04722	Search for supersymmetry in final states with jets and E_T^{miss}	174	[21]
cms_1909_03460	Search for supersymmetry with M_{T2} variable in final states with jets and E_T^{miss}	282	[22]
cms_2107_13021	Search for new particles in events with energetic jets and large E_T^{miss}	66	[23]
cms_2205_09597	Search for production of charginos and neutralinos in final states containing hadronic decays of WW, WZ, or WH and E_T^{miss}	35	[23]

Table 2: List of implemented CMS analyses which have likelihood-based signal regions (all searches at $\sqrt{s} = 13$ TeV and $\mathcal{L} = 139$ fb^{-1}).

limits on signal strength, both of which can be obtained as observed and/or expected measures. By choosing a `select` switch users can control which statistics are calculated. If no explicit choice is made the *observed upper limit* will be calculated. Finally, the `detailed` switch can be used to request calculation of all available statistics, but it should be noted that its execution can be time consuming. The option `-so` can be used to request calculation of statistics for previous `CheckMATE` runs (it requires presence of the `evaluation/total_results.dat` file in the output directory.

The second group of parameters is used to choose a method of calculation of requested statistics for the ATLAS searches (it does not affect the calculation for the CMS searches as described in the previous Section). For the default method, `simple`, calculation is performed using simplified likelihood and the `CheckMATE-pyhf` interface. The `full` switch chooses a calculation using the full likelihood and the `CheckMATE-Spey` interface. Finally, the `fullpyhf` switch requests calculation sing the full likelihood and `CheckMATE-pyhf` interface (this is somewhat less flexible regarding the output compared to the previous options). In any case, users should remember that the full likelihood calculation can be time consuming if many searches and signal regions are requested.

The results of the calculation for each of the multibin signal regions and all requested analyses are stored in the `multibin_limits/results.dat` file. In order to follow the progress of calculation the observed limits are also displayed on screen for each of the signal regions. To calculation sometimes results in bogus numbers and so as an additional precaution the CL_s results smaller than 10^{-6} are ignored. The final evaluation is decided using the upper limit on the signal strength μ (if available):

$$\begin{aligned} \mu < 1 &\implies \texttt{Exclued} \\ \mu \geq 1 &\implies \texttt{Allowed}. \end{aligned}$$

If the results for upper limit are not available the decision is made using the observed CL_s statistics at the 95% confidence level:

$$\begin{aligned} \mathrm{CL}_s < 0.05 &\implies \texttt{Exclued} \\ \mathrm{CL}_s \geq 0.05 &\implies \texttt{Allowed}. \end{aligned}$$

2.4 Evaluation time

3 Validation

Multibin signal regions are currently available in 11 ATLAS analyses and 3 CMS analyses, as listed in Tabs. 1 and 2. The searches are based on the full Run 2 luminosity of about 140 fb^{-1} at the center-of-mass energy $\sqrt{s} = 13$ TeV. In this section we briefly introduce each of the searches and

Parameter card		Terminal	X	Description and available choices
`Multibin:`	`X`	`-mb X`	`none`	No signal region combination is performed (default).
			`select`	Calculates user selected statistics.
			`scan`	Calculates observed CL_s; fast and reliable for quick assessment of exclusion.
			`detailed`	Calculates observed and expected upper limits and CL_s.
`Expected:`	`False`	`-exp`		Selects calculation of expected limits.
`CLs:`	`False`	`-cls`		Selects calculation of CL_s.
`Uplim:`	`False`	`-uplim`		Selects calculation of upper limits.
`Statonly:`	`False`	`-so`		Calculates statistical combinations without event-level analysis provided the analysis and evaluation steps were already completed.
`Model:`	`X`	`-mod X`	`simple`	The simplified likelihood model for ATLAS searches (default).
			`full`	The Spey interface to the full likelihood model for ATLAS searches.
			`fullpyhf`	The full likelihood model for ATLAS searches with `pyhf` interface.

Table 3: Summary of options related to multibin signal regions.

provide validation examples. When possible we compare full vs. simplified likelihood approach, and provide examples how the multibin approach improves exclusions compared to the best SR approach.

The validation process is organized as follows. For SUSY processes events are generated events using `MadGraph5_aMC@NLO 3.1.0` [24–26] with up to two additional partons in the final state. The NNPDF23LO [27–29] PDF set is used. The events are then interfaced to Pythia-8.3 [30, 31] for modeling of decays, hadronization and showering. The matrix element and parton shower matching was done using the CKKW-L [32] prescription and a matching scale of 1/4 of the SUSY particle mass. Inclusive signal cross sections for production of squarks and gluinos are obtained at the approximate next-to-next-to-leading order with soft gluon resummation at next-to-next-to-leading-logarithm (approximate NNLO+NNLL) [33–43], following recommendations of Ref. [44]. The signal cross sections for production of sleptons, charginos and neutralinos are computed at next-to-leading order plus next-to-leading-log precision using `Resummino` [45–51]. This setup generally follows procedures employed within LHC experiments to obtain exclusion limits used in the validation process.

For the purpose of validation we present comparisons between `CheckMATE` and official ATLAS result of both expected and observed exclusion limits. Where available, the results for both simplified and full likelihood are provided. Additionally, we also include exclusion contours using the best *expected* signal region. The latter generally shows weaker sensitivity than shape-fits, but can be advantageous in terms of evaluation speed.

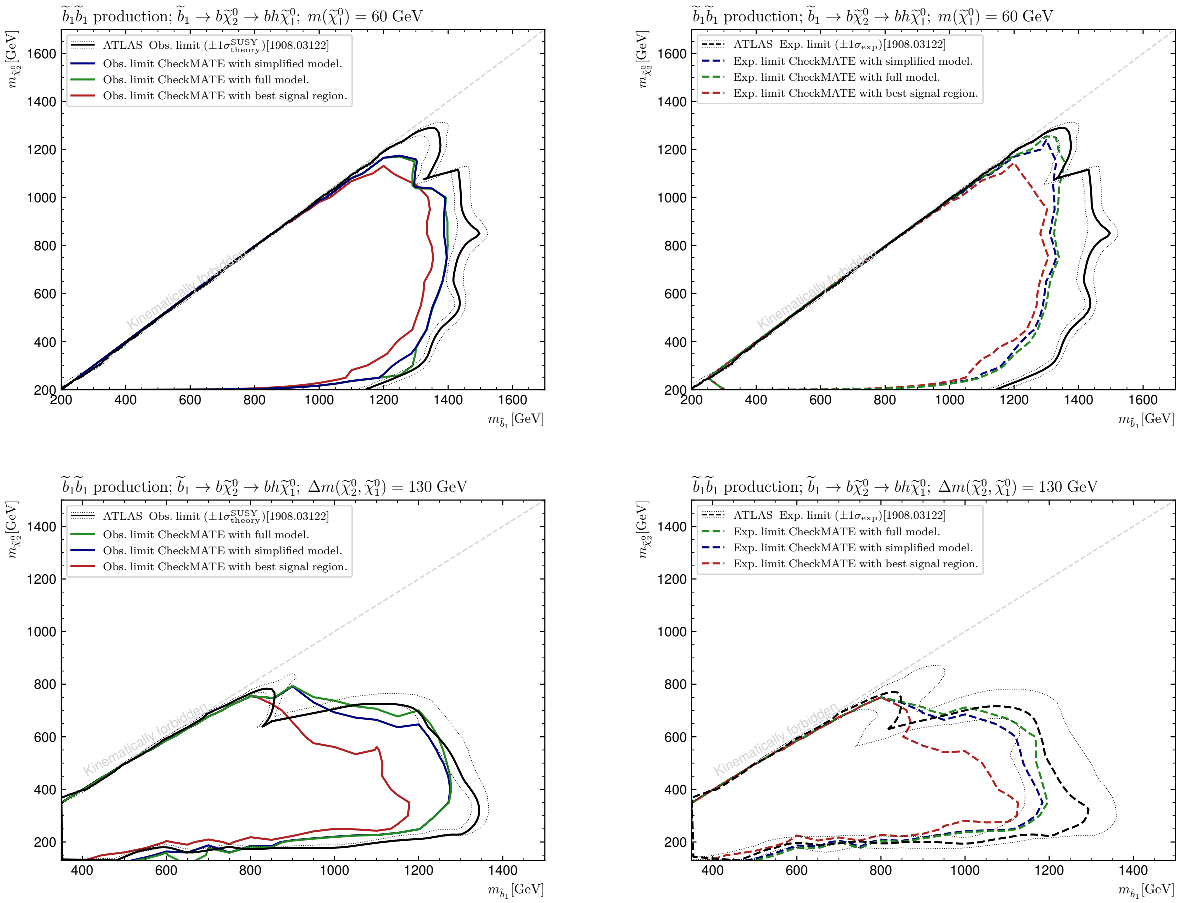


Figure 1: Validation plots for the search `atlas_1908_03122` (SUSY-2018-31). Top row: the model with $m_{\tilde{\chi}_1^0} = 60$ GeV; bottom row: the model with $\Delta m(\tilde{\chi}_2^0, \tilde{\chi}_1^0) = 130$ GeV. Left panels: observed limits; right panels: expected limits.

3.1 `atlas_1908_03122` (SUSY-2018-31)

This is a search [10] for bottom squark production in final states containing Higgs bosons, b-jets, and missing transverse momentum. The Higgs boson is reconstructed from two b-tagged jets. The final states contain at least 3 (SRC) or 4 (SRA, SRB) b-jets, no leptons and large missing transverse momentum. The signal region A is further divided into 3 bins according to effective mass, $m_{\rm eff}$, and the signal region C is divided into 4 bins of missing transverse energy significance, $\mathcal{S}$. Thus both SRA and SRC allow for a shape-fit analysis. The full likelihood model is provided.

Validation plots for this search are presented in Fig. 1. We compare bottom squark pair production, $pp \to \tilde{b}_1\tilde{b}_1^*$, and two distinct mass spectra. The first one assumes the mass of LSP to be $m_{\tilde{\chi}_1^0} = 60$ GeV and the other the mass difference between neutralinos $\Delta m(\tilde{\chi}_2^0, \tilde{\chi}_1^0) = 130$ GeV. Generally a good agreement between `CheckMATE` and ATLAS is observed for the shape-fit method with `CheckMATE` being slightly weaker. Notably, there is a very good agreement between simplified and full models. The best SR method performs well for the model with fixed LSP mass, however in the second scenario its exclusion strength can be up to 3 times weaker than shape-fits.

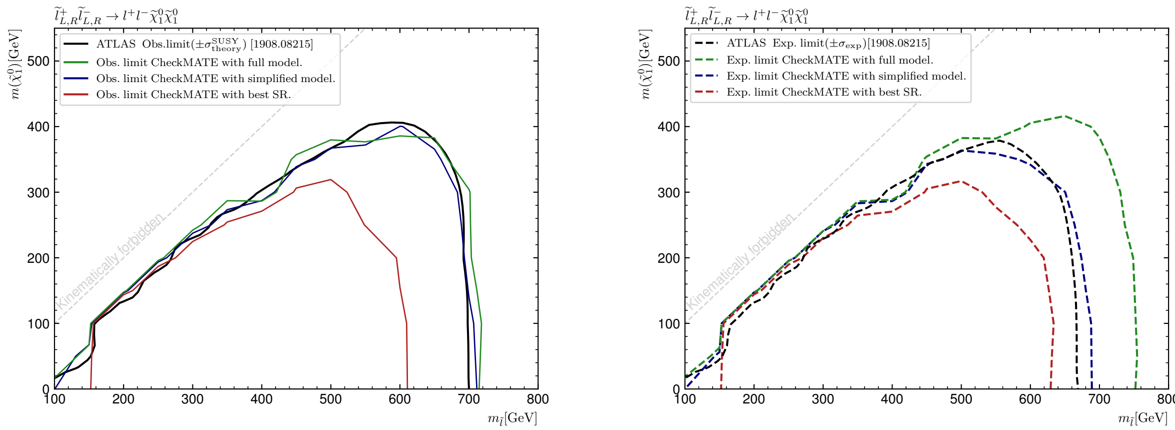


Figure 2: Validation plots for the search `atlas_1908_08215` (SUSY-2018-33). Left panels: observed limits; right panels: expected limits.

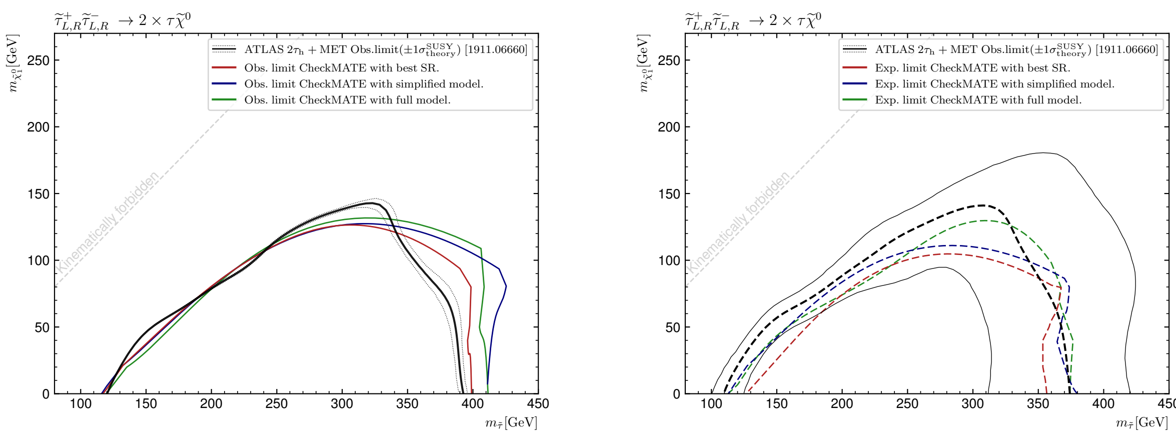


Figure 3: Validation plots for the search `atlas_1911_06660` (SUSY-2018-04). Left panels: observed limits; right panels: expected limits.

3.2 `atlas_1908_08215` (SUSY-2018-32)

This is a search [11] for production of electroweakinos and sleptons. The final states two electrons or muons (opposite sign and same or different flavour). Events are first separated into 'same flavour' and 'different flavour' events and further subdivided by the multiplicity of the non-b-tagged jets. A combined multi-bin SR is defined out of the 36 exclusive binned signal regions. The full likelihood of the model is provided.

Please check expected full result

3.3 `atlas_1911_06660` (SUSY-2018-04)

This is a search [12] for production of staus in final states with two hadronic τ-leptons and missing transverse momentum. Two orthogonal signal regions can be combined in a fit for which the full likelihood model is provided. The `CheckMATE` implementation includes one of the multijet control regions (CR-A), for which a significant contribution, up to 30%, from the signal events is expected.

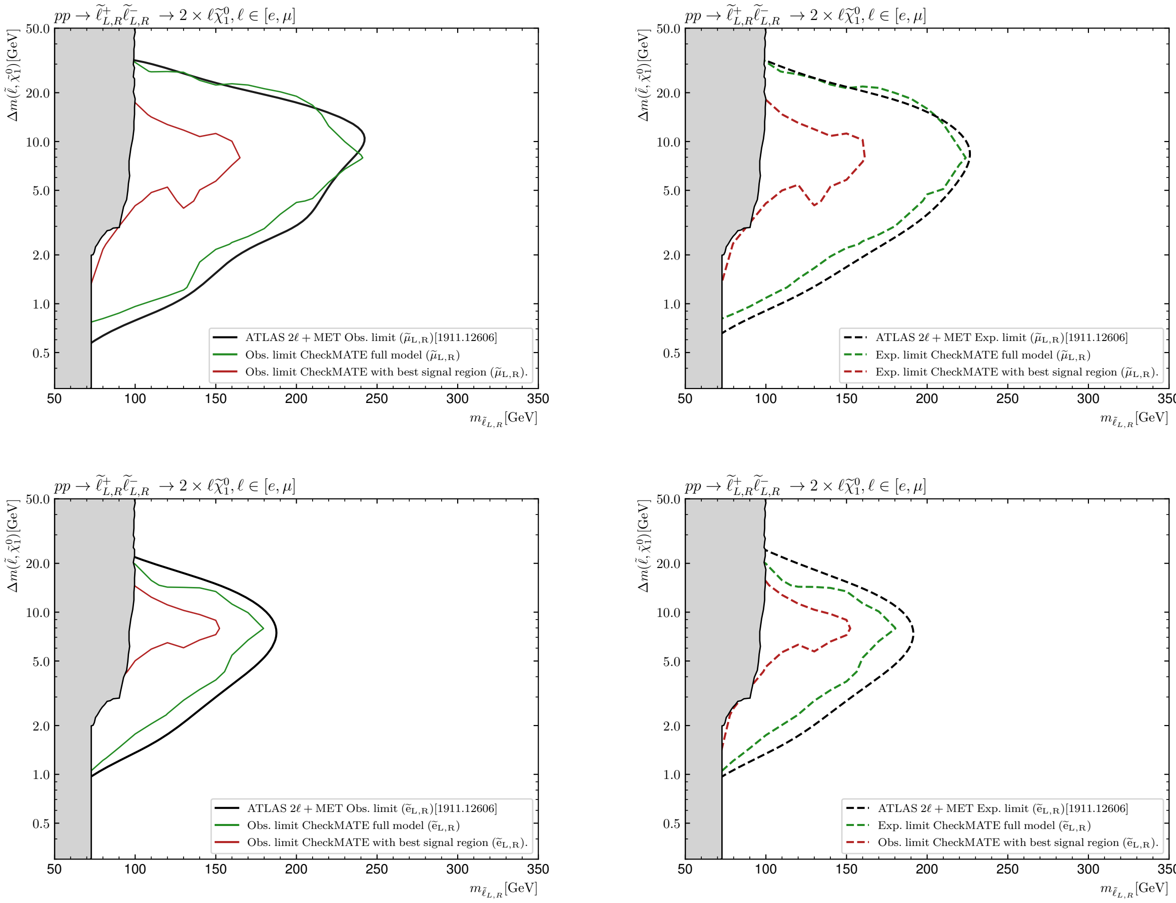


Figure 4: Validation plots for the search `atlas_1911_12606` (SUSY-2018-16). Top row: smuon search; bottom row: selectron search. Left panels: observed limits; right panels: expected limits.

3.4 `atlas_1911_12606` (SUSY-2018-16)

This is a search [13] for production of electroweakinos and sleptons in scenarios with compressed mass spectra. The final states contain two low p_T leptons (opposite sign and same or different flavour). Sensitivity of the search relies on additional initial state radiation jets which give transverse boost to the final state particles and adds missing transverse momentum. There are two multibin signal regions implemented in `CheckMATE`:[♮2] `SR-EWK` targeting production of electroweakinos and divided into 44 bins according to the lepton pair invariant mass, $E_{\mathrm{T}}^{\mathrm{miss}}$, and lepton flavour; `SR-S` targetting producrion of sleptons and divided into 32 bins. The full likelihood model is provided.

Correct labels above plots

In Figure 4, we show validation plots for slepton search regions. The electron and muon channels are shown separately. Very good agreement between ATLAS and `CheckMATE` is obtained for the shape-fit analysis. Additionally, by comparing a red exclusion curves obtained using the best-SR-method we find a clear benefit of using multibin signal regions.

[♮2]The VBF SRs are currently not available.

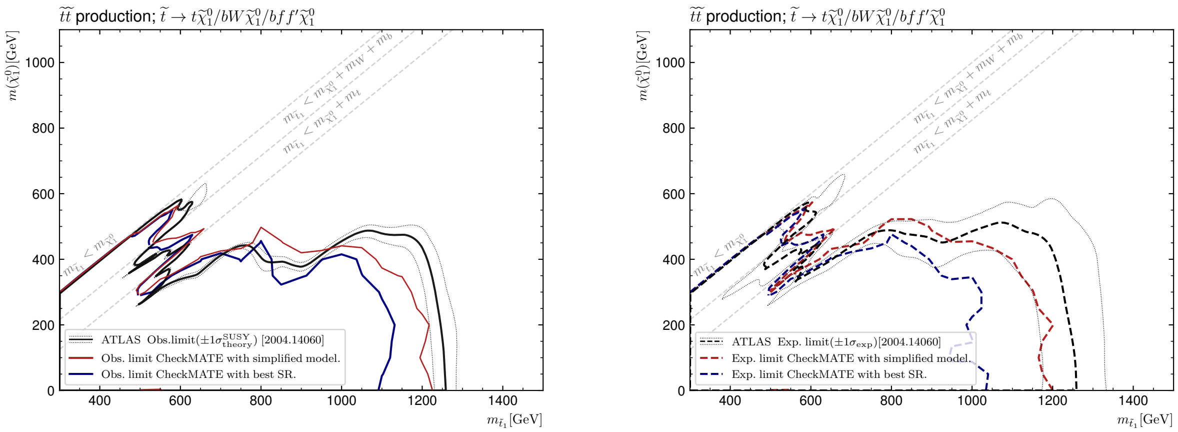


Figure 5: Validation plots for the search `atlas_2004_14060` (SUSY-2018-12). Left panels: observed limits; right panels: expected limits.

3.5 `atlas_2004_14060` (SUSY-2018-12)

This is a search [14] for hadronically decaying supersymmetric partners of top quark and up-type, 3rd generation scalar leptoquark. The final states consist of several jets, 0 leptons, large $E_{\rm T}^{\rm miss}$. Requirements for b-jets vary among signal regions. There are 3 multibin signal regions: `SRA-B` which targets scenarios with highly boosted top quarks in the final state and is divided into 6 bins according to an invariant mass of large-R jet; `SRC` for scenarios with 3-body decays of stops which is divided into 5 bins according to a recursive jigsaw reconstruction technique variable $R_{\rm ISR}$ [52]; `SRD` for scenarios with compressed spectra and 4-body decays of stops which is divided into 3 bins according to the number of identified b-jets. No likelihood model is provided and only simplified fitting is available.

Change line colors to match other plots

Validation plots for this search are shown in Figure 5. We include the full range of stop masses and decay modes. A good agreement across the parameter plane is observed. For the high-stop-mass region the `CheckMATE` result is slightly weaker than ATLAS, clearly extending the exclusion reach compared to single SR exclusion. In the more compressed scenarios the simplified fit gives a slightly too strong exclusion in some regions of the parameter space, however this is below 30% difference in the exclusion strength.

3.6 `atlas_2006_05880` (SUSY-2018-21)

This is a search [15] for supersymmetric partners of top quark decaying to a Higgs or Z boson. The final state Higgs boson is reconstructed from a pair of b-jets while the Z boson from a same-flavour opposite-sign dilepton pair. There are 3 multibin signal regions which are shape fits in $E_{\rm T}^{\rm miss}$, $E_{\rm T}^{\rm miss}$-significance and $p_{\rm T}$ of the Z candidate. No likelihood model is provided and only simplified fitting is available.

Validation plots in Figure 6 again show a good agreement, with `CheckMATE` somewhat weaker than ATLAS in the high stop-mass region. The observed limits clearly extend the reach com pared to best SR, increasing sensitivity by up to factor 2.

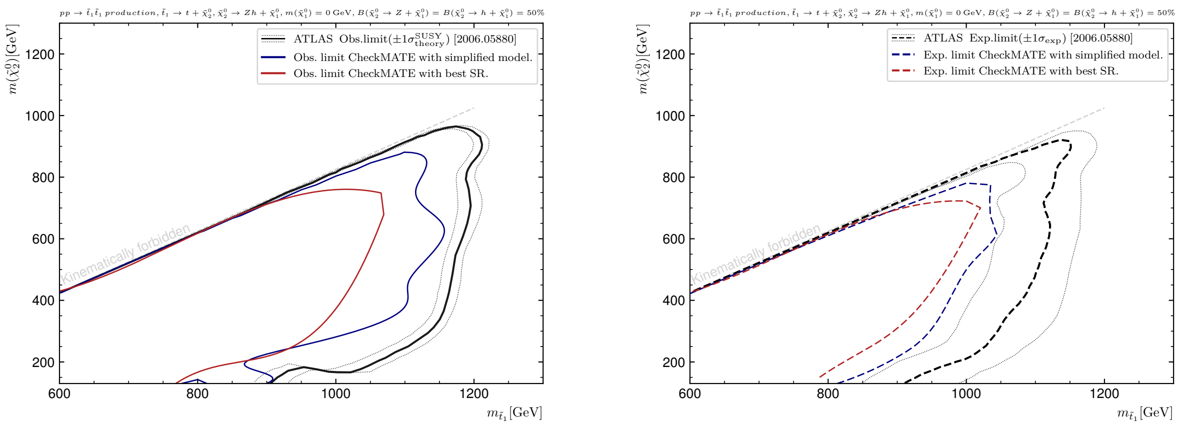


Figure 6: Validation plots for the search `atlas_2006_05880` (SUSY-2018-31). Left panels: observed limits; right panels: expected limits.

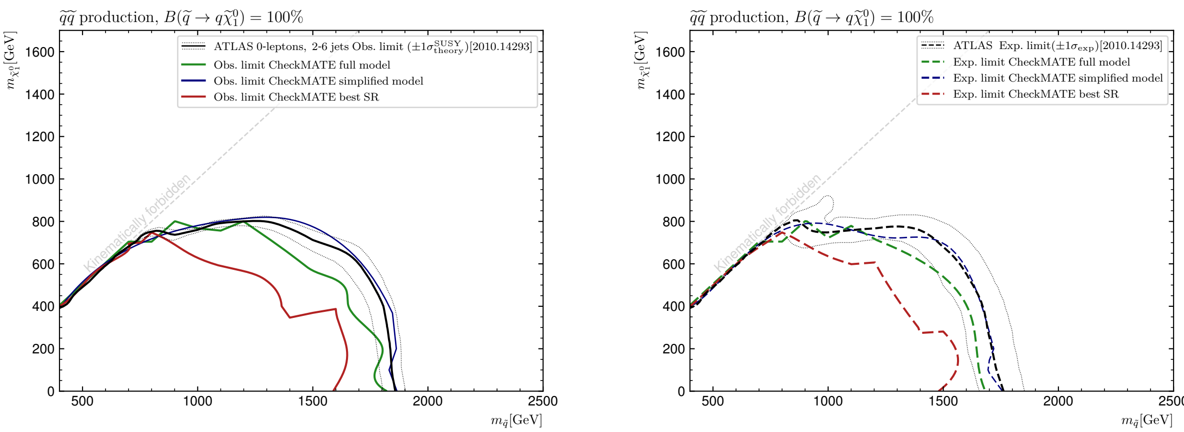


Figure 7: Validation plots for the search `atlas_2006_05880` (SUSY-2018-31). Left panels: observed limits; right panels: expected limits.

3.7 `atlas_2010_14293` (SUSY-2018-22)

This is a search [16] for squarks (1st and 2nd generation) and gluinos in final states with 2-6 jets, 0 leptons and missing transverse momentum. There are three multibin signal regions in this search: `MB-SSd` which targets production of squarks and is divided into 24 bin according to $m_{\rm eff}$, $E_{\rm T}^{\rm miss}/\sqrt{H_{\rm T}}$ and number of jets; `MB-GGd` which targets production of gluinos and is divided into 18 bin according to $m_{\rm eff}$, $E_{\rm T}^{\rm miss}/\sqrt{H_{\rm T}}$; `MB-C` which targets compressed spectra and is divided into 18 bin according to $m_{\rm eff}$, $E_{\rm T}^{\rm miss}/\sqrt{H_{\rm T}}$ and number of jets. The control regions are also implemented which enables to fully exploit the full likelihood model provided by the collaboration.

Figure 7 show validation plots for the squark pair-production process. The simplified shape-fit has excellent agreement with the official result, while the full likelihood model gives a somewhat weaker exclusion. In either case there is a clearly visible advantage over the best-SR method.

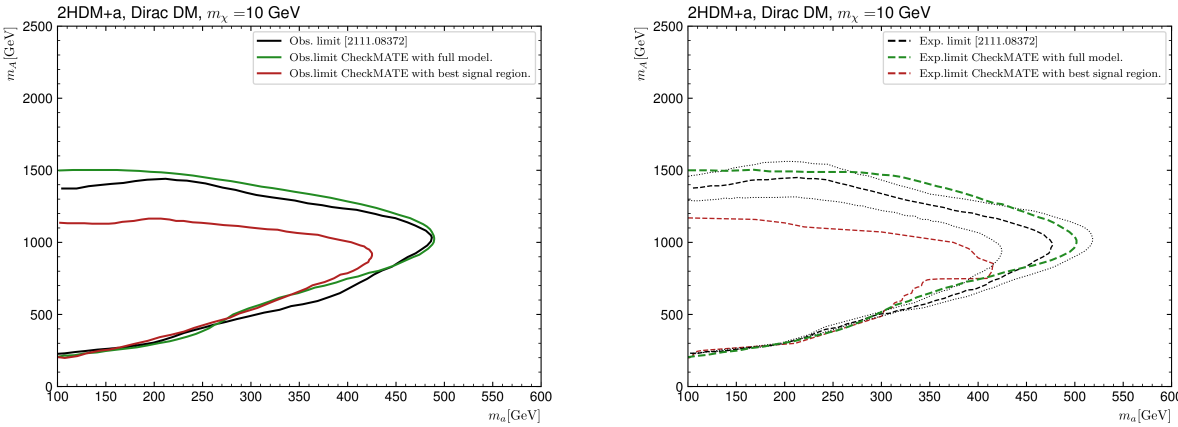


Figure 8: Validation plots for the search `atlas_2111_08372` (HIGG-2018-26). Left panels: observed limits; right panels: expected limits.

3.8 `atlas_2101_01629` (SUSY-2018-10)

This is a search [17] for squarks and gluinos in final states with one isolated lepton, jets, and missing transverse momentum. Benchmark models assume long decay chains for squarks and gluinos with charginos, neutralinos and gauge bosons in intermediate states that give rise to the final state lepton. There is one multibin signal regions that combines 26 bins defined according to a number of jets, number of identified b-jets, and m_{eff}. The full likelihood model is provided.

Strange that full is weaker than BSR. It doesn't seem so in my run. The x definition above plots is wrong

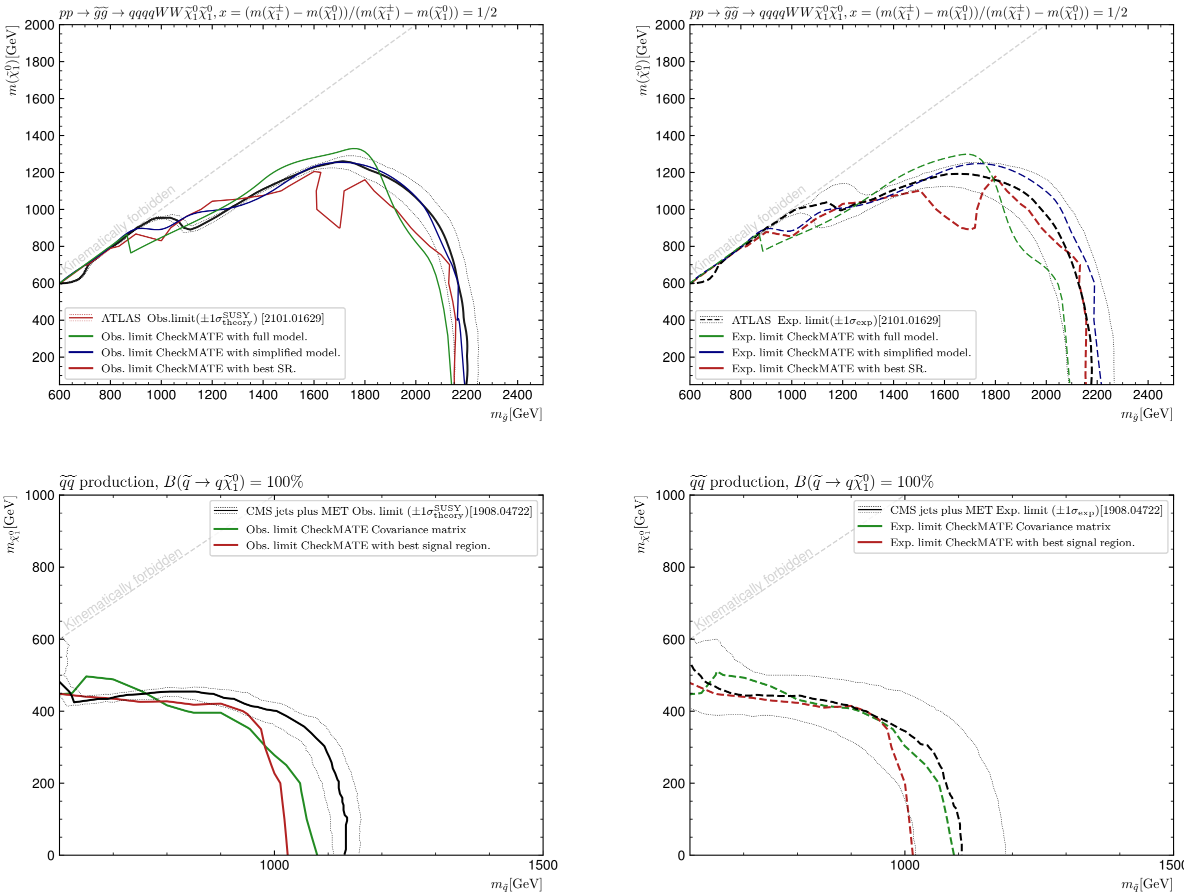
3.9 `atlas_2111_08372` (HIGG-2018-26)

This is a search [19] for invisible decays of a Higgs boson or dark matter particles produced in association with a Z boson. The final state Z boson is reconstructed from a same-flavour opposite-sign dilepton pair. One multibin signal region, optimized for the 2HDM+a model [53], is implemented in `CheckMATE`. It is divided in 22 bins according to m_{T}. The implementation uses simplified likelihood model.

As can be seen in Figure 8 we find excellent agreement between the result of the simplified shape-fit and the official result. The best-SR exclusion is significantly weaker. It should be noted that in the parts of the plot with large m_a and/or m_A the exclusion is driven by the shape-fit in the range of large m_T, which increases the sensitivity by factor 2.

3.10 `cms_1908_04722` (SUS-19-006)

This is a search [21] for supersymmetric particles in final states with jets (≥ 2) and missing transverse momentum. The search combines 174 bins simplified likelihood framework with the covariance matrix provided by the collaboration. The individual bins are defined according to a number of jets and b-jets, H_{T}, and $H_{\mathrm{T}}^{\mathrm{miss}}$. Additionally, there are 12 aggregate signal regions defined.

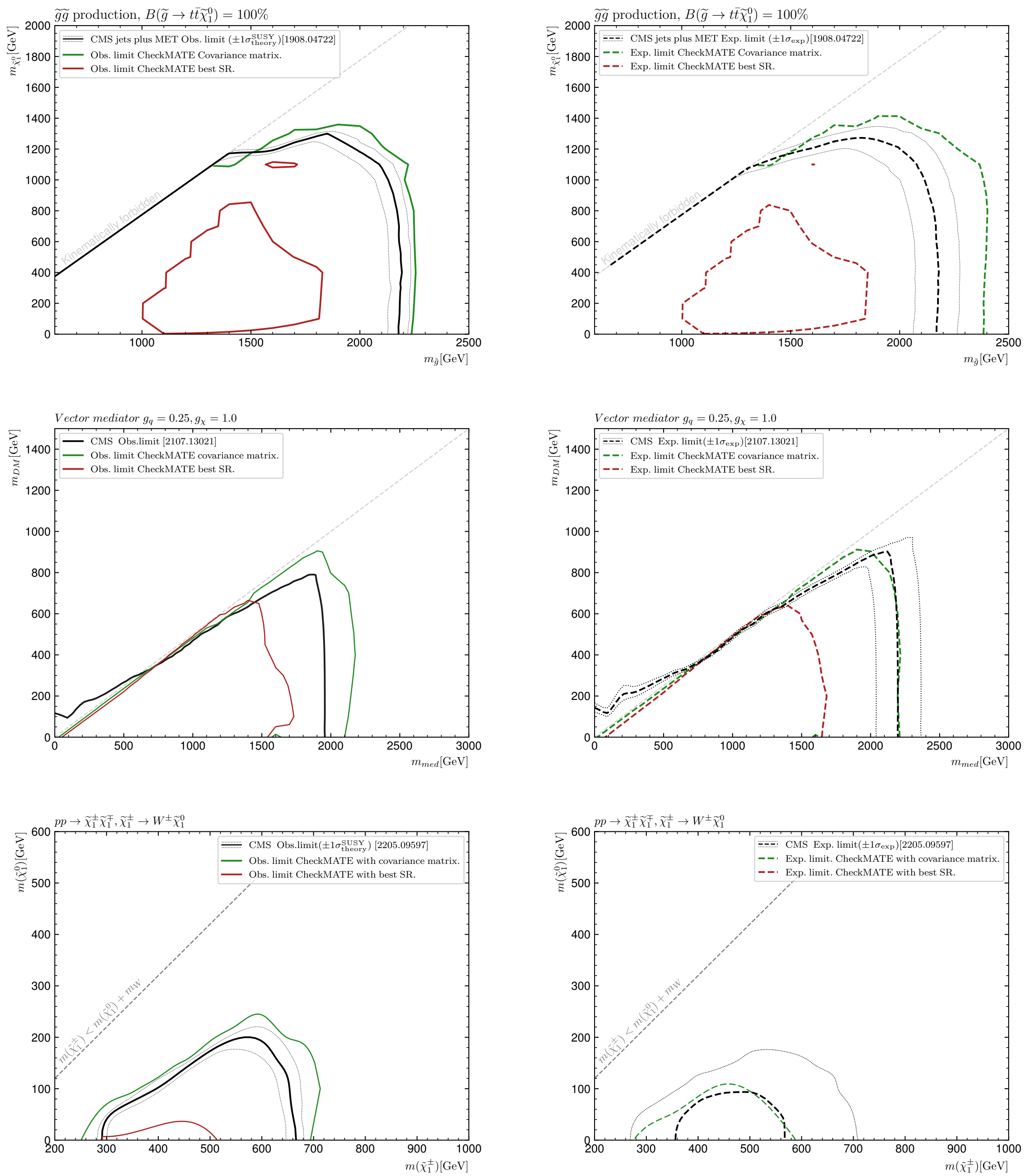


3.11 `cms_2107_13021` (EXO-20-004)

This is a search [23] for new particles in the final states with at least one jet, no leptons, and missing transverse momentum. A main focus of the analysis are invisible particles that can be dark matter candidates and that are produced with at least one ISR jet. The simplified likelihood fit is performed on 66 bins: 3 sets for different data taking periods and divided according to missing transverse energy.

3.12 `cms_2205_09597` (SUS-21-002)

This is a search [54] for charginos and neutralinos. The search looks for final states with large missing transverse momentum and pairs of hadronically decaying bosons WW, WZ and WH. This search makes use of specific algorithms (taggers) defined to identify W boson/Higgs boson candidates out of the identified signal jets. The individual bins are defined orthogonally based on the number of b-tagged jets, the number of identified "W boson candidates" and "Higgs boson candidates" as well and the missing transverse momentum. The simplified likelihood is built out of 35 signal regions. Additionally, there are 4 aggregate signal regions defined.



$\widetilde{g}\widetilde{g}$ production, $B(\widetilde{g} \to t\bar{t}\widetilde{\chi}_1^0) = 100\%$
CMS jets plus MET Obs. limit ($\pm 1\sigma_{\rm theory}^{\rm SUSY}$)[1908.04722]
Obs. limit CheckMATE Covariance matrix.
Obs. limit CheckMATE best SR.
Kinematically forbidden
$m_{\widetilde{\chi}_1^0}$[GeV]
$m_{\widetilde{g}}$[GeV]
$\widetilde{g}\widetilde{g}$ production, $B(\widetilde{g} \to t\bar{t}\widetilde{\chi}_1^0) = 100\%$
CMS jets plus MET Exp. limit ($\pm 1\sigma_{\rm exp}$)[1908.04722]
Exp. limit CheckMATE Covariance matrix.
Exp. limit CheckMATE best SR.
Kinematically forbidden
$m_{\widetilde{\chi}_1^0}$[GeV]
$m_{\widetilde{g}}$[GeV]
$Vector\ mediator\ g_q = 0.25, g_\chi = 1.0$
CMS Obs.limit [2107.13021]
Obs. limit CheckMATE covariance matrix.
Obs. limit CheckMATE best SR.
m_{DM}[GeV]
m_{med}[GeV]
$Vector\ mediator\ g_q = 0.25, g_\chi = 1.0$
CMS Exp. limit($\pm 1\sigma_{\rm exp}$)[2107.13021]
Exp. limit CheckMATE covariance matrix.
Exp. limit CheckMATE best SR.
m_{DM}[GeV]
m_{med}[GeV]
$pp \to \widetilde{\chi}_1^\pm \widetilde{\chi}_1^\mp, \widetilde{\chi}_1^\pm \to W^\pm \widetilde{\chi}_1^0$
CMS Obs.limit($\pm 1\sigma_{\rm theory}^{\rm SUSY}$) [2205.09597]
Obs. limit CheckMATE with covariance matrix.
Obs. limit CheckMATE with best SR.
$m(\widetilde{\chi}_1^\pm) < m(\widetilde{\chi}_1^0) + m_W$
$m(\widetilde{\chi}_1^0)$[GeV]
$m(\widetilde{\chi}_1^\pm)$[GeV]
$pp \to \widetilde{\chi}_1^\pm \widetilde{\chi}_1^\mp, \widetilde{\chi}_1^\pm \to W^\pm \widetilde{\chi}_1^0$
CMS Exp. limit($\pm 1\sigma_{\rm exp}$)[2205.09597]
Exp. limit. CheckMATE with covariance matrix.
Exp. limit. CheckMATE with best SR.
$m(\widetilde{\chi}_1^\pm) < m(\widetilde{\chi}_1^0) + m_W$
$m(\widetilde{\chi}_1^0)$[GeV]
$m(\widetilde{\chi}_1^\pm)$[GeV]

4 Conclusions and outlook

Acknowledgements

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