Chapter 9

Preservation and reusability

Today's particle physics experiments are designed to collect physics data over a span of several decades. They operate at scales and complexities that make it impossible for the experiments to be repeated in the foreseeable future. The data taken at these experiments and physics results derived are thus exceptionally valuable and major problems arise from a scientific reproducibility point of view. In the following, reusability problems directly related to an individual analysis are discussed, and approaches taken in view of analysis preservation and reinterpretation are presented. This chapter starts with a brief motivation for reinterpretations, followed by a description of the main ingredients necessary. The remaining sections discuss three separate efforts aiming to improve the reinterpretability of the 1ℓ search in light of new signal models.

9.1 The case for reinterpretations

9.1.1 Motivation

Designing and executing searches for BSM physics requires a substantial amount of person-power and computing resources. As laid out in detail in part II of this thesis, an analysis generally aims to design signal regions in which a given BSM signal can be efficiently discriminated against SM background. Although the careful design of such regions already requires a significant amount of resources, it constitutes only a fraction of the work necessary for concluding the search. Contributions in the signal regions from SM processes need to be estimated, usually requiring expensive MC simulation and the development of background estimation strategies. Systematic uncertainties arising from numerous sources need to be considered and their impact estimated. For the BSM signal, a similar processing pipeline involving MC simulation, event reconstruction and event selection including uncertainties needs to be executed. Furthermore, recorded data also needs to be reconstructed and processed through the analysis-specific event selection. Only after the expected and observed event rates in all regions are known, can the statistical evaluation be performed.

As shown in fig. 9.1, an analysis can thus be divided into three main processing pipelines; a background pipeline, a signal pipeline and a data pipeline. After all three processing pipelines are concluded, the next analysis step can be performed—the statistical inference, producing the final analysis results, like quantifying excesses in data or setting limits on model parameters.

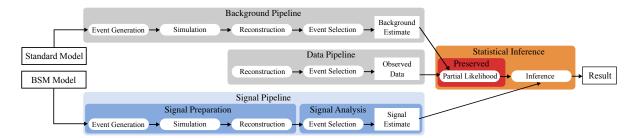


Figure 9.1: Full analysis workflow including the three main processing pipelines for deriving background and signal estimates as well as observed data rates. The outputs of the three processing pipelines are combined into a likelihood forming the basis for the statistical inference. In a Recast setup (details in text), the estimated background rates and observed data are archived, and the signal pipeline is fully preserved, such that it can be re-executed with different inputs at any time. Figure recreated from Ref. [251].

Due to the substantial amount of resources necessary for developing and performing an analysis, it is not feasible to develop dedicated searches for every possible BSM scenario. Instead, analyses are typically only interpreted in a finite set of models with a small number of free parameters that need to be varied. Still, it is likely that a given analysis is sensitive to a variety of different BSM scenarios not considered in the original publication.

Consequently, it is not surprising that there is significant interest in the HEP community to reinterpret BSM searches in different signal models. Reinterpretations of ATLAS searches for SUSY are routinely performed by various reinterpretation efforts. In the context of direct constraints on BSM physics, the search results published by the experimental collaborations represent the only windows into the LHC data that are available to the wider HEP community. Reinterpretations of BSM searches are thus the only possibility to determine the implications of LHC data for a broad range of models [250].

As will be discussed in chapter 11, reinterpretations are not only of interest for the wider HEP community, but also for the experimental collaborations themselves. Within ATLAS, reinterpretations of SUSY searches can, for example, serve as powerful tools to state a comprehensive summary of ATLAS's sensitivity to SUSY models.

9.1.2 Approaches for reinterpretations

As the event selection of an analysis is fixed, the pre-fit background estimates and observed data in the regions of interest of the analysis do not change. Hence, the data and background pipelines shown in fig. 9.1, entering the statistical inference of the analysis by means of event rates, can be archived in a format significantly smaller than the original input data. In consequence, reinterpreting a search in the light of a new signal model requires the re-execution of two main analysis ingredients with (partially) new inputs; the signal pipeline and the statistical inference.

Recently, it has become possible to preserve the partial analysis likelihood[†] built from the background estimates and observed data, including all auxiliary data and details of the statistical model used for inference in a pure-text format [149]. In fig. 9.1, this is indicated through a red rectangle. Once the signal estimates are known, a new full analysis likelihood can be built, and

[†] As before, this only refers to likelihoods built using the HISTFACTORY template.

the viability of the new signal model can be tested with respect to the analysis in question. The publication of the likelihood of the 1ℓ search will be discussed further in section 9.2.

Different approaches can be taken for rendering the signal pipeline reusable to the extent that signal estimates for a new BSM scenarios of interest can be derived. Manifestly the most precise approach involves executing the original analysis software, but using a different BSM model as input. As this requires the preservation of the entirety of the original software environment, including the workflows used in the analysis, this is arguably the most involved approach, especially since it involves executing the computationally expensive detector simulation. A framework designed to facilitate such an effort, called RECAST and originally proposed in Ref. [252], is under development and aims to provide the cyber-infrastructure needed for offering reinterpretations as a service. Through a web interface, physicists wishing to reinterpret a search with RECAST, would provide an alternative BSM model and trigger a computational workflow that would re-execute the original analysis using the new signal inputs and ultimately deliver the recasted results. An attempt to fully preserve the 1 ℓ search using the RECAST paradigm is discussed in section 9.3.

As the details of the existing Recast implementations of ATLAS searches for SUSY are not publicly available, but only meant to be interacted with through a Recast request, the exact implementation of the analysis selection is in general not available outside the ATLAS collaboration. For this reason, a number of public tools aiming to reimplement an approximated version of the event selections of a number of BSM searches at the LHC are available. Prominent examples include CheckMate [253, 254] and Madanalysis [255]. ATLAS has internally maintained a similar catalogue of its SUSY analyses and is publishing event selection snippets in C++ for many SUSY searches on Hepdata [256], a repository for high energy physics data. Recently, this package maintained by ATLAS, called SimpleAnalysis [257], has been made publicly available, allowing the C++ snippets published to be executed outside the collaboration.

A crucial step, necessary for achieving a reliable reimplementation of the signal pipeline, is the detector simulation. Executing the full detector simulation requires access to the collaborations's detector descriptio and is computationally expensive, disfavouring[†] its usage in the context of large-scale reinterpretations over a large set of models. For this reason, it is often approximated using simplified detector geometries and granularities. The most commonly used package for a fast detector simulation outside of the ATLAS collaboration is Delphes [258], which is used in, e.g., Checkmate and Madanalysis5. Other packages like, e.g., Rivet [259, 260] approximate the detector response using dedicated four-vector smearing techniques, assuming that the detector response roughly factorises into the responses of single particles. Internally, ATLAS also maintains a dedicated framework for four-vector smearing, used in scenarios where other fast simulation techniques are still too expensive. Section 9.4.2 discusses these dedicated smearing functions further.

Finally, instead of trying to estimate the signal rates of a new model using MC simulation and (reimplemented) analysis event selections, some reinterpretation efforts like, e.g., SMODELS [261, 262], use *efficiency maps* encoding the selection and acceptance efficiencies of the analysis as a function of the model parameters (typically the sparticle masses in the case of SUSY searches) and analysis selections. Such efficiency maps are routinely published on HEPDATA by ATLAS

[†] This is especially true for reinterpretation efforts outside the ATLAS collaboration, which cannot make use of the collaboration's detector description.

SUSY searches, and allow for efficient reinterpretations, as long as the signal efficiencies mostly depend on the signal kinematics and are largely independent from the specific details of the signal model [261]. For the 1ℓ search presented herein, the efficiency maps, including additional analysis data products, are available at Ref. [263].

9.2 Public full likelihood

The likelihood is arguably one of the most information-dense and important data products of an analysis. If the exact likelihood function of the original analysis is not known in reinterpretation efforts[†], approximations need to be made for the statistical inference, e.g. in terms of the correlations between event rate estimates as well as the treatment of uncertainties. Recently, ATLAS has started to publish full analysis likelihoods built using the HISTFACTORY pdf template [149]. This effort has been facilitated by the development of pyhf (cf. section 3.1), in conjunction with the introduction of a JSON specification fully describing the HISTFACTORY template. As a pure-text format, the JSON likelihoods are human- and machine-readable, highly compressible and can easily be put under version control, all of which are properties that make them suitable for long-term preservation, which is a crucial condition for reinterpretations.

The full likelihood of the 1ℓ search is publicly available at Ref. [264] and is not only heavily used in the following chapters, but also in various analysis reinterpretation and combination efforts currently ongoing in ATLAS. Several efforts outside of the ATLAS collaboration have already included the analysis likelihood into their reinterpretations, and the SMODELS [265] and MADANALYSIS5 [266, 267] collaborations have both reported significant precision improvements through its use. Furthermore, the full likelihood of the search presented herein has recently been used to demonstrate the concept of scalable distributed statistical inference on high-performance computers (HPCs) [268]. Through the funcX package [269], pyhf is used as a highly scalable function as a service to fit the entire 1ℓ signal grid of 125 signal points with a wall time of 156 s using 85 available worker nodes§.

9.3 Full analysis preservation using containerised workflows

For an analysis to be fully reusable under the RECAST paradigm, the signal pipeline of the original analysis (cf. fig. 9.1) needs to be preserved such that it can be re-executed on new inputs. As typically only the processing steps after the event reconstruction are analysis-specific, it is sufficient to preserve this part of the signal pipeline. Processing steps including and preceding the event reconstruction only involve the central ATLAS production system, introduced in section 2.2.8, and result in an ATLAS-internal data format serving as input for physics analyses. These processing steps are preserved using centrally provided ATLAS infrastructure and thus do not need to be within the scope of the preservation discussed in the following.

[†] Up until recently, the exact likelihood function was not part of the data products published by ATLAS searches for SUSY, hence approximations of the statistical models were a crucial part of most reinterpreation efforts.

Theses benchmarks use pyhf's NumPy backend and SciPy optimiser, a combination that has a slower log-likelihood minimisation time than e.g. PyTorch coupled with SciPy, as will be shown in section 10.3.

In the following, the term *signal analysis* (cf. fig. 9.1) will refer to the analysis-specific processing steps that are not handled by the central ATLAS production system, typically starting with the selection of events that have passed the reconstruction step in fig. 9.1, provided in the aforementioned internal data format. Preserving the signal analysis not only needs preservation of the full software environment required for the different processing steps, but also knowledge of the correct usage of the software through parameterised job templates together with a workflow graph connecting the different processing steps. A graph representation of the entire analysis, implemented in Recast is shown in fig. 9.2.

9.3.1 Software preservation

As much of the software is only tested, validated and deployed on a narrow set of architectures and platforms, the full software environment defining an analysis pipeline not only includes the original analysis-specific code used for object definitions, calibrations, event selection and statistical inference, but also the operating system used, and a number of low-level system libraries that the applications depend upon. Preserving the full software environment can be achieved through the use of *Docker containers* [270, 271], a technology that—except for the operating system kernel—packages the full software environment in a portable data format, including a layered file system, the operating system as well as the actual application and all of its dependencies. As opposed to full virtualisation, Docker containers do not rely on actual hardware virtualisation but share the operating system kernel with the host. As such, they only interact with the host through system calls to the Linux kernel [271], offering a highly stable interface. This makes Docker containers a well-suited solution for deploying isolated applications on a heterogeneous computing infrastructure.

Due to the specific software structure of the 1ℓ search, a containerisation requires a total of three container images. Two images contain the software necessary for performing the physics object calibrations and event selection, as well as the conversion of the information in a format that can be used by the downstream steps. The third image contains the software necessary for the statistical inference, relying on the pyhf-implementation of the HISTFACTORY models in order to benefit from the possibility of using a partial JSON likelihood to preserve background and data rates.

The Docker images are built from suitable base images containing the software environment used for deriving the published 1ℓ search results, expanded with the relevant analysis software. All docker images are subject to version control and continuous integration, such that changes to the underlying software environment can be tracked and tagged. This allows for a consistent preservation of multiple versions of the analysis pipeline.

9.3.2 Processing steps preservation

Preserving the software environment is not sufficient, as detailed instructions on how to use it have to be given. This is achieved through parameterised job templates that specify the precise commands and arguments required to re-execute the analysis code for specific processing steps. As re-executing the analysis pipeline using different signal models involves varying input parameters, all job template parameters are exposed to the user. In fig. 9.2, the parameterised

job templates including their output are shown as blue rectangles, connected together through a workflow specification represented via black arrows.

User-specifiable arguments and inputs to the event selection and physics object calibration step include the actual reconstructed MC events in the aforementioned ATLAS-internal format, obtained through the central ATLAS production system, as well as corresponding files necessary for the pile-up correction in MC. In addition, the signal process cross section as well as MC generator-level efficiencies need to be given for the correct normalisation of the estimated signal rates to the integrated luminosity of the full Run 2 dataset. For each new signal model to be tested, three MC samples need to be provided, generated with specific pile-up profiles close to the pile-up profile in data during the 2015–2016, 2017 and 2018 data-taking periods, respectively[†]. In all three jobs, the events processed are weighted according to the integrated luminosity of the data-taking period they represent within the full Run 2 dataset. A subsequent merging step uses the same docker image as the previous processing step, and serves to merge the three produced outputs into a single ROOT file that can be read by the subsequent step.

In addition, a JSON file containing theory uncertainties on the expected signal rates can be provided. These are optional and do not have to be specified if deemed to be negligible for the signal model under consideration.

The statistical inference step requires, as external input, the archived partial likelihood containing observed data as well as expected background rates including systematic variations thereof. This step generates a new full analysis likelihood and performs the necessary hypothesis tests.

9.3.3 Workflow preservation

Finally, the preserved processing steps need to be linked together, creating a parameterised workflow completely defining the analysis pipeline, starting from centrally produced MC datasets up to the statistical inference results. Within RECAST, this is achieved using the workflow description language yadage [272], capturing the full workflow in YAML format. The workflow uses the job templates and defines their processing order and dependencies.

The Recast implementation of the analysis presented in this work has been validated against original analysis inputs. The expected and observed CL_s values derived in the original analysis were successfully re-derived using the containerised workflow implementation. On a non-isolated CPU, the full preserved analysis pipeline for a single signal model can be executed with a wall time of about 50 min. Due to the highly portable nature of the containerised workflow, the pipeline can easily be run in a distributed setup, allowing scalable reinterpretations at full analysis precision.

[†] This allows to have pile-up weights relatively close to unity, avoiding unnecessary statistical dilution.

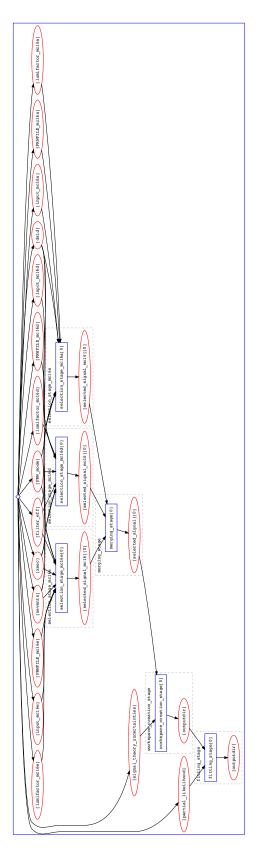


Figure 9.2: Graph of the workflow as specified for the analysis pipeline. The containerised processing steps are represented as blue rectangular selection_stage_mc16(a,d,e), merging_stage, workspace_creation_stage and fitting_stage. The first two steps perform the object calibration, event selection and merging of the three MC datasets representing the three data-taking periods 2015–2016, 2017 and 2018. The latter two steps implement the generation of the signal JSON patch as well as the final statistical inference. Compared to fig. 9.1 the first two steps nodes, while input parameters, input files and outputs are shown as red oval nodes. The workflow is comprised of four processing steps: implement the signal analysis part, while the latter two steps implement the statistical inference deriving the final results.

9.4 Truth-level analysis

A full preservation of the entire analysis pipeline, as presented in the previous section, is highly desirable as it allows for a maximum precision reinterpretation of the original analysis using a new BSM model. As the full detector simulation needs a significant amount of computing resources in addition to the non-negligible wall time of the actual preserved analysis pipeline, this approach can only be used on a limited set of models. In large-scale reinterpretations over high-dimensional parameter spaces, the amount of models that need to be sampled and investigated using the analysis is too high to employ the fully preserved analysis pipeline in every case. In order to significantly reduce the number of models that need to be passed through the full analysis pipeline, a pre-sorting of the models needs to be performed, filtering models for which (non-)exclusion based on a simplified analysis implementation is uncertain.

In the following, two major, complementary approaches to analysis simplifications are discussed, targeting both the *signal pipeline* as well as the *statistical inference* blocks in fig. 9.1. This section discusses the Simplementation of the analysis, an approach implementing the signal pipeline at *truth-level*, i.e. using the generator-level objects without running a dedicated detector simulation. An approximation of the detector response using four-vector smearing techniques is discussed.

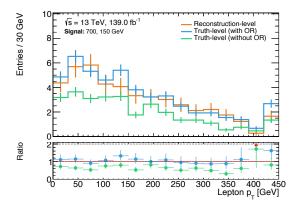
The second simplification is discussed in chapter 10, introducing a procedure for building simplified likelihoods from the full likelihoods of ATLAS SUSY searches in order to significantly lower the wall time needed for the statistical inference. In chapter 11, both approximations are combined and applied on a set of SUSY models sampled from the pMSSM.

9.4.1 Truth-level selection

All signal and control regions considered in the original 1ℓ search are implemented at truth-level using the publicly available framework SIMPLEANALYSIS. The exact implementation has been published, together with the previously discussed efficiency maps and analysis likelihod, as part of the auxiliary analysis data at Ref. [263]. In fact the SIMPLEANALYSIS implementation of the search was already used in chapter 7 for the derivation of some of the theory uncertainties.

The truth-level implementation explicitly specifies all object definitions introduced in section 4.4, even though some of them, like the lepton isolation, are technically not well-defined at truth-level. The four-vector smearing subsequently described is, however, in many cases implemented as a function of said object definitions and hence still allows to consider them to some extent. Additionally, as discussed in section 9.1, the full specification of the original analysis event selection including all object definitions allows for more straightforward reinterpretations by efforts outside of the ATLAS collaboration that generally do not have access to the original analysis software.

Following the object definitions, an overlap removal procedure following the same prescription as described in section 4.5 for the reconstruction-level analysis is performed, i.e. especially also using the same shrinking cone definitions. Since tracking information is not available at truth-level, the overlap removal step removing electrons sharing a track with a muon is approximated by using a distance parameter of $\Delta R = 0.01$ between the objects. Although often



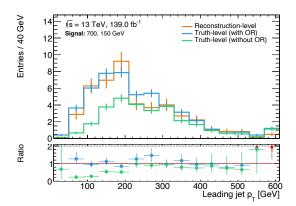


Figure 9.3: Impact of the overlap removal (OR) procedure at truth-level illustrated in the lepton and leading jet transverse momenta distributions. The truth-distributions with (blue) and without (green) overlap removal (green) are compared with a reconstruction-level (orange) distribution. The exemplary benchmark signal point with $m(\tilde{\chi}_1^{\pm}/\tilde{\chi}_2^0), m(\tilde{\chi}_1^0) = 700, 150\,\text{GeV}$ is shown in both plots. Both truth-level distributions are shown after smearing. All distributions are shown in a loose preselection requiring exactly one lepton, $E_{\text{T}}^{\text{miss}} > 50\,\text{GeV}, m_{\text{T}} > 50\,\text{GeV}$, and 2–3 jets, two of which need to be b-tagged.

neglected[†] in reinterpretation efforts outside of the collaboration, the correct implementation of the overlap removal procedure employed in the original analysis is crucial to reproduce the signal estimates of the original analysis. Figure 9.3 illustrates this by showing exemplary kinematic distributions of an exemplary signal point in configurations with and without overlap removal at truth-level, and comparing it with the distributions obtained at reconstruction-level[§]. Not implementing the overlap removal procedure of the original 1ℓ search, results in many truth-level events not passing the analysis selections because of additional objects in the final state that would otherwise have been removed through the overlap removal.

Finally, the exact implementation of all analysis observables is explicitly given, followed by the definition of all control and signal regions.

9.4.2 Truth smearing

The general assumption of the truth smearing applied in the following is that the detector response roughly factorises into the responses of single particles. This allows to use the ATLAS detector performance results in order to construct detector response maps parameterised in different observables for each physics object. Detector response maps include object reconstruction and identification efficiencies as well as scale factors to correct for differences between MC and observed data. Likewise, effects from the finite resolution of energy measurements in the detector are modelled through energy resolution maps. In the following, the four-vector components of electrons, muons, jets and $E_{\rm T}^{\rm miss}$ are smeared.

[†] The overlap removal procedures in ATLAS SUSY searches tend to be quite intricate, making them non-trivial to re-implement without ATLAS and analysis-specific knowledge.

[§] The term *reconstruction-level* here refers to distributions obtained with MC simulated datasets for which the full detector simulation and reconstruction has been run.

In the case of truth electrons, the identification efficiencies considered are parameterised in η and $p_{\rm T}$ as well as the identification working point used [212]. In η , nine fixed-width bins are used. In $p_{\rm T}$, six bins are implemented and a linear interpolation between two adjacent $p_{\rm T}$ -bins is used to get the efficiency for the given $p_{\rm T}$ of each truth electron. The probability of finding a fake electron in a truth jet is estimated through a similar two-dimensional map depending on the truth jet η and $p_{\rm T}$, again using fixed-width bins in η and a linear interpolation in $p_{\rm T}$. The range of the $p_{\rm T}$ interpolation for identification efficiencies and fake rates extends from 7 GeV to 120 GeV, covering the majority of all electrons in the analysis. If the truth $p_{\rm T}$ of the electron is outside of that range, the identification efficiency and fake rate from the respective bound of the corresponding η -bin are used. The probability for misidentifying an electron as a photon is estimated using different fixed values for the barrel and end-cap regions [211]. Finally, the transverse energy of the electron is smeared using a random number drawn from a Gaussian distribution with standard deviation corresponding to the η - and $p_{\rm T}$ -dependent energy resolution, measured in $Z \to ee$ and $J/\Psi \to ee$ events [273].

For truth muons, the identification efficiencies are also parameterised in η and $p_{\rm T}$ as well as the identification working point used [214]. Similar to truth electrons, the $p_{\rm T}$ of the muon is smeared using a Gaussian distribution with standard deviation corresponding to the momentum resolution. The momentum resolution of combined truth muons, $\sigma_{\rm CB}$, is computed from the resolutions in the ID, $\sigma_{\rm ID}$, and MS, $\sigma_{\rm MS}$, as

$$\sigma_{\rm CB} = \frac{\sigma_{\rm ID}\sigma_{\rm MS}}{\sqrt{\sigma_{\rm ID}^2 + \sigma_{\rm MS}^2}},\tag{9.1}$$

where $\sigma_{\rm ID}$ and $\sigma_{\rm MS}$ are parameterised in η and $p_{\rm T}$ and measured in $Z \to \mu\mu$ and $J/\Psi \to \mu\mu$ events [213].

The transverse momentum of truth jets is smeared using a Gaussian with standard deviation equal to the JER, provided in a map parameterised in five bins in $|\eta|$, ranging from $|\eta| = 0$ to $|\eta| = 4.5$. The jet energy resolutions are measured in dijet events [218] and provided as parameterisations of a noise N, stochastic S and constant C term for each of the seven bins in $|\eta|$, such that the resolution can be computed as

$$\frac{\sigma(p_{\rm T})}{p_{\rm T}} = \frac{N}{p_{\rm T}} \oplus \frac{S}{\sqrt{p_{\rm T}}} \oplus C. \tag{9.2}$$

Only truth jets with $10\,\mathrm{GeV} < p_\mathrm{T} < 1.5\,\mathrm{TeV}$ are smeared. For truth jets with $p_\mathrm{T} > 20\,\mathrm{GeV}$, the flavour tagging efficiency is considered using efficiencies parameterised in η , p_T and the MV2C10 efficiency working point (introduced in section 4.4) used, measured in fully reconstructed simulated $t\bar{t}$ events [224].

Finally, the smeared missing transverse energy is computed using the transverse momenta of all smeared truth objects in the event, including an approximation for the track soft term. The latter is approximated using resolution measurements from $Z \to \ell\ell$ events [227], allowing to infer a distribution of the mean soft term projected in the direction longitudinal to the total transverse momentum of all hard objects in an event, $p_{\rm T}^{\rm hard}$. The measured resolution parallel and perpendicular to $p_{\rm T}^{\rm hard}$ is then used to smear the nominal soft track value.

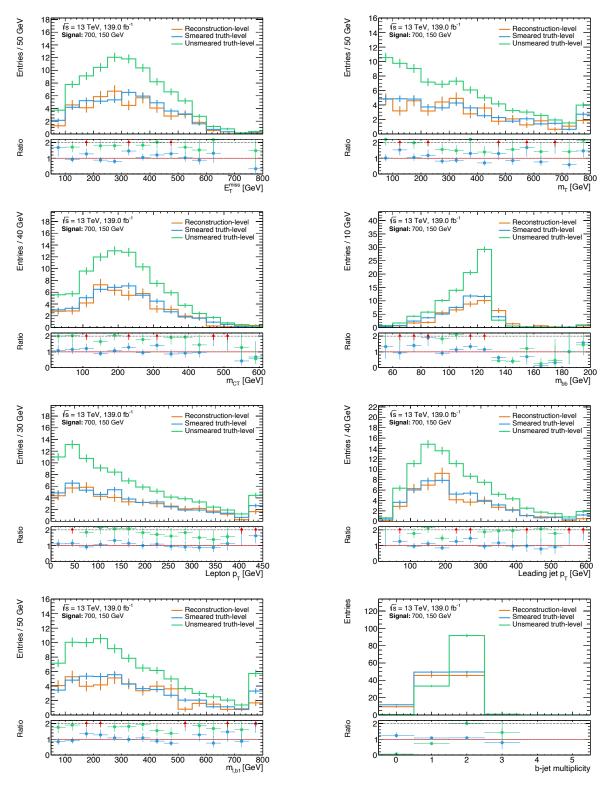


Figure 9.4: Comparisons of the kinematic distributions of key observables at (smeared) truth- and reconstruction-level. The exemplary benchmark signal point with mass parameters $m(\tilde{\chi}_1^{\pm}/\tilde{\chi}_2^0), m(\tilde{\chi}_1^0) = 700, 150 \, \text{GeV}$ is shown. The ratio pad shows the ratio of smeared and unsmeared truth-level distributions (blue and green) to reconstruction-level distributions (orange). Only MC statistical uncertainty is included in the error bars. All distributions are shown in a loose preselection requiring exactly one lepton, $E_{\text{T}}^{\text{miss}} > 50 \, \text{GeV}, m_{\text{T}} > 50 \, \text{GeV}$, and 2–3 jets, two of which need to be b-tagged. The latter requirement is dropped for the b-jet multiplicity distribution.

9.5 Validation of the truth-level analysis

9.5.1 Validation in loose preselection

The performance of the truth smearing is illustrated in fig. 9.4 in a loose preselection for an exemplary benchmark signal point. The loose preselection applied requires a final state with exactly one lepton, $E_{\rm T}^{\rm miss} > 50\,{\rm GeV},\,m_{\rm T} > 50\,{\rm GeV},\,$ and 2–3 jets, two of which need to be b-tagged. The reconstruction-level distributions are compared with the truth-level distributions before and after truth smearing. It can be observed that the truth smearing noticeably improves the agreement between the truth- and reconstruction-level distributions. While the lepton and jet reconstruction and identification efficiencies are—due to their dependence on $\eta,\,p_{\rm T}$ and individual working points—crucial for the overall agreement in shape, especially at low $p_{\rm T}$, the inclusion of flavour-tagging efficiencies significantly improves the overall agreement in normalisation.

Although some minor differences remain, a good agreement is observed overall across the relevant kinematic distributions at loose preselection level. Most of the differences remaining between smeared truth-level and reconstruction-level distributions in individual bins are well within the MC statistical uncertainties arising from the relatively limited MC statistics available.

9.5.2 Validation in signal regions

As the expected signal rates in the signal regions are ultimately what is entering the statistical inference, it is important that the good agreement observed at preselection is still present in the kinematically tighter selections of the signal regions. Additionally, it is worth investigating the agreement across all signal models considered in the original analysis, as opposed to only validating specific benchmark points. A comparison of the reconstruction-level and truth-level event rates before and after smearing in the signal regions SR-LM, SR-MM and SR-HM for all signal models considered in the 1ℓ search is shown in fig. 9.6. For the sake of conciseness, only the cumulative $m_{\rm CT}$ bins are shown in each signal region in fig. 9.6. The agreement in the individual $m_{\rm CT}$ bins in each SR-LM, SR-MM and SR-HM is provided in figs. B.1 to B.3.

The truth smearing drastically improves the agreement in event rate estimates at truth- and reconstruction-level across all SR bins. While, compared to reconstruction-level, the event rates are generally overestimated at truth-level before smearing, both tend to agree well within statistical uncertainties after smearing.

9.5.3 Validation using likelihood

Using the nominal expected event rates at (smeared) truth-level for every signal model in the original signal grid considered in the 1ℓ search, expected and observed CL_s values can be computed and exclusion contours can be derived. Figure 9.6 compares the expected and observed exclusion contours obtained using the full likelihood and reconstruction-level signal inputs with those obtained using the full likelihood and truth-level signal inputs before and after truth smearing. While all systematic uncertainties on the signal are included in the reconstruction-level contours, no signal uncertainties are considered when obtaining both the smeared and unsmeared truth-level contours. As expected from the previous validation steps

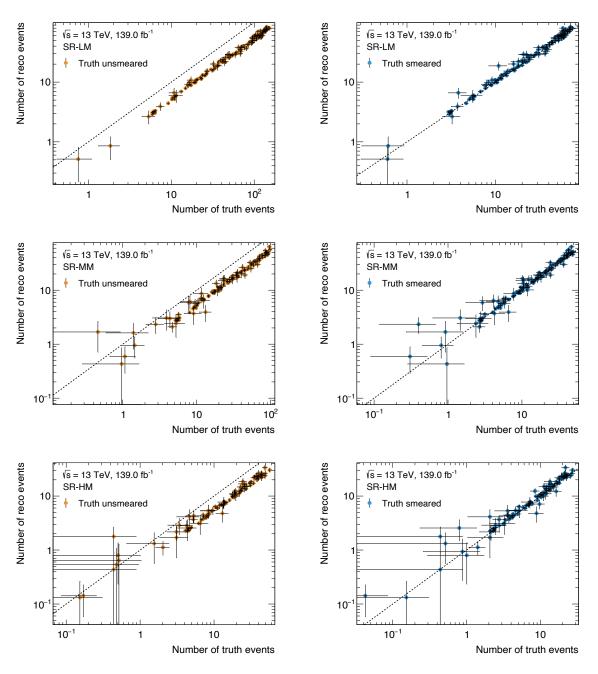


Figure 9.5: Comparison of the event rates at truth- and reconstruction-level before (left) and after (right) truth smearing. From top to bottom, the SR-LM, SR-MM and SR-HM signal regions are shown, with cumulative (integrated) $m_{\rm CT}$ bins. Every single point in the scatter plots represents a single signal model considered in the 1ℓ search. Uncertainty bars include MC statistical uncertainties.

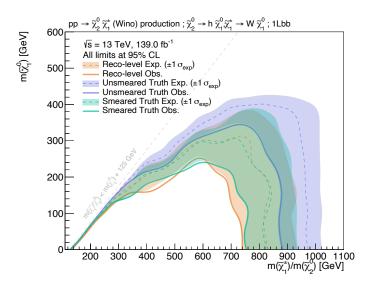


Figure 9.6: Expected and observed exclusion contours obtained with the full likelihood using reconstruction-level inputs (orange) as well as truth-level inputs before (purple) and after (green) smearing. Uncertainties include all statistical and systematic uncertainties on the background and signal for the reconstruction-level contours, but only statistical and systematic uncertainties on the background for truth-level signal inputs.

in the signal regions, the sensitivity using unsmeared truth-level signal inputs is significantly overestimated compared to the published analysis exclusion limit using reconstruction-level inputs. The smeared truth-level inputs, however, yield exclusion contours with an acceptable match compared to the reconstruction-level results.

In summary, the validation process performed at multiple selection levels of the analysis shows that the signal pipeline can be approximated reasonably well using a truth-level analysis and dedicated smearing functions. For signal models producing final states with kinematics close to those of the scenarios validated in the previous sections, this approach allows to determine the event rate estimates with high computational efficiency. In large-scale reinterpretations, the smeared truth-level analysis can be used as a basis for an efficient classification of models into two categories: models that are safely excluded or not excluded based on truth-level analysis only, and models where exclusion is in doubt and instead the precision of the full analysis pipeline using Recast is required.

Appendix B

B.1 Truth smearing

The estimated event rates in the exclusion signal regions at truth-level before and after truth smearing are compared with the reconstruction-level event rates in figs. B.1 to B.3. Each one of the 125 signal models from the simplified model signal grid corresponds to one point in the scatter plots. The smearing significantly improves the agreement between truth- and reconstruction-level event rate estimates in all signal region bins.

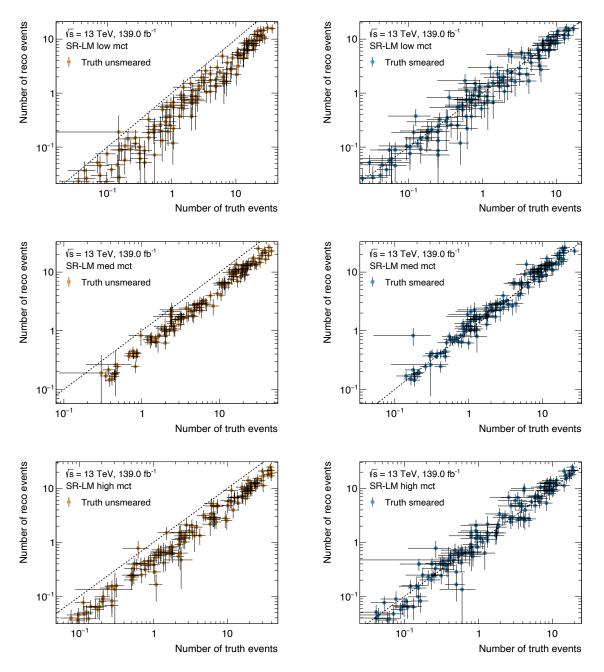


Figure B.1: Comparison of the event rates at truth- and reconstruction-level before (left) and after (right) truth smearing in SR-LM. From top to bottom, the low, medium and high $m_{\rm CT}$ bins are shown. Every single point in the scatter plots represents a single signal model considered in the original 1-lepton analysis. Uncertainties include only MC statistical uncertainties.

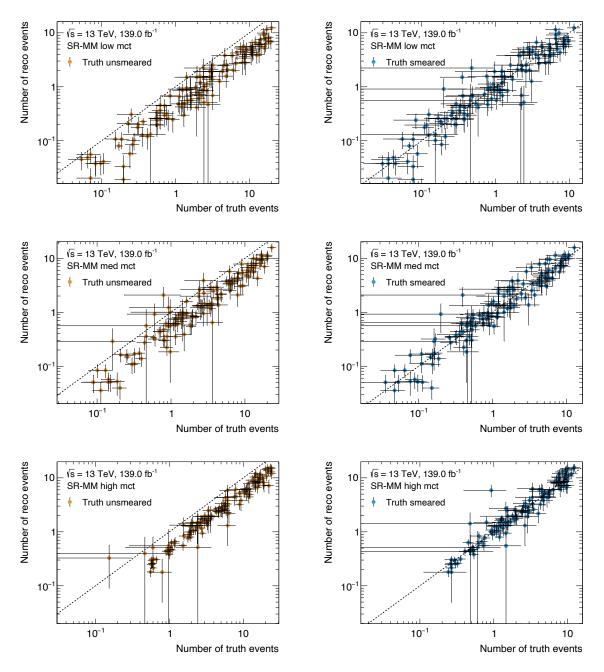


Figure B.2: Comparison of the event rates at truth- and reconstruction-level before (left) and after (right) truth smearing in SR-MM. From top to bottom, the low, medium and high $m_{\rm CT}$ bins are shown. Every single point in the scatter plots represents a single signal model considered in the original 1-lepton analysis. Uncertainties include only MC statistical uncertainties.

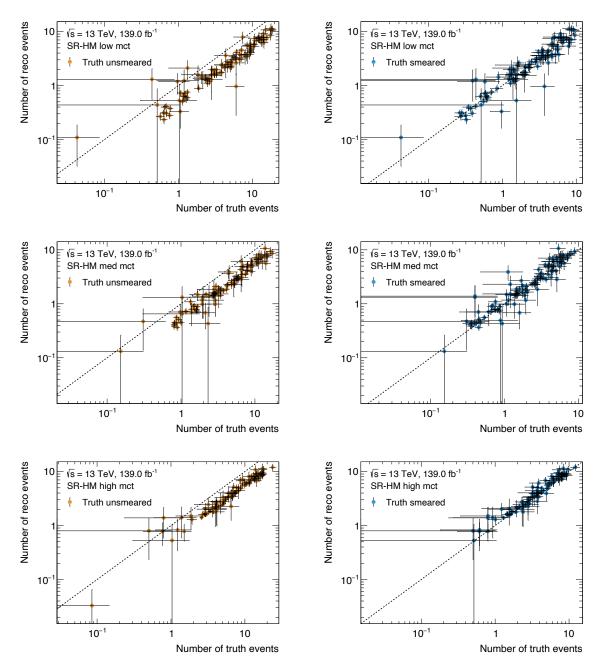


Figure B.3: Comparison of the event rates at truth- and reconstruction-level before (left) and after (right) truth smearing in SR-HM. From top to bottom, the low, medium and high $m_{\rm CT}$ bins are shown. Every single point in the scatter plots represents a single signal model considered in the original 1-lepton analysis. Uncertainties include only MC statistical uncertainties.

B.2 Simplified likelihood results

Figures B.4 and 10.5 show comparisons of the exclusion limits obtained using the full and simplified likelihoods for different ATLAS SUSY searches. In addition to the exclusion limits, the observed CL_s are given for every signal model tested. Although some likelihood simplifications needed special care (see section 10.5) and validation, a good agreement is observed throughout all analyses tested. Figures B.6 and B.7 directly compare the expected and observed CL_s values obtained using both likelihood configurations for each ATLAS SUSY search considered. Both linear- and log-scale representations are shown, revealing that the simplified likelihood tends to lead to good agreement in the CL_s values around 0.05, while slightly overestimating sensitivity in the region with $\mathrm{CL}_s \ll 0.05$, where signal models are in any case being excluded (and thus to some extent it is not important how small the CL_s value actually is).

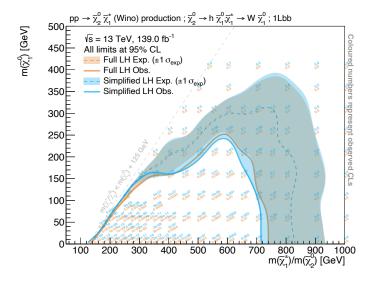


Figure B.4: Comparison of the simplified likelihood (blue contours) and full likelihood (orange contours) results for the search for electroweakinos presented previously. The observed contours are shown as solid lines, while the expected contours are shown as dashed lines. Observed CL_s values from both likelihoods are given. The uncertainty band includes all MC statistical and systematic uncertainties in the case of the full likelihood, and the simplified uncertainties in the case of the simplified likelihood.

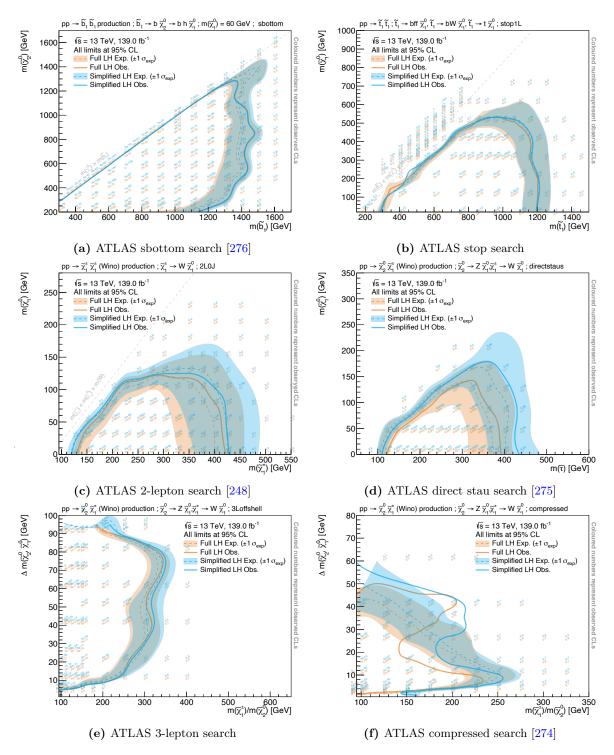


Figure B.5: Comparison of the simplified likelihood (blue contours) and full likelihood (orange contours) results for different ATLAS SUSY searches. The observed contours are shown as solid lines, while the expected contours are shown as dashed lines. Observed CL_s values from both likelihoods are given. The uncertainty band includes all MC statistical and systematic uncertainties in the case of the full likelihood, and the simplified uncertainties in the case of the simplified likelihood.

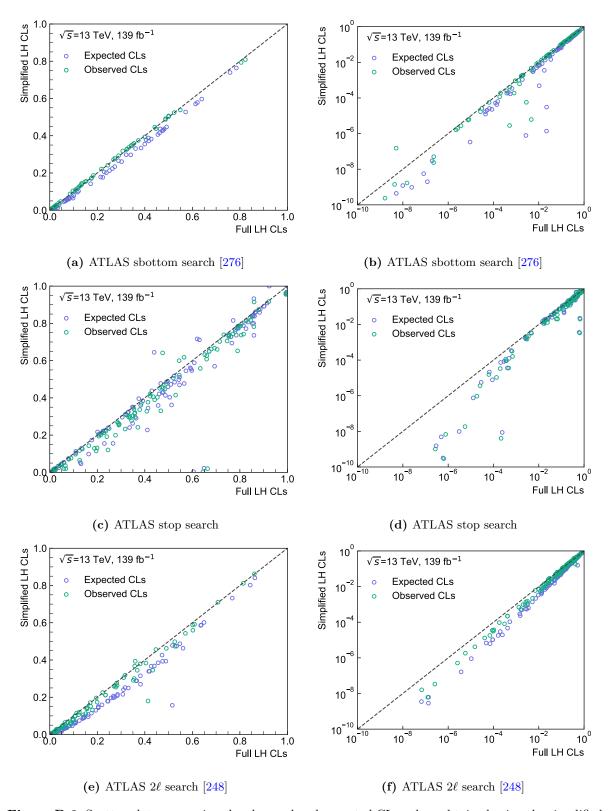


Figure B.6: Scatter plots comparing the observed and expected CL_s values obtained using the simplified and the full likelihoods for the same set of signal models originally considered in the various ATLAS SUSY searches. Both linear and logarithmic scale representations are shown on the left- and right-hand side, respectively, illustrating the full range of CL_s values. Apart from the scales, both columns show exactly the same results for each row of plots.

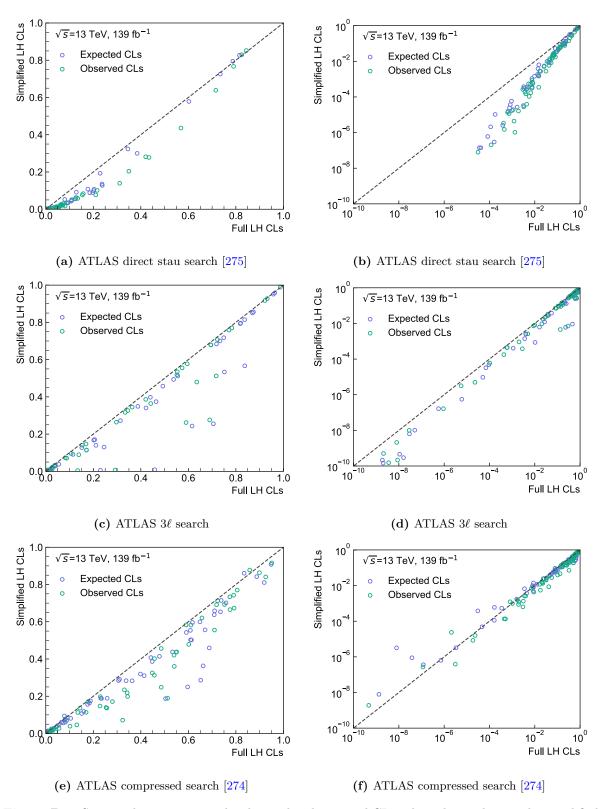


Figure B.7: Scatter plots comparing the observed and expected CL_s values obtained using the simplified and the full likelihoods for the same set of signal models originally considered in the various ATLAS SUSY searches. Both linear and logarithmic scale representations are shown on the left- and right-hand side, respectively, illustrating the full range of CL_s values. Apart from the scales, both columns show exactly the same results for each row of plots.

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