Practical Statistics for HEP



Model the distribution of observables ★ in terms of

- Physical parameters of interest p
- Other parameters of to describe detector effects (resolution, efficiency,...)



Probability density function F(x;p,q)

 normalized over allowed range of the observables x w.r.t the parameters p and q

RooFit_Basics

October 26, 2017

1 Introduction

If you want to follow this notebook you need to install ...

- ROOT (at least v6-06-06): https://root.cern.ch/building-root
- Jupyter: http://jupyter.readthedocs.io/en/latest/install.html

Alternatively, you can grab a VM Ubuntu with the above already installed from here (the admin pword is "stats"): https://cernbox.cern.ch/index.php/s/dIm4WLZU3jyjL4x

You can get this notebook from GitHub: https://github.com/nucleosynthesis/RooFitBasics

Open any notebook by typing in a terminal root --notebook

2 RooFit

RooFit is a OO analysis environment built on ROOT. It is essentially a collection of classes designed to augment root for data modeling whose aim is summarised below (shamelessly stolen from Wouter Verkerke)...

We will cover a few of the basics in the session today but note there are many more tutorials available at this link: https://root.cern.ch/root/html600/tutorials/roofit/index.html

2.1 RooFit objects

In Roofit, any variable, data point, function, PDF ... is represented by a c++ object

The most basic of these is the RooRealVar. Let's create one which will represent the mass of some hypothetical particle, we name it and give it an initial starting value and range.

RooRealVar::MH = 125 L(120 - 130)

ok, great. This variable is now an object we can play around with. We can access this object and modify it's properties, such as its value.

In particle detectors we typically don't observe this particle mass but usually define some observable which is *sensitive* to this mass. Lets assume we can detect and reconstruct the decay products of the H-boson and measure the invariant mass of those particles. We need to make another variable which represents that invariant mass

In the perfect world we would perfectly measure the exact mass of the particle in every single event. However, our detectors are usually far from perfect so there will be some resolution effect. Lets assume the resolution of our measurement of the invariant mass is 10 GeV and call it "sigma"

More exotic variables can be constructed out of these RooRealVars using RooFormulaVars. For example, suppose we wanted to make a function out of the variables which represented the relative resolution as a function of the hypothetical mass MH.

```
In [5]: RooFormulaVar func("R","@0/@1",RooArgList(sigma,mass));
    func.Print("v");

--- RooAbsArg ---
Value State: DIRTY
Shape State: DIRTY
Attributes:
Address: 0x11de8d000
Clients:
Servers:
    (0x11de8c860,V-) RooRealVar::resolution "#sigma"
    (0x11de8c368,V-) RooRealVar::m "m (GeV)"
Proxies:
    actualVars ->
    1) resolution
```

```
2) m
--- RooAbsReal ---
Plot label is "R"
--- RooFormula ---
Formula: "@0/@1"
(resolution,m)
```

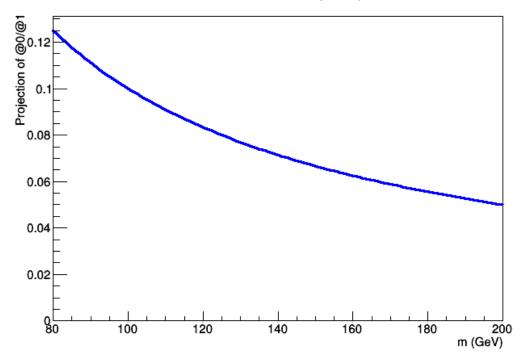
Notice how there is a list of the variables we passed (the servers or "actual vars"). We can now plot the function. RooFit has a special plotting object RooPlot which keeps track of the objects (and their normalisations) which we want to draw. Since RooFit doesn't know the difference between which objects are/aren't dependant, we need to tell it.

Right now, we have the relative resolution as $R(m, \sigma)$ whereas we want to plot $R_{\sigma}(m)$.

```
In [6]: TCanvas *can = new TCanvas();
    //make the x-axis the "mass"
    RooPlot *plot = mass.frame();
    func.plotOn(plot);

plot->Draw();
can->Draw();
```

A RooPlot of "m (GeV)"



The main objects we are interested in using from RooFit are "probability denisty functions" or (PDFs). We can construct the PDF

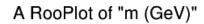
$$f(m|M_H,\sigma)$$

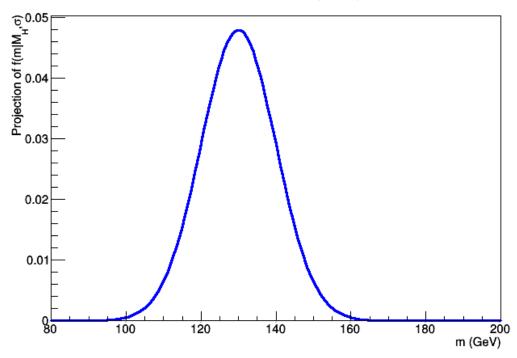
as a simple Gaussian shape for example or a RooGaussian in RooFit language (think McDonald's logic, everything is a RooSomethingOrOther)

```
In [7]: RooGaussian gauss("gauss","f(m|M_{H}, #sigma)", mass, MH, sigma);
        gauss.Print("V");
--- RooAbsArg ---
 Value State: DIRTY
  Shape State: DIRTY
 Attributes:
 Address: 0x11de8e360
  Clients:
 Servers:
    (0x11de8c368,V-) RooRealVar::m "m (GeV)"
    (0x11cf44c10,V-) RooRealVar::MH "mass of the Hypothetical Boson (H-boson) in GeV"
    (0x11de8c860, V-) RooRealVar::resolution "#sigma"
 Proxies:
    x \rightarrow m
    mean -> MH
    sigma -> resolution
--- RooAbsReal ---
 Plot label is "gauss"
--- RooAbsPdf ---
Cached value = 0
```

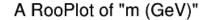
Notice how the gaussian PDF, like the RooFormulaVar depends on our RooRealVar objects, these are its servers. Its evaluation will depend on their values.

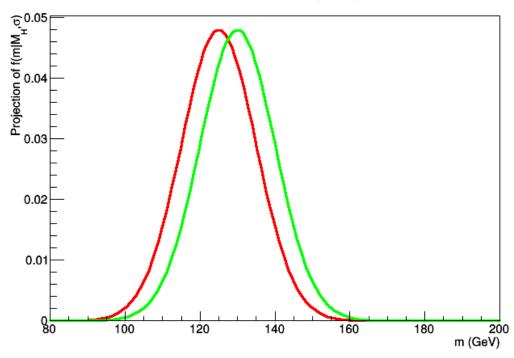
The main difference between PDFs and Functions in RooFit is that PDFs are automatically normalised to unitiy, hence they represent a probability density, you don't need to normalise yourself. Lets plot it for the current values of m and σ





If we change the value of MH, the PDF gets updated at the same time.

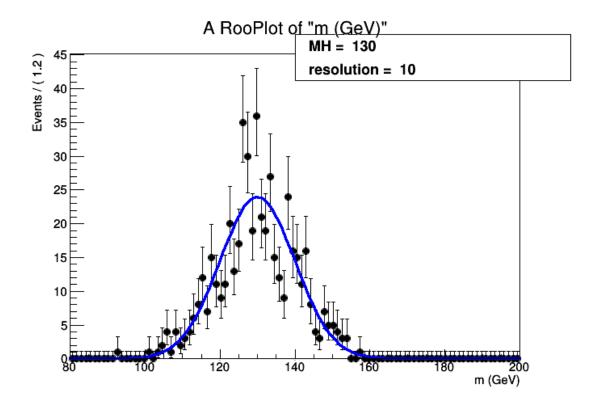




PDFs can be used to generate Monte Carlo data. One of the benefits of RooFit is that to do so only uses a single line of code!

As before, we have to tell RooFit which variables to generate in (e.g which are the observables for an experiment). In this case, each of our events will be a single value of "mass" m.

Now we can plot the data as with other RooFit objects.



Of course we're not in the business of generating MC events, but collecting real data!. Next we will look at using real data in RooFit...

2.2 RooFit datasets

A dataset is essentially just a collection of points in N-dimensional (N-observables) space. There are two basic implementations in RooFit,

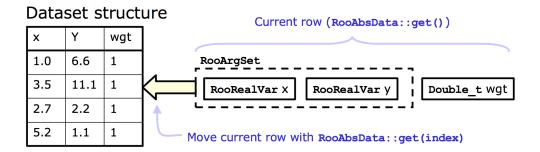
- 1) an "unbinned" dataset RooDataSet
- 2) a "binned" dataset RooDataHist

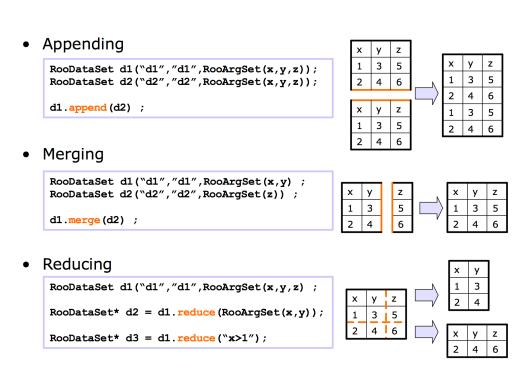
both of these use the same basic structure as below

Lets create an empty dataset where the only observable, the mass. Points can be added to the dataset one by one ...

```
In [12]: RooDataSet mydata("dummy", "My dummy dataset", RooArgSet(mass));
    // We've made a dataset with one observable (mass)

mass.setVal(123.4);
mydata.add(RooArgSet(mass));
mass.setVal(145.2);
mydata.add(RooArgSet(mass));
mass.setVal(170.8);
mydata.add(RooArgSet(mass));
```





```
mydata.Print();
RooDataSet::dummy[m] = 3 entries
```

There are also other ways to manipulate datasets in this way as shown in the diagram below Luckily there are also Constructors for a RooDataSet from a TTree and for a RooDataHist from a TH1 so its simple to convert from your usual ROOT objects.

Let's take an example dataset put together already.

```
KEY: RooWorkspace workspace;1 Tutorial Workspace
KEY: TProcessID ProcessID0;1 48737500-e7e5-11e6-be6f-0d0011acbeef
```

Inside the file, there is something called a RooWorkspace. This is just the RooFit way of keeping a persistent link between the objects for a model. It is a very useful way to share data and PDFs/functions etc among CMS collaborators.

Let's take a look at it. It contains a RooDataSet and one variable. This time we called our variable (or observable) CMS_hgg_mass, let's assume now that this is the invariant mass of photon pairs where we assume our H-boson decays to photons.

Let's have a look at the data. The RooWorkspace has several accessor functions, we will use the RooWorkspace::data one.

There are also RooWorkspace::var, RooWorkspace::function and RooWorkspace::pdf with (hopefully) obvious purposes.

```
In [15]: RooDataSet *hgg_data = (RooDataSet*) wspace->data("dataset");
    RooRealVar *hgg_mass = (RooRealVar*) wspace->var("CMS_hgg_mass");

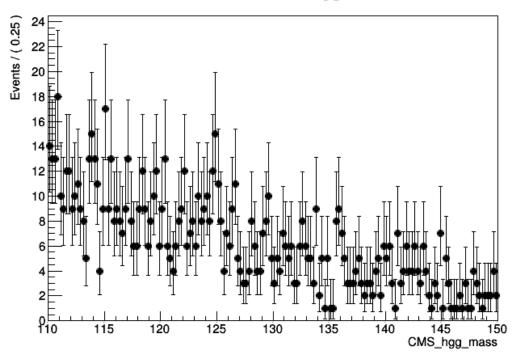
plot = hgg_mass->frame();

hgg_data->plotOn(plot,RooFit::Binning(160));

// Here we've picked a certain number of bins just for plotting purposes

plot->Draw();
    can->Update();
    can->Draw();
```

A RooPlot of "CMS_hgg_mass"



2.3 Likelihoods and Fitting to data

The data we have in our file doesn't look like a Gaussian distribution. Instead, we could probably use something like an exponential to describe it.

There is an exponential pdf already in RooFit (yep you guessed it) RooExponential. For a pdf, we only need one parameter which is the exponential slope α so our pdf is,

$$f(m|\alpha) = \frac{1}{N}e^{-\alpha m}$$

Where of course, $N=\int_{110}^{150}e^{-\alpha m}dm$ is the normalisation constant.

You can fund a bunch of available RooFit functions here: https://root.cern.ch/root/html/ROOFIT_ROOFIT_Index.html

There is also support for a generic pdf in the form of a RooGenericPdf, check this link: https://root.cern.ch/doc/v608/classRooGenericPdf.html

```
In [16]: RooRealVar alpha("alpha","#alpha",-0.05,-0.2,0.01);
    RooExponential expo("exp","exponential function",*hgg_mass,alpha);
```

We can use RooFit to tell us to estimate the value of α using this dataset. You will learn more about parameter estimation but for now we will just assume you know about maximising likelihoods. This maximum likelihood estimator is common in HEP and is known to give unbiased estimates for things like distribution means etc.

This also introduces the other main use of PDFs in RooFit. They can be used to construct likelihoods easily.

The likelihood \mathcal{L} is defined for a particluar dataset (and model) as being proportional to the probability to observe the data assuming some pdf. For our data, the probability to observe an event with a value in an interval bounded by a and b is given by,

$$P(m \in [a,b]) = \int_a^b f(m|\alpha)dm$$

As that interval shrinks we can say this probability just becomes equal to $f(m|\alpha)dm$

The probability to observe the dataset we have is given by the product of such probabilities for each of our data points, so that

$$\mathcal{L}(\alpha) \propto \prod_{i} f(m_i | \alpha)$$

Note that for a specific dataset, the *dm* factors which should be there are constnant. They can therefore be absorbed into the constant of proportionality!

The maximum likelihood esitmator for α , usually written as $\hat{\alpha}$, is found by maximising $L(\alpha)$.

Note that this won't depend on the value of the constant of proportionality so we can ignore it. This is true in most scenarios because usually only the ratio of likelihoods is needed, in which the constant factors out.

Obviously this multiplication of exponentials can lead to very large (or very small) numbers which can lead to numerical instabilities. To avoid this, we can take logs of the likelihood. Its also common to multiply this by -1 and minimize the resulting Negative Log Likelihood : $-Log\mathcal{L}(\alpha)$.

RooFit can construct the NLL for us.

Notice that the NLL object knows which RooRealVar is the parameter because it doesn't find that one in the dataset. This is how RooFit distiguishes between observables and parameters.

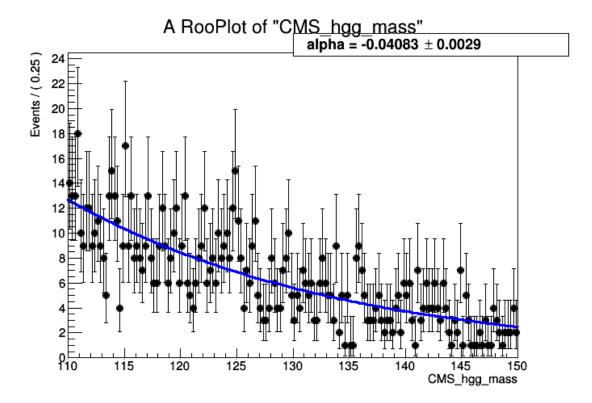
RooFit has an interface to Minuit via the RooMinimizer class which takes the NLL as an argument. To minimize, we just call the RooMinimizer::minimize() function. "Minuit" is the program and "migrad" is the minimization routine which uses gradient descent...

```
In [18]: RooMinimizer minim(*nll);
        minim.minimize("Minuit", "migrad");
 ******
      1 **SET PRINT
                              1
 ******
 *****
      2 **SET NOGRAD
 *****
PARAMETER DEFINITIONS:
   NO.
         NAME
                      VALUE
                                 STEP SIZE
                                               LIMITS
                                             -2.00000e-01 1.00000e-02
    1 alpha
                  -5.00000e-02 2.10000e-02
 ******
      3 **SET ERR
                          0.5
 ******
 ******
      4 **SET PRINT
                              1
 ******
 ******
      5 **SET STR
NOW USING STRATEGY 1: TRY TO BALANCE SPEED AGAINST RELIABILITY
 *****
      6 **MIGRAD
                         500
                                       1
 ******
 FIRST CALL TO USER FUNCTION AT NEW START POINT, WITH IFLAG=4.
 START MIGRAD MINIMIZATION. STRATEGY 1. CONVERGENCE WHEN EDM .LT. 1.00e-03
 FCN=3589.52 FROM MIGRAD
                           STATUS=INITIATE
                                                 4 CALLS
                                                                   5 TOTAL
                    EDM= unknown
                                      STRATEGY= 1
                                                      NO ERROR MATRIX
 EXT PARAMETER
                             CURRENT GUESS
                                                STEP
                                                             FIRST
 NO.
       NAME
                 VALUE
                                  ERROR
                                                SIZE
                                                          DERIVATIVE
  1 alpha
                 -5.00000e-02
                                2.10000e-02 2.24553e-01 -9.91191e+01
                              ERR DEF= 0.5
 MIGRAD MINIMIZATION HAS CONVERGED.
 MIGRAD WILL VERIFY CONVERGENCE AND ERROR MATRIX.
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
 FCN=3584.68 FROM MIGRAD
                           STATUS=CONVERGED
                                                18 CALLS
                                                                  19 TOTAL
                    EDM=1.4449e-08
                                     STRATEGY= 1
                                                      ERROR MATRIX ACCURATE
 EXT PARAMETER
                                                STEP
                                                             FIRST
 NO.
       NAME
                 VALUE
                                  ERROR
                                                SIZE
                                                          DERIVATIVE
  1 alpha
                 -4.08262e-02
                                2.91959e-03
                                            1.33905e-03 -3.70254e-03
                              ERR DEF= 0.5
EXTERNAL ERROR MATRIX.
                         NDIM= 25
                                      NPAR= 1
                                                  ERR DEF=0.5
  8.527e-06
```

RooFit has found the best fit value of alpha for this dataset. It also estimates an uncertainty on alpha using the Hessian matrix from the fit.

```
In [19]: alpha.Print("v");
--- RooAbsArg ---
  Value State: clean
  Shape State: clean
 Attributes:
  Address: 0x1224d5000
 Clients:
    (0x1224d53b0,V-) RooExponential::exp "exponential function"
    (0x7feab88fd600,V-) RooNLLVar::nll_exp_dataset "-log(likelihood)"
    (0x7feab88d9800,V-) RooExponential::exp "exponential function"
    (0x7feab88f1800,V-) RooRealIntegral::exp_Int[CMS_hgg_mass] "Integral of exponential function
  Servers:
 Proxies:
--- RooAbsReal ---
 Plot label is "alpha"
--- RooAbsRealLValue ---
 Fit range is [ -0.2 , 0.01 ]
--- RooRealVar ---
 Error = 0.00291959
```

Lets plot the resulting exponential on the data. Notice that the value of $\hat{\alpha}$ is used for the exponential.



It looks like there could be a small region near 125 GeV for which our fit doesn't quite go through the points. Maybe our hypothetical H-boson isn't so hypothetical after all!

Let's see what happens if we include some resonant signal into the fit. We can take our Gaussian function again and use that as a signal model. A reasonable value for the resolution of a resonant signal with a mass around 125 GeV decaying to a pair of photons is around a GeV.

By setting these parameters constant, RooFit knows (either when creating the NLL by hand or when using fitTo) that there is not need to fit for these parameters.

We need to add this to our exponential model and fit a "Sigmal+Background model" by creating a RooAddPdf. In RooFit there are two ways to add PDFs, recursively where the fraction of yields for the signal and background is a parameter or absolutely where each PDF has its own normalisation. We're going to use the second one.

```
const RooArgList components(hgg_signal,expo);
         const RooArgList coeffs(norm_s,norm_b);
         RooAddPdf model("model","f_{s+b}",components,coeffs);
         model.Print("v");
--- RooAbsArg ---
 Value State: DIRTY
  Shape State: DIRTY
  Attributes:
  Address: 0x1224e78b0
  Clients:
  Servers:
    (0x1224de680,V-) RooGaussian::signal "Gaussian PDF"
    (0x1224e7150,V-) RooRealVar::norm_s "N_{s}"
    (0x1224d53b0,V-) RooExponential::exp "exponential function"
    (0x1224e7500,V-) RooRealVar::norm_b "N_{b}"
 Proxies:
    !refCoefNorm ->
    !pdfs ->
      1) signal
      2)
             exp
    !coefficients ->
      1) norm_s
      2) norm_b
--- RooAbsReal ---
 Plot label is "model"
--- RooAbsPdf ---
Cached value = 0
```

Ok now lets fit the model. Note this time we add the option Extended() which tells RooFit that we care about the overall number of observed events in the data n too. It will add an additional Poisson term in the likelihood to account for this so our likelihood this time looks like,

$$L_{s+b}(N_s, N_b, \alpha) = \frac{N_s + N_b^n e^{N_s + N_b}}{n!} \cdot \prod_{i}^{n} \left[c f_s(m_i | M_H, \sigma) + (1 - c) f_b(m_i | \alpha) \right]$$

where $c = \frac{N_s}{N_s + N_b}$, $f_s(m|M_H, \sigma)$ is the Gaussian signal pdf and $f_b(m|\alpha)$ is the exponential pdf. Remember that M_H and σ are fixed so that they are no longer parameters of the likelihood.

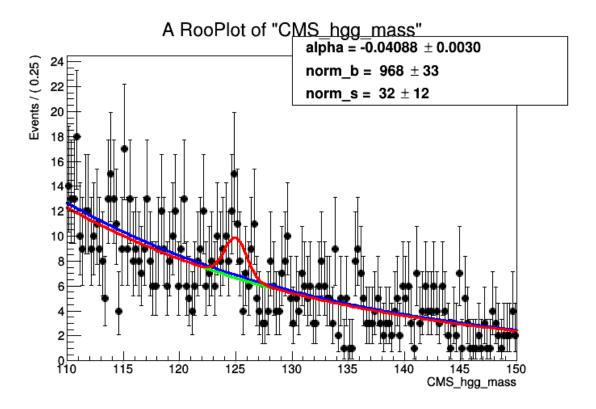
There is a simpler interface for maximum likelihood fits which is the RooAbsPdf::fitTo method. With this simple method, RooFit will construct the negative log-likelihood function, from the pdf, and minimize all of the free parameters in one step...

```
In [23]: model.fitTo(*hgg_data,RooFit::Extended());
[#1] INFO:Minization -- RooMinimizer::optimizeConst: activating const optimization
[#1] INFO:Minization -- The following expressions have been identified as constant and will be
```

```
[#1] INFO:Minization -- The following expressions will be evaluated in cache-and-track mode: (e
******
      1 **SET PRINT
                             1
*****
******
      2 **SET NOGRAD
******
PARAMETER DEFINITIONS:
   NO. NAME
                     VALUE
                                STEP SIZE
                                             LIMITS
    1 alpha
                 -4.08262e-02 2.91959e-03 -2.00000e-01 1.00000e-02
                  5.00000e+02 1.00000e+02
    2 norm_b
                                           0.00000e+00 1.00000e+03
                  5.50000e+01 9.00000e+00
                                             1.00000e+01 1.00000e+02
    3 norm_s
******
      3 **SET ERR
                         0.5
*****
******
      4 **SET PRINT
                             1
******
*****
      5 **SET STR
                           1
******
NOW USING STRATEGY 1: TRY TO BALANCE SPEED AGAINST RELIABILITY
      6 **MIGRAD
                       1500
******
FIRST CALL TO USER FUNCTION AT NEW START POINT, WITH IFLAG=4.
START MIGRAD MINIMIZATION. STRATEGY 1. CONVERGENCE WHEN EDM .LT. 1.00e-03
FCN=-2171.16 FROM MIGRAD
                           STATUS=INITIATE
                                                12 CALLS
                                                                  13 TOTAL
                   EDM= unknown
                                                     NO ERROR MATRIX
                                     STRATEGY= 1
 EXT PARAMETER
                            CURRENT GUESS
                                               STEP
                                                            FIRST
 NO.
       NAME
                VALUE
                                 ERROR
                                               SIZE
                                                         DERIVATIVE
  1 alpha
                -4.08262e-02
                               2.91959e-03
                                            3.24715e-02
                                                         8.37267e-01
  2 norm_b
                 5.00000e+02
                               1.00000e+02 2.01358e-01 -4.31189e+02
                 5.50000e+01
                               9.00000e+00 2.01358e-01 -1.12998e+01
  3 norm_s
                             ERR DEF= 0.5
MIGRAD MINIMIZATION HAS CONVERGED.
MIGRAD WILL VERIFY CONVERGENCE AND ERROR MATRIX.
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
                           STATUS=CONVERGED
FCN=-2327.53 FROM MIGRAD
                                                89 CALLS
                                                                  90 TOTAL
                   EDM=2.70696e-05
                                                      ERROR MATRIX ACCURATE
                                      STRATEGY= 1
 EXT PARAMETER
                                               STEP
                                                            FIRST
 NO.
       NAME
                                 ERROR
                                                         DERIVATIVE
                VALUE
                                               SIZE
  1 alpha
                -4.08793e-02
                               2.96856e-03
                                            1.10003e-03 -1.22544e-01
                                            5.72865e-03 -1.80553e-02
  2 norm_b
                 9.67647e+02
                               3.25523e+01
    norm_s
                 3.22534e+01
                               1.16360e+01
                                            9.71065e-03 -1.00987e-03
                             ERR DEF= 0.5
                                      NPAR= 3
EXTERNAL ERROR MATRIX.
                         NDIM= 25
                                                 ERR DEF=0.5
```

8.816e-06 1.310e-04 -1.322e-04

```
1.310e-04 1.072e+03 -1.064e+02
 -1.322e-04 -1.064e+02 1.397e+02
 PARAMETER CORRELATION COEFFICIENTS
      NO. GLOBAL
                       1
                             2
                                    3
       1 0.00378 1.000 0.001 -0.004
       2 0.27495 0.001 1.000 -0.275
       3 0.27497 -0.004 -0.275 1.000
 ******
      7 **SET ERR
                         0.5
 ******
 ******
      8 **SET PRINT
                             1
 ******
 ******
      9 **HESSE
                       1500
 ******
 COVARIANCE MATRIX CALCULATED SUCCESSFULLY
 FCN=-2327.53 FROM HESSE
                                                 16 CALLS
                                                                 106 TOTAL
                           STATUS=OK
                    EDM=2.70761e-05
                                      STRATEGY= 1
                                                      ERROR MATRIX ACCURATE
 EXT PARAMETER
                                             INTERNAL
                                                          INTERNAL
 NO.
                                             STEP SIZE
                                                            VALUE
       NAME
                 VALUE
                                 ERROR
  1 alpha
                 -4.08793e-02
                               2.96856e-03
                                             2.20007e-04
                                                          5.41516e-01
  2 norm_b
                  9.67647e+02
                               3.25747e+01
                                             2.29146e-04
                                                          1.20909e+00
  3 norm_s
                  3.22534e+01
                               1.16433e+01
                                             3.88426e-04 -5.29939e-01
                             ERR DEF= 0.5
 EXTERNAL ERROR MATRIX.
                         NDIM= 25
                                      NPAR= 3
                                                  ERR DEF=0.5
 8.816e-06 1.367e-04 -1.370e-04
 1.367e-04 1.073e+03 -1.074e+02
 -1.370e-04 -1.074e+02 1.398e+02
 PARAMETER CORRELATION COEFFICIENTS
      NO. GLOBAL
                       1
       1 0.00392 1.000 0.001 -0.004
       2 0.27718 0.001 1.000 -0.277
       3 0.27720 -0.004 -0.277 1.000
[#1] INFO:Minization -- RooMinimizer::optimizeConst: deactivating const optimization
In [24]: model.plotOn(plot,RooFit::Components("exp"),RooFit::LineColor(kGreen));
        model.plotOn(plot,RooFit::LineColor(kRed));
        model.paramOn(plot);
        can->Clear();
        plot->Draw();
        can->Update();
        can->Draw();
```



```
[#1] INFO:Plotting -- RooAbsPdf::plotOn(model) directly selected PDF components: (exp) [#1] INFO:Plotting -- RooAbsPdf::plotOn(model) indirectly selected PDF components: ()
```

What about if we also fit for the mass (M_H)? we can easily do this by removing the constant setting on MH...

NO. NAME	VALUE	STEP SIZE	LIMITS	
1 MH	1.25000e+02	1.00000e+00	1.20000e+02	1.30000e+02
2 alpha	-4.08793e-02	2.96856e-03	-2.00000e-01	1.00000e-02
3 norm_b	9.67647e+02	3.25747e+01	0.00000e+00	1.00000e+03

MINUIT WARNING IN PARAMETR ======= VARIABLE3 BROUGHT BACK INSIDE LIMITS. 3.22534e+01 1.16433e+01 1.00000e+01 1.00000e+02 4 norm_s ****** 0.5 3 **SET ERR ****** ***** 4 **SET PRINT ****** ****** ** 5 **SET STR 1 ***** NOW USING STRATEGY 1: TRY TO BALANCE SPEED AGAINST RELIABILITY ***** 6 **MIGRAD 2000 ****** FIRST CALL TO USER FUNCTION AT NEW START POINT, WITH IFLAG=4. START MIGRAD MINIMIZATION. STRATEGY 1. CONVERGENCE WHEN EDM .LT. 1.00e-03 FCN=-2327.53 FROM MIGRAD STATUS=INITIATE 10 CALLS 11 TOTAL EDM= unknown STRATEGY= 1 NO ERROR MATRIX EXT PARAMETER CURRENT GUESS STEP FIRST NO. NAMEVALUE ERROR SIZE DERIVATIVE 1 MH 1.25000e+02 1.00000e+00 2.01358e-01 1.12769e+01 -4.08793e-02 2.96856e-03 3.30048e-02 -1.22651e-01 2 alpha 3 norm_b 9.67647e+02 3.25747e+01 2.56674e-01 -1.96463e-02 3.22534e+01 1.16433e+01 3.10258e-01 -8.97036e-04 4 norm_s ERR DEF= 0.5 MIGRAD MINIMIZATION HAS CONVERGED. MIGRAD WILL VERIFY CONVERGENCE AND ERROR MATRIX. COVARIANCE MATRIX CALCULATED SUCCESSFULLY FCN=-2327.96 FROM MIGRAD STATUS=CONVERGED 65 CALLS STRATEGY= 1 EDM=1.19174e-05 ERROR MATRIX ACCURATE EXT PARAMETER STEP FIRST NO. NAME VALUE ERROR SIZE DERIVATIVE 1 MH 1.24628e+02 3.98153e-01 2.66539e-03 2.46327e-02 2 alpha -4.07708e-02 2.97195e-03 1.10093e-03 8.33780e-02 3 norm_b 9.66105e+02 3.25772e+01 5.96627e-03 1.83523e-03 4 norm s 3.39026e+01 1.17380e+01 9.60816e-03 -2.32681e-03 ERR DEF= 0.5 EXTERNAL ERROR MATRIX. NDTM= 25 NPAR= 4 ERR DEF=0.5 1.589e-01 -3.890e-05 1.462e-01 -1.477e-01 -3.890e-05 8.836e-06 -2.020e-04 2.038e-04 1.462e-01 -2.020e-04 1.073e+03 -1.072e+02 -1.477e-01 2.038e-04 -1.072e+02 1.420e+02 PARAMETER CORRELATION COEFFICIENTS NO. GLOBAL 1 2

1 0.04518 1.000 -0.033 0.011 -0.031 2 0.03317 -0.033 1.000 -0.002 0.006

```
3 0.27465 0.011 -0.002 1.000 -0.275
       4 0.27610 -0.031 0.006 -0.275 1.000
******
      7 **SET ERR
                         0.5
******
*****
      8 **SET PRINT
******
******
      9 **HESSE
                      2000
******
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=-2327.96 FROM HESSE
                           STATUS=OK
                                                23 CALLS
                                                                 89 TOTAL
                   EDM=1.19078e-05
                                                      ERROR MATRIX ACCURATE
                                     STRATEGY= 1
 EXT PARAMETER
                                            INTERNAL
                                                         INTERNAL
 NO.
       NAME
               VALUE
                                 ERROR
                                            STEP SIZE
                                                           VALUE
  1 MH
                 1.24628e+02
                              3.98106e-01
                                            5.33077e-04 -7.45154e-02
  2 alpha
                -4.07708e-02
                              2.97195e-03
                                            2.20186e-04
                                                        5.42722e-01
  3 norm_b
                 9.66105e+02
                               3.26003e+01
                                            2.38651e-04
                                                        1.20047e+00
  4 norm_s
                 3.39026e+01
                               1.17445e+01
                                            3.84326e-04 -4.87967e-01
                             ERR DEF= 0.5
EXTERNAL ERROR MATRIX.
                         NDIM= 25
                                     NPAR= 4
                                                 ERR DEF=0.5
 1.588e-01 -3.888e-05 1.304e-01 -1.304e-01
-3.888e-05 8.836e-06 -1.954e-04 1.954e-04
 1.304e-01 -1.954e-04 1.074e+03 -1.082e+02
-1.304e-01 1.954e-04 -1.082e+02 1.421e+02
PARAMETER CORRELATION COEFFICIENTS
      NO. GLOBAL
                      1
                             2
                                   3
       1 0.04274
                   1.000 -0.033 0.010 -0.027
       2 0.03314 -0.033 1.000 -0.002 0.006
       3 0.27694 0.010 -0.002 1.000 -0.277
       4 0.27806 -0.027 0.006 -0.277 1.000
[#1] INFO:Minization -- RooMinimizer::optimizeConst: deactivating const optimization
```

Notice now the result for the fitted MH is not 125 and gets added to the fitted parameters since now it is floating.

We can get more information about the fit, via the RooFitResult, using the option Save().

```
******
PARAMETER DEFINITIONS:
  NO. NAME
                  VALUE STEP SIZE
                                          LIMITS
   1 MH
                1.24628e+02 3.98106e-01
                                          1.20000e+02 1.30000e+02
   2 alpha
                -4.07708e-02 2.97195e-03 -2.00000e-01 1.00000e-02
   3 norm_b
                9.66105e+02 3.26003e+01 0.00000e+00 1.00000e+03
   4 norm s
                 3.39026e+01 1.17445e+01
                                           1.00000e+01 1.00000e+02
******
** 12 **SET ERR
                      0.5
******
******
   13 **SET PRINT
                           1
******
******
   14 **SET STR
******
NOW USING STRATEGY 1: TRY TO BALANCE SPEED AGAINST RELIABILITY
******
** 15 **MIGRAD
                      2000
                                   1
******
FIRST CALL TO USER FUNCTION AT NEW START POINT, WITH IFLAG=4.
START MIGRAD MINIMIZATION. STRATEGY 1. CONVERGENCE WHEN EDM .LT. 1.00e-03
FCN=-2327.96 FROM MIGRAD
                         STATUS=INITIATE
                                              8 CALLS
                                                               9 TOTAL
                  EDM= unknown
                                  STRATEGY= 1
                                                  NO ERROR MATRIX
                          CURRENT GUESS
                                             STEP
EXT PARAMETER
                                                         FIRST
NO. NAME
             VALUE
                              ERROR
                                             SIZE
                                                      DERIVATIVE
                             3.98106e-01 7.99293e-02 2.48316e-02
 1 MH
               1.24628e+02
                             2.97195e-03 3.30665e-02 8.31525e-02
 2 alpha
               -4.07708e-02
 3 norm_b
               9.66105e+02
                             3.26003e+01
                                          2.24827e-01 -6.61689e-04
                             1.17445e+01 3.04346e-01 -2.13755e-03
 4 norm_s
                3.39026e+01
                           ERR DEF= 0.5
MIGRAD MINIMIZATION HAS CONVERGED.
MIGRAD WILL VERIFY CONVERGENCE AND ERROR MATRIX.
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=-2327.96 FROM MIGRAD
                         STATUS=CONVERGED
                                              48 CALLS
                                                              49 TOTAL
                  EDM=4.3627e-07
                                  STRATEGY= 1
                                                  ERROR MATRIX ACCURATE
EXT PARAMETER
                                             STEP
                                                        FIRST
NO.
      NAME
             VALUE
                              ERROR
                                             SIZE
                                                      DERIVATIVE
 1 MH
                             3.98148e-01
               1.24627e+02
                                          2.66088e-03 -1.14618e-03
 2 alpha
               -4.07790e-02
                             2.97195e-03 1.10099e-03 -1.81012e-03
 3 norm_b
                9.66109e+02
                             3.25801e+01
                                          5.79949e-03 3.49697e-03
 4 norm_s
                3.39097e+01 1.17384e+01
                                          9.60079e-03 -2.05915e-04
                           ERR DEF= 0.5
EXTERNAL ERROR MATRIX.
                       NDIM= 25
                                   NPAR= 4
                                              ERR DEF=0.5
1.589e-01 -3.890e-05 1.438e-01 -1.452e-01
-3.890e-05 8.836e-06 -2.012e-04 2.028e-04
1.438e-01 -2.012e-04 1.073e+03 -1.072e+02
```

** 11 **SET NOGRAD

```
-1.452e-01 2.028e-04 -1.072e+02 1.420e+02
PARAMETER CORRELATION COEFFICIENTS
     NO. GLOBAL
                     1
                           2
                                 3
      1 0.04481 1.000 -0.033 0.011 -0.031
      2 0.03318 -0.033 1.000 -0.002 0.006
      3 0.27471 0.011 -0.002 1.000 -0.275
      4 0.27611 -0.031 0.006 -0.275 1.000
******
   16 **SET ERR 0.5
******
******
   17 **SET PRINT
                          1
******
******
   18 **HESSE
                     2000
******
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=-2327.96 FROM HESSE STATUS=OK
                                             23 CALLS
                                                             72 TOTAL
                  EDM=4.3782e-07 STRATEGY= 1
                                                 ERROR MATRIX ACCURATE
 EXT PARAMETER
                                         INTERNAL INTERNAL
 NO. NAME
                             ERROR
             VALUE
                                         STEP SIZE
                                                       VALUE
                             3.98094e-01 1.06435e-04 -7.46738e-02
  1 MH
               1.24627e+02
  2 alpha
              -4.07790e-02 2.97195e-03 4.40396e-05 5.42631e-01
               9.66109e+02 3.26025e+01 2.31980e-04 1.20049e+00
  3 norm_b
  4 norm_s
                3.39097e+01 1.17445e+01 3.84032e-04 -4.87789e-01
                           ERR DEF= 0.5
                       NDIM= 25
EXTERNAL ERROR MATRIX.
                                  NPAR= 4
                                              ERR DEF=0.5
 1.588e-01 -3.887e-05 1.246e-01 -1.246e-01
-3.887e-05 8.836e-06 -1.927e-04 1.928e-04
 1.246e-01 -1.927e-04 1.075e+03 -1.082e+02
-1.246e-01 1.928e-04 -1.082e+02 1.421e+02
PARAMETER CORRELATION COEFFICIENTS
     NO. GLOBAL
                     1
                           2
                                 3
      1 0.04196 1.000 -0.033 0.010 -0.026
      2 0.03314 -0.033 1.000 -0.002 0.005
      3 0.27693 0.010 -0.002 1.000 -0.277
      4 0.27795 -0.026 0.005 -0.277 1.000
[#1] INFO: Minization -- RooMinimizer:: optimizeConst: deactivating const optimization
 RooFitResult: minimized FCN value: -2327.96, estimated distance to minimum: 4.3782e-07
              covariance matrix quality: Full, accurate covariance matrix
              Status : MINIMIZE=0 HESSE=0
   Constant Parameter
                       Value
          resolution 1.0000e+00
```

23

Floating Parameter InitialValue FinalValue +/- Error GblCorr.

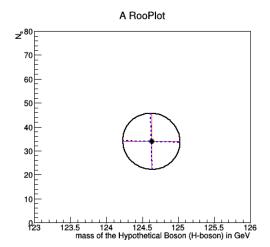
```
MH 1.2463e+02 1.2463e+02 +/- 3.98e-01 <none>
alpha -4.0771e-02 -4.0779e-02 +/- 2.97e-03 <none>
norm_b 9.6611e+02 9.6611e+02 +/- 3.26e+01 <none>
norm_s 3.3903e+01 3.3910e+01 +/- 1.17e+01 <none>
```

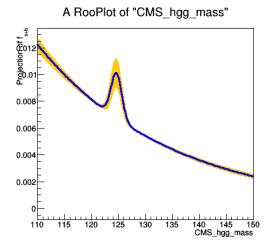
For example, we can get the Correlation Matrix from the fit result... Note that the order of the parameters are the same as listed in the "Floating Parameter" list above

4x4 matrix is as follows

1	0	1 l	2	3 l
0	1	-0.03282	0.009538	-0.02623
1	-0.03282	1	-0.001978	0.005439
2	0.009538	-0.001978	1	-0.2769
3	-0.02623	0.005439	-0.2769	1

And there even some fancy ways to visualise these results ...





A nice feature of RooFit is that once we have a pdf, data and results like this, we can import this new model into our RooWorkspace and show off our new discovery to our LHC friends (if we weren't about 5 years too late!). We can also save the "state" of our parameters for later, by creating a snapshot of the current values.

```
In [29]: wspace->import(model);
         RooArgSet *params = model.getParameters(*hgg_data);
         wspace->saveSnapshot("nominal_values",*params);
         wspace->Print("V");
[#1] INFO:ObjectHandling -- RooWorkspace::import(workspace) importing RooAddPdf::model
[#1] INFO:ObjectHandling -- RooWorkspace::import(workspace) importing RooGaussian::signal
[#1] INFO:ObjectHandling -- RooWorkspace::import(workspace) importing RooRealVar::MH
[#1] INFO:ObjectHandling -- RooWorkspace::import(workspace) importing RooRealVar::resolution
[#1] INFO:ObjectHandling -- RooWorkspace::import(workspace) importing RooRealVar::norm_s
[#1] INFO:ObjectHandling -- RooWorkspace::import(workspace) importing RooExponential::exp
[#1] INFO:ObjectHandling -- RooWorkspace::import(workspace) importing RooRealVar::alpha
[#1] INFO:ObjectHandling -- RooWorkspace::import(workspace) importing RooRealVar::norm_b
RooWorkspace(workspace) Tutorial Workspace contents
variables
(CMS_hgg_mass,MH,alpha,norm_b,norm_s,resolution)
p.d.f.s
RooExponential::exp[x=CMS_hgg_mass c=alpha] = 0.00248636
RooAddPdf::model[ norm_s * signal + norm_b * exp ] = 0.00240205
RooGaussian::signal[ x=CMS_hgg_mass mean=MH sigma=resolution ] = 5.34013e-110
```

```
-------
RooDataSet::dataset(CMS_hgg_mass)

parameter snapshots
------
nominal_values = (MH=124.627 +/- 0.398094,resolution=1[C],norm_s=33.9097 +/- 11.7445,alpha=-0.04
```

3 Removing Nuisance Parameters

In HEP, we often have the case where there are some parameters of the model which are physics parameters of interest, while others are known as nuisance parameters. In some cases, those parameters may have external constraints, coming from other data or some theoretical reasoning. This is how we often treat systematic uncertainties but we won't cover those today.

There are two schools of thought for removing nuisance parameters

• Frequentists use profiling

datasets

• Bayesians use marginalisation

In our case, the hypothesis mass M_H might be the thing which we can write papers on and win Nobel prizes for while we're not nearly so interested in the values of N_s , α or N_b .

For simplicity, we will assume that the values of α and N_b are fixed (maybe from theory or from a large Monte Carlo simulation) and so the only remaining nuisance paraemeter is N_s .

The profile likelihood is one which removes the nuisances parameters by fitting them away. Note this is a major divide for Bayesians and Frequentist since removing nuisance parameters for Bayesians involves integrating (or marginalising) over them.

The profile likeihood is written as,

$$\mathcal{L}_p(M_H) = \mathcal{L}_{s+b}(M_H, \hat{N}_s)$$

where the double hat notation, $\hat{\cdot}$, denotes the values of the nuisance parameter which maximises L_{s+b} at a given value of M_H .

RooFit has a useful class under the RooStats libraries for profile likelihoods: ProfileLikelihoodCalculator: https://root.cern.ch/doc/v606/classRooStats_1_1ProfileLikelihoodCalculator.html

```
In [31]: MH.setRange(123,126);
    RooStats::ProfileLikelihoodCalculator plc(*hgg_data,model,RooArgSet(MH));
```

According to Wilks' theorem, -2 times the log of profile likelihood ratio,

$$-2\log\lambda = -2\lograc{\mathcal{L}(M_H)}{\mathcal{L}(\hat{M}_H)}$$

should be distributed as a χ^2 with the number degrees of freedom equal to the number of parameters (in our case 1). This means that we can obtain the 1σ (or 68%) uncertainty by finding the interval for which

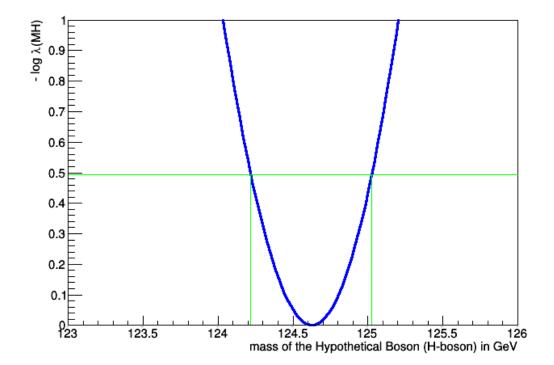
$$-\log \lambda(M_H) < 0.5$$

We can tell RooFit to find that interval for us,

```
In [32]: plc.SetConfidenceLevel(0.68);
        RooStats::LikelihoodInterval *interval = plc.GetInterval();
        std::cout << "\n\t hat{MH} = "
            << ((RooRealVar*)interval->GetBestFitParameters()->find("MH"))->getVal()
            << std::endl;
        std::cout << "\t 68% interval = ("
            << interval->LowerLimit(MH) << "," << interval->UpperLimit(MH) << ")"</pre>
            << std::endl;
[#1] INFO:Minization -- p.d.f. provides expected number of events, including extended term in li
[#0] PROGRESS: Minization -- ProfileLikelihoodCalcultor:: DoGLobalFit - find MLE
[#0] PROGRESS: Minization -- ProfileLikelihoodCalcultor:: DoMinimizeNLL - using Minuit / Migrad wi
[#1] INFO: Minization -- RooMinimizer::optimizeConst: activating const optimization
[#1] INFO:Minization -- The following expressions have been identified as constant and will be
[#1] INFO: Minization -- The following expressions will be evaluated in cache-and-track mode: (s
[#1] INFO:Minization --
 RooFitResult: minimized FCN value: -2327.96, estimated distance to minimum: 5.65025e-10
               covariance matrix quality: Full, accurate covariance matrix
               Status: MINIMIZE=0
   Floating Parameter FinalValue +/- Error
  -----
                        1.2463e+02 +/- 3.94e-01
                   MH
               norm_s 3.3910e+01 +/- 1.13e+01
        hat\{MH\} = 124.627
        68\% interval = (124.22, 125.026)
```

We can see where these values come from by drawing the negative of the profile likelihood ratio.

```
[#1] INFO:Minization -- RooProfileLL::evaluate(nll_model_dataset_Profile[MH]) Creating instance
[#1] INFO:Minization -- RooProfileLL::evaluate(nll_model_dataset_Profile[MH]) determining minimu
[#1] INFO:Minization -- RooProfileLL::evaluate(nll_model_dataset_Profile[MH]) minimum found at (
.
[#1] INFO:Minization -- RooProfileLL::evaluate(nll_model_dataset_Profile[MH]) Creating instance
[#1] INFO:Minization -- RooProfileLL::evaluate(nll_model_dataset_Profile[MH]) determining minimu
[#0] ERROR:InputArguments -- RooArgSet::checkForDup: ERROR argument with name MH is already in t
[#1] INFO:Minization -- RooProfileLL::evaluate(nll_model_dataset_Profile[MH]) minimum found at (
```



. . .

We can also obtain a Bayesian posterior density by using Bayes' theorem ...

$$P(M_H|\text{data}) = \frac{\int P(\text{data}|M_H, N_s)\pi(N_s|M_H)dN_s}{P(\text{data})}$$

where $\pi(N_s|M_H)$ is the (condidtional) prior probability density for our parameters. You might notice that $P(\text{data}|M_H, N_s)$ is nothing more than our likelihood function $\mathcal{L}(M_H, N_s)$!

Notice that I can use "=" here because we normalise according to P(data), which is the integral over the likelihood (multiplied by the prior) with respect to all of its parameters.

We can get RooFit to calculate this posterior using the BayesianCalculator class but first, for this time, we are going to create a ModelConfig which keeps track of which parameters are POIs and which are nuisances/observables. This is useful when sharing your model between collegues.

There are a few things to set up since we're using variables inside the workspace. First, lets set our two background parameters to constant, this time, directly in the workspace

And we will load the nominal values from the fit before...

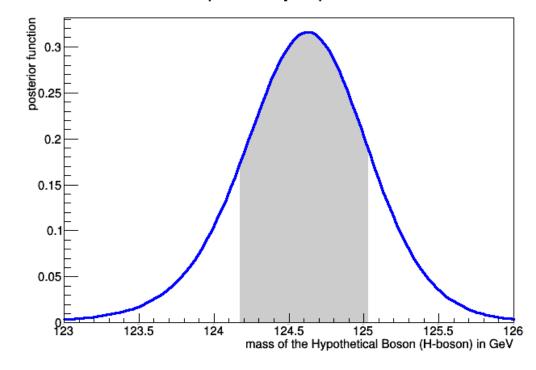
For Bayesian results, we need to set the prior density function (π). For now, let's assume no prior knowledge of the parameters - i.e the prior is constant within the range of the parameters and 0 elsewhere.

Note that choosing a suitable prior is a debated subject amongst Bayesians since the results can depend on what you choose as a prior. Worse still, if a flat prior is chosen, say for M_H , should it be flat in M_H , or flat in M_H^2 (eg since $M_H = 2\lambda v^2$ and maybe λ is the fundamental thing)?

```
Prior PDF: RooUniform::flat_prior[ x=(MH,norm_s) ] = 1
```

Now we can create the calculator and plot the posterior pdf...

Posterior probability of parameter "MH"



This was the "shortest" interval, but we can also find the other valid intervals [a,b] which satisfy $P(M_H \epsilon [a,b]) = 0.68$. Let's compare the Bayesian 68% credible interval with our 65% confidence interval from the profile likelihood scan...

They agree pretty well for our analysis but beware that this is not always the case!

You will learn a more about Likelihoods and their use in Hypothesis Testing (Frequentist/Basyesian intervals, coverage and credibility, setting limits, discovery...) in future statistics Lectures. There are many more useful toos for performing them with the RooStats library https://twiki.cern.ch/twiki/bin/view/RooStats/WebHome - check them out!