Chapter 7

Systematic uncertainties

Several sources of systematic uncertainties need to be considered in the following. As laid out in chapter 3, they enter the likelihood as nuisance parameters and can be interpreted as a loss of information on the signal strength parameter. In the following, they are separated into experimental uncertainties, arising e.g. from finite detector resolution, and theoretical uncertainties due to modelling of the physics processes during simulation.

7.1 Experimental uncertainties

Experimental uncertainties arise from the methods used to reconstruct, identify and calibrate the physics objects used in the 1ℓ search. They are evaluated using up and down variations provided either as variational weights in the case of efficiency uncertainties, or as additional variational samples derived by re-executing the entire object reconstruction pipeline with varied parameters.

7.1.1 Pile-up reweighting and luminosity

The MC simulated events used in the 1ℓ search were largely already generated before the full Run 2 dataset was recorded, and therefore before the full pile-up profile in data was known. For this reason, the number of average interactions $\langle\mu\rangle$ per bunch crossing in MC is in general not identical to that in data, necessitating a reweighting procedure in MC. In order to account for differences in the measured inelastic pp cross section [239] and the one obtained from MC simulation, a scale factor of 1.03 is applied before the reweighting procedure. As MC samples are generated with integer values of $\langle\mu\rangle$ only, the scale factor is applied to data instead. The uncertainty on the pileup reweighting is evaluated by varying the data scale factor by ± 0.04 and deriving variational pileup weights.

As detailed in section 2.1.2, the total integrated luminosity relies on the measurement of the bunch luminosity which, in turn, needs precise measurements of the visible inelastic cross section σ_{vis}, as well as the visible pile-up parameter μ_{vis}. Uncertainties on the measurement of the total recorded cross section are dominated by the uncertainties on σ_{vis} that is measured during special vdM scans. For the full Run 2 dataset, an overall luminosity uncertainty of $\pm 1.7\%$, is considered for all MC processes not normalised to data using a CR, derived using the methods described in Ref. [100].

7.1.2 Triggers

As all selections considered in the analysis apply a minimum requirement of $E_{\mathrm{T}}^{\mathrm{miss}} > 240\,\mathrm{GeV}$, thus targeting a region where the $E_{\mathrm{T}}^{\mathrm{miss}}$ triggers are fully efficient (see section 4.7). For this reason, no trigger scale factors and associated uncertainties are needed. Instead, only a 2% normalisation uncertainty correlated over all bins is considered in order to cover differences between the trigger plateaus due to MC statistical uncertainties.

7.1.3 Leptons

A large number of uncertainties on electrons arise from energy scale and resolution measurements [208, 210]. They are assumed to be fully correlated in η and are summed in quadrature, resulting in one nuisance parameter for the energy scale and one for the resolution. Uncertainties on muons arise from calibrations of the muon momentum scale and resolution, and are evaluated using variations in the smearing of the ID and MS tracks as well as the momentum scale, resulting in a total of five Gaussian-constrained nuisance parameters entering the likelihood [211]. Additional lepton-related uncertainties considered in the following originate from measurements of the reconstruction, identification and isolation efficiencies. Two more uncertainties arising from track-to-vertex association and bad muon identification efficiencies are considered in the case of muons.

7.1.4 Jets

The calibration of the jets to the absolute JES is subject to uncertainties arising e.g. from the *in situ* measurements, pile-up effects or flavour-dependence [216], encoded in a large set of 125 parameters. The full detail contained in the complete set of uncertainty components offers far greater statistical precision than needed for the 1ℓ search. As the majority of the parameters (a total of 98) stems from *in situ* measurements, an eigenvector decomposition is performed on the covariance matrix of these components [240], allowing to determine the 15 principal orthogonal components (including a residual term adding the remaining terms in quadrature), with minimal loss in bin-by-bin correlation information. Five additional parameters evaluating uncertainties arising from *in situ* η-intercalibrations of forward jets with respect to central jets are kept separate due to their two-dimensional dependence on p_{T} and η [216]. Effects from pile-up are described by four additional nuisance parameters. Uncertainties arising from differing detector responses to gluon- and quark-initiated jets as well as flavour-related differences are accounted for by two more nuisance parameters. Uncertainties from jets that are not contained in the calorimeters and *punch-through* into the MS are evaluated with an additional parameter. A last parameter encodes the uncertainty arising from the calibration of MC samples reconstructed using ATLFAST-II instead of the full detector simulation.

Systematic uncertainties on the JER arise from measured differences between data and MC simulation, noise from pile-up, and *in situ* measurements of the jet p_{T} imbalance. A similar eigenvector decomposition as for part of the JES uncertainties is used, reducing the set of nuisance parameters considered in the following to 13 [216]. Finally, uncertainties related to the efficiency of jet vertex tagging are evaluated using a weight systematic.

7.1.5 Flavour tagging

Uncertainties on the flavour tagging efficiency originate from e.g. modelling uncertainties, as well as uncertainties on the reconstruction of physics objects. Similar to the JER and JES uncertainties, the full set of nuisance parameters that would in principle need to be included in order to consider the full bin-by-bin correlations and p_{T} and η dependence of the flavour-tagging uncertainties, is reduced to a more manageable size using an eigenvector decomposition. This leads to a total of five nuisance parameters encoding uncertainties on the b-tagging efficiency, c-jet and light-jet mis-tagging rate as well as the extrapolation to high-p_{T} jets [222, 223].

7.1.6 Missing transverse energy

The uncertainties on $E_{\mathrm{T}}^{\mathrm{miss}}$ are evaluated using the systematic variations of all calibrated objects as inputs to the $E_{\mathrm{T}}^{\mathrm{miss}}$ calculation. Additional uncertainties arise from the calculation of the track soft term. In the following, uncertainties on the soft term scale and resolution are considered, resulting in one nuisance parameter for the soft term scale and two nuisance parameters—corresponding to the perpendicular and parallel components—for the soft term resolution uncertainty. All track soft term uncertainties are derived by comparing MC simulation to $Z \to \mu\mu$ events [224].

7.2 Theoretical uncertainties

As discussed in section 2.2.8, due to finite order calculations, the different steps of the MC simulation generally introduces a certain number of unphysical scales and parameters. In order to quantify the uncertainties arising from the ad-hoc values of these, the MC simulation generally needs to be re-run with systematically varied parameter values. Since varied MC simulation parameters affect the event kinematics even before reconstruction and calibration, it is computationally very expensive to produce a full set of variations for each MC simulated dataset used in the nominal analysis.

In the following, different approaches are used to derive the theory uncertainties. For some of the variational MC datasets, the full MC simulation chain was run with reduced statistics. For others, different MC datasets produced with a different set of MC generators and tunes were available. For still others, variations were already processed during the initial MC simulation of the nominal sample and subsequently stored as variational weights. Finally, some of the variational MC datasets were simulated at MC truth-level, i.e. without detector simulation. The latter approach was used especially in the case of SUSY signal samples, where the impact of the full detector simulation compared to truth-level comparisons is expected to be small in the context of theory uncertainties. Additionally, a full simulation of MC datasets for all parameter variations and all signal points considered, would be computationally unfeasible.

For background processes that are normalised to data in a dedicated CR, the theory uncertainties are evaluated on the transfer factors. For a process p, a control region CR_i, and a destination region R_j, the transfer factor reads

$$f_p(\mathrm{CR}_i \to \mathrm{R}_j) = \frac{N_p^{\mathrm{MC}}(\mathrm{R}_j)}{N_p^{\mathrm{MC}}(\mathrm{CR}_i)}, \tag{7.1}$$

where $N_p^{\mathrm{MC}}(\mathrm{R}_j)$ and $N_p^{\mathrm{MC}}(\mathrm{CR}_i)$ are the expected event rates for the process p in CR_i and R_j, respectively. The systematic uncertainty on the transfer factor is then given by

$$\Delta f_p^{\mathrm{syst}} = \frac{f_p^{\mathrm{variation}}}{f_p^{\mathrm{nominal}}} - 1, \tag{7.2}$$

with $f_p^{\mathrm{variation}}$ and f_p^{nominal} the transfer factors from the variational and nominal samples, respectively. If the MC datasets used for deriving the variational and nominal transfer factors are statistically independent, a statistical component of the uncertainty is derived using the individual statistical uncertainties on the background estimate,

$$\Delta f_p^{\mathrm{stat}} = (\Delta f_p^{\mathrm{syst}} + 1)\sqrt{\sum_{n \in \boldsymbol{N}} (\frac{\sigma_n}{n})^2}, \tag{7.3}$$

where n runs over the set of expected event rates and σ_n is the absolute MC statistical uncertainty associated to each expected event rate n. In the following, the control region used to evaluate the uncertainties on the transfer factors is taken to be the sum of all CRs introduced in section 6.2. This approach not only significantly improves the statistics in the region used for normalisation, but also results in a consistent treatment across all theoretical uncertainties on all relevant processes.

For backgrounds directly estimated from MC simulation, the systematic uncertainty on the expected event rate in each region R_i is given by

$$\Delta n_p^{\mathrm{syst}}(\mathrm{R}_i) = \frac{n_p^{\mathrm{syst}}(\mathrm{R}_i) n_p^{\mathrm{nominal}}(\mathrm{P})}{n_p^{\mathrm{nominal}}(\mathrm{R}_i) n_p^{\mathrm{syst}}(\mathrm{P})} - 1, \tag{7.4}$$

where the region P is a so-called *loose preselection* with minimal analysis selection criteria, used for normalisation of the event rates to be compared. If not otherwise indicated, the loose preselection used for normalisation requires exactly one isolated lepton, 2–3 jets of which at least one is b-tagged, $E_{\mathrm{T}}^{\mathrm{miss}} > 220\,\mathrm{GeV}$ and $m_{\mathrm{T}} > 50\,\mathrm{GeV}$.

Apart from the hard scattering and parton showering uncertainties on top processes, all other theoretical uncertainties enter the likelihood as asymmetric correlated shape uncertainties. The hard scattering and parton showering uncertainties on top processes described below are estimated using MC generator comparisons and thus need to be symmetrised. The shape information is however still kept, i.e. the uncertainties are not one-sided.

7.2.1 Background

$t\bar{t}$ and single top

Theory uncertainties on the estimate of $t\bar{t}$ and single top processes arise for example from the simulation of the hard scattering between the interacting partons. These are evaluated by comparing the estimates from the nominal MC datasets generated using POWHEG and PYTHIA8 with those from alternative datasets generated using MADGRAPH_AMC@NLO and PYTHIA8. An uncertainty resulting from the hadronisation and fragmentation scheme chosen in PYTHIA8 is estimated by comparison to a MC dataset generated using POWHEG and HERWIG++ [241]. Uncertainties arising from ISR are evaluated at full reconstruction level by varying up and down by a factor of two the unphysical renormalisation μ_{R} and factorisation μ_{F} scales as well as the parameters controlling the showering and ME+PS matching [242]. Likewise, uncertainties arising from simulation of FSR are estimated by varying the effective coupling α_s^{FSR} [242].

Uncertainties also originate from the PDF set used during generation of the nominal MC dataset. As detailed in table 4.1, the NNPDF3.0NLO is used for the simulation of both $t\bar{t}$ and single top processes. An envelope around the variational expected event rates obtained from the NNPDF3.0NLO uncertainties are used to compute an uncertainty on the transfer factor.

Beyond LO single top production diagrams, interference appears between Wt and $t\bar{t}$ production. Two approaches are commonly used to try and isolate the Wt channel: diagram removal (DR) and diagram subtraction (DS) [243]. While the former removes all diagrams in the NLO Wt amplitude that are doubly resonant (meaning that they involve an intermediate top quark that can be on-shell), the latter introduces subtraction terms in the NLO Wt cross section cancelling the $t\bar{t}$ contribution [243]. As the DR scheme is used for estimating the event rate of the Wt channel in the analysis, a comparison with an estimation using the DS scheme allows to derive an uncertainty associated to the interference.

W/Z + jets

For W/Z + jets processes, simulated using SHERPA 2.2.1, four different unphysical scales can be varied in order to evaluate uncertainties on the modelling. The renormalisation μ_{R} and factorisation μ_{F} scales are both independently and together varied up and down by a factor of two, resulting in a total of seven combined variations. Three envelopes are determined from varying only μ_{R}, only μ_{F} or μ_{R} and μ_{F} together, allowing to determine three separate uncertainties. The CKKW ME+PS matching scheme also uses an unphysical scale for determining the overlap between jets from the ME and the PS. The nominal value of 20 GeV for the merging scale is varied to 30 GeV and 15 GeV for the up and down systematic variations, respectively. Finally, the scale used for resummation of soft gluon emission, μ_{QSF}, is varied up and down by a factor of two, and the effect on the expected event rates are determined.

An additional uncertainty arises from the choice of PDF set used for simulating W/Z + jets. It is evaluated by propagating the PDF error set (containing slightly different parameterisations of the PDF) to the analysis observables. Uncertainties due to the choice of the strong coupling constant $\alpha_s(m_Z) = 0.118$ for fitting the PDFs are estimated by comparing with variations using $\alpha_s(m_Z) = 0.119$ and $\alpha_s(m_Z) = 0.117$, and added in quadrature to the PDF uncertainty.

As $Z+$jets is not normalised to data in a dedicated CR but to its nominal SM cross section, an additional normalisation uncertainty corresponding to the theoretical uncertainty on the cross section is considered.

Other backgrounds

For diboson, multiboson and $t\bar{t}+V$ processes, uncertainties arising from the unphysical scales μ_{F}, μ_{R} as well as μ_{QSF} and the CKKW ME+PS matching scale are considered using the same prescription described above for $W/Z+$jets. For these three processes as well as for the other minor backgrounds $V+h$ and $t\bar{t}+h$, an additional uncertainty on the SM cross section used for normalisation is taken into account.

7.2.2 Signal

Theoretical uncertainties on the SUSY signal processes arise from the unphysical factorisation, renormalisation and CKKW-L ME+PS merging scales. These are evaluated using a similar procedure as for background processes, varying the different scales up and down by a factor of two and comparing the expected signal rates. An additional uncertainty on PS originating from the chosen Pythia8 tune is estimated by varying up and down the chosen value for α_s^{ISR}.

As detailed in section 4.3.1, the cross section of electroweakino pair production is calculated using Resummino. A theoretical uncertainty on the cross section is considered in the following, but does not enter the statistical fit procedure as nuisance parameter. Instead, in addition to the set of observed CL_s values using the nominal cross section, two additional variational sets are derived using signal cross sections fixed at their $\pm 1\sigma$ variations. This allows to draw a cross section uncertainty band on the observed exclusion contour.

Due to the large number of MC samples, all theory uncertainties on SUSY signal processes are evaluated at MC truth-level only. As the VRs typically have relatively low signal contamination and thus low signal MC statistics available for evaluating theory uncertainties, requirements on observables with negligible impact on the shapes of the theoretical uncertainties are loosened. In the on-peak VRs, the requirements loosened are $m_{\mathrm{T}} > 60\,\mathrm{GeV}$ and $E_{\mathrm{T}}^{\mathrm{miss}} > 140\,\mathrm{GeV}$. The same loosened selection is applied in SRs in cases where the MC statistical uncertainty is too high for a reliable estimation of the theoretical uncertainties. In the off-peak VRs, the requirements loosened are $m_{\mathrm{T}} > 60\,\mathrm{GeV}$ and $E_{\mathrm{T}}^{\mathrm{miss}} > 60\,\mathrm{GeV}$ and $m_{\mathrm{CT}} > 60\,\mathrm{GeV}$. Overall, the theoretical uncertainties on the expected signal rate range from about 10% in phase space regions with large mass splitting between $\tilde{\chi}_1^{\pm}/\tilde{\chi}_2^0$ and $\tilde{\chi}_1^0$ to about 25% in regions with small mass splittings.

7.3 Impact on signal regions

Table 7.1 shows a breakdown of the dominant systematic uncertainties on the background prediction in the SRs, obtained after a background-only fit in the CRs with subsequent extrapolation to the SRs. The total uncertainty in the SRs amounts to 15% in SR-LM and increases to 25% in SR-MM and 34% in SR-HM. Theoretical uncertainties have the largest contribution to the total uncertainty. For SR-LM, the largest uncertainty, amounting to 10% of the total background estimate, originates from the $t\bar{t}$ parton shower uncertainty. For SR-MM

Table 7.1: Breakdown of the dominant systematic uncertainties on background estimates in the various exclusion signal regions (m_{CT} bins summed up). As the individual uncertainties can be correlated, they do not necessarily add up in quadrature to the total background uncertainty. The percentages show the size of the uncertainty relative to the total expected background. Table adapted from Ref. [170].

Signal Region	SR-LM	SR-MM	SR-HM
Total background expectation	27	8.6	8.1
Total uncertainty	±4 [15%]	±2.2 [25%]	±2.7 [34%]
Theoretical systematic uncertainties			
$t\bar{t}$	±2.6 [10%]	±0.6 [7%]	±0.33 [4%]
Single top	±0.8 [2.7%]	±1.1 [12%]	±1.9 [23%]
W+jets	±0.23 [0.9%]	±0.07 [0.8%]	±0.19 [2.3%]
Other backgrounds	±0.13 [0.5%]	±0.15 [1.7%]	±0.08 [1.0%]
MC statistical uncertainties			
MC statistics	±1.7 [6%]	±1.1 [13%]	±1.2 [14%]
Uncertainties in the background normalisation			
Normalisation of dominant backgrounds	±1.3 [5%]	±1.6 [18%]	±1.3 [16%]
Experimental systematic uncertainties			
$E_{\mathrm{T}}^{\mathrm{miss}}$/JVT/pile-up/trigger	±1.8 [7%]	±0.4 [4%]	±0.4 [5%]
Jet energy resolution	±1.6 [6%]	±0.5 [6%]	±0.4 [5%]
b-tagging	±1.1 [4%]	±0.29 [3.4%]	±0.13 [1.5%]
Jet energy scale	±0.9 [3.2%]	±0.9 [10%]	±0.29 [4%]
Lepton uncertainties	±0.32 [1.2%]	±0.09 [1.0%]	±0.19 [2.3%]

(SR-HM), the single top generator uncertainties are the largest ones with 10% (21%) of the total background estimate. Theoretical uncertainties on W + jets and other minor backgrounds have only small to negligible effects. The experimental uncertainties in general have less impact on the total uncertainty than the theoretical ones, with the largest experimental uncertainties contributing only 5–10% depending on the SR. The dominant experimental uncertainties arise from the JES and JER as well as $E_{\mathrm{T}}^{\mathrm{miss}}$ modelling and pile-up effects. The MC statistical uncertainties contribute 5–18%, depending on the SR.

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