

DISSERTATION

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**End to end optimization in a search for  
boosted Higgs boson pair production in  
the  $bbbb$  final state via  
vector-boson-fusion (VBF) production  
using the run 2 dataset with the ATLAS  
detector**

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For the attainment of the academic degree doctor rerum naturalium

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## Abstract

I am an abstract.



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# List of abbreviations

**ATLAS**    The Atlas Experiment  
**pdf**        probability density function



# Chapter 1

## Theory

Where to start? Sometimes it seems like that particle physics is bringing it all together, as it tries to give a comprehensive picture of the world by describing the structure of matter from quantum mechanics to cosmology. So I would say to start shallow (since we are experimentalists) at the very beginning, and then dive a bit deeper into Standard Model to have a plausible thread how the need and the development of the Higgs mechanism came about. The following is mainly based on [1, 2] and intended to make the calculation of cross sections plausible.

### 1.1 Feynman rules from field theory

The fact that elementary particles can seemingly be born out of nothing and die again led to the development of their currently most successful description through quantum field theories. Heuristically it can be understood by the uncertainty principle, which states that energy can vary greatly on short time scales, and by special relativity, which allows the property energy to be converted into the property mass. This marriage between quantum mechanics and special relativity is what drove the development of quantum field theory.

can be deduced through perturbation theory, just on term, The conventional strategy is perturbation theory with the free fields as starting point, treating the interaction as a small perturbation

To make a field one assigns a quantity to some region in spacetime, e.g.  $\phi(\mathbf{x}, t)$ . A Lagrangian  $L(\phi(\mathbf{x}, t))$  then governs the dynamics, like excitations or interactions of this field, which can e.g. represent the birth and death of particles or interactions by the exchange of a particle between them. One formulation of quantum field theory is by use of the path integral formulation. It then basically boils down to integrals of the form  $\int D\phi e^{i \int d^4x L(\phi(\mathbf{x}, t))}$ . Where  $\int D\phi$  is the integral over all possible paths/ways a particle could take. Through back and forth expansions of the  $e$  functions the integral can be solved and the result is a probability - the amplitude  $\mathcal{M}$  of e.g. an interaction between two particles, like scattering, usually depicted in the form of Feynman Diagrams. As this follows a pattern the formalism can be contracted into the infamous Feynman rules (for details see [2]).

## 1.2 Probability of a process

Probes of elementary particle interactions are accessible via bound states, decays and scattering. The first can be studied within classical quantum mechanics whereas the latter uses the preceding. Since this work deals with a collider experiment I think its at least useful to see how one can calculate in principle a cross section  $\sigma$ . It is a measure of how possible an interaction is when shooting something at each other. Calculating reaction rates in quantum mechanics is done by Fermi's golden rule. Here the relativistic version for a scattering process like  $1 + 2 \rightarrow 3 + 4 + \dots + n$  is given [2]

$$\sigma = \frac{S\hbar^2}{4\sqrt{(p_1 \cdot p_2)^2 - (m_1 m_2 c^2)^2}} \int |\mathcal{M}|^2 (2\pi)^4 \delta^4(p_1 + p_2 - p_3 \dots - p_n) \times \prod_{j=3}^n 2\pi \delta(p_j^2 - m_j^2 c^2) \Theta(p_j^0) \frac{d^4 p_j}{(2\pi)^4}. \quad (1.2.1)$$

$S$  is a statistical factor accounting for identical particles (e.g.  $a \rightarrow b + b + c + c + c$ , then  $S = (1/2!)(1/3!)$ ),  $p_i$  are four momenta of particle  $i$  over which one integrates,  $\mathcal{M}(p_1, \dots, p_n)$  is the amplitude of the process calculable with the Feynman rules, the  $\delta^4$  ensures energy and momentum conservation, the last  $\delta$  ensures that particles are on their mass shell ( $E_j^2/c^2 - \mathbf{p}_j^2 = m_j^2 c^2$ ) and the Heaveside  $\Theta$  makes sure that

outgoing energies are positive  $p_j^0 = E_j/c > 0$ . With this, a particle physicist can calculate the probability of any process at a collider experiment.

## 1.3 The Standard Model

### 1.1

dirac, require local gauge invariance  $\rightarrow$  qed Lagrangian

gauge field blah only about Lagrangians, no field solutions needed

## 1.4 Statistics

Every scientific investigation starts with a hypothesis that is to be tested empirically. The main objective is to evaluate if the proposed hypothesis agrees or disagrees with observed data, to either accept or reject it against the null-hypothesis. The metric at hand to do so is the p-value that arises within hypothesis testing.

In the field of high-energy physics, a framework based on likelihood statistics has been developed specifically for this task. This section begins to lay out the mathematical fundamentals of the approach and explains its implementation in PYHF. The following is based on [3–5].

### 1.4.1 Building the likelihood

The statistical model must take into account how compatible the observed collision events are with the theoretical predictions. This can be described by a likelihood  $L(\mathbf{x}|\boldsymbol{\phi})$  that is just a probability for an observation  $\mathbf{x}$  under a given set of parameters  $\boldsymbol{\phi}$ . Since we are dealing with a counting experiment the tool at hand will be bins of a histogram  $\mathbf{h} = (h_1, \dots, h_N)$ .

It is useful to subdivide a measurement  $\mathbf{x} = (\mathbf{n}, \mathbf{a})$  further into a quantity of interest  $\mathbf{n}$ , (e.g. the invariant mass of a particle) and *auxiliary* measurement histograms  $\mathbf{a}$  that help to constrain the model. Additionally in the context of hypothesis testing it is useful to split the set of parameters  $\boldsymbol{\phi} = (\boldsymbol{\psi}, \boldsymbol{\Theta})$  into so called parameters of interest  $\boldsymbol{\psi}$  and nuisance parameters  $\boldsymbol{\Theta}$ . For this section the parameter of interest will be only one parameter, the signal strength  $\mu$ .

The bin heights (counts) can then be expressed in terms of the amount of signal  $s_i(\boldsymbol{\Theta})$  and background  $b_i(\boldsymbol{\Theta})$  in them depending in some way on the nuisance parameters. The prediction (expectation value) of the  $n_i$  can then be expressed as

$$\langle n_i(\mu, \boldsymbol{\Theta}) \rangle = \mu s_i(\boldsymbol{\Theta}) + b_i(\boldsymbol{\Theta}), \quad (1.4.1)$$

and similar for the  $a_i$

$$\langle a_i(\boldsymbol{\Theta}) \rangle = u_i(\boldsymbol{\Theta}). \quad (1.4.2)$$

As we are expecting the bin counts to occur with a constant mean rate and independent of time compared to the last event, each bin follows a Poisson distribution

$$\frac{r^k e^{-r}}{k!}. \quad (1.4.3)$$

$r$  is the expected rate of occurrences, which translates as our prediction, whereas  $k$  are the actual measured occurrences. Accounting for all the bins  $N$  by multiplying them together yields

$$L(\mu, \Theta) = \prod_{j=1}^N \frac{(\mu s_j(\Theta) + b_j(\Theta))^{n_j}}{n_j!} e^{-(\mu s_j(\Theta) + b_j(\Theta))} \prod_{k=1}^M \frac{u_k(\Theta)^{a_k}}{a_k!} e^{-u_k(\Theta)}. \quad (1.4.4)$$

The last product can also be thought of penalizing the likelihood if e.g. an auxiliary measurement displays a very improbable value for a quantity. To test for a hypothesized value of  $\mu$ , the best choice according to the Neyman-Pearson lemma, is the profile likelihood ratio that reduces the dependence to the parameter(s) of interest

$$\lambda(\mu) = \frac{L(\mu, \hat{\Theta})}{L(\hat{\mu}, \hat{\Theta})} \quad (1.4.5)$$

The denominator is the unconditional maximum likelihood estimation so that  $\hat{\mu}$  and  $\hat{\Theta}$  both are free to vary to maximize  $L$ , whereas the numerator is the found maximum likelihood conditioned on some chosen  $\mu$  and the set nuisance parameters  $\hat{\Theta}$  that maximize the likelihood for that particular  $\mu$ . This definition gives  $0 \leq \lambda \leq 1$ . For a  $\lambda \approx 1$  the hypothesized value of  $\mu$  shows good agreement to the Poissonian model.

### 1.4.2 From test statistic to p-value

Transforming the profile likelihood into a test statistic  $t_\mu$  is practical to calculate p-values

$$t_\mu = -2 \log \lambda(\mu). \quad (1.4.6)$$

This translates as  $t_\mu \rightarrow 0$  as good agreement,  $t_\mu \rightarrow \infty$  as bad agreement to the model. A right-tail p-value can then be calculated from the probability density

function of  $t_\mu$ :  $\text{pdf}(t_\mu) = f(t_\mu | \mu)$

$$p_\mu = \int_{t_{\mu,obs}}^{\infty} f(t_\mu | \mu) dt_\mu \quad (1.4.7)$$

$t_{\mu,obs}$  is the test statistic  $t_\mu$  evaluated at the observed data. This is like plugging into the Poisson distributions the same values for  $r$  as for  $k$  in eq. 1.4.3. Just like a probability density function for a standard normal distribution, intuitively the pdf is just, how probable a particular value of the test statistic  $t_\mu$  is under a fixed value of the signal strength (how often it occurs compared to all other values  $t_\mu$  can have).

This particular form is handy because there exist approximations for  $f(t_\mu | \mu)$  [3]. Wald [6] proved that in the large sample limit the test statistic follows a normalized sum of squared distances between the tested parameter of interest  $\mu_i$  and its maximum likelihood estimate  $\hat{\mu}_i$ . The result was extended by Wilk [7] for any number of parameters of interest so the test statistic becomes

$$t_\mu = \sum_i \frac{(\mu_i - \hat{\mu}_i^2)}{\sigma_i^2} + \mathcal{O}(1/\sqrt{N}). \quad (1.4.8)$$

The  $\hat{\mu}_i$  are in the large sample limit normally distributed with mean  $\mu'$  (true values) and standard deviation  $\sigma_i$ . This is the definition of a non-central chi-squared distribution with degrees of freedom  $i$  equal to the parameters of interest (see section 3.1 in [3]). For one parameter of interest the distribution reads

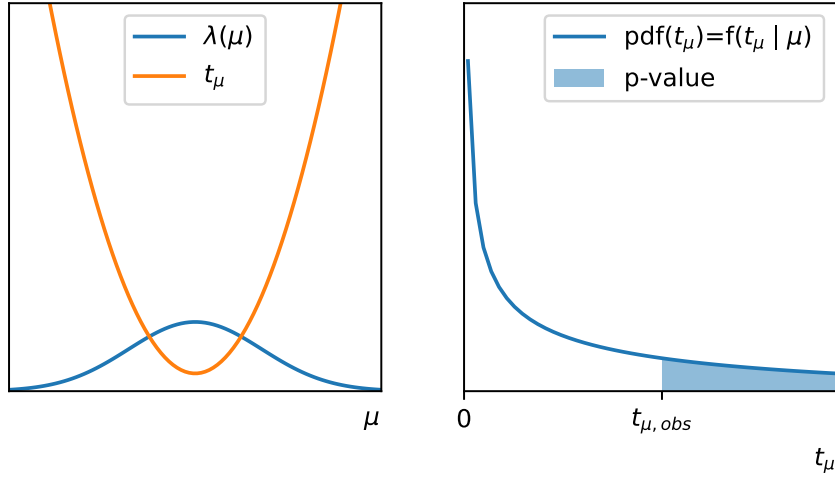
$$f(t_\mu | \mu) = \frac{1}{2\sqrt{t_\mu}} \frac{1}{\sqrt{2\pi}} \left[ \exp\left(-\frac{1}{2}(\sqrt{t_\mu} + \sqrt{\Lambda_\mu})\right) + \exp\left(-\frac{1}{2}(\sqrt{t_\mu} - \sqrt{\Lambda_\mu})\right) \right], \quad (1.4.9)$$

with non-centrality parameter

$$\Lambda_\mu = \frac{(\mu - \mu')^2}{\sigma^2}. \quad (1.4.10)$$

Figure 1.1 illustrates the different steps. Being able to calculate p-values allows now to state how likely it is that the proposed hypothesis is reflected by the observed data. Put differently, if the experiment would be repeated the p-value represents





**Figure 1.1:** A sketch to follow the steps to calculate p-values. (**left**) The profile likelihood (■) has essentially some hill-like form with a maximum at  $\lambda(\hat{\mu}, \hat{\Theta})$ ,  $t_\mu$  (■) is  $-2\ln(\lambda)$ . (**right**) For one parameter of interest in the large sample limit  $f(t_\mu | \mu)$  follows a non-central chi-squared distribution with one degree of freedom, equation 1.4.9. The blue shaded area under the pdf is a right hand sided p-value.

the probability of that the outcome favors the alternative hypothesis over the null hypothesis.

In the scientific community a widely accepted threshold for this is a p-value of 0.05. Though particle physicists only claim discovery of a new phenomenon for  $p < 2.87 \times 10^{-7}$  (5 standard deviations of the standard normal distribution). One caveat here is that this particular form of  $t_\mu$  assumes  $\mu$  can also be negative, which can be non-physical depending on the impact of a new process. Test statistics and their pdf approximations considering the different cases are covered in [3].

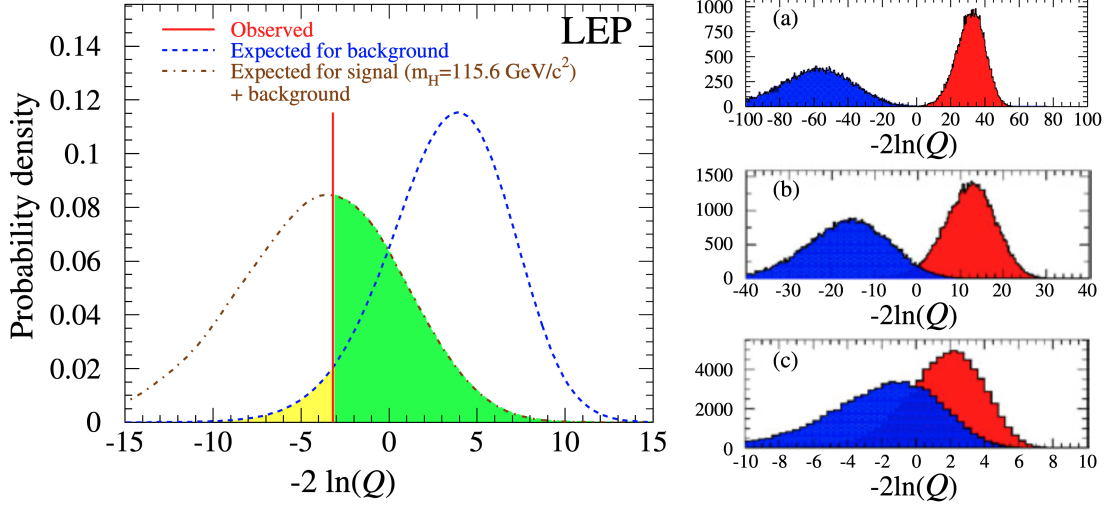
### 1.4.3 The $\text{CL}_s$ value

Particle physicists are usually interested in two things when making statistical tests for discovery of new phenomena: how well is the modeling of backgrounds (things we know) and if there is evidence in the observations for a new phenomenon. This means one needs to test two hypotheses: a background only ( $b$ ) and a signal plus background ( $s + b$ ) hypothesis. Each will result in a p-value on their own.

For example  $p_b = 0$  would mean that the backgrounds are perfectly reflected by the observations and a  $p_{s+b} < 0.05$  could be a sign of e.g. new physics. To combine these two metrics into a single score, particle physicists came up with the pseudo Confidence Level/p-value called  $CL_s$  incorporating also the goodness of the modeling of the backgrounds

$$CL_s = \frac{p_{s+b}}{1 - p_b} = \frac{\int_{t_{\mu,obs}}^{\infty} f(t_{\mu} | \mu) dt_{\mu}}{1 - \int_{t_{\mu,obs}}^{\infty} f(t_{\mu} | \mu) dt_{\mu}}. \quad (1.4.11)$$

Intuitively the numerator is again just the value for the alternative hypothesis whereas the denominator penalizes  $CL_s$  if the modeling of the backgrounds is not reflected in the observations. This can also be understood visually from the first figure of the heavily cited  $CL_s$  paper that introduced the quantity [8] (see description of fig. 1.2).



**Figure 1.2:** Probability density functions of test statistics from a Higgs search at LEP illustrating the calculation of p-values ( $\lambda$  becomes  $Q$ ). **(left)** The pdf's of the test statistic  $f(t_\mu | \mu)$  of the signal + background ( $\text{green}$ ) and background only ( $\text{blue}$ ) hypotheses. The p-value is calculated by integration from  $t_{\mu,obs}$  (the red observed line) to infinity (see eq. 1.4.7). The green shaded area corresponds to  $p_{s+b}$  whereas the yellow area corresponds to  $1 - p_b$  since the integral over one whole pdf is 1. **(right)** Degradation of search sensitivity from (a) to (c). Note that the colors of the pdf's change here to signal + background ( $\text{blue}$ ) and background only ( $\text{red}$ ). For example putting the observation ( $t_{\mu,obs}$ ) on the x-axis at 0 in these plots, one would get for plot (a)  $p_b \approx 1$  and  $p_{s+b} \approx 0$  resulting in a  $CL_s \approx 0$ , whereas with increasing overlap the  $CL_s$  value increases and the sensitivity decreases. From [8].

#### 1.4.4 The HistFactory model

A model used widely to achieve the preceding for a typical ATLAS analysis is called HistFactory [9] and is implemented within PYHF [10]. This follows closely the introduction to the model within the documentation of PYHF [5]. HistFactory draws the name from the idea that the problem is reducible to a small number of basic components. In order to build a likelihood like eq. 1.4.4 it is again useful to think of another splitting of the nuisance parameters  $\phi$  into

$$L(\mathbf{x}|\phi) = \underbrace{L(\mathbf{x}|\underbrace{\boldsymbol{\psi}}_{\text{nuisance parameters}}, \underbrace{\boldsymbol{\theta}}_{\text{parameters of interest}})}_{\text{nuisance parameters}} = \underbrace{L(\mathbf{x}|\underbrace{\boldsymbol{\eta}}_{\text{constrained}}, \underbrace{\boldsymbol{\chi}}_{\text{free}})}_{\text{constrained}} \quad (1.4.12)$$

free parameters  $\boldsymbol{\eta}$ , for example a cross section of a process and constrained parameters  $\boldsymbol{\chi}$ , that incorporate systematic uncertainties. The likelihood can then be modeled with Poissonians for each of the channels  $c$  (e.g. signal regions), bins  $b$  and constraint terms  $c_\chi$  that again penalize the likelihood

$$L(\boldsymbol{n}, \boldsymbol{a} | \boldsymbol{\eta}, \boldsymbol{\chi}) = \underbrace{\prod_{c \in \text{channels}} \prod_{b \in \text{bins}_c} \text{Pois}(n_{cb} | \nu_{cb}(\boldsymbol{\eta}, \boldsymbol{\chi}))}_{\text{Simultaneous measurement of multiple channels}} \underbrace{\prod_{\chi \in \boldsymbol{\chi}} c_\chi(a_\chi | \chi)}_{\text{constraint terms for auxiliary measurements}}. \quad (1.4.13)$$

The  $n_{cb}$  is the observation and  $\nu_{cb}(\boldsymbol{\eta}, \boldsymbol{\chi})$  the prediction. The  $c_\chi$  are calculated from auxiliary measurements  $a_\chi$  to constrain  $\chi$  and can be any function (e.g. Gaussian, Poissonian,...) we believe the parameter to be distributed.

The prediction is a sum of nominal bin height estimates  $\nu_{scb}^0$  over all samples  $s$  (e.g.  $t\bar{t}$ , multijet-background etc.). These nominal bin height estimates can be modified within associated errors. This enters the likelihood through the constraint terms  $c_\chi$  and multiplicative  $\kappa_{scb}$  and additive modifiers  $\Delta_{scb}$

$$\nu_{cb}(\boldsymbol{\phi}) = \sum_{s \in \text{samples}} \nu_{scb}(\boldsymbol{\eta}, \boldsymbol{\chi}) \quad (1.4.14)$$

$$= \sum_{s \in \text{samples}} \underbrace{\left( \prod_{\kappa \in \boldsymbol{\kappa}} \kappa_{scb}(\boldsymbol{\eta}, \boldsymbol{\chi}) \right)}_{\text{multiplicative modifiers}} \left( \nu_{scb}^0(\boldsymbol{\eta}, \boldsymbol{\chi}) + \underbrace{\sum_{\Delta \in \boldsymbol{\Delta}} \Delta_{scb}(\boldsymbol{\eta}, \boldsymbol{\chi})}_{\text{additive modifiers}} \right). \quad (1.4.15)$$

To understand this approach let us consider one systematic. If we would modify the nominal bin height estimate  $\nu_{scb}^0$  by some factor (modifier) while the penalization stays small (constraint term), it can be beneficial for our goal of maximizing the likelihood. This means we find the most likely/compatible value to the observed data within our modeling of the errors.

In HistFactory there are by convention four types  $\{\gamma, \alpha, \lambda, \mu\}$  of such multiplicative rate modifiers that will be explained throughout the rest of this section.

There are free rate modifiers  $\lambda$  and  $\mu$  that affect all bins equally, like the cross section of a process or the luminosity

$$\nu_{scb}(\mu) = \mu \nu_{scb}^0. \quad (1.4.16)$$

These are bin-independent and shape(of the histogram)-preserving normalization factors and could be for example the signal strength from above.

In addition  $\gamma_b$  denotes bin-wise parameters (uncorrelated shape)

$$\nu_{scb}(\gamma_b) = \gamma_b \nu_{scb}^0. \quad (1.4.17)$$

These are useful for example to include the Monte Karlo uncertainties or a per bin data-driven background estimate. This type without a constraint term has to be used with care as if there is only one sample or channel, the fit would always match the data perfectly, which of course is not of much use.

Further there are bin-independent (shape factors) nuisance parameters  $\alpha$  that enter the modeling through an interpolation function  $\eta$  instead of being the factor itself. There is the multiplicative version

$$\nu_{scb}(\alpha) = \eta(\alpha) \nu_{scb}^0, \quad (1.4.18)$$

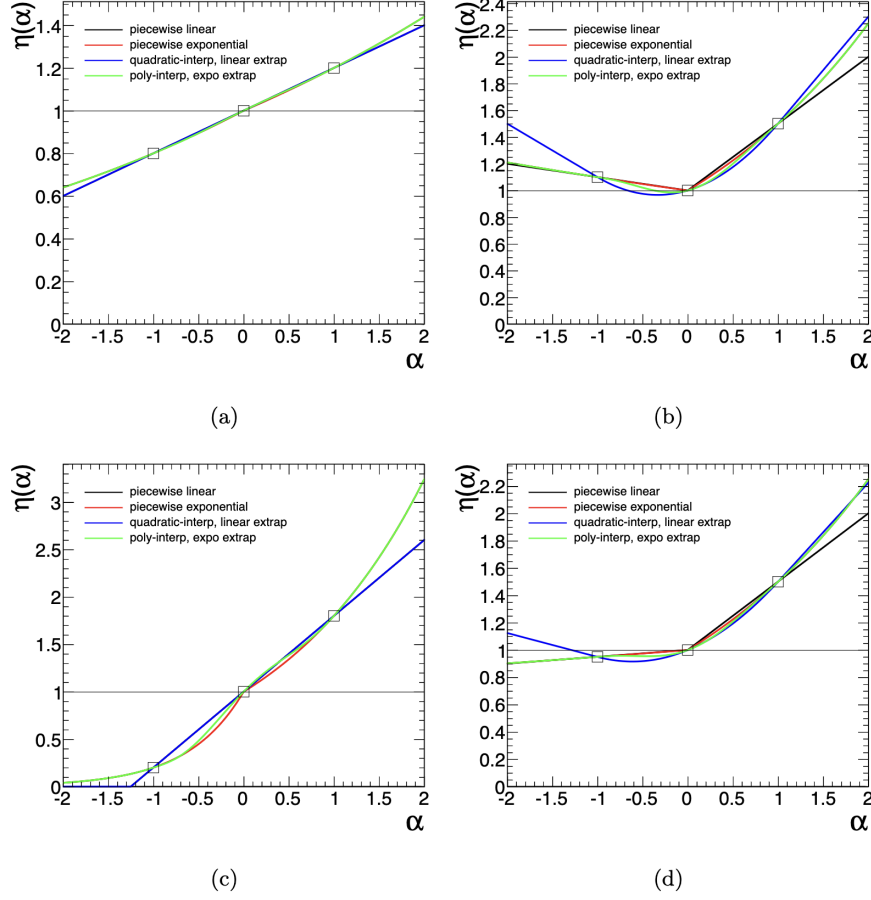
and the additive version

$$\nu_{scb}(\alpha) = \nu_{scb}^0 + \eta(\alpha), \quad (1.4.19)$$

with some constraint term  $c_\alpha(\alpha)$ . This is useful if systematic uncertainties are to be included. In an ATLAS analysis typically this is done by plugging in the upper ('1up') and lower ('1down') standard deviation values (pretending they were the nominal values entering the calculation) and observe the impact it has on a final quantity. The interpolation function transports this knowledge into the likelihood model, by scaling the nominal value  $\nu_{scb}^0$  and at the same time applying a penalization  $c_\alpha$  according to our modeling of the errors. The following illustrates this.

In HistFactory there exists four of such interpolation functions. For those exist an identity operator

$$\eta_0 = \eta(\alpha = 0) = \begin{cases} 1, & \text{multiplicative modifier, } (\kappa) \\ 0, & \text{additive modifier, } (\lambda). \end{cases} \quad (1.4.20)$$



**Figure 1.3:** The four Interpolation functions  $\eta(\alpha)$  for different up and down standard deviation values. For example in (a) the bin height will be scaled with a factor of 0.8 for an  $\alpha = -1$  (1.2 for an  $\alpha = 1$ ). From [9].

One of these interpolation function that scales the bin height linear over the known deviations  $\eta_{-1} = \nu_{scb}^{\text{down}}$  and  $\eta_1 = \nu_{scb}^{\text{up}}$  is

$$\eta_{\text{linear}}(\alpha) = \begin{cases} \alpha(\eta_0 - \eta_1), & \alpha > 0 \\ \alpha(\eta_0 - \eta_{-1}), & \alpha < 0 \end{cases} \quad (1.4.21)$$

An illustration of this can be found in fig. 1.3(a). For the other ones the reader is referred to e.g. [11]. Remember  $\alpha$  is the nuisance parameter and not the function  $\eta(\alpha)$  and there is an associated constraint term  $c_\alpha$  to each  $\alpha$  that uses

**Table 1.1:** Modifiers and constraint terms used in HistFactory implemented by pyhf. Note that the interpolation functions are called  $f_p$  and  $g_p$  here instead of  $\eta$  as chosen in the full text. From [5]

Description	Modification	Constraint Term $c_\chi$	$c_\chi$ input
Uncorrelated Shape	$\kappa_{scb}(\gamma_b) = \gamma_b$	$\prod_b \text{Pois}(r_b = \sigma_b^{-2}   \rho_b = \sigma_b^{-2} \gamma_b)$	$\sigma_b$
Correlated Shape	$\Delta_{scb}(\alpha) = f_p(\alpha   \Delta_{scb, \alpha=-1}, \Delta_{scb, \alpha=1})$	$\text{Gaus}(a = 0   \alpha, \sigma = 1)$	$\Delta_{scb, \alpha=\pm 1}$
Normalisation Unc.	$\kappa_{scb}(\alpha) = g_p(\alpha   \kappa_{scb, \alpha=-1}, \kappa_{scb, \alpha=1})$	$\text{Gaus}(a = 0   \alpha, \sigma = 1)$	$\kappa_{scb, \alpha=\pm 1}$
MC Stat. Uncertainty	$\kappa_{scb}(\gamma_b) = \gamma_b$	$\prod_b \text{Gaus}(a_{\gamma_b} = 1   \gamma_b, \delta_b)$	$\delta_b^2 = \sum_s \delta_{sb}^2$
Luminosity	$\kappa_{scb}(\lambda) = \lambda$	$\text{Gaus}(l = \lambda_0   \lambda, \sigma_\lambda)$	$\lambda_0, \sigma_\lambda$
Normalisation	$\kappa_{scb}(\mu_b) = \mu_b$		
Data-driven Shape	$\kappa_{scb}(\gamma_b) = \gamma_b$		

Gaussian and Poissonian modeling. The standard normal Gaussian implementation is straightforward as the nuisance parameter is scaled to the standard deviation values as described before  $\text{Gauss} = (\alpha | a, \sigma = 1)$ .

For a poissonian constraint to a multiplicative factor  $\gamma_b$ , with a nominal (most probable) value  $\gamma_0 = 1$ , we must scale the Poisson distribution with a factor  $f$  so it reflects the original bin-height uncertainty  $\sigma$ . We basically need to multiply all parameters of the Poisson distribution with a factor  $f$  and then solve for the one with the desired uncertainty. Since the Variance of a Poissonian like eq. 1.4.3 is just the rate parameter  $\lambda$  it follows

$$\text{Var}(\text{Pois}(k = f\gamma_0, \lambda = f\gamma)) = \lambda \stackrel{\gamma=\gamma_0}{=} f\gamma_0 = (f\sigma)^2 \quad \rightarrow \quad f = (1/\sigma^2). \quad (1.4.22)$$

This completes all the requirements needed for the creating of histfactory models which are summarized in table 1.1.





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