Upper limit for High mass X→WW search

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Abstract

1 Introduction

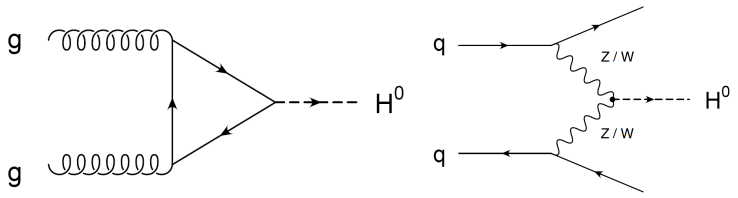
In this report we will study the statistical approach to the upper limit computation for a high energy physics search for a new particle. We will use data from the 2015 run of the CMS experiment at the LHC and the corresponding Monte Carlo (MC) simulations.

We will search for a new signal in the $WW \to 2l2\nu$ final state. This channel is also a decay channel for the Standard Model Higgs boson (H). We will however search for an additional particle, named X in the following, that is supposed to be heavier than H. We will scan a wide range of masses for X and, if we do not find a compelling evidence for a signal, we will set an upper limit on the cross section of X.

2 The physics case

In this experience we will search for the existence of a new hypothetical high mass particle, named X. **We expect this particle to be a heavy variant of the Standard Model Higgs boson**. For this reason we hypothesize that X shares with H the production mechanism. This is a reasonable assumption that is verified in several new physics models. In particular we assumes that X can be produced via two main production mechanisms, called gluon fusion (ggF) and vector boson fusion (VBF), represented by the diagrams in Fig. 1.

The details and precise meaning of the Feynman dagrams of Fig. 1 are not relevant for this exercise, the relevant piece of information is that two



(a) ggF (b) VBF

Figure 1: Feynmann diagrams of the two main production mechanisms for X.

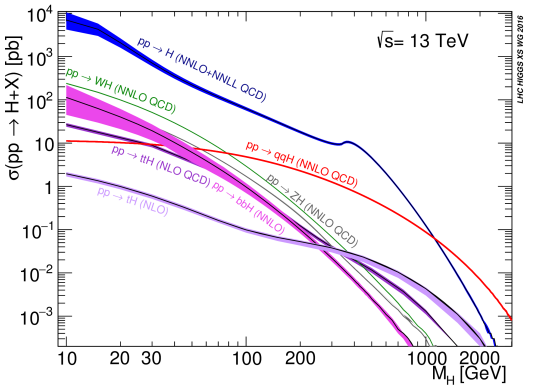


Figure 2: Standard model Higgs boson cross section as a function of the mass of the Higgs boson. The ggF mechanisms is labeled $pp \to H$, the VBF mechanism is labeled $pp \to qqH$. Also other, sub-leading mechanisms are reported, which we will neglect.

mechanisms are available and that they are marked by a substantial difference: **the ggF shows no other particles in the final state beyond X, the VBF has two quarks in addition to the X in the final state**. Although it should be noted that a precise calculation shows that additianal particles in the form of hadronic jets can also arise in ggF, it remains true that events arising from the two mechanisms are different when it comes to the number of jets produced in addition to the X particle.

The production cross section for the Higgs boson as a function of its mass is reported in Fig. 2. Although we now know the mass of the Higgs boson to be 125 GeV, this plot is useful because it can be used as a model for the expected cross section for X.

We will assume that the cross section σ for each of the production channels of X scales with a common factor μ of the corresponding Higgs boson cross section:

$$\sigma_{X[ggF,VBF]}(M) = \mu(M)\sigma_{H[ggF,VBF]}(M) \tag{1}$$

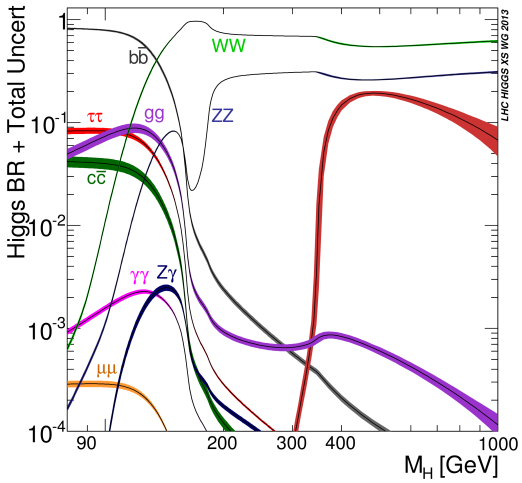


Figure 3: Standard model Higgs boson cross section as a function of the mass of the Higgs boson. The ggF mechanisms is labeled $pp \to H$, the VBF mechanism is labeled $pp \to qqH$. Also other, sub-leading mechanisms are reported, but we will neglect them.

where M is the mass of X, and obvious meaning of the other symbols. This is a reasonable assumption, verified by several new physics models. We notice that **the relative importance of the VBF mechansm grows with the X mass**, and becomes dominant above ∼1.5 TeV.

We will assume that, like H, also X has several decay channels. We assume that X has the same branching ratios of H, which are summarized in Fig. 3. It should be noted that **the WW decay channel is the one with the highest branching ratio**.

3 Data sample and analysis strategy

Owing to the large branching fraction in the WW final state we choose this channel for our search. In other words we search for the decay X→WW. The W bosons are themselves unstable. 30% of the times a W boson decays to a charged lepton (electron, muon, tauon) and a neutrino (10 % for each of the three lepton species). The remaining 70% of the times the W boson decays to a pair of hadrons. In this exercise we will concentrate on the leptonic decays of the W bosons. The reason of this choice will become clearer when we discuss backgrounds, but let us mention already that requiring leptons in the final state allows a dramatic reduction of background processes. To summarise, **we search for the H→WW→ $2l2\nu$ decay chain**.

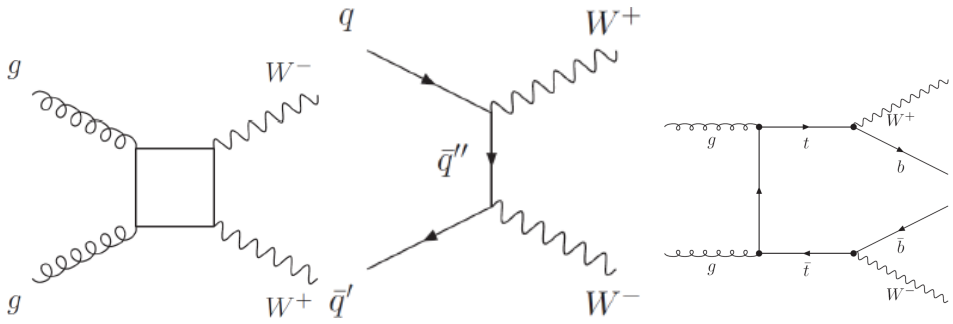


Figure 4: Gluon initiated (a) and quark initiated (b) WW. Top pair production (c).

We will use data collected by the CMS experiment in the 2015 data taking at the LHC. These data correspond to an integrated luminosity of 2.3 fb^{-1}. We will base our analysis on data reconstructed with the official CMS software and Simulations for both the signal and the background processes. These data come in the form of ROOT trees.

For each event the tree stores several event variables, in particular:

- reconstructed leptons kinematic variables;
- the reconstructed missing transverse energy;
- the reconstructed jet kinematic variables.
- several weights, used both to improve the Data/Simulation agreement and to normalize the simulation to the data luminosity.

3.1 Main backgrounds

A background process in a high energy physics analysis is a physics process that yields a final state that resembles that of the signal. In the case of this analysis there are two main background processes:

- production of two W bosons without an intermediate X;
- production of a pair of top quarks, $t\bar{t}$. The top quark decays to a b quark and a W boson.

The Feynman diagrams of these two processes are reported in Fig. 4 for the interested reader.

We apply a series of cuts to reduce their contribution as much as possible. $t\bar{t}$ is reduced by requiring that jets in the event are not compatible with being

originated from b quarks, using dedicated jet-tagging techniques. WW is reduced with kinematic cuts on the leptons.

Other subleading sources of background originate from processes in which at least one of the leptons is not a real lepton, but is identified as such by the reconstruction algorithms. The control of these backgrounds is a crucial part of the analysis, but is beyond the scope of this exercise. The cuts to be applied will be provided by the teachers.

3.2 Main discriminating variable

After the selection cuts mentioned above we end up with a sample that is primarily composed of WW and $t\bar{t}$. In order to further discriminate a possible signal we use a kinematic variable called $m_{T,i}$. This variable is the invariant mass of the 4-momentum resulting from the sum of the two lepton 4-momenta and the MET 4-momentum. Since we are unable to reconstruct the longitudinal component of the neutrinos momenta, this variable is the closest approximation of the resonance invariant mass that we can reconstruct in a signal event, and it retains a significant discriminating power with respect to backgrounds.

The distribution of $m_{T,i}$ is shown in Fig. 5 after the selection cuts. The data point are show on top of the stack of the backgrounds. The shape of a signal for X mass of 1 TeV is also shown (multiplied by 10). The rightmost bin of each distribution is an overflow bin. The fact that the signal shape does not peak at 1 TeV is due to $m_{T,i}$ lacking the contribution from the longitudinal momenta of neutrinos.

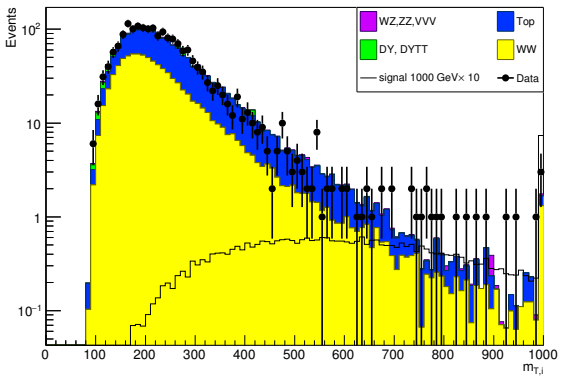


Figure 5: $m_{T,i}$ in data and simulation for 2015 data after selection cuts.

Exercise 1:

Write a code that builds the stack of backgrounds to obtain a plot similar to Fig. 5.

A set of root files is provided, together with a root macro (`HWWYields.C`) implementing selection cuts.

Each root file contains a root tree named `latino`. This tree holds several variables, including $m_{T,i}$ in a branch called `mTi`.

Eight data files are provided, corresponding to two distinct data taking periods (called `Run2015C` and `Run2015D`) and four triggers. Data from CMS are in fact divided into different streams depending on the triggers each event fires. In this analysis we use events with at least two electrons (`DoubleEG`), at least two muons (`DoubleMu`), at least an electron and a muon (`MuonEG`) or at least a muon (`SingleMuon`). The latter is used only to recover an inefficiency in the other triggers.

Simulated events (MC) are produced for several physics processes, including $t\bar{t}$, WW, Z$\to \tau\tau$, and other subleading processes. Simulated samples for different mass hypotheses for X are also provided. For each mass hypothesis two different files are provided, one containing the simulation of the ggF production mechanism and the other containing the simulation for the VBF production mechanism.

Simulated events are weighted with several weights that are aimed at bringing data and MC in close agreement. We will not discuss these weight in detail. We will just discuss an important weight contained in the branch named `baseW`. This variable is used to equalize the luminosity of all samples to 1/fb.

Running `HWWYields.C` results in a root file (`yields.root`) containing one histogram for each background, one for each signal and one for the data. The variable plotted and the binning are controlled in the first few lines of `HWWYields.C`.

Please write a root macro that builds a stack of all the backgrounds, superimposes the data and one signal for reference.

3.3 Cut based analysis

In order to check whether the data are consistent with the signal+background hypothesis or with the background only hypothesis, we can proceed to counting events passing our selection. Let N_{obs} be the data events after the selection, ν_b be the expected number of background evens and ν_s be the expected number of signal events for an X signal with mass M. We expect N_{obs} to follow the Poisson statistics with an average of $\nu_b+\nu_s$ in the signal+background

hypothesis and ν_b in the background only hypothesis.

The best estimate that we can give of the number of signal events, based on a single experiment, is

$$\hat{\nu}_s = N_{obs} - \nu_b \tag{2}$$

where the dependency on the mass hypothesis is there to remind us that the analysis cuts can be different depending on the mass of the signal we search for.

In order to understand whether the obtained value of $\hat{\nu}_s$ is significantly different from 0 we should compare it with the statistical fluctuation of the expected background. Only if $\hat{\nu}_s$ is larger than several standard deviations (5) of the expected background we can claim a discovery.

Following this discussion we are left with an open question: should we ad any other selection cuts to our selection to improve the analysis sensitivity to a signal?

Exercise 2

For each X mass hypothesis find the cut on $m_{T,i}$ which maximises the sensitivity

Fig. 5 shows that $m_{T,i}$ has a good discriminating power. In particular if we only count events above a certain optimal value of $m_{T,i}$ we should be able to improve the sensitivity to a signal.

The student should find, for each X mass hypothesis, the value of $m_{T,i}$ ($m_{T,i}^{cut}$) such that by integrating events with $m_{T,i} > m_{T,i}^{cut}$ the ratio of expected number of signal events ν_s and the statistical fluctuation of background events $\sqrt{\nu_b}$ ($\nu_s/\sqrt{\nu_b}$) is maximised.

4 Upper limit with approximate formulae

Upon completion of Exercise 2 the student has found the optimal value in $m_{T,i}$ where one should cup in order to find a possible signal. The optimal position of the cut depends on the mass of the hypothesized signal.

We now aim at finding the upper limit for each mass hypothesis. We refer to Cowan's book equation 9.39. The upper limit at 95% confidence level on the number of signal events (ν_{up}) can be found as:

$$\nu_{up} = \hat{\nu}_s + \delta_{\hat{\nu}_s} \cdot \Phi^{-1}(0.95) \tag{3}$$

where $\hat{\nu}_s$ is given by Eq. 2, $\delta_{\hat{\nu}_s}$ is the error on $\hat{\nu}_s$, Φ^{-1} is the inverse cumulative distribution of the Gaussian.

Eq. 3 **holds under the assumption that the distribution of $\hat{\nu}_s$ is Gaussian**. However $\hat{\nu}_s$, as defined in Eg. 2 comes as the difference between a random variable distributed according to Poisson distribution (N_{obs}) and a number. The assumption that $\hat{\nu}_s$ is Gaussian is only valid in case N_{obs} has a relatively large expectation value, so that the difference between Poisson and Gaussian distribution can be neglected.

How do we estimate $\delta_{\hat{\nu}_s}$? If we know the number of expected background events with no error, then $\delta_{\hat{\nu}_s} = \sqrt{N_{obs}}$, following Poisson statistics.

However we usually have an uncertainty on the estimation of the number of background events δ_{ν_b}. This kind of uncertainty is systematic, contrary to the uncertainty on N_{obs}, which is statistical instead. It is not obvious how to combine the two uncertainties into $\delta_{\hat{\nu}_s}$.

In the following we will make a common choice, which consists in combining the two uncertainties as one would do if they were both statistical. It then follows that

$$\delta_{\hat{\nu}_s} = \sqrt{N_{obs} + \delta^2_{\nu_b}}. \tag{4}$$

Let us discuss in some more detail the meaning of our choice of summing in quadrature the genuinely statistical uncertainty on N_{obs} and the systematic uncertainty δ_{ν_b}. By doing this we are effectively expressing our degree of belief in our estimate of the background in the form of a Gaussian with average ν_b and standard deviation δ_{ν_b}. Indeed, if you assume that the true value of the expected number of background events is distributed as a Gaussian of standard deviation δ_{ν_b} around the average ν_b, then the variance of $\hat{\nu}_s$ is indeed given by Eq. 4.

In other words we are weighting the probability that we are wrong about our estimate of the number of background events in a Gaussian way with respect to our best estimate δ_{ν_b}. It should be somewhat clear from the choice of words in the two past sentences that we are to some extent entering the realm of Bayesian probability, in that we are using a PDF, a Gaussian in this case, to measure how sure we are of our background estimate.

It should be clear that using a Gaussian to describe our degree of belief in the background estimate, as an effective way of modeling the systematic uncertainties is not the only option. Other systematic uncertainties may be better modeled by different PDFs, such as Uniform, of lognormal. It is in general a good practice (although not always done in practice) to test the robustness of a result against the (somewhat arbitrary) choice of the PDF that models the systematic uncertainties.

Exercise 3

Derive an upper limit on the signal strength μ using Eq. 3

Using the signal and background yields obtained from the mass dependent cuts of Exercise 2, the student should plot the expected and observed limit.

The systematic uncertainty on the background should be taken to be a (reasonable) 10% of ν_b.

The **expected limit is the limit you expect to put in the background only hypothesis**. It can be derived very simply by assuming $\hat{\nu}_s$=0. This however does not give you any sense of how the statistical fluctuations in the number of observed events may affect the limit.

In order to have such an idea the student should make several "toy" experiment, i.e. they should simulate what the result of an experiment could be in a background only hypothesis. In our simple case this boils down to throwing several random numbers according to the Poisson distribution around ν_b. Each random extraction i would yield a number N^i_{obs}. For each N^i_{obs} the student should compute the upper limit according to Eq. 3. The expected limit can be extracted by taking the median of the limits obtained in all the toy extractions. Similarly a 1 and 2 sigma band can be extracted by taking the 2.5% percentile (2σ down), 34% (1σ down), 84% (1σ up), 97.5% (2σ up) of the distribution of expected limits from toys for each mass.

The observed limit is the limit obtained from data, using N_{obs} from data. The student should finally obtain a plot similar to the one shown in Fig. 6.

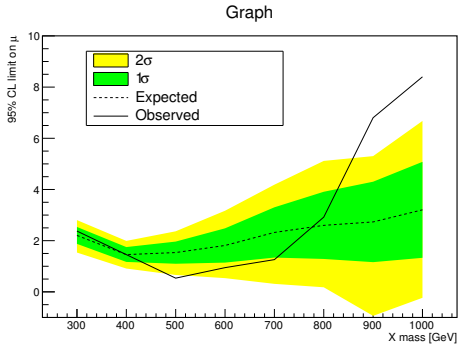


Figure 6: Expected and observed limit. The result of Exercise 3 should be something of this form.

5 Maximum likelihood estimator of the signal strength

In this paragraph we will introduce the maximum likelihood fit as a way to estimate the signal strength in the presence of systematic uncertainties. We spell out since the beginning that the systematic uncertainties will be included in the fitting procedure in the form of parameters for which an external constraint is imposed in the fit. Parameters in a maximum likelihood fit which represent systematic uncertainties are called **nuisance parameters**, to distinguish them from the parameters for which we do not put external constraints, such as the signal strength (μ) in our case, which are known as **parameters of interest (POI)**.

Let us assume that the random variable that we measure in our experiment is N_{obs}. We expect it to be Poisson-like distributed around $\nu_b + \mu \cdot \nu_s$, where ν_s is the number of signal events we expect for the signal, if X is actually the SM H (remember Eq. 1). In this case the likelihood function $\mathcal{L}(\mu)$ is simply:

$$\mathcal{L}(\mu) = \frac{(\nu_b + \mu \cdot \nu_s)^{N_{obs}}}{N_{obs}!} e^{-(\nu_b + \mu \cdot \nu_s)} \tag{5}$$

Maximizing $\mathcal{L}(\mu)$ with respect to μ gives the best fit value for μ, $\hat{\mu}$. The result is the already known result of Eq 2, which we can express in terms of μ as

$$\hat{\mu} = \frac{N_{obs} - \nu_b}{\nu_s}. \tag{6}$$

We can introduce our degree of belief in the knowledge of the background distribution in the form of a nuisance parameter with an external constraint in the likelihood $\mathcal{L}(\mu)$. Let us for example assume that we know the normalization of the background with a relative uncertainty δ_{ν_b}/ν_b, and let us introduce the nuisance parameter μ_b, which is a multiplier of ν_b in much the same way as μ is multiplier for the number of expected signal events.

In order to add a constraint on μ_b in the likelihood we simply have to multiply the likelihood of Eq. 5 by a Gaussian constraint on μ_b with standard deviation δ_{ν_b}/ν_b. The new likelihood function is now function of both μ (the POI) and μ_b (a nuisance parameter), and reads:

$$\mathcal{L}(\mu; \mu_b) = \frac{1}{2\pi \frac{\delta_{\nu_b}}{\nu_b}} e^{-\frac{(\mu_b - 1)^2}{2(\frac{\delta_{\nu_b}}{\nu_b})^2}} \times \frac{(\mu_b \cdot \nu_b + \mu \cdot \nu_s)^{N_{obs}}}{N_{obs}!} e^{-(\mu_b \cdot \nu_b + \mu \cdot \nu_s)}, \tag{7}$$

where the initial part before the $\times$ symbol is the Gaussian constraint on μ_b.

The reader might be surprised by the fact that by maximizing Eq. 7 we are effectively fitting two parameters (the POI μ and the nuisance μ_b) with a single measurement (N_{obs}). One should remember, however, that the second constraint effectively comes from the assumed shape of the distribution of the nuisance parameter, a Gaussian in this case.

The likelihood function of Eq. 7 can be easily extended to the case in which our measurement consists of a vector of n random variables $\vec{N}_{obs} = (N^1_{obs}...N^n_{obs})$. We would like to draw the reader's attention on the fact that this is exactly the case we have when we measure number of events in a binned histograms with n bins, such as in Fig. 5. To extend Eq. 7 to handle this case, one simply needs to introduce a product of Poisson distributions, one for each of the n bin.

Similarly Eq. 7 can be easily extended to the case in which we have more nuisances. For example, our background could be (and most likely will be) composed by several contributions (e.g. one for each different background process), each with their own normalization uncertainty. In this case one simply add each nuisance as a multiplicative constraint in the likelihood. Also, the functional form of each constraint could be different for the different constraints.

Although the formalism introduced in this paragraph might sound like an overkill for a simple measurement counting experiment such as the one we are considering in this experiment, this formalism allows for handling of arbitrary number of bins and arbitrary number of nuisances. Consider for example that the H$\rightarrow$ WW analysis in CMS has around 100 bins, a variable number of POIs, ranging from 1 to 10 depending on the particular quantity that is measured, and several tens of nuisance parameters.

6 The profile log likelihood ratio (LLR) statistics

When making minimizations or maximizations, derivatives are involved. The derivative of a product (Eq. 7) can be cumbersome to compute. We notice that any monotonic function of Eq. 7 would show minima and maxima in the same spots of the dependand variables as Eq. 7. We then can choose to use the negative logarithm of the likelihood function (negative log-likelihood, NLL). The logarithm turns the product into a sum (easier to derive), and the negative sign in front allows us to search for minima instead of maxima (for some reason physicists prefer minima over maxima). We then introduce

$L(\mu;\mu_b)$ as:

$$L(\mu;\mu_b) = -\ln(\mathcal{L}(\mu;\mu_b)). \tag{8}$$

We use a single POI and a single nuisance in Eq. 8 just for simplicity. The generalization to multiple POIs and nuisances is straightforward.

Based on $L(\mu;\mu_b)$ we can construct a **test statistic** (i.e. a function of the stocastic variables we measure) $\lambda(\mu)$, called log-likelihood ratio (LLR) as forllows:

$$\lambda_\mu(N_{obs}) = \frac{\mathcal{L}(\mu;\hat{\hat{\mu}}_b)}{\mathcal{L}(\hat{\mu};\hat{\mu}_b)}. \tag{9}$$

Some explanation on the symbols is required: $\hat{\mu}$ **is the best fit of the signal strength** μ, our POI. Similarly, $\hat{\mu}_b$ **is the best fit of the nuisance** μ_b. In other words, given our measurement of N_{obs}, the ($\hat{\mu}$,$\hat{\mu}_b$) pair is the minimum of the NLL function 8, or, equivalently, the maximum of the likelihood 7. Suppose now that we choose a particular value of the POI, a value of our choice and we call it μ: then $\hat{\hat{\mu}}_b$ **is the value of the nuisance** μ_b **which minimizes the NLL function 8 for our chosen value of** μ.

The reason why we go through the burden of constructing $\lambda_\mu(N_{obs})$ is simply that, by the Neyman-Pearson lemma, this test statistics gives the best power to discriminate the background only and the signal + background hypotheses.

Let us now see how we can use the LLR, or small modifications of it, for the task of either measuring the significance of a possible signal, or setting an upper limit.

6.1 LLR for significance estimation

We can use a test statistic that is based on the LLR to test the significance of a $\hat{\mu} > 0$ result from the best fit of our data. The test statistics that we are going to use is q_0 defined as follows:

$$q_0 = \begin{cases} -2\ln\lambda_0(N_{obs}) & \hat{\mu} \geq 0 \\ 0 & \hat{\mu} < 0 \end{cases} \tag{10}$$

What does this mean in practice? First of all, we are testing against the background only hypothesis, so we use the LLR for the case $\mu = 0$, $\lambda_0(N_{obs})$ (as we were mentioning before, we can compute the LLR for any choice of μ). Then, since we regard only upward fluctuations of the data as possible signals, we distinguish the cases in which the best fit value for the signal strength $\hat{\mu}$ is larger (possible signal) or smaller (background underfluctuation) than 0. Finally, why the logarithm, the 2 and the minus sign. The logarithm and

the minus sign have the purpose of simplifying the computation and turning a search for maxima into a search for minima, similarly to Eq. 8. This, together with the factor 2 allows for nice "asymptotic" properties of q_0. In particular, for large samples, the distribution of q_0 is Gaussian, with average 0 and standard deviation 1.

This means that, given the value of q_0 for our dataset, one can simply compute the p-value as:

$$p = 1 - \Phi(\sqrt{q_0}), \tag{11}$$

where Φ is the cumulative distribution of a Gaussian with average 0 and standard deviation 1. Similarly the "number of sigmas" of the signal is

$$Z = \sqrt{q_0} \tag{12}$$

6.2 Setting up a model in RooFit

Based on out previous discussion, it is clear that the first step to use the LLR as a means to measure the significance of a signal is to setup a maximum likelihood fit of the POI with constraints on the nuisances.

Stated differently, we want to setup a parametric model which describes our data. The parameters of the model will be the POI and the nuisances. This can be achieved in a relatively easy way in `RooFit`. In order to make the code more generic, we will drop the simplification of the single counting analysis, and we will assume that our measurement consists of a set of event counts, $\vec{N}_{obs} = (N^1_{obs}...N^n_{obs})$, which is represented practically by a histogram, a `TH1` in `ROOT` language. Of course, the simple counting experiment can be simply modeled in this framework as a single-bin histogram.

The following is a guide describing the `RooFit` code used to implement the ML fit we are interested in. The code implementing the fit is in the `HWWWorkspace.C` file.

Let us call `h_data` a histogram of event counts in a certain variable ($m_{T,i}$ for example) after selection. Our task is to write a parametric model that describes that histogram as the sum of different signal and background components.

For the signal and each background we are able to derive from simulation the expected shape and normalization in the relevant variable in the form of a histogram. We can thus derive from simulation the `TH1s` represented by the following variables: `ww`, `top`, `dytt`, `vv`, `sig`. The variable names correspond to the process that is represented by each variable.

From each of those variable we derive a binned PDF (represented by instances of class `RooHistPdf`). The variable names of these PDFs in `HWWWorkspace.C`

are: pdf_ww, pdf_top, pdf_dytt, pdf_vv, pdf_s, again with hopefully obvious meaning of the names.

We also single out variables (instances of class RooRealVar) representing the normalization of each process (nu_ww, nu_top, nu_dytt, nu_vv, nu_s). Also, and most importantly, we introduce instances of class RooRealVar to describe the POI (mu) and a nuisance representing a multiplier for each background process (mu_ww, mu_top, mu_dytt, mu_vv). We describe introduce formulas for the normalization of each signal and background, so that, for example, the normalization of the WW background is represented by variable norm_ww which is the product mu_ww*nu_ww. Similarly for the signal and the other backgrounds.

Finally, the model that we will use to fit the data is represented by the variable model (an instance of class RooAddPdf), which effectively represents the expression:

model=norm_s*pdf_s+ norm_ww*pdf_ww+ norm_top*pdf_top+ norm_dytt*pdf_dytt+ norm_vv*pdf_vv.

In the file HWWWorkspace.C we also prepare the nuiscne constraints, to be used later. These have the form of Gaussian distribution of the mu_ parameters.

Everything is saved in an instance of RooWorkspace and returned to the calling code, for later use.

Exercise 4

Observed significance with LLR

6.3 LLR for upper limit

Exercise 5

Upper limit with LLR