# $\begin{array}{c} {\bf Implementation~of~full~and~simplified~likelihoods~in}\\ {\bf CheckMATE} \end{array}$

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December 21, 2023

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 CheckMATE and user switches for controlling their execution.

#### 2.1 ATLAS

The functionality of combining signal regions for recasting in ATLAS searches can be implemented either using 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  $\mu$  is the parameter of interest. Depending on the user choices output can contain information about expected and observed upper limit on  $\mu$ , with 2- $\sigma$  bounds, along with observed and expected CL<sub>s</sub> 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. <sup>\$1</sup> 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

<sup>&</sup>lt;sup>‡1</sup>Installation of Spey is straightforward: pip install spey. Please refer to the Spey online documentation for more details [9].

Name	Description	#SR	$N_{\mathrm{bin}}$	Full	Ref.
atlas_1908_03122	Search for bottom squarks in final states with Higgs bosons, $b$ -jets and $E_{\rm T}^{\rm miss}$	2	7	✓	[10]
atlas_1908_08215	Search for electroweak production of charginos and sleptons in final states with 2 leptons and $E_{\rm T}^{\rm miss}$	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 $E_{\rm T}^{\rm miss}$	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 $E_{\rm T}^{\rm miss}$	3	60	✓	[16]
atlas_2101_01629	Search for squarks and gluinos in final states with one isolated lepton, jets, and $E_{\rm T}^{\rm miss}$	1	26	✓	[17]
atlas_2106_01676	Search for chargino—neutralino production in final states with 3 leptons and $E_{\rm T}^{\rm miss}$	2	72	✓	[18]
atlas_2111_08372	Search for associated production of a Z boson with an invisibly decaying Higgs boson or dark matter candi-	1	22	×	[19]
atlas_2202_07953	dates Search for invisible Higgs-boson decays in vector-boson fusion	1	16	×	[20]

**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<sup>-1</sup>).

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. [21]. This assumes correlation between background contributions that can be modelled using the multivariate Gaussian distribution:

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

where the product runs over all bins and  $\mu$  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,  $\theta_i$  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,

Name	Description	$N_{\mathrm{bin}}$	Ref.
cms_1908_04722	Search for supersymmetry in final states with jets and $E_{\rm T}^{\rm miss}$	174	[22]
cms_1909_03460	Search for supersymmetry with $M_{\rm T2}$ variable in final states with jets and $E_{\rm T}^{\rm miss}$	282	[23]
$cms_2107_13021$	Search for new particles in events with energetic jets and large $E_{\mathrm{T}}^{\mathrm{miss}}$	66	[24]
cms_2205_09597	Search for production of charginos and neutralinos in final states containing hadronic decays of $WW,WZ,$ or $WH$ and $E_{\rm T}^{\rm miss}$	35	[24]

**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<sup>-1</sup>).

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 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  $\mu$  (if available):

$$\mu < 0 \implies \texttt{Exclued}$$
 $\mu \ge 0 \implies \texttt{Allowed}.$ 

If the results for upper limit are not available the decision is made using the observed  $\mathrm{CL}_s$  statistics at the 95% confidence level:

$${
m CL}_s < 0.05 \implies {
m Exclued}$$
  ${
m CL}_s \geq 0.05 \implies {
m Allowed}.$ 

## 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<sup>-1</sup> at the center-of-mass energy  $\sqrt{s} = 13$  TeV. In this section we briefly introduce each of the searches and

Parameter card Ten		Terminal	Х	Description and available choices	
Multibin:	Х	-mb X	none	No signal region combination is performed (default).	
			select	Calculates user selected statistics.	
			scan	Calculates observed $\mathrm{CL}_s$ ; fast and reliable for quick assessment of exclusion.	
			detailed	Calculates observed and expected upper limits and $\mathrm{CL}_s$ .	
Expected:	False	-exp		Selects calculation of expected limits.	
CLs:	False	-cls		Selects calculation of $\widetilde{\mathrm{CL}}_s$ .	
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 [25–27] with up to two additional partons in the final state. The NNPDF23LO [28–30] PDF set is used. The events are then interfaced to Pythia-8.3 [31,32] for modeling of decays, hadronization and showering. The matrix element and parton shower matching was done using the CKKW-L [33] 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) [34–44], following recommendations of Ref. [45]. 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 [46–52]. This setup generally follows procedures employed within LHC experiments to obtain exclusion limits used in the validation process.

## 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,  $m_{\text{eff}}$ , 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.

## 3.2 atlas\_1911\_06660 (SUSY-2018-04)

This is a search [12] for production of staus in final states with two hadronic  $\tau$ -leptons and missing transverse momentum. Two orthogonal signal regions can be combined in a fit for which the full likelihood model is provided.

#### 3.3 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: \$\Psi^2\$ SR-EWK targeting production of electroweakinos and divided into 44 bins according to the lepton pair invariant mass,  $E_{\rm T}^{\rm miss}$ , and lepton flavour; SR-S targetting production of sleptons and divided into 32 bins. The full likelihood model is provided.

## 3.4 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  $R_{\rm ISR}$  [53]; 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.

#### 3.5 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.

#### 3.6 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.

<sup>&</sup>lt;sup>‡2</sup>The VBF SRs are currently not available.

## 3.7 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  $m_{\text{eff}}$ . The full likelihood model is provided.

## 3.8 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 [54], is implemented in CheckMATE. It is divided in 22 bins according to  $m_{\rm T}$ . The implementation uses simplified likelihood model.

## 3.9 atlas\_2202\_07953 (EXOT-2020-11)

This is a search [20] for invisible decays of a Higgs boson produced vector boson fusion. The final state consists of two forward jets consistent with a vector boson signature and missing transverse momentum. There is one multibin signal region divided into 16 bins according to a number of jets, invariant mass of the leading jets pair  $m_{jj}$  and their angular separation. The implementation uses simplified likelihood model.

## 3.10 cms\_1908\_04722 (SUS-19-006)

This is a search [22] for supersymmetric particles in final states with jets ( $\geq 2$ ) 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,  $H_{\rm T}$ , and  $H_{\rm T}^{\rm miss}$ . Additionally, there are 12 aggregate signal regions defined.

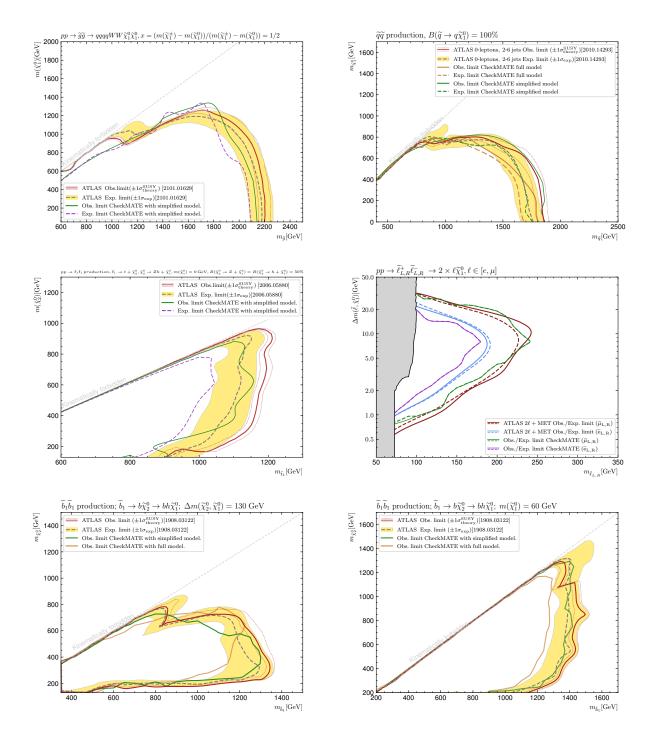
#### 3.11 cms\_2107\_13021 (EXO-20-004)

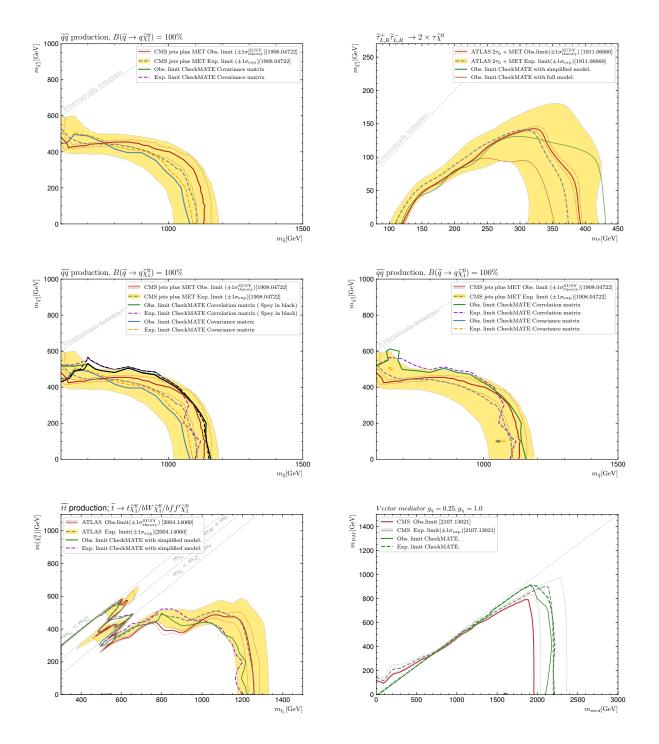
This is a search [24] for new particles in the final states with at least one jet, no leptons, and missing transverse momentum. A main focus of the analysis are invisible particles that can be dark matter candidates and that are produced with at least one ISR jet. The simplified likelihood fit is performed on 66 bins: 3 sets for different data taking periods and divided according to missing transverse energy.

#### 4 Conclusions and outlook

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