Automated Matrix‑Element Re‑Weighting in Effective Field Theories

Master’s Thesis

Christopher Robert Jacobsen  
Niels Bohr Institute  
November 2015

Advisor  
 Jørgen Beck Nielsen  
 Niels Bohr Institute

# Abstract

**TOC**

# Introduction

In the search for physics beyond the standard model it is necessary to compare the predictions of a candidate theoretical model to experimental data, in order to ascertain the likelihood of the candidate’s veracity. Most models have parameters that influence or determine the behavior of the model, and often the exact values of these parameters are not known in advance. It is common to fit the model to data, to find the set of parameter values that give the best match to experimental data, and in conjunction with error estimates determine confidence limits for the model parameters.

Monte-Carlo event-generators and detector simulators are used to generate model events for a specific set of model parameters, which can then be compared to experimental data for various observables. To test another set of model parameters, new events must typically be generated, and this cycle of changing parameters and re-generating events can be highly time consuming.

For example, to generate one-million events with the Sherpa event generator takes about 10 minutes on a fast desktop computer. Thereafter, the events need to be run through a detector simulator, which will take significantly longer. For ATLAS detector simulations, one million events will take the fastest simulator (ATLFASTIIF) about 14 days, and the slowest (GEANT4) about four years [1].

Reweighting is a technique that can be used to very quickly recalculate event-distributions for different model parameter values from an existing event dataset. Event generation and detector simulation do not need to be repeated for each model parameter configuration. One can create new event-distributions in milliseconds instead of days or weeks. Clearly reweighting is a

Reweighting works by determining, with the help of an event generator, the functional dependency of the squared matrix-element for each event on the model parameters. By definition, this functional dependency is a quadratic function of the model parameters and can be stored for later retrieval as a set of quadratic coefficients for each event.

As the probability of an event is proportional to its squared matrix element, we can calculate the relative change in frequency for each generated event to a new set of model parameters, by comparing the squared matrix-elements of the new and old model parameters. Reweighting then uses this relative change factor as an event-weight when constructing event-distributions for our model. In this manner, we can construct equivalent event-distributions for any set of model parameters.

The primary goal of this project is to develop a generic software tool that enables the use of matrix-element reweighting. Specifically, to use the Sherpa Monte-Carlo event generator [2] to determine the matrix-element dependencies on model parameters, and embed these in generated event files, so that they can be used later for reweighting of observable event-distributions.

The secondary goal of this project is to test the reweighting workflow with effective field theory and dimension six-operators, and to test the fitting characteristics of reweighted events to standard-model (SM) pseudo-data. This will involve creating libraries of methods and classes for performing reweighting and fitting.

The tertiary goal of this project is to examine the fitting performance of different observables, specifically testing optimal observables. Additionally, to test the fit characteristics of binned and unbinned fits.

In the remainder of this section we examine reweighting in more detail, and introduce the different third-party software that went into this project.

In section 2, we introduce and describe SherpaWeight, the application that was developed to meet our primary goal.

In section 3, we introduce effective field theory (EFT) for dimension-six operators, and describe and test our implementation of the model.

In section 4, we describe and test our reweighting implementation.

In section 5, we introduce and describe optimal observables.

In section 6, we describe our choice of observables, binning, and our attempts to optimize binning.

In section 7, we fit the EFT model to SM pseudo-data for 21 different observables, including optimal observables, using both binned and unbinned fits.

Finally, our conclusions can be found in section 8.

## Reweighting details

We will now look a bit deeper into the details of reweighting. According to Fermi’s golden rule, the probability of a scattering process is proportional to its squared matrix-element (aka amplitude):

|  |  |  |
| --- | --- | --- |
|  |  | (1.1) |

Where is the differential cross-section, essentially the probability of the event; i, and f are the initial and final states; and H is the Hamiltonian of the system. The probability of a scattering process will also include a final-state density term. For proton-proton collisions, the probability of extracting the incoming partons in the initial state from colliding protons must also be included. For convenience, we will often refer to the squared matrix-element as simply the matrix-element or ME.

Theoretical model parameters are generally added linearly to a model’s Lagrangian, such that Lagrangian model terms are scaled by the value of the model parameter. Changes to model parameters will only affect the Lagrangian and thus the Hamiltonian. All states and other factors affecting the probability of the event are unchanged.

For model parameters linear in the Lagrangian, the squared matrix-element will by definition be quadratic in terms of these parameters. In the case of a single linear model parameter the squared matrix-element can be written as:

|  |  |  |
| --- | --- | --- |
|  |  | (1.2) |

Where A, B, and C are quadratic coefficients, which we will call reweight coefficients. If is zero in the standard-model (SM), then the A coefficient becomes equivalent to the SM squared matrix-element.

For two or more model parameters cross-terms are added:

|  |  |  |
| --- | --- | --- |
|  |  | (1.3) |

We can write this in matrix-form as:

|  |  |  |
| --- | --- | --- |
|  |  | (1.4) |

Where is a vector of model parameters prefixed with value of 1 in the first index, and **F** is an upper triangular matrix of reweight coefficients, corresponding to the a, b, c and d coefficients in (1.3). is a zero-order coefficient, are the first-order coefficients, are the second-order coefficients, and are the cross-term coefficients.

The number of reweight-coefficients depends upon the number of model parameters, that we wish to be able to reweight events with, and is given by:

|  |  |  |
| --- | --- | --- |
|  |  | (1.5) |

Where NF is the number of reweight-coefficients and NP is the number of reweight-parameters.

### Calculating the reweight-coefficients

If we can determine the reweight-coefficient matrix F for each event, then we can recalculate the matrix-element for that event for any model parameter values. Fortunately, Monte-Carlo generators like Sherpa are capable of calculating the matrix-element value for a given event and set of model parameters. We can use linear algebra to solve for the unknown reweight-coefficients by by calculating matrix-elements for each event for NF independent evaluations of model parameters.

This is achieved by placing the NF elements of the triangular matrix **F** into a vector , in row-column order:

|  |  |  |
| --- | --- | --- |
|  |  | (1.6) |

Similarly, we can construct an evaluation vector with matching model parameters corresponding to the terms in :

|  |  |  |
| --- | --- | --- |
|  |  | (1.7) |

The matrix-element equation for a single event now becomes a simple linear equation:

|  |  |  |
| --- | --- | --- |
|  |  | (1.8) |

We can write the NF independent evaluations and calculated matrix-elements in matrix form, giving us an equation we can solve by linear algebra:

|  |  |  |
| --- | --- | --- |
|  |  | (1.9) |

Defining as the vector of calculated ME-values, and **A** as the matrix of model parameter evaluations, we can acquire our unknown reweight coefficients by:

|  |  |  |
| --- | --- | --- |
|  |  | (1.10) |

This only requires that **A** is constructed in such a manner that it can be inverted, i.e. that the NF model parameter evaluations are independent.

With the aid of a Monte-Carlo generator, one can thus calculate matrix-elements for different reweight-parameter evaluations and solve for the reweight-coefficients of any generated event. The calculated reweight-coefficients can be stored separately or embedded within the generated event file.

### Using reweight-coefficients to reweight event-distributions

With the reweight-coefficients for each event one can calculate the matrix-element for that event using (1.8) for any set of reweight-parameter values. This does not give the new probability or differential cross-section for the event, but one can use it to compare the relative probabilities of the event at two different sets of reweight-parameter values:

|  |  |  |
| --- | --- | --- |
|  |  | (1.11) |

If one also knows the the reweight-parameter values used to generate the events, we can calculate the relative probability of an event for any set of reweight-parameter values to its probability when generated.

Normally all generated events in a dataset have equal probability, and are placed in event-distributions with equal weights of one. To reweight an event-distribution, one can simply use the relative probability, compared to the probability when generated, to weight the event. A relative increase in probability for an event will result in it being given a proportionally higher weight in the distribution, and correspondingly for a relative decrease.

Given the reweight-coefficients for each event, and the values of the reweight-parameters for the generated events, one can reweight all event-distributions for the dataset to a new set of reweight model parameter values.

A word of caution: one cannot reweight events if those events are not present in the dataset. One can reweight an event to zero probability, but one cannot give a probability to an event that is not present. So it is essential when reweighting that the dataset not be generated with a set of model parameters that effectively zero terms of the Lagrangian that will later be reweighted.

## Software tools

This project has the primary focus of developing a software tool that automates the calculation of reweight-coefficients using the Monte-Carlo event-generator Sherpa. In this section, we briefly introduce Sherpa as well as the other major software tools that were used in this project.

### Sherpa

Sherpa is a Monte-Carlo event generator for the **S**imulation of **H**igh-**E**nergy **R**eactions of P**A**rticles. It is an open-source project developed by the Sherpa Team, a global group of physics researchers and students. Information, documentation, and download links for Sherpa are available on Sherpa’s web-site [2].

Sherpa can be downloaded from its web-site and built locally on Linux and Mac OS operating systems. For Mac OS, we recommend using the software package tool Homebrew [3] and the HEP software repository for Homebrew [4], to download and install the latest version of Sherpa easily.

There are various build-options that can be used when building Sherpa. For reference purposes, we used the following build-options for Sherpa for this project:

|  |  |
| --- | --- |
| --enable-pyext | Enables Python support. Required for UFO model support. |
| --enable-root | Enables writing and reading of ROOT event files. |
| --enable-hepmc2 | Enables writing and reading of HepMC event files. |
| --enable-gzip | Enables support for gzipped event files. |
| --enable-lhapdf | Enables support for PDFs from the LHAPDF library. |
| --enable-mpi | Enables support for OpenMPI multi-processor computing. |

Sherpa can be used both as a command line tool and as a C++ library. In both instances, Sherpa uses a text file it calls a run card to setup and configure event generation. The run card file can contain many different parameters, and we refer the reader to the documentation for Sherpa for details. Figure 1.1 shows an example run card for Sherpa.

The command line for Sherpa is generally fairly simple:

|  |
| --- |
| Sherpa –f run\_card\_filename |

Without the –f option Sherpa will look for a run-card called Run.dat. There are many other options described in the documentation.

Sherpa also provides a set of C++ classes that can be dynamically linked to by an application. These classes are not documented, however, and it is up to the user to read the header files and source code for Sherpa to determine how they may be used.

Beware: this is not a task for the light-hearted. In this project, much time was used reading and understanding Sherpa source code. It is not well commented, and is written in a highly compact and difficult to read form. Further, there is no guarantee of backwards compatibility of the C++ code with future versions of Sherpa.

|  |
| --- |
| !------ Run parameters (Sherpa 2.2.0 manual 5.1) ------  (run){  EVENTS 10000  EVENT\_OUTPUT HepMC\_GenEvent[events]  OUTPUT 2 ! output info and error messages but not events  PRETTY\_PRINT Off ! disable color messages  }(run)  !------ Beam parameters (Sherpa 2.2.0 manual 5.2) ------  (beam){  BEAM\_1 2212; BEAM\_ENERGY\_1 6500  BEAM\_2 2212; BEAM\_ENERGY\_2 6500  ! BEAM\_REMNANTS 0 ! disable beam remnants - only hard process  }(beam)  !------ ISR parameters (Sherpa 2.2.0 manual 5.3) ------  (isr){  PDF\_LIBRARY CT10Sherpa  PDF\_SET ct10  }(isr)  !------ Models (Sherpa 2.2.0 manual 5.4) ------  (model){  MODEL SM  CKMORDER 1 ! enable quark-mixing using CABIBBO parameter (default = 0.2272)  }(model)  !------ Matrix elements (Sherpa 2.2.0 manual 5.5) ------  (me){  ME\_SIGNAL\_GENERATOR Comix  ! SCALES VAR{Abs2(p[0]+p[1])} ! required if SHOWER\_GENERATOR is None  ! ME\_QED Off ! disable FSR - only hard-process  }(me)  !------ Processes (Sherpa 2.2.0 manual 5.6) ------  (processes){  Process 93 93 -> 24 23  End process  }(processes)  !------ Selectors (Sherpa 2.2.0 manual 5.7) ------  (selector){  PT 24 10.0 E\_CMS  PT 23 10.0 E\_CMS  }(selector)  !------ Parton showers (Sherpa 2.2.0 manual 5.10) ------  (shower){  ! SHOWER\_GENERATOR None ! disable parton showers - only hard-process  }(shower)  !------ Multiple interactions (Sherpa 2.2.0 manual 5.11) ------  (mi){  MI\_HANDLER None ! disable multiple interactions  }(mi)  !------ Hadronization (Sherpa 2.2.0 manual 5.12) ------  (fragmentation){  ! FRAGMENTATION Off ! disable hadronization - only hard-process  }(fragmentation) |

Figure 1.1: Example Sherpa run card file.  
This file instructs Sherpa to generate 10000 events from proton-proton collisions at  = 13 TeV, with the process . Run parameters are grouped into different sections, and are either listed on a line by themselves, or may be separated by semi-colons on the same line. Section-names, parameters and parameter values are case-sensitive. Comments begin with either an exclamation mark (!) or a hash (#). Multiple whitespace characters (spaces and tabs) are treated as one.

As this project took place over the span of a year, work began with Sherpa version 2.1.1 and continued with Sherpa version 2.2.0, upon its release in July 2015. These two versions are significantly different in many aspects, and much of the programming work done with 2.1.1 had to re-done with 2.2.0. The biggest change that affected this project was the change of supported models.

Sherpa 2.1.1 supports among others, the standard model, an anomalous gauge coupling model, and user defined models via a specially defined FeynRules export format. Sherpa 2.2.0 only supports the standard model and user-defined FeynRules UFO models, a completely different FeynRules model format than used in the previous version.

### FeynRules and Mathematica

FeynRules is a software package that allows the calculation of Feynman rules in momentum space for *any* QFT physics model. It is used together with Mathematica, a commercially available multi-purpose mathematics software system. FeynRules is an open-source project maintained by a global group of physics researchers and students. Information, documentation, and download links for FeynRules are available on FeynRules web-site [5]. Some additional instructions on using FeynRules, which is well worth reading, is given in [6] and [7].

FeynRules allows the user to define a QFT physics model using FeynRules methods and definitions. The model can be tested for Hermiticity along with many other tests. Models can be exported in several different formats for use by event-generators.

We used FeynRules to define a working Effective Field Theory model for three dimension-six operators, and exported this model to Sherpa using two different model formats: a special FeynRules-Sherpa model format, and the FeynRules UFO model format [8]. The first is a custom format only useable by Sherpa version 2.1.1 and earlier. The second is an open format supported by many event-generators, and supported by Sherpa version 2.2.0.

We recommend using the UFO model format together with Sherpa 2.2.0, as we encountered many problems using the special FeynRules-Sherpa model with Sherpa 2.1.1. Specifically, FeynRules had difficulty compiling dimension-six operators into the specialized Sherpa export format.

We discuss using FeynRules to implement our EFT model further in section 3.1.

For this project we used FeynRules version 2.0.32 through 2.3.7, and recommend using version 2.3.7 which was the final version we used and it worked without issue. We did encounter some issues with earlier versions.

### HepMC

HepMC is a C++ library for reading and writing object-orientated event records for use by high energy physics Monte-Carlo event-generators. HepMC is an open-source project and the HepMC file format is supported by many tools and event-generators. The library and its documentation can be downloaded from its web-site [9].

We used HepMC for storing this project’s generated events, as it is a open format, is supported by Sherpa, compresses well using gzip, and supports the addition of reweight-coefficients to the event records.

We used version 2.06.08 of HepMC.

### ROOT

ROOT is a large library of C++ classes and methods that provides data analysis, statistics, mathematics, and physics functionality. ROOT is developed and maintained by CERN and the source code is freely available for download. Both the documentation and installation links are available on ROOT’s web-site [10].

For Mac OS users, we again recommend using Homebrew to install ROOT quickly and easily.

We used ROOT for event and data storage, constructing and storing histograms, performing binned and unbinned fits, and drawing figures. We also used ROOT for four-momentum vector calculations on event data.

ROOT is a large and comprehensive library, that is easy to get started with, but hard to master. The documentation is pretty good for most downloadable software projects, using automated tools to create the documentation from the source code. However, the documentation can be quite thin is many areas, and the user is left reading header files and source code to understand the underlying functionality. In this project, much time was used in understanding and reading the source code for histograms (TH1D), profiles (TProfile), and all the many layers of fitting and function minimization classes and helper methods.

We used version 5.34.32, the last available version of ROOT when the project started. Since then, ROOT version 6 has been released. As version 6 had no new functionality that we required, and we were familiar with version 5, we continued using the version we began the project with.

More details are given on how we implanted key functionality in this project using ROOT in various sections of this report.

# SherpaWeight

SherpaWeight is the name of the software tool developed in this project for calculating reweight-coefficients for events, using Sherpa to calculate the matrix-elements, and to embed the coefficients with the events in an output event file.

It is the intention from the outset of this project that this tool be made as generic as possible and to be shared upon completion with the high energy physics community for use in the search for physics beyond the standard model. SherpaWeight was also required to be compatible with future-extensions, such as new file or model support. Thus the code of SherpaWeight must be written to a high standard.

SherpaWeight is a command-line application, designed to implement the following functionality:

1. Read events from a number of supported input file formats, that is easily extendable. Currently three event file formats are supported: HepMC, gzipped HepMC, and Sherpa-ROOT.

Note that the events do not need to be generated by Sherpa.

1. Initialize the Sherpa framework using a user-provided run-card file that details the model, processes, and other criteria that Sherpa requires to generate matrix-elements for events.
2. From the same run-card used to initialize the Sherpa framework, read from a SherpaWeight specified section, the names of the model-parameters for which reweight-coefficients should be calculated for, as well as their evaluation center- and delta-values.
3. Calculate the number of reweight-coefficients NF, and construct NF independent sets of parameter evaluation values, using the evaluation range for each parameter. Using the NF sets of evaluation values, construct the NF×NF matrix from (1.10).
4. For each of the NF sets of parameter evaluation values, set the corresponding model parameters in the Sherpa framework, and then iterate through all events acquiring the matrix-element from the Sherpa framework and adding it to a vector for each event.
5. iterate through all events the vector for that event along with the matrix and (1.10) to acquire the vector of reweight-coefficients for each event.
6. Generate a new event file of the same format as the input event file, copying all the event data and embedding the calculated reweight-coefficients for each event in its event record.

## Developing SherpaWeight

SherpaWeight was developed using C++11 and a selection of classes from the Sherpa, HepMC and ROOT libraries. It was developed on Mac OS X, using the clang compiler and XCode for editing, debugging and build configuration. It is easily portable to Linux, and can be built with a simple makefile.

In developing SherpaWeight it was necessary to gain an intimate knowledge of how some of the key classes in Sherpa works, particularly how its framework is initialized and prepared for generating events, as well as how it calculates matrix-elements. As mentioned earlier, the source code for Sherpa is not documented, and is written in a terse manner making it difficult to read. Much time was spent digging through the layers of Sherpa to understand why something did not work as expected. Further, as we began using Sherpa fully, we found that it contained many bugs or undocumented setup requirements, which if you were lucky would result in an exception being thrown, but more often than not would result in a direct crash or hang.

The first issue to resolve was how to get the matrix-element for an event from the Sherpa framework. Fortunately, Sherpa includes with its source code an example C++ class, called MEProcess, with the required functionality, and an example application showing how to use it. Unfortunately, the MEProcess class did not work properly for processes that include a decay specification. Eventually, we figured out how to modify the MEProcess to support all possible processes, and created our own class based upon MEProcess to do the matrix-element calculations.

The second issue we had to overcome was the issue of setting the reweight model-parameters for each evaluation in step 5 above. We discovered to our dismay, that the Sherpa framework only allows the setting of model-parameters during the frameworks initialization, and that the framework can only initialized once per execution of an application.

This resulted in us dividing the functionality of SherpaWeight into two applications: SherpaWeight and SherpaME. SherpaME is a standalone application that simply calculates the matrix-elements for the events in a given input event file and stores the results in a ROOT data file. SherpaWeight sets up the running environment for SherpaME, including the values of the reweight model-parameters, and calls SherpaME to calculate the matrix-elements for that specific configuration. SherpaWeight calls SherpaME NF times, once for each set of parameter evaluation values, reading the matrix-elements from the ROOT data file generated by SherpaME.

### Calculation of independent evaluations

For the calculation of the independent sets of parameter evaluation values, we were inspired by the code used by AfterBurner, an application developed at NBI by Jørgen Beck Hansen and some of his students.

It constructs a NF×NP matrix, where each row is a set of evaluation values for the NP reweight model-parameters. It fills the first row with all zeroes, then next NP rows with a diagonal NP×NP matrix of +1, and the following next NP rows with a diagonal diagonal NP×NP matrix of −1, and the remaining rows with the vector , rotated by 1 in each subsequent row.

For NP = 1 we get 3 independent rows:

|  |  |  |
| --- | --- | --- |
|  |  | (2.1) |

For NP = 2 we get 6 independent rows:

|  |  |  |
| --- | --- | --- |
|  |  | (2.2) |

For NP = 3 we get 10 independent rows:

|  |  |  |
| --- | --- | --- |
|  |  | (2.3) |

And so on.

To support different parameter ranges, SherpaWeight enables uses to define a center-value and delta-value for each reweight-parameter. SherpaWeight multiplies each column of the simple ±1 matrixes derived above by the delta-value for the corresponding parameter, and adds the center-value. In this way the parameter values are transformed in each column from ±1 to for the parameter.

The resulting parameter evaluation matrix is power and cross-term expanded into the evaluation matrix, which is inverted to get the matrix.

## Using SherpaME

The command line for SherpaME is:

|  |
| --- |
| SherpaME inputFile outputFile <Sherpa command line options> |

The inputFile argument is the file path to an event file, in either HepMC, gzipped HepMC, or Sherpa-ROOT format. The outputFile argument is the file path to a ROOT data file in which will be written a table of matrix-element values and event ids for each event. If the output file already exists, it will be overwritten.

Any valid Sherpa command line option can be appended to the command line following the first two arguments, and will be passed unmodified to the Sherpa framework.

## Using SherpaWeight

The command line for SherpaWeight is:

|  |
| --- |
| SherpaWeight inputFile outputFile <Sherpa command line options> |

The inputFile argument is the file path to an event file, in either HepMC, gzipped HepMC, or Sherpa-ROOT format. The outputFile argument is the file path to store a copy of the input events with the reweight-coefficients embedded in each event record. If the output file already exists, it will be overwritten. The output file will be created in the same format as the input file. The output file path may not be the same as the input file path.

Any valid Sherpa command line option can be appended to the command line following the first two arguments, and will be passed unmodified to the Sherpa framework. Typically, this might be used to specify the run-card for SherpaWeight to use, otherwise it will look for a Run.dat file in the same folder where SherpaWeight is run from.

In addition, SherpaWeight requires a (SherpaWeight) section to be present in the run card file that Sherpa will use for calculating matrix elements, which is Run.dat by default, unless specified using a Sherpa command line option. The (SherpaWeight) section follows the same rules for all sections in a Sherpa run-card file. Everything following a comment is ignored and blank lines are ignored. Each entry in the (SherpaWeight) section corresponds to a desired reweight parameter, and has the the following format:

|  |
| --- |
| <parameter-name> <center-value> <delta-value> |

<parameter-name> is the name of a model-parameter to be used for reweighting. <center-value> and <delta-value> are floating-point numbers that specify the center-and delta-value used for evaluating this parameter to determine the reweight-coefficients for each event.

If the model is a UFO model, where parameters are stored in blocks in a (ufo) section, the parameter-name is the block-name for the parameter, followed by the parameter-number in square brackets. For example, eftcoef[0] is the parameter-name for the zeroth parameter in the eftcoef block. Alternatively, a user-friendly name can be placed in a comment following the parameter values in a section, and in this case, the name in the comment can be used directly. Note that the first word in the comment will be treated as the name.

SherpaWeight creates a temporary folder called SherpaWeight.tmp in the running folder, in which it places log files and other temporary files, such as the output ROOT data file from SherpaME. This folder is not removed when SherpaWeight exits, so its contents can be used to help debug any issues that may have occurred. Users are free to delete this folder manually.

# Effective Field Theory

To test re-weighting we have chosen to apply it to effective field theory (EFT), specifically three dimension-six operators. Effective field theory extends the standard model while respecting gauge symmetries. It can be used to search for physics beyond the standard model by searching for new interactions of known particles. The EFT framework is considered cleaner and simpler to that of anomalous couplings, as it does not use an arbitrarily chosen form factor, but takes a model-independent approach to the physics of non-standard interactions. In this section, we will primarily follow the theoretical arguments laid forth by [11] and [12].

In the standard model (SM), all operators are of dimension four, except the quadratic term in the Higgs potential. The principle idea of EFT is to simply add operators of higher dimension with unknown coefficients that define the strength of the operators and its corresponding interactions. By dimensional analysis, the operator coefficients will be of inverse powers of mass, and a mass scale can be defined to help characterize the coefficients. The following is the EFT extension to the SM for dimension-six and dimension-eight operators:

|  |  |  |
| --- | --- | --- |
|  |  | (3.1) |

Where and are dimensionless coefficients to dimension-six operators and dimension-eight operators respectively.

EFT assumes that is large compared to experimental energies, and the higher dimensional operators are thus suppressed at the lower experimental energies. An effective field theory is essentially a low-energy approximation to new physics, below the new physics scale .

Operators of lower dimensionality will clearly dominate the EFT extension, and we will concentrate on dimension-six operators only. In addition, we feel that the scale , essentially just introduces an unnecessary complication, and can be absorbed into the coefficients themselves. This gives us:

|  |  |  |
| --- | --- | --- |
|  |  | (3.2) |

Where are the coefficients to the dimension-six operators . have mass-dimension −2 (M−2).

There are several dimension-six operators, that could affect a given physical process. For example, there are 59 independent B- and L-conserving dimension-six operators for one generation of quarks and leptons. We will focus on interactions with electroweak vector bosons, particularly self-interactions, as interactions with fermions are constrained by other processes. Assuming C and P conservation, there are only three independent dimension-six operators for EW self-interactions:

|  |  |  |
| --- | --- | --- |
|  |  | (3.3) |
|  |  | (3.4) |
|  |  | (3.5) |

Where is the Higgs doublet field and

|  |  |  |
| --- | --- | --- |
|  |  | (3.6) |
|  |  | (3.7) |
|  |  | (3.8) |

Where is the covariant derivative. and are respectively the field-strengths tensors of the and gauge-bosons. and are respectively the weak and U(1) Y coupling constants at the Z pole. are the Pauli-sigma matrixes, and is the Levi-Civita symbol.

and are defined by requiring:

|  |  |  |
| --- | --- | --- |
|  |  | (3.9) |

Note that is a 2×2 matrix, thus the use of trace in (3.3).

The coefficients corresponding to the three operators , and are defined as , , and respectively.

## Implementing a UFO model for EFT in FeynRules

To use the EFT model in Sherpa, we need to construct a Universal FeynRules Output (UFO) model [8]. Sherpa 2.2.0 can use a UFO model to generate a Sherpa model dynamic library for event generation. Note that before version 2.2.0 of Sherpa, this was not possible. We used FeynRules 2.3.7 to generate a UFO model for EFT, and detail our implementation in this section.

We copied the SM FeynRules file (SM.fr) to a new file (SM+EFT.fr) so that we could add our dimension-six operators to the existing SM definition. We defined each new coefficient and operator using the FeynRules extension to Mathematica. Then we checked that our implementation was Hermitian. Finally, we exported our model to the UFO format.

The following is the code used to setup the three external coefficients for our EFT model:

|  |
| --- |
| (\* \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* \*)  (\* \*\*\*\*\* Parameters \*\*\*\*\* \*)  (\* \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* \*)  M$Parameters = {  (\* SM paramters are here \*)  (\* Effective Field Theory External Parameters \*)  (\* Coefficients for dimension 6 electroweak-boson self-interactions" \*)  ocWWW == {  ParameterType -> External,  BlockName -> EFTCOEF,  OrderBlock -> 1,  Value -> 0,  TeX -> Subscript[oc, WWW],  Description -> "Subscript[O,WWW] coefficient"  },  ocW == {  ParameterType -> External,  BlockName -> EFTCOEF,  OrderBlock -> 2,  Value -> 0,  TeX -> Subscript[oc, W],  Description -> "Subscript[O,W] coefficient"  },  ocB == {  ParameterType -> External,  BlockName -> EFTCOEF,  OrderBlock -> 3,  Value -> 0,  TeX -> Subscript[oc, B],  Description -> "Subscript[O,B] coefficient"  },  }; |

A parameter block called EFTCOEF was defined, with three parameters: ocWWW, ocW, and ocB, corresponding to our three EFT model coefficients. The o-prefix was used in-order to lengthen the parameter name and avoid any possible conflicts with pre-existing names.

The following is the code used for our three dimension-six operators:

|  |
| --- |
| (\* Effective Field Theory - Dimension 6 Operators \*)  LOD6 := Block[{mu,nu,rho,ii,jj,kk,feynmangaugerules,Bhat,What},  feynmangaugerules = If[Not[FeynmanGauge], {G0|GP|GPbar ->0}, {}];  What[mu\_,nu\_,ii\_,jj\_] :=  Module[{aa}, -I/2 gw PauliSigma[aa,ii,jj] FS[Wi,mu,nu,aa]];  Bhat[mu\_,nu\_] := -I/2 g1 FS[B,mu,nu];  ExpandIndices[ocWWW What[mu,nu,ii,jj] What[nu,rho,jj,kk]  What[rho,mu,kk,ii], FlavorExpand->True] +  ExpandIndices[ocW DC[Phibar[ii],mu] What[mu,nu,ii,jj]  DC[Phi[jj],nu], FlavorExpand->True] +  ExpandIndices[ocB DC[Phibar[ii],mu] Bhat[mu,nu] DC[Phi[ii],nu],  FlavorExpand->True]  /. feynmangaugerules ];  LSM\_EFT:=LSM + LOD6; |

A block called LOD6 was defined to contain the dimension-six operators. An optional feynmangaugerules substitution rule is created to support both unitary and Feynman gauge, removing ghost particles when unitary gauge is selected. Note that we only used unitary gauge for this project.

The What and Bhat methods correspond to the and equations given in (3.7) and (3.8). g1 and gw are respectively the U(1) Y coupling constant and weak coupling constant at the Z pole. The PauliSigma method returns the specified index (ii,jj) of the specified (aa) Pauli-sigma matrix. The FS FeynRules method constructs the field strength tensors.

Note that there is a sign difference between the implementation of the What and Bhat methods and the and equations. This is due to the sign difference in the covariant derivative in (3.6) and the definition of the FeynRules covariant derivative method DC:

|  |  |  |
| --- | --- | --- |
|  |  | (3.10) |

This results in a change of sign in the derivation of and following (3.9).

The FeynRules method ExpandIndexes is used to contract the indexes of the three dimension-six operators. The trace given in (3.3) is acquired by contracting implicit indexes of the three 2×2 terms in a circular fashion.

Finally, our dimension-six operator Lagrangian (LOD6) is appended to the existing SM Lagrangian (LSM) to create our SM+EFT Lagrangian (LSM\_EFT).

### Generating the UFO model.

To generate the UFO model from FeynRules, the following commands were run from Mathematica:

|  |
| --- |
| $FeynRulesPath = SetDirectory["Path/feynrules-2.3.7"];  << FeynRules`  SetDirectory[NotebookDirectory[]]  LoadModel["SM+EFT.fr"]  FeynmanGauge = False;  LoadRestriction["Sherpa\_Massless.rst"]  FeynRules[LOD6]  CheckHermiticity[LOD6]  WriteUFO[LGauge, LHiggs, LFermions, LYukawa, LOD6] |

The first few lines load the FeynRules package and our SM+EFT model into Mathematica, ensuring that the gauge is unitary. The LoadRestriction command loads an additional model setup file, discussed in section 3.1.2, which enforces some initial conditions for compatibility with Sherpa. The FeynRules and CheckHermiticity commands validate that our Lagrangian for dimension-six operators can be understood by FeynRules and that it is Hermitian. Finally, the WriteUFO command is used to create a UFO model comprising of the four SM Lagrangians and our dimension-six Lagrangian.

Note: One could have called WriteUFO with only LSM\_EFT as a parameter, but this can cause the command to fail as it runs out of memory. By handling each Lagrangian separately, WriteUFO accomplishes the same result but processes each Lagrangian separately.

The resulting UFO model is created in a “SM+EFT\_UFO” sub-folder and contains several python files listed in Table 3.1.

Table 3.1: UFO model files.

|  |  |
| --- | --- |
| Filename | Contents |
| particles.py | Particles defined using the Particle class. |
| parameters.py | Parameters, like masses, coupling constants, etc., defined using the Parameter class. |
| vertices.py | Interactions defined using the Vertex class. |
| couplings.py | Coupling terms for the defined vertices. |
| CT\_couplings.py | Counter-coupling-terms for the defined vertices. |
| lorentz.py | Lorentz structures for the model. |
| coupling\_orders.py | Coupling order for e.g. QCD and QED. |
| decays.py | Decay widths for various particles. |
| propagators.py | Propagator definitions. |
| \_\_init\_\_.py | Model independent files containing various UFO model methods. |
| function\_library.py |
| object\_library.py |
| write\_param\_card.py |

The most interesting of these files are parameters.py, vertices.py and couplings.py. parameters.py contains the definitions of our 3 EFT model parameters, as well as other external SM parameters. vertices.py contains the definitions of all the SM and EFT model vertices. couplings.py contains the coupling constants used by vertices.py.

A quick overview of the differences in file contents between SM and SM+EFT is given in Table 3.2. As we have dimension-six operators in our EFT-model, some of the vertices are for five or six-particle interactions. The additional vertices added by our EFT model are listed in Table 3.3.

Table 3.2: Major differences between SM and SM+EFT UFO models

|  |  |  |
| --- | --- | --- |
| Filename | SM | SM+EFT |
| parameters.py | 12 external parameters | 15 external parameters |
| vertices.py | 66 vertices  3 legs: 58  4 legs: 8 | 87 vertices  3 legs: 58+1=59  4 legs: 8+3=11  5 legs: 11  6 legs: 6 |
| couplings.py | 43 couplings | 83 couplings |

Table 3.3: List of additional vertices added by the EFT model

|  |  |
| --- | --- |
| Vertex Legs | Particles |
| 3 |  |
| 4 | , |
| 5 | ,  , |
| 6 |  |

Most of the additional vertices added by our EFT model include Higgs particles, which are rather rare. So we do not expect much affects from these at experimental energies. Further, in our evaluation of this model, we will concentrate on known processes, such as WZ-production, where these additional vertices will play no role.

The most significant change is the modifications to the couplings of the existing SM vertices, caused by the introduction of our dimension-six operators, where the three new EFT parameters now play a role.

### Generating a Sherpa-compatible UFO model

Built-in Sherpa models treat many of the particles as massless by default in the hard-process calculation. The so-called *jet* particle container (pdg code 93), is often used to represent incoming partons in Sherpa process definitions, and automatically contains the pdg codes of all massless quarks and the gluon.

With UFO models, particles are not massless by default, and it is up to the model to set the mass to zero, for it to be treated as massless and to be included automatically in the *jet* particle container.

To accomplish this, a set of restraints or initial model values can be set after loaded the FeynRules model file, using the LoadRestrictions command. We defined such a set of initial conditions in the file Sherpa\_Massless.rst:

|  |
| --- |
| (\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*)  (\* Restriction file for SM.fr \*)  (\* Only t-quarks are massive \*)  (\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*)  M$Restrictions = {  Me -> 0, yme -> 0, ye -> 0, (\* massless electron \*)  MMU -> 0, ymm -> 0, ym -> 0, (\* massless muon \*)  MTA -> 0, ymtau -> 0, ytau -> 0, (\* massless tau \*)  MU -> 0, ymup -> 0, yup -> 0, (\* massless u-quark \*)  MD -> 0, ymdo -> 0, ydo -> 0, (\* massless d-quark \*)  MS -> 0, yms -> 0, ys -> 0, (\* massless s-quark \*)  MC -> 0, ymc -> 0, yc -> 0, (\* massless c-quark \*)  MB -> 0, ymb -> 0, yb -> 0 (\* massless b-quark \*)  } |

This completes our UFO model creation. In section 3.3, we will continue to refine our UFO model setup, by adjusting its external parameters to match Sherpa defaults.

## Using the EFT UFO model with Sherpa

Sherpa 2.2.0 supports the importing of UFO models, by using the script *Sherpa-generate-model* and passing the path to the UFO model files generated by FeynRules. This script converts the python files into C++ files, compiles them, and links them into a Sherpa model dynamic library, which it installs in the current Sherpa installation folder. There is, however, three catches.

The first catch, is that various other software packages must be pre-installed in order for the script to run. These include python, scons, cmake, and automake, as well as these packages dependencies. Further, Sherpa must be compiled with the ‑‑enable‑pyext option.

The second catch, is that the folder name is used to create the model name as well as a matching C++ class name. The folder name SM+EFT\_UFO is not compatible with these scripts, as it is not a valid C++ class name. Thus, the folder name was changed to SM\_EFT, dropping the UFO suffix.

The third catch, is that there is a bug in one of the scripts included with Sherpa that prevents linking on Mac OS X with the clang compiler. We have reported this bug to the Sherpa team, and it will likely be fixed in the next version. However, until then, this is easily fixed by modifying the Sherpa file:

<Sherpa installation>/lib/python2.7/site-packages/ufo\_interface/sconstruct\_template  
Find the line:  
 vars.Add('CXX','The C++ Compiler','g++ -Wl,--no-as-needed')  
and delete the “-Wl,--no-as-needed” part, resulting in:  
 vars.Add('CXX','The C++ Compiler','g++')

Sherpa-generate-model not only generates the Sherpa model dynamic library, it also generates an example Sherpa run-card, showing how to select the EFT model, and to define the external parameters for this model. Below are the most relevant elements from the generated example run-card for our model:

|  |
| --- |
| (run){  # model setup  MODEL SM\_EFT  # me generator setup  ME\_SIGNAL\_GENERATOR Comix  }(run)  (ufo){  block yukawa  6 172  block ckmblock  1 0.227736  block mass  23 91.1876  6 172  25 125  block sminputs  1 127.9  2 1.16637e-05  3 0.1184  block eftcoef  1 0  2 0  3 0  decay 23 2.4952  decay 24 2.085  decay 6 1.50833649  decay 25 0.00407  }(ufo) |

In the (run) section, the MODEL parameter is set to the name of the model built by the script, which in our case is SM\_EFT. The ME\_SIGNAL\_GENERATOR parameter is set to Comix. Comix is the only built-in only Sherpa signal generator that can be used with UFO models. Strictly speaking it is not necessary to specify Comix, as Sherpa will use it automatically for UFO models.

The (ufo) section is the most important section when working with UFO models. It defines all the UFO model external parameters. For our model, the most interesting are the three EFT model parameters, specified in the eftcoef block. However, the other parameters are set to their UFO model defaults, which are different than the defaults used for Sherpa’s built-in models.

To be compatible with the built-in Sherpa models, we need to add a few entries and modify the (ufo) section parameters, as follows:

|  |
| --- |
| (run){  # model setup  MODEL SM\_EFT  # me generator setup  ME\_SIGNAL\_GENERATOR Comix;  # set stable to 0 for those particles  # with a non-zero decay-width  STABLE[6] 0  STABLE[23] 0  STABLE[24] 0  STABLE[25] 0  # disable ghost particles  # these are not used by the model anyway (unitary gauge)  ACTIVE[82] 0  ACTIVE[250] 0  ACTIVE[251] 0  ACTIVE[9000001] 0  ACTIVE[9000002] 0  ACTIVE[9000003] 0  ACTIVE[9000004] 0  }(run)  (ufo){  block yukawa  6 173.21 # ymt  block ckmblock  1 0.2272 # cabi  block mass  23 91.1876 # MZ  6 173.21 # MT  25 125 # MH  block sminputs  1 128.8022421894320 # aEWM1  2 1.197448274494500E-05 # Gf  3 0.118 # aS  block eftcoef  1 0 # ocWWW  2 0 # ocW  3 0 # ocB  decay 23 2.4952  decay 24 2.085  decay 6 2.0  decay 25 0.00407  }(ufo) |

The STABLE and ACTIVE parameters in the (run) section, are strictly speaking not necessary. However, they do ensure that the default setup for our UFO model is identical to that of the Sherpa built-in SM.

The parameters in the (ufo) section have been updated to match the defaults used by Sherpa 2.2.0. Comments have been added to help the reader identify the parameters in each block.

Note that one parameter is not the same as the Sherpa default, and that is the Cabbibo angle (cabi), which defines the CKM matrix. In Sherpa, the default CKM matrix is a unit matrix, disabling quark-mixing. However, in this project, when working with built-in models, we always enable quark-mixing and set the Sherpa parameter CKMORDER = 1, which effectively sets the Cabbibo angle to 0.2272. Thus for compatibility, we have also configured all EFT models to use the same value.

Note that for our SM+EFT UFO model, the CKM matrix is given by:

|  |  |  |
| --- | --- | --- |
|  |  | (3.11) |

Where is the Cabbibo angle of 0.2272.  
However, in Sherpa, the CKM matrix for built-in models is instead approximated by the leading order terms of the Taylor-series expansion of cosine and sine:

|  |  |  |
| --- | --- | --- |
|  |  | (3.12) |

The difference is rather small, but it could lead to small differences between the events generated for the built-in SM and those for the SM+EFT UFO model.

## Validating EFT model using WZ production

In order to test that we have built the EFT model correctly, we need to compare the output generated by this model with an equivalent model. Fortunately, Sherpa has a built-in model that is compatible with EFT: anonymous gauge couplings (AGC). The coefficients of EFT are convertible to equivalent parameters in AGC. We can generate events with both models using equivalent parameters, and compare the cross-sections as well as the distributions of several different observables.

Without getting into too much details on the AGC model, the built-in Sherpa model SM+AGC has five C- and P-conserving parameters that can be converted to our three EFT parameters and visa-versa: . Other AGC parameters are available, but they violate C- and/or P-conservation. The relationships between the two sets of model parameters is given by:

|  |  |  |
| --- | --- | --- |
|  |  | (3.13) |
|  |  | (3.14) |
|  |  | (3.15) |

Where and and . Note that . AGC parameters for the SM are .

These relationships are only valid below the scale of new physics , and only if we restrict ourselves exclusively to dimension-six operators. They also require that we treat the anomalous couplings as constants independent of energy.

UFO models, such as our EFT model, are only supported in Sherpa 2.2.0. Unfortunately, the built-in AGC model is only supported in earlier versions of Sherpa, such as version 2.1.1. Thus we will have to generate and compare events from two different versions of Sherpa. These versions of Sherpa have slightly different defaults, such as particle masses, and parton PDF. For example, the default PDF in Sherpa 2.1.1 is CT10, but in Sherpa 2.2.0 it is NNPDF30. These differences need to be aligned in order to reduce differences between the two versions. In general, we have chosen to align to Sherpa version 2.2.0 where possible. Section 3.3.3 contains more details on the run-cards used and the alignment choices made.

We have chosen parton-level WZ-production for comparing models, as this process includes many of the vertices affected by EFT and AGC.

TODO: Add tree diagrams.

TODO: say something more about the process.

For observables, we will focus on three phase-space observables, PT(Z) – the transverse momentum of Z, M(WZ) – the invariant mass of the WZ-pair, and y(Z) – the rapidity of Z.

### Sherpa 2.2.0 SM (UFO) vs. Sherpa 2.1.1 SM (AGC)

We need to gauge any differences between the built-in Sherpa 2.1.1 SM and our UFO SM implementation, so as to ensure that the SM parts of our two models are nearly identical, before we can measure the non-SM parts. To do this events were generated using Sherpa 2.2.0 with our EFT UFO model and with Sherpa 2.1.1 with its built-in SM+AGC model, where all model parameters were set to their SM values. A summary of the generated event datasets is shown in Table 3.4.

Figure 3.1 shows a comparison of the events generated by the two models for our three chosen observables. For comparison, the histograms for each model have been scaled to a luminosity 10 fb−1. Various comparison statistics have been generated and are both shown in the figure and summarized in Table 3.5. Note that the errors shown in the figure are scaled by the same factor used to scale the content to the common luminosity.

The first comparison statistic is a Kolmogorov-Smirnov test [REF], that gives the probability of equality for two distributions. Second, is a standard -test between the two distributions. A ratio of the two distributions is shown in the lower-half of the figure, and two -fits are performed to two horizontal-lines, one fixed to a value of one, and the other parameterized by a free constant. The fit results give a third and fourth comparison statistic. The fit parameter of the second fit result also gives us a fifth statistic.

Note that bins with less than 10 events, before luminosity scaling, are excluded from the statistics, and marked on the figure with a circle around the bin value (unless the bin is empty). This is done to ensure that bins with low statistics do not bias the results. Most of our observables have long sparse tails in either end of their data range that result in low statistic bins. The count of 10 was chosen as it is more than 3 sigma from the value zero, given errors.

Table 3.4: Sherpa event datasets for testing parton-level WZ-production with SM models.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Dataset | Sherpa version | Number of Events | Cross-section [pb] | Effective Luminosity [fb−1] |
| SM‑EFT | 2.2.0 | 1M | 18.543 ± 0.015 | 53.929 ± 0.044 |
| SM‑AGC | 2.1.1 | 1M | 18.554 ± 0.016 | 53.897 ± 0.046 |

Table 3.5: Comparison statistics of SM+EFT to SM+AGC model with SM model parameters.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Observable | Kolmogorov- Smirnov |  | Ratio Fit to 1 | Ratio Fit to c | Ratio Fit to c Value |
| PT(Z) | 0.752 | 0.9597 | 0.9807 | 0.9822 | 1 ± 0.0014 |
| M(WZ) | 0.754 | 0.8803 | 0.9035 | 0.9029 | 1 ± 0.0014 |
| y(Z) | 0.0491 | 1.24 | 1.211 | 1.216 | 1 ± 0.0014 |

The PT(Z) observable indicates a very good match between the two models, with Kolmogorov-Smirnov probabilities of 0.75 and results fairly close to 1. However, both the M(WZ) and y(Z) observables match less well, though still fairly good. For these two observables, the small differences between the two models are often outside the error-bars, resulting in a poorer statistical match. All-in-all, there is a good match between the two SM models. Differences for PT(Z) are within expected statistical fluctuations and less than two sigma. The small but larger difference in M(WZ) and y(Z) are less than three sigma, and thus not large enough to conclude that the two models are not equivalent.

The larger differences in M(WZ) and y(Z) could be systematic, possibly caused by a slightly different phase-space integration optimization prior to the generation of the events in the two datasets.

TODO: discuss M(WZ) having no angular component. What does y(Z) have?

We conclude that the SM-parts of the two models are close to equivalent, with only a small systematic error.

### SM+EFT vs. SM+AGC

We can now compare and validate the non-SM part of our SM+EFT model with the SM+AGC model, confident that the SM-parts of the two models are nearly equivalent. To test our three EFT parameters, separately and together, we generated four datasets for each model using equivalent EFT and AGC model parameters, as shown in Table 3.6 and Table 3.7. We chose EFT parameters that approximately double the SM cross-section for 1M events, to ensure datasets with a visible and quantifiable difference from the SM.

Table 3.6: Equivalent EFT and AGC model parameters for testing the SM+EFT model.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| EFT Test | EFT Model Parameters | | | AGC Model Parameters | | | |
| **[GeV−2]** | **[GeV−2]** | **[GeV−2]** |  |  |  |  |
|  | 3×10−5 | 0 | 0 | 0.127275 | 0 | 0 | 0 |
|  | 0 | 5×10−5 | 0 | 0 | 0.207879 | 0.161544 | 0.161544 |
|  | 0 | 0 | 9×10−4 | 0 | 0 | 2.907787 | −0.834044 |
| all | 3×10−5 | 5×10−5 | 9×10−4 | 0.127275 | 0.207879 | 3.069330 | −0.672500 |

Table 3.7: Sherpa event datasets for testing parton-level WZ-production for SM+AGC and SM+EFT models.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| EFT Test | Dataset | Sherpa version | Number of Events | Cross-section [pb] | Effective Luminosity [fb−1] |
|  | EFT cWWW | 2.2.0 | 1M | 30.426 ± 0.027 | 32.867 ± 0.029 |
| AGC lambda | 2.1.1 | 1M | 30.466 ± 0.027 | 32.823 ± 0.029 |
|  | EFT cW | 2.2.0 | 1M | 30.717 ± 0.027 | 32.555 ± 0.029 |
| AGC g1 | 2.1.1 | 1M | 30.715 ± 0.027 | 32.557 ± 0.029 |
|  | EFT cB | 2.2.0 | 1M | 31.671 ± 0.026 | 31.575 ± 0.026 |
| AGC kappa | 2.1.1 | 1M | 31.725 ± 0.026 | 31.521 ± 0.026 |
| all | EFT all | 2.2.0 | 1M | 42.805 ± 0.038 | 23.362 ± 0.021 |
| AGC all | 2.1.1 | 1M | 42.829 ± 0.038 | 23.349 ± 0.021 |

Table 3.8: Comparison statistics of SM+EFT to SM+AGC model with equivalent model parameters.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| EFT Test | Observable | Kolmogorov-Smirnov |  | Ratio Fit to 1 | Ratio Fit to c | Ratio Fit to c Value |
|  | PT(Z) | 0.877 | 1.042 | 1.046 | 1.040 | 1 ± 0.0015 |
| M(WZ) | 0.285 | 1.026 | 1.058 | 1.047 | 0.99 ± 0.0014 |
| y(Z) | 0.560 | 1.081 | 1.094 | 1.090 | 1 ± 0.0014 |
|  | PT(Z) | 0.891 | 0.9811 | 0.9863 | 0.9843 | 1 ± 0.0015 |
| M(WZ) | 0.990 | 1.015 | 1.029 | 1.024 | 1 ± 0.0014 |
| y(Z) | 0.798 | 1.030 | 1.066 | 1.071 | 1 ± 0.0014 |
|  | PT(Z) | 0.935 | 0.9757 | 1.025 | 1.015 | 1 ± 0.0014 |
| M(WZ) | 0.105 | 0.9191 | 0.9685 | 0.9587 | 1 ± 0.0014 |
| y(Z) | 0.147 | 1.101 | 1.093 | 1.084 | 1 ± 0.0014 |
| all | PT(Z) | 0.693 | 1.065 | 1.064 | 1.061 | 1 ± 0.0015 |
| M(WZ) | 0.761 | 0.9599 | 0.9924 | 0.9853 | 1 ± 0.0014 |
| y(Z) | 0.383 | 0.9523 | 0.944 | 0.946 | 1 ± 0.0014 |

Comparisons of the resulting distributions for our four tests are shown in Figure 3.2 through Figure 3.5, and the comparison statistics are summarized in Table 3.8. See section 3.3.1 for comments on the comparison statistics. Note that the errors shown in the figures are scaled by the same factor used to scale the content to the common luminosity.

For all tests and observables, the resulting comparisons shows a very high degree of equivalence. Kolmogorov-Smirnov probabilities vary from ca. 0.10 to 0.99. results vary from ca. 0.92 to 1.10 with p-values from 0.06 to 0.96. Most observables have differences less than two sigma, and a few have less than three.

The comparison results are slightly better than when only the SM-parts were compared in section 3.3.1, particularly for y(Z). This might possibly indicate that the “noise” from the differences in SM-parts has been reduced by the the addition of equivalent EFT and AGC distributions.

We conclude, that our EFT model and the AGC model are statistically equivalent. We can now use our UFO EFT model trusting in its implementation.

|  |  |
| --- | --- |
| (a) |  |
| (b) |  |
| (c) |  |

Figure 3.1: Comparison of SM (EFT) to SM (AGC) for parton-level WZ-production for: (a) PT(Z), (b) M(WZ) and (c) y(Z).  
The upper-half of each sub-figure shows the event distributions for both models scaled to a luminosity of 10 fb−1 from 1M generated events, as well as Kolmogorov-Smirnov and comparison statistics. The lower-halves show the ratio of the two distributions, as well as fit results for fitting the ratio to one and to a constant. Bins with less than 10 events (before luminosity scaling) are excluded from all statistics and marked with circles. Events were generated using SM values for model parameter using the SM+EFT (Sherpa 2.2.0) and SM+AGC (Sherpa 2.1.1) models. Bin widths are (a) 1 GeV/c, (b) 2 GeV/c2 and (c) 0.05.

|  |  |
| --- | --- |
| (a) |  |
| (b) |  |
| (c) |  |

Figure 3.2: Comparison of SM+EFT to SM+AGC for parton-level WZ-production, with and set to equivalent non-SM values, for: (a) PT(Z), (b) M(WZ) and (c) y(Z).  
See Table 3.6 for model parameter values. The upper-half of each sub-figure shows the event distributions for both models scaled to a luminosity of 10 fb−1 from 1M generated events, as well as Kolmogorov-Smirnov and comparison statistics. The lower-halves show the ratio of the two distributions, as well as fit results for fitting the ratio to one and to a constant. Bins with less than 10 events (before luminosity scaling) are excluded from all statistics and marked with circles. Events were generated for SM+EFT and SM+AGC using Sherpa version 2.2.0 and 2.1.1 respectively. Bin widths are (a) 1 GeV/c, (b) 2 GeV/c2 and (c) 0.05.

|  |  |
| --- | --- |
| (a) |  |
| (b) |  |
| (c) |  |

Figure 3.3: Comparison of SM+EFT to SM+AGC for parton-level WZ-production, with , and set to equivalent non-SM values, for: (a) PT(Z), (b) M(WZ) and (c) y(Z).  
See Table 3.6 for model parameter values. The upper-half of each sub-figure shows the event distributions for both models scaled to a luminosity of 10 fb−1 from 1M generated events, as well as Kolmogorov-Smirnov and comparison statistics. The lower-halves show the ratio of the two distributions, as well as fit results for fitting the ratio to one and to a constant. Bins with less than 10 events (before luminosity scaling) are excluded from all statistics and marked with circles. Events were generated for SM+EFT and SM+AGC using Sherpa version 2.2.0 and 2.1.1 respectively. Bin widths are (a) 1 GeV/c, (b) 2 GeV/c2 and (c) 0.05.

|  |  |
| --- | --- |
| (a) |  |
| (b) |  |
| (c) |  |

Figure 3.4: Comparison of SM+EFT to SM+AGC for parton-level WZ-production, with and set to equivalent non-SM values, for: (a) PT(Z), (b) M(WZ) and (c) y(Z).  
See Table 3.6 for model parameter values. The upper-half of each sub-figure shows the event distributions for both models scaled to a luminosity of 10 fb−1 from 1M generated events, as well as Kolmogorov-Smirnov and comparison statistics. The lower-halves show the ratio of the two distributions, as well as fit results for fitting the ratio to one and to a constant. Bins with less than 10 events (before luminosity scaling) are excluded from all statistics and marked with circles. Events were generated for SM+EFT and SM+AGC using Sherpa version 2.2.0 and 2.1.1 respectively. Bin widths are (a) 1 GeV/c, (b) 2 GeV/c2 and (c) 0.05.

|  |  |
| --- | --- |
| (a) |  |
| (b) |  |
| (c) |  |

Figure 3.5: Comparison of SM+EFT to SM+AGC for parton-level WZ-production, with all parameters set to equivalent non-SM values, for: (a) PT(Z), (b) M(WZ) and (c) y(Z).  
See Table 3.6 for model parameter values. The upper-half of each sub-figure shows the event distributions for both models scaled to a luminosity of 10 fb−1 from 1M generated events, as well as Kolmogorov-Smirnov and comparison statistics. The lower-halves show the ratio of the two distributions, as well as fit results for fitting the ratio to one and to a constant. Bins with less than 10 events (before luminosity scaling) are excluded from all statistics and marked with circles. Events were generated for SM+EFT and SM+AGC using Sherpa version 2.2.0 and 2.1.1 respectively. Bin widths are (a) 1 GeV/c, (b) 2 GeV/c2 and (c) 0.05.

### Sherpa run-cards for event generation of parton-level WZ-production

To ensure alignment between events generated with Sherpa 2.1.1 and 2.2.0, we chose to align Sherpa 2.1.1 run-cards to the Sherpa 2.2.0 defaults, except with regards to the parton PDF.

For the parton PDF we chose to use the Sherpa 2.1.1 default, as NNPDF30 is not available in Sherpa 2.1.1. One could use the LHAPDF library to import NNPDF30 into Sherpa 2.1.1, but experience has proven that this is not so easy a task. Many internal parameters are tuned to the PDF automatically, when a built-in PDF is used. When using LHAPDF to load an external PDF, one must tune these parameters oneself. Further, in our experience Sherpa tends to crash when using a PDF via the LHAPDF library.

The following run-cards were used for generating events for WZ-production in Sherpa 2.1.1 and Sherpa 2.2.0.

#### Sherpa 2.1.1 SM+AGC run-card

This run card was used for both Sherpa 2.1.1 SM and SM+AGC event generation, by appropriately setting the AGC parameters.

|  |
| --- |
| (run){  # general settings  EVENTS 0;  EVENT\_OUTPUT HepMC\_GenEvent[AGC\_211]  PRETTY\_PRINT Off  # me generator setup  ME\_SIGNAL\_GENERATOR Amegic;  SCALES VAR{Abs2(p[0]+p[1])};    # model setup  MODEL SM+AGC  CKMORDER 1  LAMBDA\_GAMMA = 1.272753587483230E-01 # cWWW = 3E-5  LAMBDA\_Z = 1.272753587483230E-01  KAPPA\_GAMMA = 4.069330406875000E+00 # cB = 9E-4  KAPPA\_Z = 3.275001296830000E-01  G1\_Z = 1.207879459844000E+00 # cW = 5E-5  UNITARIZATION\_SCALE = 1E9  UNITARIZATION\_SCALE3 = 1E9  UNITARIZATION\_SCALE4 = 1E9  # align particle defaults to Sherpa version 2.2.0  MASS[6] 173.21; WIDTH[6] 2.0; STABLE[6] 0  WIDTH[15] 2.26735e-12;  MASS[23] 91.1876; WIDTH[23] 2.4952; STABLE[23] 0  MASS[24] 80.385; WIDTH[24] 2.085; STABLE[24] 0  STABLE[25] 0  # set PDF to Sherpa version 2.1.1 default  PDF\_LIBRARY CT10Sherpa  PDF\_SET ct10  # generate only parton-level process  MI\_HANDLER None  FRAGMENTATION Off  SHOWER\_GENERATOR None  ME\_QED Off  BEAM\_REMNANTS 0  # LHC beam setup (13 TeV)  BEAM\_1 2212; BEAM\_ENERGY\_1 6500;  BEAM\_2 2212; BEAM\_ENERGY\_2 6500;  }(run)  (processes){  Process 93 93 -> 24 23  End process;  }(processes) |

The relevant AGC model parameters are set via LAMBDA\_GAMMA, LAMBDA\_Z, KAPPA\_GAMMA, KAPPA\_Z, and G1\_Z. The default values used by the SM are 0 for the lambda parameters, and 1 for the kappa and G1 parameters.

The three UNITARIZATION\_SCALE parameters are used by the SM+AGC model to set an upper energy cut-off that the ACG contributions are valid up to. As no such cut-off is applied to our UFO model, we have effectively disabled this by setting the AGC energy cut-off to 109 GeV, well above any energy in our project.

The signal generator (ME\_SIGNAL\_GENERATOR) is set to Amegic, as this is required to use the SM+AGC model.

SCALES, defines the renormalization and factorization scale, and is set to the invariant mass of the two incoming partons. The scale must be manually set when disabling showers.

CKMORDER is set to 1, to disable a unitary CKM matrix, as described in section 3.2.

The MASS, WIDTH, and STABLE parameters are used to align the particle configuration to that used in Sherpa 2.2.0.

The remaining parameters, setup a 13 TeV proton-proton beam, set the process to WZ-production, and disable all but parton-level particles in the output file.

#### Sherpa 2.2.0 UFO SM+EFT run-card

This run card was used for both Sherpa 2.2.0 SM and SM+EFT event generation, by appropriately setting the EFT parameters.

|  |
| --- |
| (run){  # general settings  EVENTS 0;  EVENT\_OUTPUT HepMC\_GenEvent[EFT\_220]  PRETTY\_PRINT Off  # me generator setup  ME\_SIGNAL\_GENERATOR Comix;  SCALES VAR{Abs2(p[0]+p[1])};    # model setup  MODEL SM\_EFT  # set PDF to Sherpa version 2.1.1 default  PDF\_LIBRARY CT10Sherpa  PDF\_SET ct10  # set stable to 0 for those particles with a non-zero decay-width  STABLE[6] 0  STABLE[23] 0  STABLE[24] 0  STABLE[25] 0  # disable ghost particles, which are not used by the model anyway (unitary gauge)  ACTIVE[82] 0  ACTIVE[250] 0  ACTIVE[251] 0  ACTIVE[9000001] 0  ACTIVE[9000002] 0  ACTIVE[9000003] 0  ACTIVE[9000004] 0  # generate only parton-level process  MI\_HANDLER None;  FRAGMENTATION Off;  SHOWER\_GENERATOR None;  ME\_QED Off  BEAM\_REMNANTS 0  # LHC beam setup (13 TeV)  BEAM\_1 2212; BEAM\_ENERGY\_1 6500;  BEAM\_2 2212; BEAM\_ENERGY\_2 6500;  }(run)  (processes){  Process 93 93 -> 24 23  End process;  }(processes)  (ufo){  block yukawa  6 173.21 # ymt  block ckmblock  1 0.2272 # cabi  block mass  23 91.1876 # MZ  6 173.21 # MT  25 125 # MH  block sminputs  1 128.8022421894320 # aEWM1  2 1.197448274494500E-05 # Gf  3 0.118 # aS  block eftcoef  1 3E-5 # ocWWW  2 5E-5 # ocW  3 9E-4 # ocB  decay 23 2.4952  decay 24 2.085  decay 6 2.0  decay 25 0.00407  }(ufo) |

The three EFT model parameters are set via the eftcoef block parameters in the (ufo) section. The standard model values for all three parameters is zero.

The signal generator (ME\_SIGNAL\_GENERATOR) is set to Comix, as this is required to use a UFO model.

SCALES, defines the renormalization and factorization scale, and is set to the invariant mass of the two incoming partons. The scale must be manually set when disabling showers.

The parton PDF is set to CT10 to align to the default PDF used by Sherpa 2.1.1. The STABLE and ACTIVE parameters align the UFO model to the same defaults used by Sherpa 2.2.0 built-in models, as discussed in section 3.2.

The remaining parameters, setup a 13 TeV proton-proton beam, set the process to WZ-production, and disable all but parton-level particles in the output file.

# Implementing Reweighting

SherpaWeight can be used to add reweight coefficients to the event datasets. However, we also need a library of routines that can read our event data and the added reweight coefficients, and generate reweighted event histograms for any specified set of model parameters. We developed such a reweighting library and made use of our EFT model to test both SherpaWeight and the reweighting library.

In this section, we will give a brief overview of this reweighting library and test its capability to reweight EFT event data to SM model parameters, comparing the reweight result to SM event data. Further, we will give some notes on developing reweighting code using ROOT.

The library of reweighting and histogram support methods was developed in C++ with the assistance of ROOT and HepMC libraries. All the classes and methods are generic and can be re-used in any application. To test the routines, we developed a test application called ReweightEFT.

The reweighting library contains the following functionality:

1. Classes to create a generic set of observables and generic methods for filling histograms or profiles with observable data.

Note that we desire to examine different observables both in histogram but also profile form. A profile is a histogram displaying the mean and error-of-the-mean of the content in each bin, instead of simply the sum. We use ROOT’s TProfile and TH1D classes to store profiles and histograms respectively.

In general, we use the term histogram to refer to both histograms and profiles.

1. Classes to define model event datasets, including cross-section information.
2. Methods to load observable histograms from event datasets, with optional cache support for higher performance on subsequent runs (important). HepMC and gzip compressed HepMC event files are supported.

In addition to the observable histogram, these methods also construct reweight-coefficient histograms from the reweight-coefficients stored with each event. Thus a set of observable and reweight-coefficient histograms are constructed for each model dataset and observable.

1. A method for scaling the luminosity of a histogram to any specified value, based upon the cross-section and number of events in the model dataset definition.

This method takes care to scale the errors such that the result after scaling is a pseudo-dataset, aka. an Asimov dataset. See the discussion in sections 4.2 and 4.3.2.

1. A method to create a reweighted histogram from the set of reweight-coefficient histograms and a set of model parameters.

Care must be taken in how the errors are defined for the resulting reweighted histogram. Our method recalculates the errors following reweighting, resulting in a pseudo-dataset, aka. an Asimov dataset. See the discussion in sections 4.2 and 4.3.3.

1. Methods for creating comparison figures, calculating ratios of histograms, and comparison statistics.

These methods were also used in section 3.3 to construct the comparison figures used there.

1. General histogram helper methods, such as logging histogram data, measuring different histogram statistics, loading and saving histograms to ROOT data files.

We will not describe in detail all of the above functionality, however, source code is available for download as described in the introduction. In section 4.3, notes are given regarding the implementation of certain key elements of reweighting using ROOT classes.

## Adding reweight-coefficients to SM+EFT datasets

Before we can reweight the events in a dataset, reweight-coefficients must be calculated and stored with the events. Here is where SherpaWeight is used.

Adding the reweight-coefficients to events is simply a matter of running SherpaWeight with an input and output event file and adding a (SherpaWeight) section to the run-card used to generate the events, as described in 2.3.

We chose to test reweighting using the same SM+EFT generated events used in section 3.3 for parton-level WZ-production, specifically the dataset where all EFT parameters were set to non-SM values.

The following (SherpaWeight) section was added to the run-card used to generate SM+EFT events detailed in section 3.3.3.2:

|  |
| --- |
| (SherpaWeight){  ocWWW 0 1E-5  ocW 0 1E-5  ocB 0 1E-4  }(SherpaWeight) |

Here we made use of SherpaWeight’s support for using the comment following a (ufo) block parameter as the name of the parameter. As a reminder, the two terms following the parameter name are the center-value and the delta-value.

Running SherpaWeight on the 1M event file for SM+EFT, ran through 10 different configurations of EFT parameters for all events, and took about 53 minutes, on a 2.8 GHz Mac Book Pro with SSD hard-drive. Note that reading and writing 1M HepMC events are the main bottlenecks.

## Comparison of reweighted EFT to SM for WZ-production

In this section, we examine the results of reweighting a SM+EFT dataset, generated with non-SM parameter values, to a reweighted dataset with SM parameter values. We compare the reweighted SM dataset with a generated SM dataset, using the same observables and comparison statistics used previously in section 3.3.

We have chosen to again use parton-level WZ-production as the test process, using the same SM+EFT dataset used previously in section 3.3. Specifically, the dataset where all EFT parameters are set to non-SM values. The selected EFT parameters used in this dataset more than double the cross-section of 1M generated events from 18 to 42 pb, so this dataset should be a good test of reweighting.

Reweighting was tested with 21 different observables (see Table 6.1), however, in this section we will only present the results for PT(Z) – the transverse momentum of Z, M(WZ) – the invariant mass of the WZ-pair, and y(Z) – the rapidity of Z. The results for the other observables are nearly identical to these three and to save space, these three will be used as representative.

The datasets we used are shown in Table 4.1. We reweighted the “EFT (all)” dataset, using the SM values of zero for all three EFT parameters. The reweight result was compared to a “SM-EFT” dataset that was generated separately with these same SM parameter values. Figure 4.1 shows the comparison results, with both datasets scaled to a luminosity of 10 fb−1. The corresponding comparison statistics are summarized in Table 4.2. See section 3.3 for a description of the comparison statistics.

Table 4.1: Sherpa event datasets for testing reweighting of parton-level WZ-production.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Dataset | EFT Model Parameters | | | Number of Events | Cross-section [pb] | Effective Luminosity [fb−1] |
| **[GeV−2]** | **[GeV−2]** | **[GeV−2]** |
| EFT (all) | 3×10−5 | 5×10−5 | 9×10−4 | 1M | 42.805 ± 0.038 | 23.362 ± 0.021 |
| SM‑EFT | 0 | 0 | 0 | 1M | 18.543 ± 0.015 | 53.929 ± 0.044 |

Table 4.2: Comparison statistics of reweighting EFT events with SM model parameters to generated SM events, excluding low-statistic bins.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Observable | Kolmogorov- Smirnov |  | Ratio Fit to 1 | Ratio Fit to c | Ratio Fit to c Value |
| PT(Z) | 0.999 | 0.1856 | 0.1991 | 0.1949 | 1 ± 0.0033 |
| M(WZ) | 0.854 | 0.2663 | 0.3400 | 0.3345 | 0.99 ± 0.0033 |
| y(Z) | 0.978 | 0.3029 | 0.3152 | 0.3084 | 1 ± 0.0033 |

The comparison results indicate a very high equivalence between reweighted EFT-to-SM events and directly generated SM events. The results are much lower than 1, giving p-values of 1 in every case. Note that the error-bars in the comparison figures in this section are larger than those shown for the same observables in section 3.3. This could help explain why the results are so low.

Bin-errors in this section have been recalculated after luminosity scaling and reweighting. The resulting distributions thus represent pseudo-data, otherwise known as an Asimov dataset, as the errors match those that would be given to the content if it had been measured or generated directly at the given luminosity. The simple reason for this is that bin-errors cannot be reweighted, and thus one must recalculate the bin-errors after reweighting. It follows that the generated SM dataset must have its errors recalculated as well, so that the comparison is pseudo-data to pseudo-data.

As before, bins with less than 10 events before luminosity scaling or reweighting are excluded from the comparison statistics, and marked with circles on the figures. We can see that these low-statistic bins result in many outliers in the ratio comparison, with large error-bars. In the three observables shown, these outliers also appear to cluster more to one side of the horizontal line drawn at a ratio of 1, than being evenly spread.

We can infer that we have a very good match in areas of high-statistics, but have problems in areas of low-statistics. This is one of the fundamental problems with reweighting. It is impossible to reweight an empty bin, and reweighting a bin with low-statistics is less certain to give a correct result.

Statistically, though including the low-statistic bins does not make much difference in the results. The comparison statistics calculated from all bins, including those with low-statistics, are shown in Table 4.3. The results are fairly much the same as those where low-statistic bins are excluded – all p-values are still 1. Even though the statistic increases from the outliers, so do the number of degrees of freedom. Statistics obviously does not tell the whole picture; one must also visually assess the results.

Table 4.3: Comparison statistics of reweighting EFT events with SM model parameters to generated SM events, including low-statistic bins.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Observable | Kolmogorov- Smirnov |  | Ratio Fit to 1 | Ratio Fit to c | Ratio Fit to c Value |
| PT(Z) | 0.999 | 0.144 | 0.1756 | 0.1723 | 1 ± 0.0033 |
| M(WZ) | 0.796 | 0.234 | 0.7493 | 0.7342 | 0.99 ± 0.0033 |
| y(Z) | 0.976 | 0.3033 | 0.3413 | 0.3344 | 1 ± 0.0033 |

We conclude that reweighting produces highly accurate results in areas of high statistics.

TODO: break the single figure into 3 larger figures.

|  |  |
| --- | --- |
| (a) |  |
| (b) |  |
| (c) |  |

Figure 4.1: Comparison of an EFT dataset reweighted to SM vs. a SM dataset, for parton-level WZ-production, for: (a) PT(Z), (b) M(WZ) and (c) y(Z).  
See Table 4.1 for model parameter values for each dataset. The upper-half of each sub-figure shows the event distributions for both models scaled to a luminosity of 10 fb−1 from 1M generated events, as well as Kolmogorov-Smirnov and comparison statistics. The lower-halves show the ratio of the two distributions, as well as fit results for fitting the ratio to one and to a constant. Bins with less than 10 events (before luminosity scaling) are excluded from all statistics and marked with circles. Bin widths are (a) 1 GeV/c, (b) 2 GeV/c2 and (c) 0.05.

## Notes on reweighting using ROOT

### Histograms and profiles

As previously mentioned, ROOT classes TH1D and TProfile were used to store and provide the main functionality for histograms and profiles. Generally, the classes were used as is, however, some instances helper methods were developed to handle special cases, such as luminosity scaling and re-weighting.

Each bin of a TH1D histogram contains two simple sums of the event-weights for the bins events:

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | (TH1D and TProfile) | (4.1) |
|  |  | (TH1D and TProfile) | (4.2) |

The bin content of a TH1D is given by , and the bin error by . The sum can be disabled, resulting in the bin error being defined as , but generally we always enabled it.

For both TH1D and TProfile, the effective number of entries in a bin is:

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | (TH1D and TProfile) | (4.3) |

In the case where all event-weights are 1, then .

Each bin of a TProfile profile contains the same sums as a TH1D, as well as two others containing summing the y-values associated with each bin-event:

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | (TProfile) | (4.4) |
|  |  | (TProfile) | (4.5) |

The bin content of TProfile is defined as the weighted mean of the bins y-values. The default bin error is by default defined to be the standard-deviation-of-the-mean (SDOM) given by:

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | (TProfile) | (4.6) |
|  |  | (TProfile) | (4.7) |

Note TProfile supports different bin error definitions, with SDOM as the default, which we use exclusively in this project.

### Scaling luminosity

To compare the event counts of different Monte-Carlo datasets, either to each other or to experimental data, they must first be scaled to a common luminosity. Normally, model data is scaled to the luminosity of experimental data. In our case, all our data is MC-generated, and we chose to compare at a luminosity of 10 fb−1.

The effective luminosity of a generated dataset is given by:

|  |  |  |
| --- | --- | --- |
|  |  | (4.8) |

Where is the number of events generated and is the integrated cross-section for the generated events. Note that the effective luminosity for a dataset is unchanged, even if events are later cut by additional selection criteria.

To scale a dataset from its effective luminosity to a desired luminosity L, one scales the effective number of events in the dataset by the scaling factor:

|  |  |  |
| --- | --- | --- |
|  |  | (4.9) |

TH1D and TProfile have a method called Scale that on the surface would appear to be useful for doing the luminosity scaling. Scale modifies the the sums stored in TH1D and TProfile in the following manner:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  |  | (TH1D) | (4.10) |
|  |  | (TProfile) |

Firstly, the Scale method does not actually change number of effective entries defined by (4.3). Secondly, it scales the mean bin values for a TProfile, which are independent of luminosity, and should not change.

To perform luminosity scaling we implemented our own method called ScaleHistToLuminosity, which scales all sums identically:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  |  | (TH1D) | (4.11) |
|  |  | (TProfile) |

This simulates a change to the number of events that went into a sum, but does not change to the distribution of weights or y-values for those events. It has the desired effect that the number of effective entries in each bin is scaled by , and the mean values for a TProfile are not affected.

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | (TH1D and TProfile) | (4.12) |

Our method also scales bin-errors in a way that maintains a pseudo-dataset, or Asimov dataset as introduced previously. That is the resulting bin-errors are as if the dataset had been generated at the desired luminosity in the first place. The scaled bin errors are:

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | (TH1D) | (4.13) |
|  |  | (TProfile) | (4.14) |

For TH1D bins, our method scales bin errors with, instead of with as implemented by the Scale method. For TProfile bins, the bin errors scale with . Normally, we are scaling to a lower luminosity than the datasets’s effective luminosity. In this case , and we are reducing the number of effective events, and the errors on TH1D bins are reduced, and those on TProfiles are increased.

### Reweighting histograms

To create a reweighted histogram or profile, we can simply use the relative probability for an event, for a given set of reweight-parameter values, as the weight of each the event, as described in section 1.1.2. However, there is a much faster method to create reweighted histograms and profiles, without running through all the events each time the model parameters are changed. This is particularly important when fitting reweighted models to data, as fits need to iterate through many different candidate parameter values to find the ones that minimize the desired objective. This faster method is described in this section, as well as how to calculating bin-errors for reweighted event distributions.

The matrix element for a given event can be calculated from (1.6) through (1.8), repeated here for convenience:

|  |  |  |
| --- | --- | --- |
|  |  | (1.6) |
|  |  | (1.7) |
|  |  | (1.8) |

Where is the reweight-coefficient vector for each event, and is an evaluation vector derived from appropriate combinations of the values of the reweight-parameters. Both vectors contain NF terms. We can use SherpaWeight to calculate and embed the reweight-coefficient vector for each event in the datasets we wish to reweight.

The event-weight for each event is given by:

|  |  |  |
| --- | --- | --- |
|  |  | (4.15) |

Where and are respectively the reweighted and generated matrix-elements. The generated matrix-element is calculated by using the same reweight-parameter values that the events were generated with.

Note that both and are constant for each event, and event-weights only depend upon the evaluation vector , which depends upon reweight-parameters. If we take the evaluation vector out of (4.15), we end up with a constant weight for each coefficient, and we can create separate histograms and profiles for each reweight-coefficient using this constant weight. As these reweight-coefficient histograms are independent of the choice of reweight-parameters, they do not need to be recalculated

Then to acquire a final reweighted event-distribution, we simply multiply each reweight-coefficient histogram by its corresponding term in the evaluation vector and sum all the histograms together. This simple weighted-sum operation can be repeated for each iteration of reweight-parameter values, without loading the event dataset. It is extremely fast, taking only milliseconds to construct a reweighted event-distribution.

One would be tempted to use the class methods Scale and Add available in TH1D and TProfile to perform the weighted-sum of coefficient histograms. However, they both suffer from the same issues introduced in the previous section. ROOT’s methods are principally designed to be mathematically correct for the purposes of applying equations to histograms, and propagating errors. However, we want to construct a final reweighted histogram from the weighted-sum of several other histograms, in such a way that the reweighted result is equivalent to the result that we would have achieved if constructing the histogram in one pass. In particular, we want the number of effective entries to be the same, whether we calculate a reweighted histogram directly, or via a weighted-sum of histograms.

As an example, if we subtract a histogram from itself using ROOT’s methods, we will not get an empty histogram, with all internal sums empty. Sums of squares will remain, and for TProfile in particular the number of effective entries will double. We need to be able to handle negative as well as positive contributions to the number of effective entries to get the correct result. ROOT’s methods are not designed for this.

In fact, it is impossible to obtain the same bin errors when using a weighted-sum of coefficient histograms as compared to constructing a single histogram directly, using TH1D and TProfile. This is because only sums, such as S1, S3 and S4, that use event-weights linearly can be constructed identically by both methods. The sum S2, which squares the event-weights is different when calculated by the two methods. This is shown in the following equations for a linear and quadratic sum of weights:

|  |  |  |
| --- | --- | --- |
|  |  | (4.16) |
|  |  | (4.17) |

Where is an event index, and is a reweight-coefficient index. is an arbitrary term, which is 1 in S1 and S2 and and in S3 and S4.nOn the left, the sums are acquired by calculating the weight using the reweight-parameters and the coefficients for each event, and summing over events. On the right, the sums are acquired by using the reweight-coefficients alone as the weight, summing over events, and then creating a weighted-sum using the reweight-parameters. The right-hand-side represents our optimized reweighting method.

Fortunately, we are not interested in a reweighted histogram, where the bin-errors are calculated from our weights. We are interested in reconstructing a new dataset that is representative of what would have been generated with the new set of reweight-parameter values was used. We require a pseudo-dataset where the bin-errors correspond to the errors that would be there if the bin was filled with weights of one.

We developed our own methods called HistReweightAdd and CalculateReweightHist to perform the weighted-sum of histograms and create the resulting reweighted histogram. These resulting weighting can be summarized as follows:

|  |  |  |
| --- | --- | --- |
|  |  | (4.18) |
|  |  | (4.19) |
|  |  | (4.20) |
|  |  | (4.21) |

Effectively, we perform the weighted-sums as described, but do so by modifying the internal sums maintained within TH1D and TProfile. Only S2 is treated differently, and is set to the same value as S1, which is equivalent to creating a distribution with event-weights of 1. This has the effect that the bin-errors for a reweighted TH1D is simply , and the SDOM for a TProfile is calculated using . This gives us the pseudo-data result that we want.

# Optimal Observables

In this section we introduce a new observable type, called optimal observables, which we will use later during our fit analysis. Optimal observables are designed to give the smallest possible statistical error on model parameters. They are very useful for determining values or constraints for a set of model parameters from experimental data, or calculating theoretical sensitivities.

## Derivation of first-order optimal observables

In the following, we present the derivation of optimal observables given in [13] and [14]. Optimal observables can be used with any process where the differential cross-section is dependent upon a set of parameters with small values. For a given process the differential cross-section is given by:

|  |  |  |
| --- | --- | --- |
|  |  | (5.1) |

Where is the set of all measured phase-space variables, for example, the incoming and outgoing four-momenta for the process. For an isolated hard-process, is equivalent to the matrix-element for the process.

is a polynomial of second-order in terms of EFT parameters as well as TGC parameters:

|  |  |  |
| --- | --- | --- |
|  |  | (5.2) |

Where are the model parameters, is the differential cross-section in the SM, and and are the first and second-order modifications. For an isolated hard-process, this equation is essentially equivalent to (1.3) presented in our discussion on reweighting, where in (1.3) is in (5.3).

One way one can measure the parameters is to look for a set of observables whose expectation values are sensitive to the dependence of on :

|  |  |  |
| --- | --- | --- |
|  |  | (5.3) |

Where is the total cross-section. Restricting ourselves to first-order, for the time-being, and combining (5.2) and (5.3) we get:

|  |  |  |
| --- | --- | --- |
|  |  | (5.4) |

With:

|  |  |  |
| --- | --- | --- |
|  |  | (5.5) |
|  |  | (5.6) |
|  |  | (5.7) |
|  |  | (5.8) |

Where is the expectation value for no model parameters, or for EFT, when all parameter values are zero. is the sensitivity of to .

Solving (5.4) for the parameters, we get estimators for whose covariance matrix, using matrix notation, is:

|  |  |  |
| --- | --- | --- |
|  |  | (5.9) |

Where N is the number of events, c is a constant matrix, and is the the covariance matrix of the observables, expanded around its value in the SM:

|  |  |  |
| --- | --- | --- |
|  |  | (5.10) |

For observables, if we chose:

|  |  |  |
| --- | --- | --- |
|  |  | (5.11) |

This gives us from (5.6) and (5.10) the covariance matrixes:

|  |  |  |
| --- | --- | --- |
|  |  | (5.12) |
|  |  | (5.13) |

The observables in (5.11) are “optimal” in that for , the errors on the parameters (5.13) are as small as they can be for a probability distribution [16]. Further, phase space cuts, detector efficiency and acceptance effects cancel in the ratio in (5.11), and thus do not affect the optimal observables. However, detector resolution effects, if significant, may distort the distributions and in a way that does not cancel in the ratio, and should still be taken into account, to avoid biasing the estimators.

## Derivation of second-order optimal observables

We can also define a second-order optimal observable. By definition, (5.2) is a second-order Taylor series expansion of around . The optimal observable for given in (5.11) is seen to be the first-order term for , divided by the zeroth-term. As the first-order term is the partial-derivative of with regards to , and is most sensitive to , it makes sense that the optimal observable for would contain it. We can generalize this observation to define an optimal observable for .

|  |  |  |
| --- | --- | --- |
|  |  | (5.14) |
|  |  | (5.15) |

Where and are the first- and second-order optimal observables.

A detailed analysis on higher-order optimal observables is given in [17], where it is shown that although first-order optimal observables can be conclusively shown to give the least statistical error, the same cannot be said of second-order optimal observables. Higher-order optimal observables can be increased in sensitivity by expanding around a good estimate for In our case, is small and expanding around zero is a good estimate, so we expect that second-order optimal observables will still give a low statistical error, if not the minimum.

## Optimal observables and reweight coefficients

For a single event is proportional to the squared matrix-element for that event. Comparing the above equations to those for reweighting in section 1.1.1 (being careful not to confuse the phase-space used here with the model parameter used there), we find that , and are proportional to the terms of the reweight-coefficient matrix **F**. Thus for each event the first- and second-order optimal observables for a given reweight-parameter are given by:

|  |  |  |
| --- | --- | --- |
|  |  | (5.16) |
|  |  | (5.17) |

As the reweight-coefficient matrix **F** is constant for a specific event, so are and fixed for this event, just as all other observables are. Like all other observables, and have their own event distributions for a given process. Further, these event-distributions depend upon all model-parameters, not just the model-parameter associated with the optimal observable. The reweight-coefficients for an event given by the matrix, not only determine the values of the optimal observables for that event, they also determine the weight of the event for a given set of model-parameters.

## Optimal observables in this project

In section 7, when we perform our fit analysis for reweighted EFT, we will examine the fit characteristics of optimal observables for our three EFT model parameters.

As stated above, the expectation values of an optimal observable is sensitive to the dependence of on . Therefore, we will also use the mean of each optimal observable , plotting it versus the invariant mass of events, as another set of observables for our fit analysis.

TODO: add figures

TODO: add talk about dividing by invariant mass.

# Chosen observables for parton-level WZ-production

In the following section we will measure the fit characteristics of reweighting EFT to SM data. To do so we need to select some observables to perform fits with. In addition to a handful of phase-space observables, we will also examine optimal observables. We also need to select for each observable, the range and bin sizes, in an as objective a way as possible, as these will affect the fit results to some degree.

We will continue to use the SM and EFT data samples used previously. Both samples contain 1M events, which we will scale to a luminosity of 10 fb–1. Using only the SM data sample to determine data range and binning, the chosen observables and their characteristics are shown in Table 6.1.

We have chosen 3 phase-space observables, PT(Z) – the transverse momentum of Z, M(WZ) – the invariant mass of the WZ-pair, and y(Z) – the rapidity of Z. We have also added the first- and second-order optimal observables for the 3 EFT model parameters cWWW, cW, and cB to our table of observables.

Since fitting to the mean of the optimal observables should give the least statistical error, we have included in our table of observables, profile histograms of the mean of each optimal observable plotted against the invariant mass of the hard-process. Note the Mandelstam variable s used here corresponds to the hard-process and not the proton beams.

In addition, as each optimal observable is a function of the invariant mass, we have divided out that dependency for each event, and included profile histograms of the mean across events of each optimal observable divided by their invariant mass dependency, again plotted against the invariant mass. These profiles should be nearly constant, or asymptotic to a constant at high energy.

In summary, the selected objectives can be divided into two broad groups: event-counted objectives stored in histograms, and mean-objectives, which are stored in profiles that are effectively equivalent to a data graph with vertical error bars.

Table 6.1: Observables for parton-level WZ-production, characteristics and selected range.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Observable** | | **Units y-axis** | **Units x-axis** | **Mean a (x-axis)** | **Std. Dev. a (x-axis)** | **IQR a (x-axis)** | **Selected Range (x-axis)** | **Under/ overflow Count b** |
| **Phase-space observables** | | | | | | | | |
| 1 | PT(Z) |  | GeV/c | 54.6 | 42.5 | 41.7 | 0 to 750 | 0 / 8.2 |
| 2 | M(WZ) = |  | GeV/c2 | 325 | 167 | 138 | 0 to 3000 | 0 / 6.3 |
| 3 | y(Z) |  |  | 1.24×10−4 | 2.02 | 3.21 | −5 to +5 | 0 / 0 |
| **Optimal observables** | | | | | | | | |
| 4 |  |  | GeV2 | −1340 | 5660 | 3210 | (−6 to 1) ×104 | 6.7 / 0.2 |
| 5 |  |  | GeV4 | 8.13×108 | 4.90×1010 | 8.35×107 | (0 to 14) ×1011 | 0 / 9.5 |
| 6 |  |  | GeV2 | −5540 | 26700 | 7280 | (−12 to 1) ×105 | 7.6 / 0 |
| 7 |  |  | GeV4 | 3.93×108 | 1.86×1010 | 8.08×107 | (0 to 53) ×1010 | 0 / 9.8 |
| 8 |  |  | GeV2 | 184 | 574 | 418 | (−1 to 5) ×103 | 0.2 / 8.2 |
| 9 |  |  | GeV4 | 6.78×105 | 2.76×106 | 4.00×105 | (0 to 13) ×107 | 0 / 9.1 |
| **Mean optimal observables vs. invariant mass** | | | | | | | | |
| 10 | vs | GeV2 | GeV | Same as M(WZ) | | | | |
| 11 | vs | GeV4 | GeV |
| 12 | vs | GeV2 | GeV |
| 13 | vs | GeV4 | GeV |
| 14 | vs | GeV2 | GeV |
| 15 | vs | GeV4 | GeV |
| **Mean optimal observables divided by powers of invariant mass vs. invariant mass** | | | | | | | | |
| 16 | vs |  | GeV | Same as M(WZ) | | | | |
| 17 | vs |  | GeV |
| 18 | vs |  | GeV |
| 19 | vs |  | GeV |
| 20 | vs |  | GeV |
| 21 | vs |  | GeV |

1. For all events including those outside the selected range.
2. SM data sample at 10 fb–1.

## Data range

Most of our observables have long tails approaching a sparse distribution of single events separated by areas with no events. Once binned, these sparse areas will result in bins with low statistics and empty bins. When fitting, all bins are treated equally and if we have a relatively high number of low statistic bins, these can dominate the fit results. With some fit objectives, such as minimizing χ2, empty data bins are skipped, reducing the degrees of freedom for the fit.

One can solve such problems, by using different bin sizes across the data range to ensure that no bins have low statistics. This is discussed in the next section. For simplicity though, we have chosen to use equal-width bins for our histograms, thus sparse data tails remain an issue, and the data range must be carefully chosen.

To set the data range in a somewhat objective manner, we have chosen ranges that exclude less than 10 events on either end, after scaling to the test luminosity of 10 fb–1. Thus the underflow and overflow bins will have less than 10 events. Why use 10 events as the criteria? Simply because, a bin with 10 events and thus an error of has more than a 3 sigma probability of not having a true value of zero. Bins with less than 10 events have a small but significant probability of being zero.

In addition, we have set the range based solely upon the SM data sample, that is the data sample that we are fitting to and not the EFT data sample that we are reweighting. A common range and bin size must be used to perform binned fits. Normally one bins one’s data (the SM sample) according to its characteristics, and then bins the model (the reweighted EFT sample) equivalently.

## Binning for binned fits

All choices in binning affect fit results to some degree, and unfortunately it is not easy to gauge these effects. We desire that fit results remain fairly stable as a function of binning near our binning choice.

We have several choices when binning our data. The **first choice** is whether a single bin-width should be used across the entire range, equivalent to dividing the data range equally into a specified number of bins, or whether different bin-widths should be used through the data range.

The choice of a single bin-width is obviously the simplest. However, as mentioned in the previous section, our observables often have areas of sparse events at one or both ends of their data range. These areas will contain bins that are empty or with low statistics. One cannot reweight an empty bin, and bins with low statistics have larger relative errors. When fitting, all bins are treated equally and if we have a relatively high number of low statistic bins, these can dominate the fit results. Also with some fit objectives, such as minimizing χ2, empty data bins are skipped, reducing the degrees of freedom for the fit.

One can solve such problems, by using different bin sizes across the data range to ensure that no bins have low statistics. Thus there will be more bins in areas of high density and fewer in areas of low density. One can divide each bin’s height by its bin width, to create a density distribution, but this is not necessary for fitting, and will cannot be used with a likelihood fit objective that compares event counts. However, gauging the binning effects of a specific choice of variable bin-widths on a fit result is not an easy task.

For this project, we have chosen for simplicity to use equal-width bins for our histograms, despite the potential benefits of variable bin-widths. This means that we must be aware of the sparse regions in our data, and take care to handle empty and low-statistic bins appropriately. This is discussed further in the sections describing the fits performed.

One potential compromise between variable and fixed bin-widths, is to use fixed bin-widths, and then to fill in empty bins with events from adjacent non-empty bins, spreading the events evenly across the empty areas. This has the same affect of creating wider pseudo-bins locally where the density is lower, without actually changing the binning scheme. This obviously can only be done on model histograms and not data histograms, as data should never be modified. This technique is used where appropriate, and discussed further in sections describing the fits performed.

One can also obviously avoid low-statistic and empty bins by using more events, or fewer number of bins.

### Optimal number of bins

The **second choice**, when binning our data using fixed bin-widths, is the number of bins to use across the data range. There are widely different suggestions on how to determine the optimal number of bins for a given data set [REF]. For example, there is the very simple square root choice, used by Microsoft Excel:

|  |  |  |
| --- | --- | --- |
|  |  | (6.1) |

where *K* is the number of bins, and *N* the number of data points. For 1M data points, this gives *k* = 1000.

There is *Rice’s rule*, for approximately normal distributions:

|  |  |  |
| --- | --- | --- |
|  |  | (6.2) |

which gives k = 200 for 1M data points.  
There is *Scott’s normal reference rule* for normal distributions:

|  |  |  |
| --- | --- | --- |
|  |  | (6.3) |

where *W* is the optimal width and is the standard deviation of the data sample.  
For non-normal distributions, there is the *Freedman-Diaconis rule* [REF]:

|  |  |  |
| --- | --- | --- |
|  |  | (6.4) |

where IQR is the interquartile range of the data sample.  
The above rules are straight-forward to calculate, and the results for Scott’s and Freedman-Diaconis rule are included in table [REF].

Somewhat more complicated are functions that when minimized give the optimal bin-width, or in our case the optimal number of bins. Here are two such functions, based upon minimizing the mean integrated square error (MISE). That is, they try to minimize the mean error between a binned histogram and the true continuous distribution it estimates. Since the true distribution is not known, they estimate the true distribution from the data itself.

The first method [REF], minimizes the MISE cost function given by:

|  |  |  |
| --- | --- | --- |
|  |  | (6.5) |

Where is the mean events per bin, is the variance in the events per bin, are the number of events in bin , and is the total number of bins.

The second method, know as the cross-validation method [REF], minimizes:

|  |  |  |
| --- | --- | --- |
|  |  | (6.6) |

During testing, it was found that both functions effectively generate the same minimization curve, differing only in scale and offset, but having the same shape and minimal point. The scale of the cross-validation function was fairly independent of the observable, whereas the scale of the MISE cost function was highly dependent upon the observable chosen, mostly due to the higher power of the term in the denominator. Therefore, we chose to only minimize the cross-validation function.

The results of Scott’s and the *Freedman-Diaconis rule* along with the results of minimizing the cross-validation function are shown in Table 6.2. The following section details how the cross-validation function was minimized.

#### Minimizing the cross-validation function

Initially, we attempted to use ROOT’s fit methods to minimize the cross-validation function. To keep the function smooth, minimization was performed on a continuous number of bins, and all but the last bin were equal in size. For example, to achieve 12.2 bins, the range was divided by 12 equal sized bins, and one extra bin that was 0.2 the size of the other bins. As a cross-check, to ensure that we were minimizing the proper function parameter, we also ran the minimization using continuous bin-widths, instead of the number of bins. Fortunately, the results of minimizing the cross-validation function using either the number of bins or the bin-width as the function parameter were identical, as one would expect.

Using ROOT’s fit methods and its default Minuit minimizer, we attempted to find the optimal number of bins between 10 and 1M. The cross-validation function for most observables descends rapidly to a nearly constant plateau after about 100 bins. This plateau is nearly flat, descending very slowly as the number of bins increase, wobbling through numerous local minima, to an ultimate global minimum, before rising very slowly afterwards. See Figure [REF] for an example minimization curve.

The nearly flat nature of this plateau, often resulted in ROOT’S fit function converging on some local minima. Hesse errors were enabled to make a parabolic estimate of the errors, and these were always close to the order of the entire allowed range of the number of bins. However, it was unclear whether we could rely on the error estimates at all, as they are dependent upon a Gaussian distribution around the converged upon parameter result, and the corresponding definition of the equivalent height in the cost function corresponding to the desired confidence level. The fit results were also fairly dependent upon the tolerance setting for the minimizer, the fit range, and the initial step.

We suspected that perhaps the issue is the continuous nature of the fit parameter, as opposed to the integer nature of the number of bins the original cross-validation objection function was derived with. In an attempt to solve this, we changed the objective function to return an interpolated result between the two nearest integer values for the number of bins. For example, if the minimizer requested 12.2 bins, we would calculate the cross-validation function for 12 and 13 bins, and return a weighted average using 80% of the 12 result and 20% of the 13 result. This helped smooth the minimization function somewhat, but not sufficiently that it helped solve the issues we were having in getting consistent fit results.

In the end, we concluded that using a minimizer to find the optimal number of bins was overly complicated and untrustworthy given the circumstances. Instead, we programmed a very simple scan of the cross-validation function across an allowed range of the number of bins using only integer values in steps that were humanly selected. For example, in the 10s we scanned by steps of 5, in the 100s by steps of 25, in the 1000s by steps of 250, and so on. We scanned from 10 to 1M bins and recorded the point with the minimal cross-validation value. The cross-validation results from this simple scan are shown in Table 6.2.

For the phase-space observables, reasonably low number of bins is chosen by this method. However, for the optimal observables, particularly the second-order, the number of bins is very high. The minimization plateau of two of second order optimal observables, was observed to continue descend past our upper limit of 1M bins. This casts some doubt on the usability of the cross-validation method for our data. The long flat plateau in its entirety can be seen as roughly the functions minimum, indicating that any number of bins from somewhere between 100 and 1000 to 1M could conceivably be used.

### Selection of the number of bins

The different results for optimal bins by Scott’s rule, the Freedman-Diaconis rule, and by minimizing the cross-validation function, are fairly varied. The broad minimization plateau for the cross-validation, suggests that a broad range of number of bins will be effectively the same. So despite all the mathematics to predict the optimal number of bins, we will end up choosing the number ourselves, guided by the mathematical suggestions.

The fewer bins we have the faster the performance of the model fits we will perform in the next section. In that interest, we have chosen to limit the number of bins to a maximum of 10000, which is a quite likely limit for most data samples. Finally, we have chosen numbers of bins that are rounded to humanly pleasing numbers, that fit the range nicely, and that are close to the suggested values. Considering the broad minimization plateau of the cross-validation function, this should not change the fit result significantly. The selected number of bins is shown in Table 6.2.

For the mean-value observables using profile histograms, the number of bins is selected to match the observable the mean is plotted against. In our case this is invariant mass, which is the same as M(WZ).

Table 6.2: Observables for parton-level WZ-production, optimal bins by different methods, and selected bins.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Observable** | | **Optimal Bins** | | | **Selected Bins** |
| **Scott’s** | **Freedman- Diaconis** | **Cross-Validation** |
| **Phase-space observables** | | | | | |
| 1 | PT(Z) | 952 | 1700 | 900 | 750 |
| 2 | M(WZ) = | 709 | 1510 | 1750 | 1500 |
| 3 | y(Z) | 139 | 153 | 175 | 200 |
| **Optimal observables** | | | | | |
| 4 |  | 394 | 1220 | 2000 | 2000 |
| 5 |  | 16300 | 1.68×107 | > 1E6 | 10000 |
| 6 |  | 6110 | 39200 | 17500 | 10000 |
| 7 |  | 16200 | 6.53×106 | > 1E6 | 10000 |
| 8 |  | 338 | 812 | 1250 | 1000 |
| 9 |  | 6190 | 74900 | 325000 | 10000 |
| **Mean optimal observables vs. invariant mass** | | | | | |
| 10 | vs | Same as M(WZ) | | | |
| 11 | vs |
| 12 | vs |
| 13 | vs |
| 14 | vs |
| 15 | vs |
| **Mean optimal observables divided by powers of invariant mass vs. invariant mass** | | | | | |
| 16 | vs | Same as M(WZ) | | | |
| 17 | vs |
| 18 | vs |
| 19 | vs |
| 20 | vs |
| 21 | vs |

## Binning for unbinned fits

One way to minimize the effects of binning on fit results is to do unbinned fits. In unbinned fits, only the model events are binned, and the individual likelihood for all data events is calculated and the sum maximized. We also performed unbinned fits on event counted observables in the following sections. The advantage of unbinned fits is that one no longer needs to bin the fit model with the same binning used for the fit data, one can use much higher resolution binning, improving the precision of the result.

For our unbinned fits, we have used 100K bins for the 1M model events for each observable.

# Fitting EFT to SM for parton-level WZ-production

Now that we have the reweighting tools to construct the observable plots for any defined set of EFT model parameters, we can now measure the fit characteristics of reweighting EFT to SM data at the parton-level. Specifically, we can measure how well reweighted EFT data fits the SM data for each selected observable, using a fit algorithm to determine the EFT model parameters that fit best. We are primarily interested in the error to the parameters, as the true value is zero for all three parameters cWWW, cW, and cB.

For the fits we used the same parton-level WZ-production pseudo-data generated by Sherpa used previously. The SM events are used as the fit-data, and the EFT events are reweighted and used as the fit-model. The SM and EFT data samples both have 1M events and their total cross-sections are 18.554 ± 0.016 pb and 42.805 ± 0.038 pb respectively. The data samples are scaled to a luminosity of 10 fb−1, and Asimov bin errors are used as discussed in section 4.2. Note that the fit will only use the errors on the fit-data, that is the SM data.

We used ROOT’s fit methods to perform all fits, and describe the details in section 7.3. We fit all objectives detailed in section 6, fitting each to each EFT parameter individually, as well as fitting to all 3 parameters simultaneously.

We performed two kinds of fits: binned and unbinned. Binned fits use the same binning for both the fit data and model, and are the traditional form of fit. For unbinned fits, we only bin the model, and maximize the log-likelihood of all 1M data events.

The choice of binning for binned and unbinned fits is described in detail in sections 6.2 and 6.3. Unbinned fits should be less affected by the choice of binning. Unfortunately, unbinned fits are far slower as all 1M fit-data events must be iterated through for each parameter selection during the fit process, as opposed to iterating through typically less than 1000 bins. Unbinned fits can only be done on event-counted observables.

For binned fits we used two different fit objectives: maximize log-likelihood (or rather minimize negative log-likelihood) for event-counted observables, and minimize for mean-observables.

Note that the likelihood function for binned fits uses Poisson statistics to calculate the likelihood. However, the likelihood function for unbinned fits requires the fit-model histogram to be normalized to a constant value, and does not take the relative number of events into consideration.

It should be noted that in all cases fit data corresponding to empty bins in the fit model are skipped by the fit process, as it is impossible to reweight an empty bin. Empty bins in the fit data are also skipped when minimizing , as there is no error for an empty bin to calculate the denominator of the value.

## Binned fit results

The binned fit results are shown in Table 7.1, Table 7.2 and Table 7.3 for each of the EFT model parameters.

Table 7.1: Binned fit results for cWWW

| **Observable** | | **Fit only cWWW** | | | **Fit All** | | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Value**  **[10−6 GeV2]** | **95% CL**  **[10−6 GeV2]** |  | **Value**  **[10−6 GeV2]** | **95% CL**  **[10−6 GeV2]** |  |
| **Phase-space observables** | | | | | | | |
| 1 | PT(Z) | −0.26 | 0.64  (−0.43,+0.96) | 0.26 | 0.051 | 1.2  (−0.85,+0.77) | 0.26 |
| 2 | M(WZ) = | −1.80 | 0.24  (−0.23,+0.24) | 0.41 | −1.0 | 2.0  (−0.93,+2.9) | 0.41 |
| 3 | y(Z) | −0.98 | 1.5  (−1.1,+4.6) | 0.6 | 0.45 | 5.7  (−4,+3.4) | 0.6 |
| **Optimal observables** | | | | | | | |
| 4 |  | −0.31 | 0.55  (−0.44,+0.9) | 0.36 | 0.43 | 1.6  (−1.7,+0.91) | 0.36 |
| 5 |  | −0.27 | 0.54  (−0.4,+0.88) | 0.023 | 0.21 | 1.6  (−1.1,+0.75) | 0.023 |
| 6 |  | −0.30 | 0.50  (−0.39,+0.91) | 0.081 | −0.43 | 1.5  (−0.65,+1.5) | 0.081 |
| 7 |  | −0.26 | 0.55  (−0.41,+0.85) | 0.024 | 0.13 | 1.5  (−1,+0.8) | 0.024 |
| 8 |  | −0.28 | 0.56  (−0.45,+0.88) | 0.39 | 0.30 | 2.0  (−1.6,+1) | 0.39 |
| 9 |  | −0.27 | 0.56  (−0.41,+0.96) | 0.062 | 0.38 | 1.2  (−1.4,+0.65) | 0.062 |
| **Mean optimal observables vs. invariant mass** | | | | | | | |
| 10 | vs | 0.011 | 0.018 | 7.5 | −0.00070 | 0.023 | 3.1 |
| 11 | vs | 0.0100 | 0.0015 | 780 | −0.00080 | 0.002 | 210 |
| 12 | vs | 0.0097 | 0.0029 | 210 | −0.00077 | 0.0039 | 60 |
| 13 | vs | 0.0098 | 0.0024 | 310 | −0.00078 | 0.0032 | 87 |
| 14 | vs | 0.012 | 0.032 | 3.2 | −0.00045 | 0.038 | 1.7 |
| 15 | vs | 0.012 | 0.029 | 3.8 | −0.00054 | 0.034 | 2 |
| **Mean optimal observables divided by powers of invariant mass vs. invariant mass** | | | | | | | |
| 16 | vs | 0.011 | 0.018 | 7.5 | −0.00070 | 0.023 | 3.1 |
| 17 | vs | 0.0100 | 0.0015 | 780 | −0.00080 | 0.002 | 210 |
| 18 | vs | 0.0097 | 0.0029 | 210 | −0.00077 | 0.0038 | 60 |
| 19 | vs | 0.0098 | 0.0024 | 310 | −0.00078 | 0.0032 | 87 |
| 20 | vs | 0.012 | 0.032 | 3.2 | −0.00045 | 0.038 | 1.7 |
| 21 | vs | 0.012 | 0.029 | 3.8 | −0.00054 | 0.034 | 2 |

Table 7.2: Binned fit results for cW

| **Observable** | | **Fit only cW** | | | **Fit All** | | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Value**  **[10−6 GeV2]** | **95% CL**  **[10−6 GeV2]** |  | **Value**  **[10−6 GeV2]** | **95% CL**  **[10−6 GeV2]** |  |
| **Phase-space observables** | | | | | | | |
| 1 | PT(Z) | −0.11 | 0.26 (−0.25,+0.26) | 0.26 | −0.16 | 0.40 (−0.37,+0.68) | 0.26 |
| 2 | M(WZ) = | −2.00 | 0.33 (−0.32,+0.34) | 0.41 | −1.9 | 1.9 (−0.78,+2.1) | 0.41 |
| 3 | y(Z) | −0.41 | 0.74 (−0.71,+0.78) | 0.60 | −2.0 | 4.6  (−1.8,+9.3) | 0.60 |
| **Optimal observables** | | | | | | | |
| 4 |  | −0.11 | 0.22 | 0.36 | 0.011 | 0.83 (−0.5,+1.1) | 0.36 |
| 5 |  | −0.094 | 0.22 (−0.22,+0.23) | 0.023 | −0.011 | 0.60 (−0.39,+0.84) | 0.023 |
| 6 |  | −0.088 | 0.20 | 0.081 | 0.084 | 1.0 (−0.48,+0.93) | 0.081 |
| 7 |  | −0.093 | 0.22 | 0.024 | −0.044 | 0.44 (−0.36,+0.74) | 0.024 |
| 8 |  | −0.095 | 0.22 | 0.39 | −0.011 | 0.70 (−0.46,+1) | 0.39 |
| 9 |  | −0.083 | 0.22 (−0.21,+0.22) | 0.062 | 0.015 | 0.71 (−0.43,+0.82) | 0.062 |
| **Mean optimal observables vs. invariant mass** | | | | | | | |
| 10 | vs | 0.870 | 0.035 | 3.1 | 0.870 | 0.036 | 3.1 |
| 11 | vs | 0.8600 | 0.0032 | 210 | 0.8500 | 0.0033 | 210 |
| 12 | vs | 0.8400 | 0.0061 | 60 | 0.8400 | 0.0062 | 60 |
| 13 | vs | 0.8500 | 0.0051 | 87 | 0.8400 | 0.0051 | 87 |
| 14 | vs | 0.850 | 0.059 | 1.7 | 0.860 | 0.060 | 1.7 |
| 15 | vs | 0.860 | 0.053 | 2.0 | 0.870 | 0.054 | 2.0 |
| **Mean optimal observables divided by powers of invariant mass vs. invariant mass** | | | | | | | |
| 16 | vs | 0.870 | 0.035 | 3.1 | 0.870 | 0.036 | 3.1 |
| 17 | vs | 0.8600 | 0.0032 | 210 | 0.8500 | 0.0033 | 210 |
| 18 | vs | 0.8400 | 0.0061 | 60 | 0.8400 | 0.0062 | 60 |
| 19 | vs | 0.8500 | 0.0051 | 87 | 0.8400 | 0.0051 | 87 |
| 20 | vs | 0.850 | 0.059 | 1.7 | 0.860 | 0.060 | 1.7 |
| 21 | vs | 0.860 | 0.053 | 2.0 | 0.870 | 0.054 | 2.0 |

Table 7.3: Binned fit results for cB

| **Observable** | | **Fit only cW** | | | **Fit All** | | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Value**  **[10−6 GeV2]** | **95% CL**  **[10−6 GeV2]** |  | **Value**  **[10−6 GeV2]** | **95% CL**  **[10−6 GeV2]** |  |
| **Phase-space observables** | | | | | | | |
| 1 | PT(Z) | 2.5 | 11  (−11,+10) | 0.26 | −2.3 | 20  (−17,+26) | 0.26 |
| 2 | M(WZ) = | 54 | 19  (−21,+17) | 0.39 | −51 | 55  (−41,+66) | 0.41 |
| 3 | y(Z) | 12 | 22  (−24,+20) | 0.6 | −61 | 230  (−190,+200) | 0.6 |
| **Optimal observables** | | | | | | | |
| 4 |  | 3.8 | 7.7  (−7.8,+7.6) | 0.36 | 7.5 | 35  (−22,+33) | 0.36 |
| 5 |  | 4.2 | 9.5  (−9.7,+9.2) | 0.023 | 5.6 | 31  (−20,+31) | 0.023 |
| 6 |  | 3.2 | 7.8  (−7.9,+7.7) | 0.081 | 0.91 | 17  (−14,+21) | 0.081 |
| 7 |  | 3.8 | 8.9  (−9.1,+8.7) | 0.024 | 3.4 | 25  (−17,+27) | 0.024 |
| 8 |  | 3.4 | 7.7  (−7.8,+7.6) | 0.39 | 5.6 | 34  (−20,+34) | 0.39 |
| 9 |  | 2.9 | 8.8  (−9,+8.6) | 0.062 | 6.1 | 30  (−21,+28) | 0.062 |
| **Mean optimal observables vs. invariant mass** | | | | | | | |
| 10 | vs | −12.0 | 2.0 | 7.2 | −0.45 | 2.5 | 3.1 |
| 11 | vs | −12.00 | 0.17 | 750 | −1.80 | 0.24 | 210 |
| 12 | vs | −12.00 | 0.33 | 200 | −1.80 | 0.45 | 60 |
| 13 | vs | −12.00 | 0.27 | 300 | −1.80 | 0.37 | 87 |
| 14 | vs | −11.0 | 3.2 | 3.1 | 2.1 | 3.8 | 1.7 |
| 15 | vs | −12.0 | 2.9 | 3.7 | 1.4 | 3.5 | 2 |
| **Mean optimal observables divided by powers of invariant mass vs. invariant mass** | | | | | | | |
| 16 | vs | −12.0 | 2.0 | 7.3 | −0.45 | 2.5 | 3.1 |
| 17 | vs | −12.00 | 0.17 | 750 | −1.80 | 0.24 | 210 |
| 18 | vs | −12.00 | 0.33 | 200 | −1.80 | 0.45 | 60 |
| 19 | vs | −12.00 | 0.27 | 300 | −1.80 | 0.37 | 87 |
| 20 | vs | −11.0 | 3.2 | 3.1 | 2.1 | 3.8 | 1.7 |
| 21 | vs | −12.0 | 2.9 | 3.7 | 1.4 | 3.5 | 2 |

## Unbinned fit results

Table 7.4: Unbinned fit results for cWWW

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Observable** | | **Fit only cWWW** | | **Fit All** | |
| **Value [10−6 GeV2]** | **95% CL [10−6 GeV2]** | **Value [10−6 GeV2]** | **95% CL [10−6 GeV2]** |
| **Phase-space observables** | | | | | |
| 1 | PT(Z) | −0.70 | 0.30 | −0.036 | 0.51 |
| 2 | M(WZ) = | −5.5 | 0.14 | −0.52 | 0.66 |
| 3 | y(Z) | −10 | 0.0089 | 10 | 1.7 |
| **Optimal observables** | | | | | |
| 4 |  | 6.3 | 0.16 | −5.0 | 0.37 |
| 5 |  | −0.0014 | 0.54 | −0.0017 | 0.78 |
| 6 |  | 0.77 | 0.36 | 1.1 | 0.37 |
| 7 |  | 0.0014 | 0.52 | −0.0012 | 0.76 |
| 8 |  | 6.1 | 0.16 | −4.0 | 0.42 |
| 9 |  | 0.34 | 0.53 | 0.55 | 1.1 |

Table 7.5: Unbinned fit results for cW

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Observable** | | **Fit only cW** | | **Fit All** | |
| **Value [10−6 GeV2]** | **95% CL [10−6 GeV2]** | **Value [10−6 GeV2]** | **95% CL [10−6 GeV2]** |
| **Phase-space observables** | | | | | |
| 1 | PT(Z) | −0.53 | 0.22 | −0.67 | 0.31 |
| 2 | M(WZ) = | −7.9 | 0.22 | −3.3 | 0.64 |
| 3 | y(Z) | −10 | 0.014 | −10 | 0.45 |
| **Optimal observables** | | | | | |
| 4 |  | 10 | 0.0098 | 1.0 | 0.67 |
| 5 |  | 0.043 | 0.23 | 0.12 | 0.39 |
| 6 |  | 0.035 | 0.22 | 0.81 | 0.85 |
| 7 |  | 0.055 | 0.23 | 0.14 | 0.40 |
| 8 |  | 10 | 0.011 | 0.85 | 0.67 |
| 9 |  | 0.13 | 0.23 | 0.28 | 1.1 |

Table 7.6: Unbinned fit results for cB

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Observable** | | **Fit only cB** | | **Fit All** | |
| **Value [10−6 GeV2]** | **95% CL [10−6 GeV2]** | **Value [10−6 GeV2]** | **95% CL [10−6 GeV2]** |
| **Phase-space observables** | | | | | |
| 1 | PT(Z) | 14 | 10 | −10 | 16 |
| 2 | M(WZ) = | 430 | 9.7 | 340 | 21 |
| 3 | y(Z) | −1000 | 1.6 | −870 | 34 |
| **Optimal observables** | | | | | |
| 4 |  | 81 | 7.6 | −420 | 20 |
| 5 |  | 0.092 | 9.4 | 3.9 | 18 |
| 6 |  | −3.9 | 8.8 | 27 | 27 |
| 7 |  | −0.055 | 9.3 | 4.5 | 18 |
| 8 |  | 65 | 8.8 | −450 | 15 |
| 9 |  | 81 | 7.6 | −420 | 20 |

## Analysis of fit results

TODO:

* Binned mean optimal observables had the best overall resolution, i.e. lowest CL.
* Mean optimal observables and mean optimal observables divided by powers of invariant mass gave the same results, to two significant digits. Neither is better than the other. [Double check this is not a bug].
* Unbinned results are inconsistent. Sometimes CL is low, sometimes high. Often fit value is much greater than CL, meaning that the true value of zero is very unlikely. Could this be due to only fitting shape? The results for binned were worse for 100K bins (those shown) than 10K bins. Shouldn’t higher resolution be better.
* Ran fits as described, as well as with empty-bins merged with non-empty bins. The difference on the fit results was very little, only changing the second significant digit of the CL on a small handful of observables. Decided to leave zero-bin-merging out of the final results.

## Notes on using ROOT to fit data

In general, we have used as much as possible ROOT’s default fit configuration. It was necessary to increase the tolerance setting from its default of 0.1 to 25 for unbinned fits, in order for some of the unbinned fits to converge, possibly due to the increased scale of the log-likelihood measurements from summing 1M likelihoods as opposed to 100 to 10000.

TODO: add more details

# Conclusion

# References

[1] Almalioglu Yasin, Salzburger Andreas, and Ritsch Elmar, "Performance Improvements for the ATLAS Detector Simulation Framework," (2013) [10.5281/zenodo.7558](http://dx.doi.org/10.5281/zenodo.7558).

[2] “Sherpa”, 2014-2015. <https://sherpa.hepforge.org/trac/wiki>.

[3] “Homebrew – The missing package manager for OS X”, 2015. <http://brew.sh/>.

[4] David C. Hall, “homebrew-hep”, 2014-2015. <http://davidchall.github.io/homebrew-hep/>.

[5] “FeynRules”, 2014-2015. <http://feynrules.irmp.ucl.ac.be/>.

[6] Adam Alloul, Neil D. Christensen, Céline Degrande, Claude Duhr, and Benjamin Fuks, "FeynRules 2.0 - A complete toolbox for tree-level phenomenology," Comput.Phys.Commun. **185**, 2250-2300 (2014).

[7] Neil D. Christensen and Claude Duhr, "FeynRules - Feynman rules made easy," Comput.Phys.Commun. **180**, 1614-1641 (2009).

[8] Celine Degrande, Claude Duhr, Benjamin Fuks, David Grellscheid, Olivier Mattelaer, and Thomas Reiter, "UFO - The Universal FeynRules Output," Comput.Phys.Commun. **183**, 1201-1214 (2012).

[9] “HepMC Event Record”, 2015. <http://lcgapp.cern.ch/project/simu/HepMC/>.

[10] “ROOT a data analysis framework”, 2014-2015. <https://root.cern.ch/>.

[11] Celine Degrande, Nicolas Greiner, Wolfgang Kilian, Olivier Mattelaer, Harrison Mebane, Tim Stelzer, Scott Willenbrock, and Cen Zhang, "Effective Field Theory: A Modern Approach to Anomalous Couplings," Annals Phys. **335**, 21-32 (2013).

[12] K. Hagiwara, S. Ishihara, R. Szalapski, and D. Zeppenfeld, "Low energy effects of new interactions in the electroweak boson sector," Physical Review D **48** (5), 2182-2203 (1993).

[13] Markus Diehl, Otto Nachtmann, and Felix Nagel, "Triple gauge couplings in polarized e- e+ ---> W- W+ and their measurement using optimal observables," Eur.Phys.J. **C27**, 375-397 (2003).

[14] Otto Nachtmann and Felix Nagel, "Optimal observables and phase-space ambiguities," Eur.Phys.J. **C40**, 497-503 (2005).

[15] M. Dobbs and L. Lefebvre, "Prospects for Probing the Three Gauge-boson Couplings in W + Photon Production at the LHC," (2002).

[16] M. Diehl and O. Nachtmann, "Optimal observables for the measurement of three gauge boson couplings in e+ e- ---> W+ W-," Z.Phys. **C62**, 397-412 (1994).

[17] M. Diehl and O. Nachtmann, "Anomalous three gauge couplings in e+ e- ---> W+ W- and 'optimal' strategies for their measurement," Eur.Phys.J. **C1**, 177-190 (1998).

# Source code

Source code for all the applications and libraries developed for this project are publicly available for download from GitHub at <https://github.com/christopher-jacobsen>. Relevant repositories are prefixed with Physics-Thesis.