RooFit/RooStats Analysis Report

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Abstract

I have started to use a new and highly flexible tool called RooStats, which makes use of a Workspace container created within RooFit, to do statistical tests on the validity of a user created model hypothesis. In earnest, some crude assumptions have been made, which will be discussed here and addressed with further experience. This first report is aimed at bringing together the initial stages of my work.

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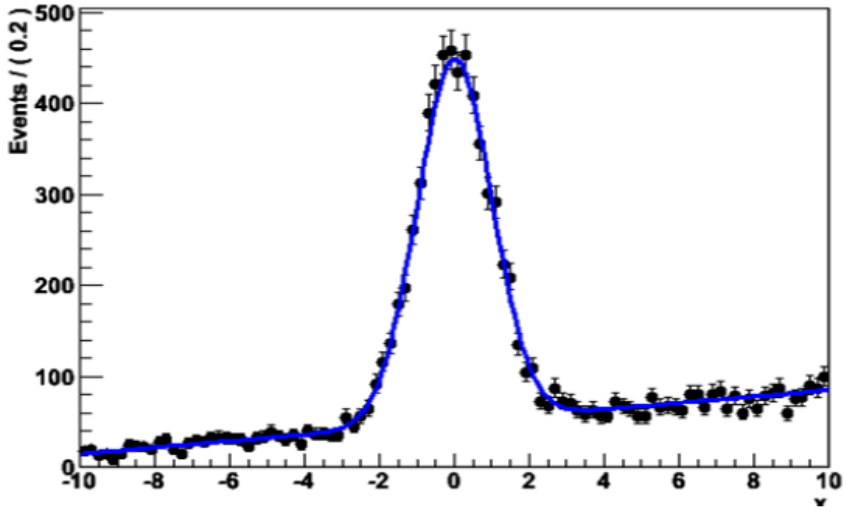

Figure 1: A simple PDF Function Created in RooFit

1 RooFit

RooFit focuses on the need for a practical way to create a probability density function in ROOT, providing ways not just to code simple problems, but to enable use of non-trivial or even multidimensional functions that were usually too problematic to include previously.

The implementation of RooFit, compliments the already existing ROOT Libraries, creating practically no overlap of functionality (See Figure 2).I will not go through the tools in great detail here, but I do feel some points are worth mentioning in this report, any further information can be easily located in the comprehensive RooFit Manual, which is easy to follow even for newcomers.

RooFit's core design philosophy is to represent the relations between variables and functions in the same way that you would associate client and server links between objects, orientated around the framework of object-orientated data modelling. As all objects in RooFit are self documenting, it enables objects to have unique identifiers and complex descriptions right from the get go, and the relation between these objects made clear.

As well as creating your desired model, with signal and as many background components as required, one is able to make uses of data in this environment in several ways. The simplest way is to generate toy monte carlo events about your model, including statistical fluctuations to a user preset degree. If one wishes to take a more frequentist approach they can simply create more of these toy monte carlo sets but the advantage of this system is that one is not restricted to using a strictly frequentist OR bayesian approach when coming to analysis as they can include components that en-

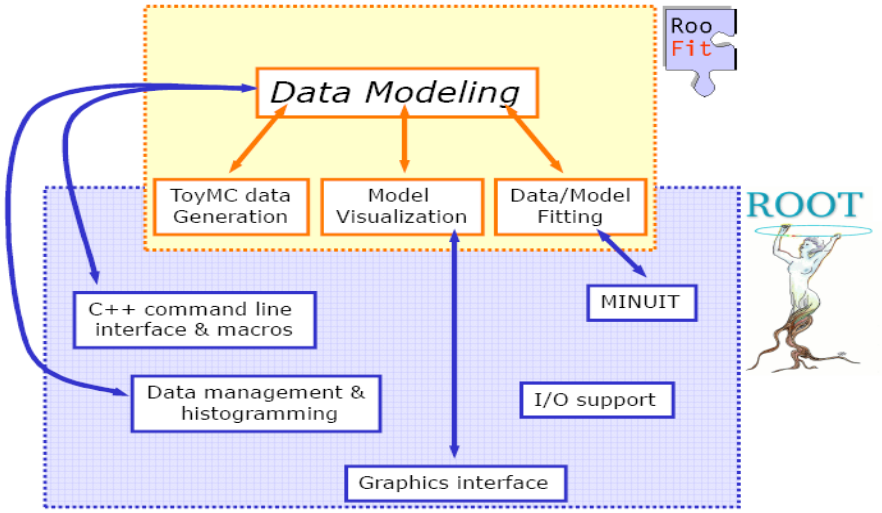

Figure 2: A Diagram of the Extension of RooFit to ROOT.

able you to later run separate or even hybrid analyses. Another method for including data, which is of more interest in this report for it's future connotations, is the ability to import unbinned/binned data from ROOT TTrees. It will initially be seen that from an invariant mass search which was performed on offical monte carlos samples, RooFit/RooStats can then be used to try and determine any significance of such a search unbiasedly, only assuming the shape of the Signal Peak and Background. However the further reaches of this second method is it's ability to eventually be used with real data, allowing RooStats to be used to it's full potential with multiple physics channels and datasets.

The end product of the RooFit endeavour is to create a Workspace, which RooFit uses as a generic container class for all the objects of your project, easing the task of your analysis projects organisation. The hand over from RooFit to RooStats is here, with RooFit writing the final composite model and it's components, the data, and any priors or details specified, to the Workspace for Roostats to later read out as required for the analysis technique chosen.

2 RooStats

RooStats is a collaborative project between ATLAS, CMS, and ROOT, to provide a consolidated set of statistical tools. It was created for want of several features that centre around the ability to have sound statistical interpretations of data in an analysis, and be able to combine different analysis's with and even across the experiments involved. When one has a problem,

it is undesirable to recode the problem each time you want to compare it to another analysis, or even just look at it with another method, there is always some information that may be being lost. Roostats is designed for the purpose of only having the problem coded once, and then it has the ability to compare the statistical methods, generalise, and bring together the statistical tools within ROOT. Currently at the time of writing this report, the RooStats manual is still under construction, however its synopsis will still be short, as the important details are included where relevant throughout the rest of the report.

On the premise of eventually wanting to combine channels, it is prudent to mention the basics of how this would be done. In the example of a simple likelihood analysis you would have the form in Equation 1, and naively this can be simply extended to a binned likelihood for multiple channels by the order of Equation 2. Finally extending the latter to include observables for the signal and background events, with distributions f_s, and f_b respectively, one obtains Equation 3.

$$L_i(n_i|r, s_i, b_i) = \frac{e^{-rs_i-b_i}}{n_i!}(rs_i + b_i)^{n_i} \tag{1}$$

$$L(r) = \prod_i L_i(n_i|r, s_i, b_i) \tag{2}$$

$$L(\overrightarrow{x}|r, s, b, \overrightarrow{O_s}\overrightarrow{O_b}) = \frac{e^{-rs-b}}{n!}(rs + b)^n \prod_{j=1}^{n}(rsf_s(\overrightarrow{x_j}|\overrightarrow{O_s}) + bf_b(\overrightarrow{x_j}|\overrightarrow{O_b})) \tag{3}$$

Once a statistical problem has been described, various methods can then be easily applied using RooStats, with the results of which are simultaneous enabling ease of comparison for different methods. An overview of the classes currently in RooStats can be seen in Figure 3.

3 My Analysis

3.1 Aim

My Aim is to use the tools mentioned above to search for a High Mass Di-Lepton Resonance with the ATLAS Detector at CERN, initially looking at e^+e^- but with the view to combining this with the $\mu^+\mu^-$ and $\gamma\gamma$ channels at a later stage. For the purpose of this report, I will be using the example of the Graviton, which is the subject of my PhD Thesis. This provides the need to create a model, which incorporates many interesting parameters, like the Mass, and coupling k/M_{pl}, as well as difficult parameters in regards to statistical tests, such as the width of the expected signal SigSigma, which

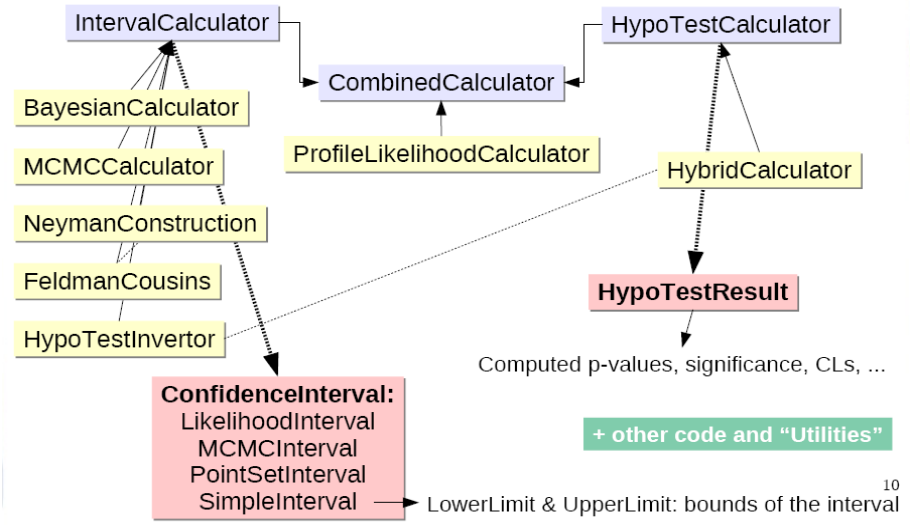

Figure 3: A Diagram of the Extension of RooFit to ROOT.

for the graviton is very narrow and so causes problems for certain fitting methods as will be shown.

The initial aims will be to create a robust model for my analysis, trying various statistical tests to verify this, and extract significances and exclusion limits for both the official, and in situ generated, monte carlo data. This includes the extraction of limits for various volumes of integrated luminosity, and how this plot changes relative to the parameters of my model.

3.2 My Model

3.2.1 Signal

Assuming one knows the shape of your signal peak, which I have rather naively extracted from the truth of my official monte carlo sample, one can create a signal peak trivially using RooFit as shown in Figure 4. Note here I have assumed a Breit Wigner signal shape.

3.2.2 Background

Currently for the Background to my model I am only considering the Drell-Yan process, as this is the dominant irreducible background to my signal. Note that here I have used a Landau function, which may have to be revisited as it causes complications in the fitting process which will be seen. The function has to be repeatedly integrated each time, in cases of tests that use a large numbers of toy monte carlo samples.

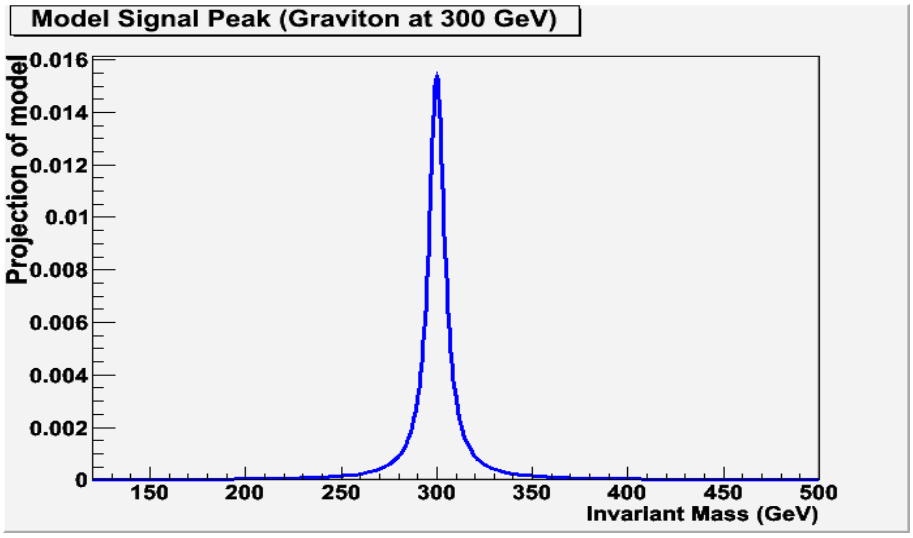

Figure 4: Model Signal Peak (BreitWigner::sigPdf(mass,trueMass[300,150,450],sigSigma[10]))

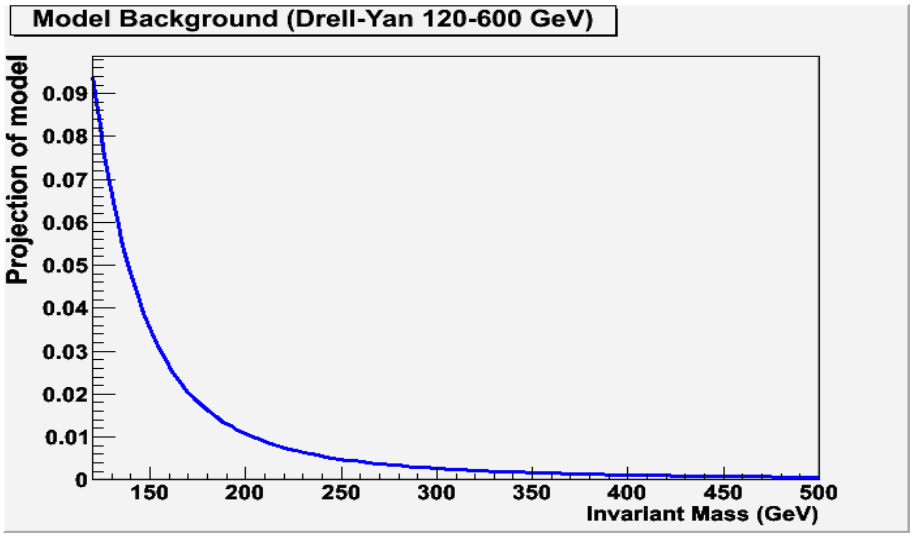

Figure 5: Model Background (Landau::bkgPdf(mass,c0[100],c1[10])

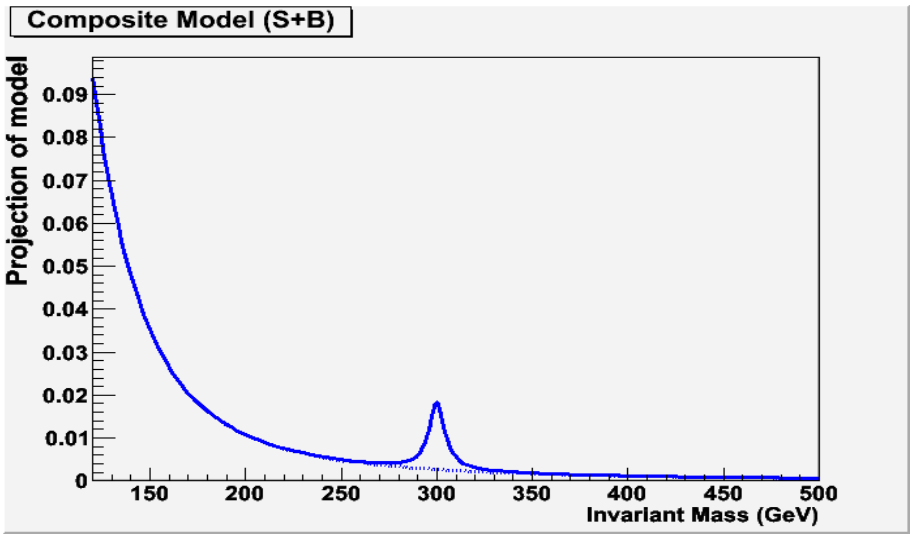

Figure 6: Composite Model (SUM::model(S[300]*sigPdf,B[3000]*bkgPdf"))

3.2.3 Composite

The composite model is a predefined combination of the two separate pdfs. The ratio of signal/background has to initially be set, but can be scanned across with the RooStats tests. I set the ratio to that roughly expected, but give a range either side of these values to allow some freedom. Note that one can immediately see the model's signal and background components separated by a dashed line so that one can see the proportion of background under the signal peak easily. Ranges can be given to the number of Signal and Background events, the Width of the signal peak, and indeed almost any of the parameters shown. Below is a full model and list of parameters written into the Workspace for the proceeding tests.

// Observable
mass[120,500]

// Signal & Background Pdf's
BreitWigner::sigPdf(mass,trueMass[300,150,450],sigSigma[5,20])
Landau::bkgPdf(mass,c0[100],c1[10]
SUM::modelSB(S[300,0,600]*sigPdf,B[3000,0,30000]*bkgPdf

// Background Only Pdf
ExtendPdf::modelBkg(bkgPdf,B)

// Priors for Signal
Uniform::priorS(S)

```
Uniform::priorMass(trueMass)
PROD::priorPOI(priorS,priorMass)

// Priors for Nuisance Parameters
Gaussian::prior_sigSigma(sigSigma,15,2)
Uniform::prior_B(B)
PROD::priorNuisance(prior_sigSigma,prior_B)

// Full Model Including Systematics
PROD::model(modelSB,priorNuisance)

// Definition of Observables and Parameters of Interest
defineSet("observables","mass")
defineSet("parameters","B,sigSigma")
defineSet("POI","S,trueMass")
// Note for POI, the S and trueMass can be taken separately or together.
```

3.3 Data Sources

The test data for this report will come from two separate sources. The first is generated binned monte carlo data, created around the model with preset error fluctuations, that RooFit will perform and write into the WorkSpace. This will be used for Bayesian approaches, however for the Frequentist methods RooStats is able to actually repeat this monte carlo generation with different random seeds, to get the preset required number of toy monte carlos in those examples. The second source of data will be that of the official monte carlo samples for the Graviton (Signal), and Drell-Yan (Background) which I intend to test my user made model against, as if I were looking at real data. A plot of the initial data written into the Workspace for both the model generated monte carlo, and the official monte carlo can be found in Figures 7, and 8, respectively. Note that these plots are data with Signal + Background in them.

4 Statistical Tests used in this Report

4.1 Profile Likelihood Calculator

The Profile Likelihood Calculator is a bayesian interval estimation and hypothesis testing method using MINUIT/MINOS, which essentially requires a fit to be made to the model twice, once with everything floating, and once with the signal fixed to zero. It incorporates Wilks' theorem that states; asymptotically the distribution of Equation 5 approaches a chi-square distribution, with the number of degrees of freedom equal to the number of parameters of interest.

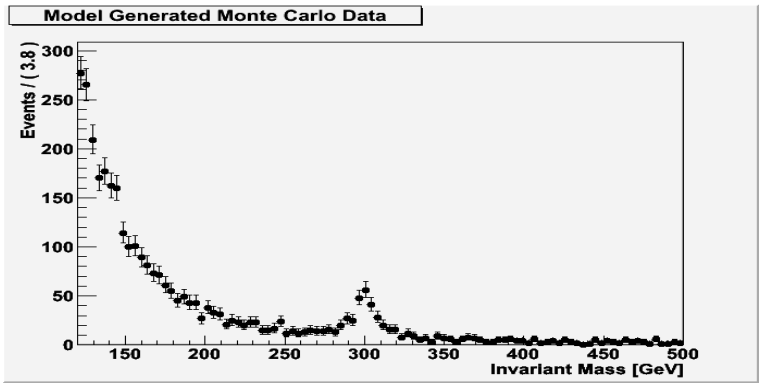

Figure 7: Monte Carlo Data, Generated around the Model

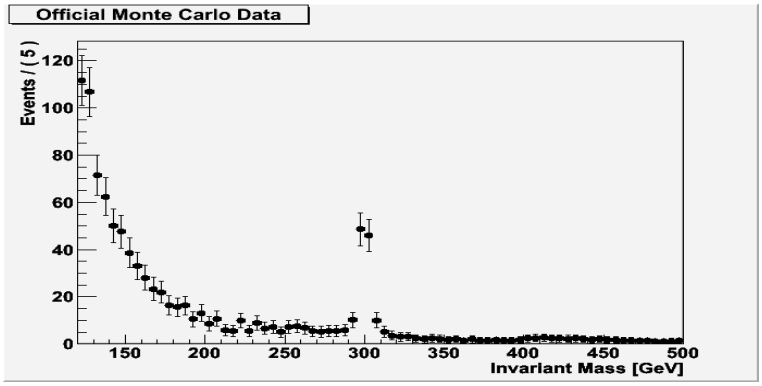

Figure 8: Official Monte Carlo Data

$$\ell = \frac{L(x|\theta_{rO}, \hat{\hat{\theta}}_s)}{L(x|\hat{\theta}_r, \hat{\theta}_s)} \tag{4}$$

$$-2log\lambda(\theta_O) = -2log\frac{f(x|\theta_O)}{f(x|\theta_{best}(x))} \tag{5}$$

4.2 Hybrid Calculator

The Hybrid Calculator, is a Frequentist hypothesis testing calculator with Bayesian integration of nuisance parameters. This method is based on sampling toy monte carlos around a test statistic, Q, for the Background Only, and Signal+Background Hypothesis. The test statistic is the likelihood ratio by default, shown in equation 6, but can optionally be set to the number of events, or the profile likelihood ratio which are all performed in this report. The test returns a HypoTestResult with the hypothesis p-values; CLb, CLsb, and the ratio of these which gives you CLs along with it's significance.

This test is based on the Frequentist method as it uses a preset number of toy monte carlo (usually around 5000), bus has a Bayesian element in the form of Cousins-Highland integration of the nuisance parameters. Note that the toys are created by generating data around their pdf's while varying the nuisance parameters.

$$Q = \frac{L(s+b)}{L(b)} \tag{6}$$

4.3 Three Test Comparison

One can also perform multiple tests and plot them on the same graph for comparison of methods. Looked at here with be the 2D Profile Likelihood (Blue Contour), Feldman Cousins (Red Boxes), and Markov Chain Monte Carlo (MCMC)(Black Outline Contour) methods. The 2D Profile Likelihood is simply the intersection of two 1D Profile Likelihood tests, one for each of the parameters of interest, and seems therefore to be the most robust of the tests looked at here. Feldman Cousins uses Neyman construction with likelihood ratio ordering rule, WILL ADD TO AT A LATER DATE. MCMC is a Bayesian Approach that incorporates Markov Chain Monte Carlo, WILL ADD TO AT LATER DATE.

4.4 Combination Run

The only original test in this report, written by the author to try and emulate a H to $\tau\tau$ example for combining the WorkSpaces containing different datasets, based around the same model albeit optimised for the test mass hypothesis of the WorkSpace. The aim of this test was to be two-fold; Firstly, for the case where the data set is monte carlo generated around the model within each WorkSpace, the Combination Run macro plots signal significance from the profile likelihood tests for each WorkSpace. The result of this should be interpreted as the expected significance if the signal were found at that mass, with a given integrated luminosity ($200pb^{-1}$ for all cases here). The Second use of this macro is if instead of monte carlo data generated around the model each time, one used the Official Monte Carlo data with Signal at 300 GeV for all of the Workspaces, while still varying the models Signal peak trueMass, then the result should be interpreted as the expected significance one would see given some integrated luminosity, if the Graviton existsed at 300 GeV.

5 Statistical Testing

5.1 Simple Example

First of all I give the example of a very simple model created in RooFit, with the results which using the suite of statistical tests I will be doing on my own model are shown in Appendix A. Here all of the tests seem to work well, and all are performed without warnings or errors in the terminal output.

5.2 Model + Generated Data

Here I introduce my own Model based on the Physics of the Graviton to e^+e^-, using Monte Carlo generated about it as the dataset, I will only include here the main points for discussion, but all relevant plots can be found in Appendix B.

5.2.1 Hybrid Calculator

Upon running the Hybrid Calculator, for every Toy Monte Carlo Generated, one receives the output line "INFO:NumericIntegration – RooRealIntegral :: init(bkgPdf_Int[mass]) using numeric integrator RooIntegrator1D to Calculate Int(mass)" This I have pinned down to the use of a Landau Function for the background, and while everything still works it slows the process down. As well as the problem of using the Landau function, from Figure 16 one can see that if the nuisance parameters are not considered in the hypothesis fit something goes wrong, but in reality it would make more sense to always include nuisance parameters where possible, especially as the point in the Hybrid Calculator is to be Hybrid by integrating those parameters out. My initial thoughts on another reason for this though could be because the signal width, sigSigma, is so small, that it gets to the point where you can find a fit anywhere, the width of the signal peak approaches the width of a bin, so any tiny fluctuation above normal becomes a possible fit, and you cannot get a good fit anywhere. Indeed by increasing the sigSigma to an unreasonably large value that no longer represents the physics, the Hybrid Calculator returns a more sensible plot with nuisance parameters turned off. In Figures 17 & 18 there is good overlap between the distributions and one gets an 89% signal result confidence level, with σ:1.21177, and a test significance (1-Cb) of 0.8872 which seems positive. But the test statistics now seem to have a flat distribution, where as I would have expected them, possible falsely so, to be of the same distribution shape as the case where the prior nuisance is turned off. The reason for this I can only attribute to being because the Signal and Background event priors are Uniform, and I do not know whether this a correct assmuption, or the prior for the number of signal/background events should be distributed in the same form as that of their respective pdf, i.e. for the Breit Wigner signal shape, should the

prior S distribution be Uniform, or also of a Breit Wigner Shape? Initially experimenting by using a Landau function as the Prior for B, as well as the Background Pdf, seems to disrupt most of the statistical tests.

5.2.2 Three Test Comparison

The most robust of the tests seems to be the 2D profile Likelihood test as it consistently succeeds to give a contour. In Figure 19 it can be seen that the possible mass range is very limited as you would expected for such an obvious signal, whereas the amount of signal can vary +/- 50 events. The main problems are faced with the other two tests, where varying the sigSigma appropriately to allow random walks through the parameter space seems to be the trouble with constant warnings during the MCMC fit saying that the sigSigma parameter keeps going out of bounds, meaning that the test is trying to vary it to explore the parameter space fully and is unable because of the narrow range it is allowed. Using a BreitWigner function for the Signal Shape may also partly be the problem as the RooStats tests seem to favour Gaussian shapes, I have still been unable to solve this problem. Also again using the Landau function to describe the background seems to slow down the process.

5.2.3 Combination Run

This macro is successful in producing the distribution of significances and is what one would expect, with the significance continually rising with Signal Peak Mass, as this in turn means a lower background around the peak and so clearer signal. However I am uncomfortable with just how high the significances are, and I fear this is simply due to the nature of the signal being too obvious over the background, which is an inherent issue in this search, if the parameters are as expected, then there is no trouble what so ever to find the resonance.

5.3 Model + Official Monte Carlo Data

Here I will repeat the same tests as in the previous section but using instead for data, the Official Monte Carlo of the 300 GeV Graviton and 120-500 GeV Drell-Yan Channel. As before only points of interest will be discussed here, and all relevant plots can be found in Appendix C.

5.3.1 Hybrid Calculator

Once again performing the test without nuisance parameters returns a non-sense result, the distributions are well separated with no overlap around the test statistic, and a significance of infinite is returned. Including the nuisance parameters produces a plot that does make sense, but has the unexpectedly

flat distributions once again. The result for the likelihood ratio (test statistic = 1) returns a no signal result unfortunately, but with a CLsb:0 which usually means and indeed as the macro recommends, maybe more toy monte carlo should be used (even though I was already using 5000). The result for the number of events (test statistic = 2) returns a positive signal result with 65% confidence level, σ:1.88671 and test significance = 0.9704.

5.3.2 Three Test Comparison

In the case of the Official Graviton Sample in Figure 27, more or less the same results are found, with the allowed mass being in a narrow region while the number of signal events has some possible range, only this time the number of signal events are lower, which merely reflects the differences in the official to crudely model generated monte carlo.

5.3.3 Combination Run

The Combination macro in this case should be interpreted as the returned profile likelihood significance for the model, given the existence of a 300 GeV Graviton. As expected in Figure 28 the significance at model masses far away from 300 GeV on both sides are low, being highest at the correct mass, and interestingly +/- 50 GeV of the trueMass in the dataset. To better visualise the models within each workspace here, you may find the model and data for each WorkSpace the macro used, in Appendix D. One final thing I tried, as the significances seemed uncomfortably high, was to say, what if the number of signal events were actually far less than we expected, 25% of what the Official monte carlo was saying, which approached the generated monte carlo of the model case (See Figure 37, Appendix D). The effect of using this reduced dataset can be seen in Figure 29 (Back in Appendix C), and shows much lower significances but still of the same form, showing that even though the significances were very high in the previous case, the plot does change logically with reduced data so the tests do appear to be correct. It simply means that other than something going wrong, the inherent problem of the signal being very clear over the background gives these very high significances.

6 Summary of Current Questions, Issues & Problems

- Landau Function representing Background pdf causes problems. What substitute could be used? Maybe doing a manual fit would expose where/why the fit is going wrong? (Talk to Samir Ferrag)

- Narrow Width of Signal Peak creates difficulty fitting. How can this be solved while remaining true to Physics? Initial thoughts further reduce the size of the binning so width is comparatively large.
- Signal is very clear over background, so always going to get high significances. As it is clear that the search would be trivial, need to turn attention to minimum number of signal events to reach 3σ, 5σ discovery, given the user made model. This is next step.
- Leading on from the previous point, use more Official samples as they arrive at different masses and width's, how does this change?
- Why does distribution around the test statistic in the Hybrid test go from a gaussian (like) distribution to a completely flat distribution when the (admittedly uniform) prior nuisance parameters are included. As this is of importance what form should the Prior B and Prior S have? (Ask Glen Cowan).
- All of the above, will hopefully result in the FC and MCMC tests finally working for my model as these are the tests that properly scan parameter space, and so I am keen to fix, as testing different parameter hypothesis' is my long term aim for the project, aided greatly with the eventual arrival of the new Graviton samples.

References

[1] RooFit Users Manual v2.07, written by W. Verkerke, D. Kirkby. Document version 2.07-29-11. Jan 2006.

[2] First RooStats Tutorial 15/10/09 & 16/10/09 hosted by Gregory Schott: http://indico.cern.ch/conferenceOtherViews.py?view=standard&confId=68912

[3] Statistical Lectures given by Luca Lista on 18/11/09 & 19/11/09 at CERN, Agenda: http://indico.cern.ch/conferenceDisplay.py?confId=73545

[4] Second RooStats Tutorial 26/11/09 & 27/11/09 hosted by Gregory Schott: http://indico.cern.ch/conferenceOtherViews.py?view=standard&confId=72320

A Simple Model

In this Appendix you can find the Figures relating to the Simple Model Example.

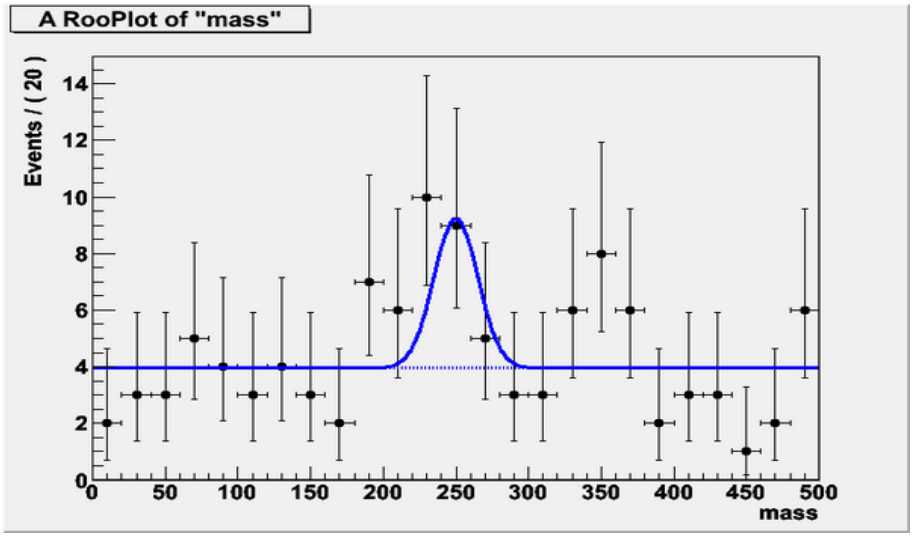

Figure 9: Simple Model

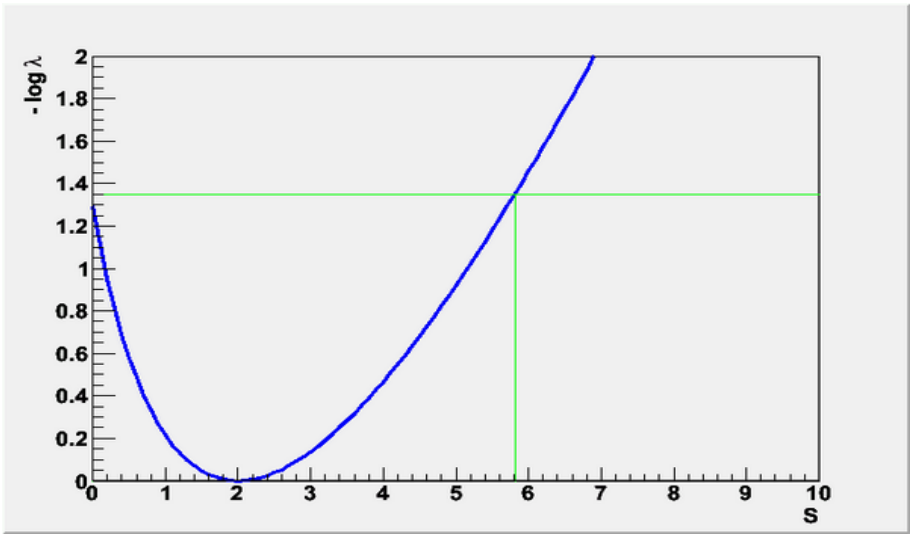

Figure 10: Profile Likelihood Test on Simple Model with Significance 3.27176σ

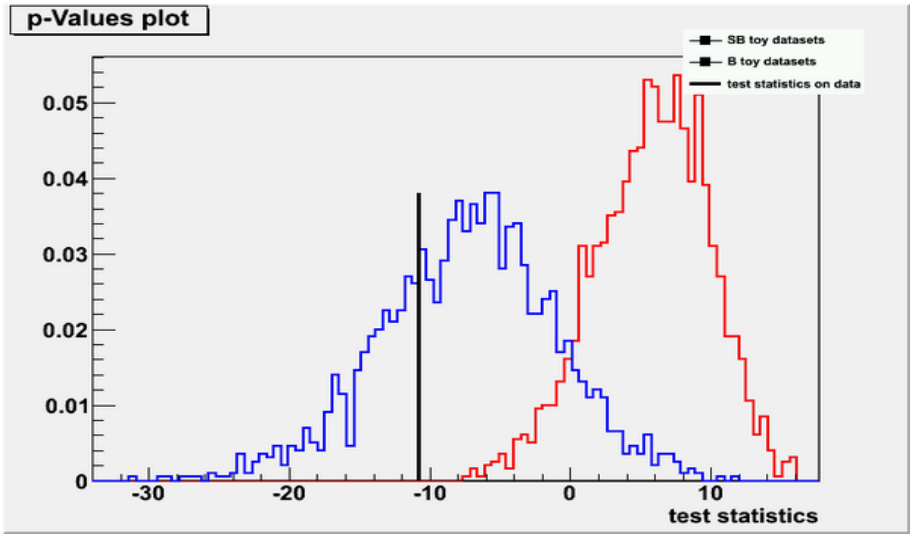

Figure 11: Hybrid Calculator Test on Simple Model, for 5000 toy monte carlo, giving p-value S+B:0.6694, p-value B:0.023, CLs:0.685159, at a significance of 1.99539σ

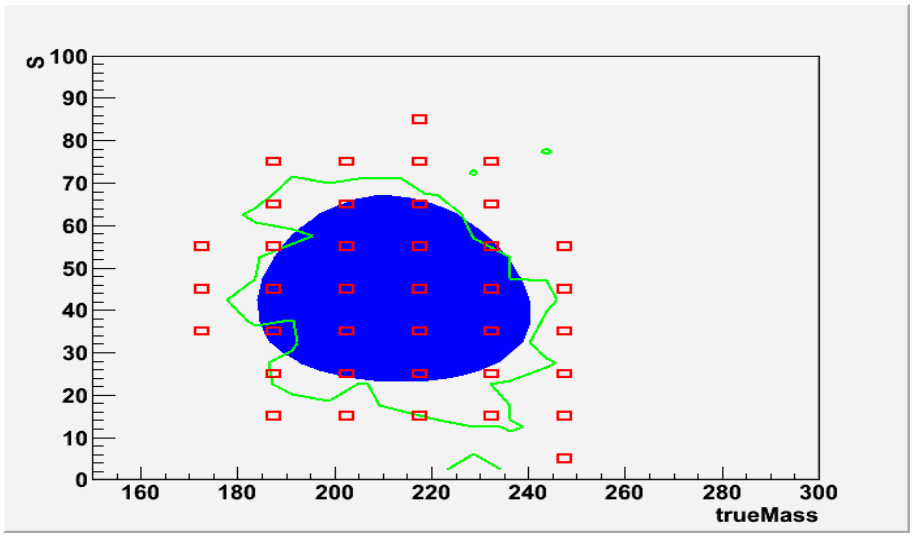

Figure 12: A comparison of the 2D Profile Likelihood, Feldman Cousins, and MCMC tests

B Model + Generated Data

In this Appendix you can find the Figures relating to My Model with generated Monte Carlo used for the dataset.

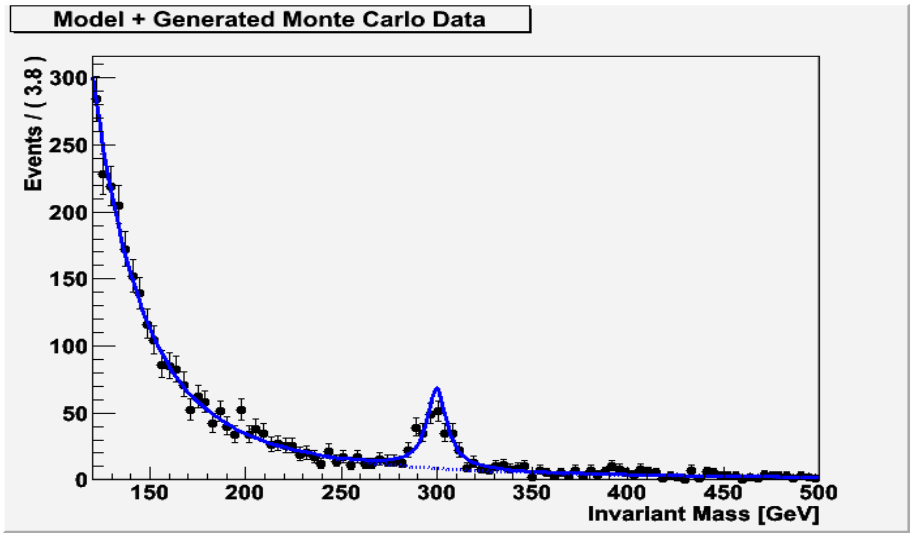

Figure 13: Model + Generated Monte Carlo Data

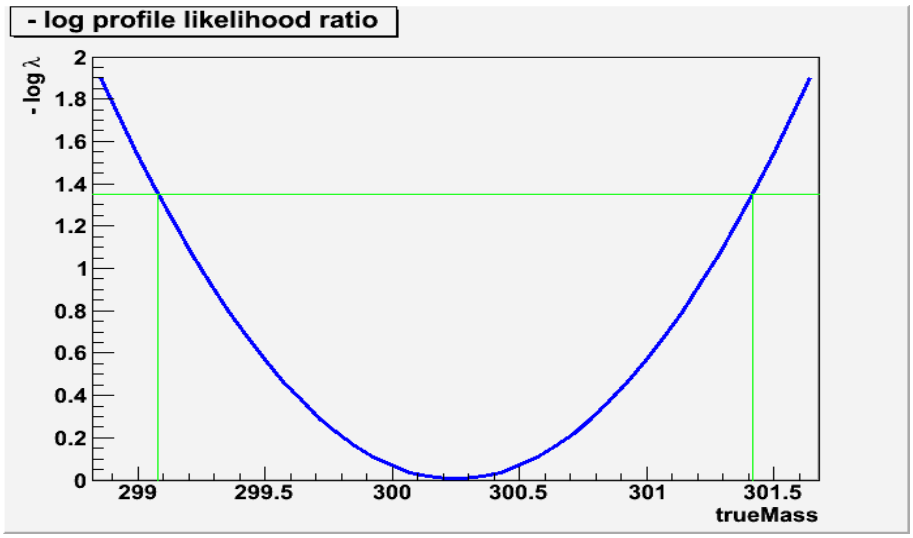

Figure 14: ProfileLikelihood Test with trueMass as Parameter of Interest, at 90% two-sided upper CL interval [299.078;301.419], test gives a significance estimation of 17σ

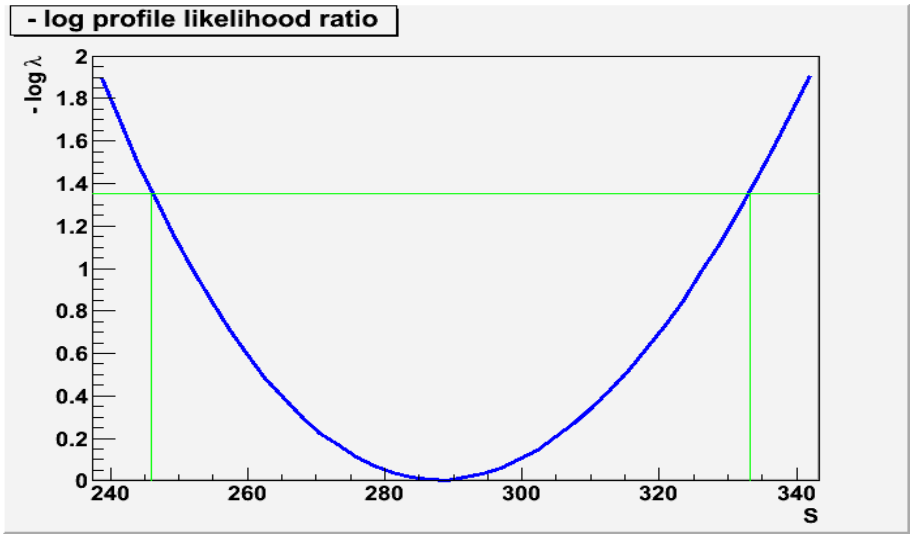

Figure 15: ProfileLikelihood Test with Number of Signal Events as Parameter of Interest, at 90% two-sided upper CL interval [212.036;298.392], test gives a significance estimation of 17σ

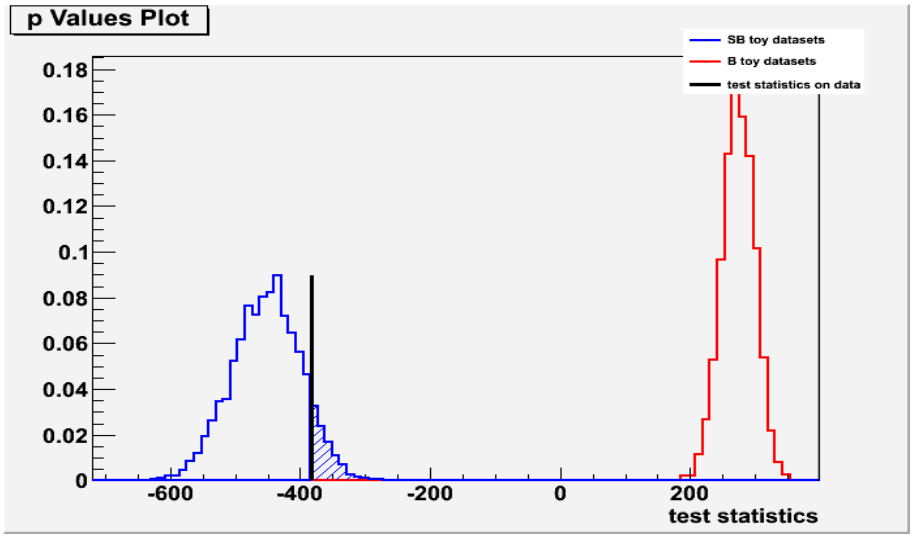

Figure 16: Hybrid Calculator with test stat = 1 (Likelihood Ratio), 5000 toy monte carlo samples were used, and Nuisance Parameters turned OFF. The calculator tests the hypothesis at specific values of the parameters; SignalWidth(15GeV), SignalN(300), BkgN(3000), and gives a significance estimation of infσ, for CLb:1, CLsb:0.089 CLs:0.089

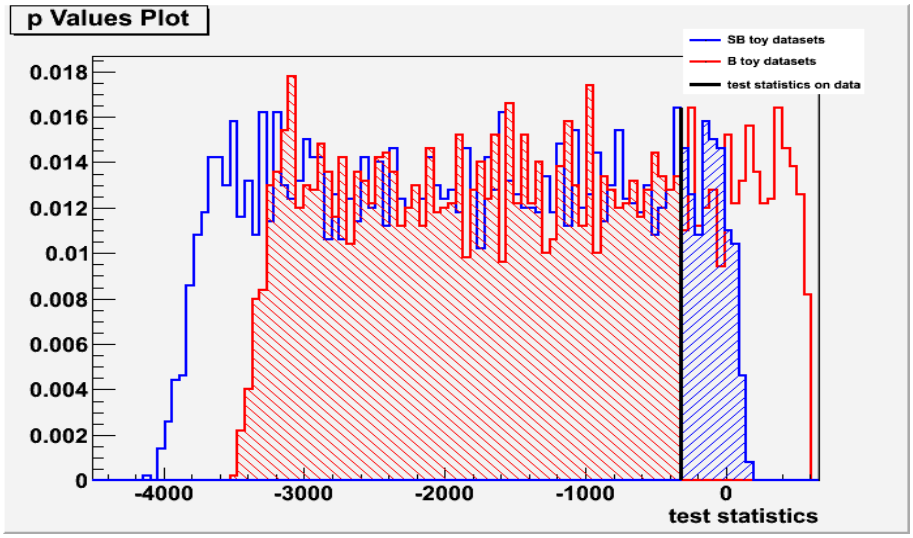

Figure 17: Hybrid Calculator with test stat = 1 (Likelihood Ratio), 5000 toy monte carlo samples were used, and Nuisance Parameters turned ON. The calculator tests the hypothesis at specific values of the parameters; SignalWidth(15GeV), SignalN(300), BkgN(3000), and gives a significance estimation of 0.723σ, for CLb:0.2348, CLsb:0.0986 CLs:0.42029

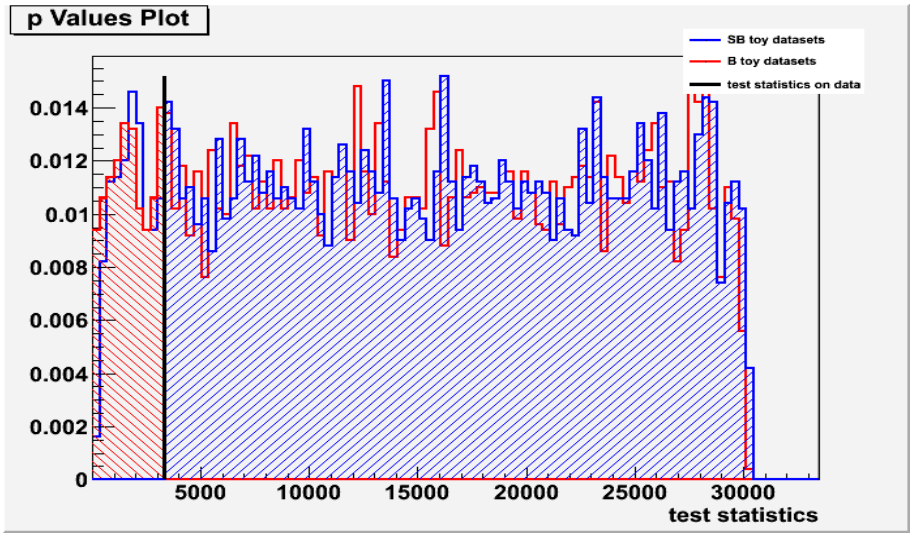

Figure 18: Hybrid Calculator with test stat = 2 (Number of Events), 5000 toy monte carlo samples were used, and Nuisance Parameters turned ON. The calculator tests the hypothesis at specific values of the parameters; SignalWidth(15GeV), SignalN(300), BkgN(3000), and gives a significance estimation of 1.21177σ, for CLb:0.1128, CLsb:0.1004, CLs:0.89

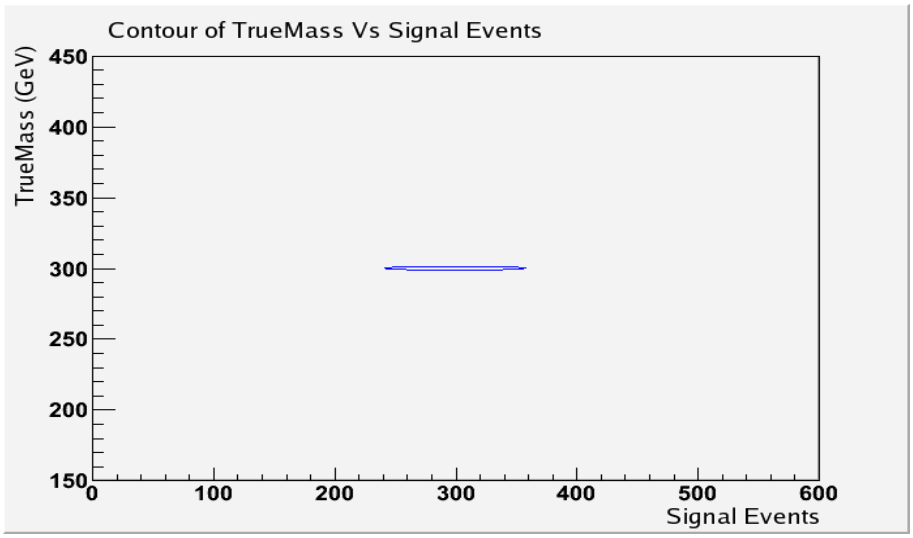

Figure 19: Three Tests, however only the 2D Profile Likelihood Test was successful, shown is the 90% confidence interval

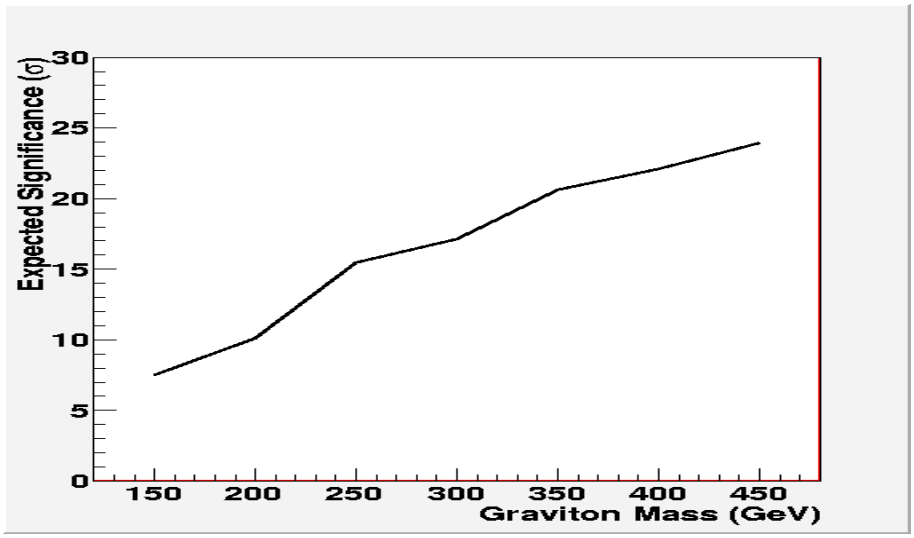

Figure 20: Combination of WorkSpaces to give model significance with varying Graviton Mass

C Model + Official Monte Carlo Data

In this appendix you can find the Figures relating to My Model with the Official Graviton and Drell-Yan Monte Carlo samples used for the dataset.

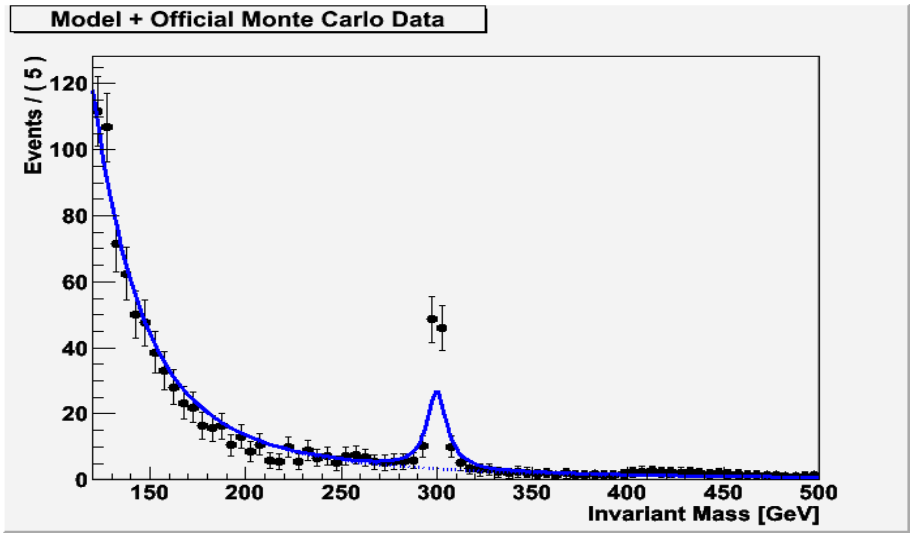

Figure 21: Model + Official Monte Carlo Data

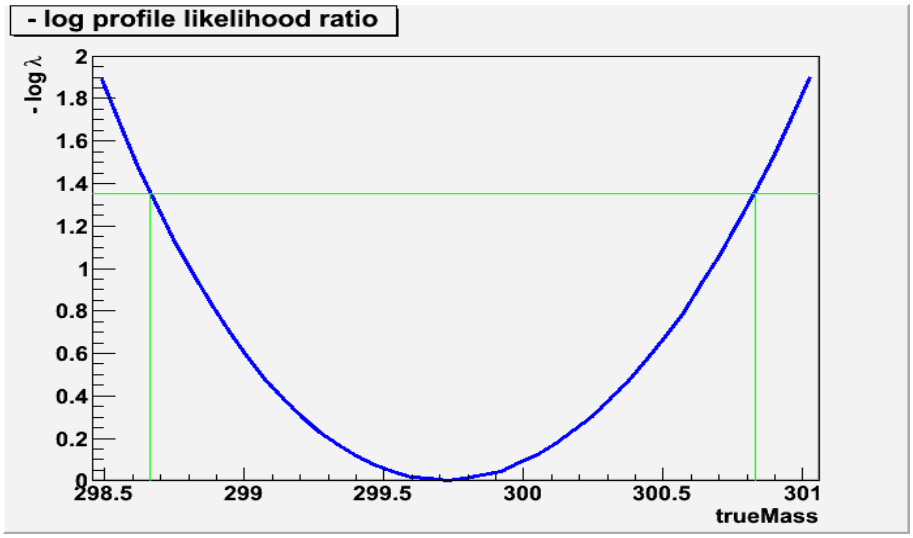

Figure 22: ProfileLikelihood Test trueMass as Parameter of Interest, at 90% two-sided upper CL interval [298.478;301.033], test gives a significance estimation of 18σ

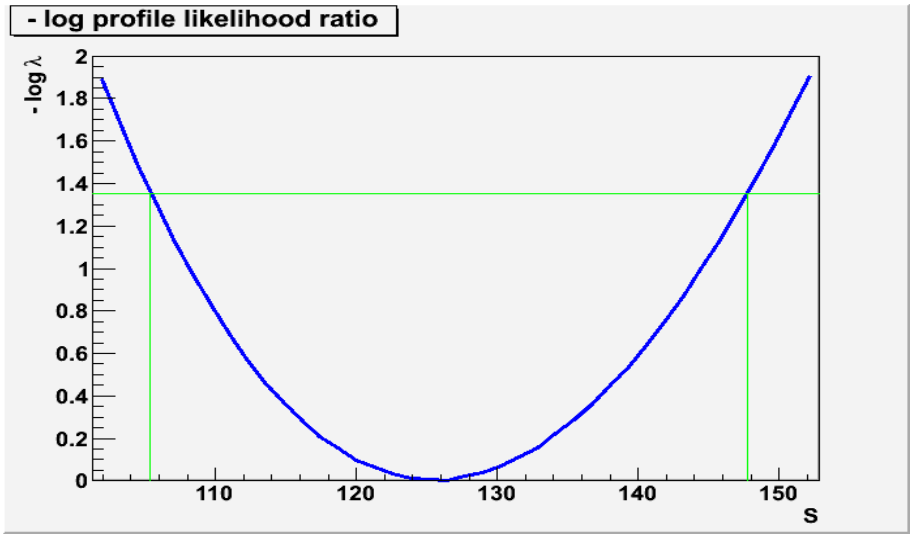

Figure 23: ProfileLikelihood Test with Number of Signal Events as Parameter of Interest, at 90% two-sided upper CL interval [101.726;152.301], test gives a significance estimation of 18σ

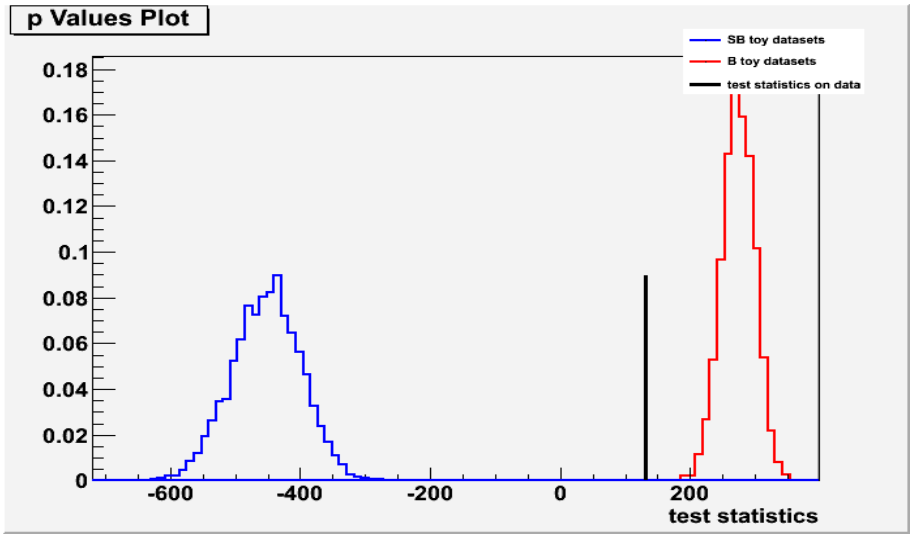

Figure 24: Hybrid Calculator with test stat = 1 (Likelihood Ratio), 5000 toy monte carlo samples were used, and Nuisance Parameters turned OFF. The calculator tests the hypothesis at specific values of the parameters; SignalWidth(15GeV), SignalN(100), BkgN(1000), and gives a significance estimation of infσ, for CLb:1, CLsb:0 CLs:0

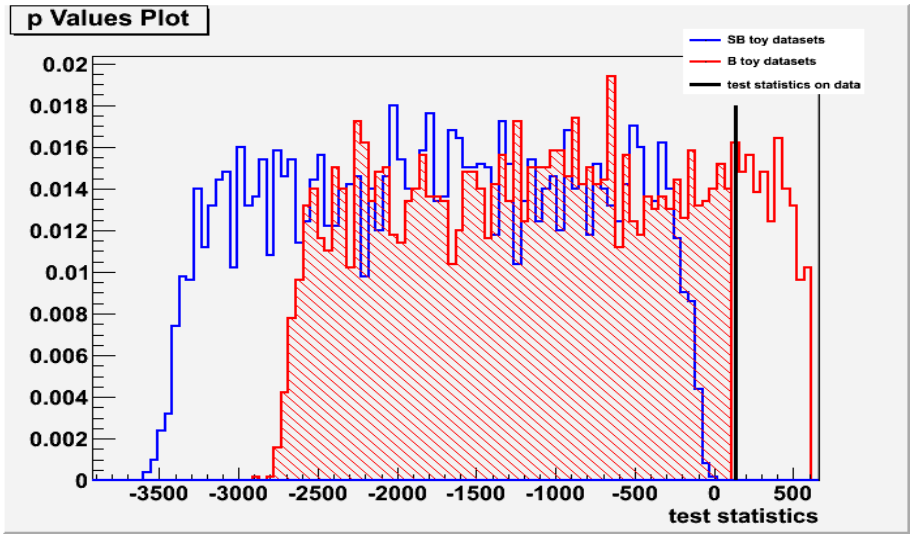

Figure 25: Hybrid Calculator with test stat = 1 (Likelihood Ratio), 5000 toy monte carlo samples were used, and Nuisance Parameters turned ON. The calculator tests the hypothesis at specific values of the parameters; SignalWidth(15GeV), SignalN(100), BkgN(1000), and gives a significance estimation of 1.0696σ, for CLb:0.1424, CLsb:0 CLs:0

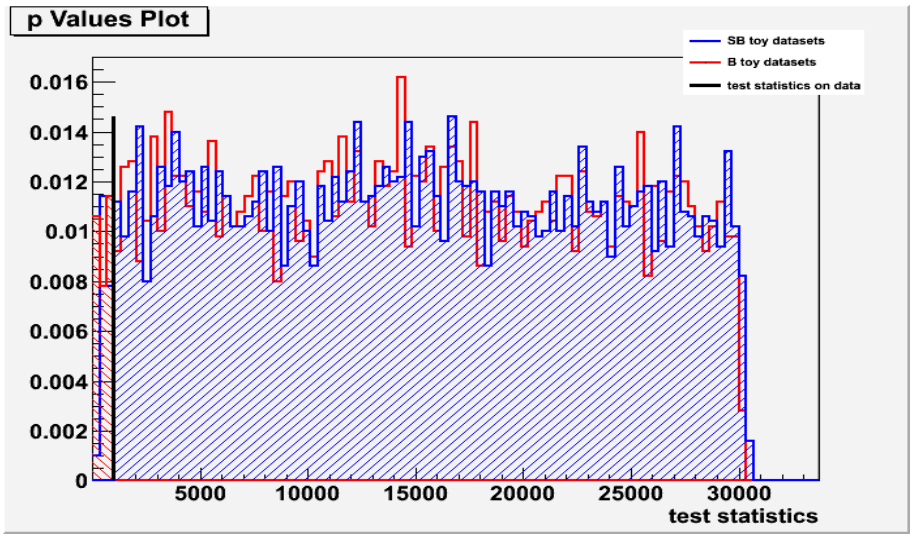

Figure 26: Hybrid Calculator with test stat = 2 (Number of Events), 5000 toy monte carlo samples were used, and Nuisance Parameters turned ON. The calculator tests the hypothesis at specific values of the parameters; SignalWidth(15GeV), SignalN(100), BkgN(1000), and gives a significance estimation of 1.88671σ, for CLb:0.0296, CLsb:0.0194, CLs:0.6554

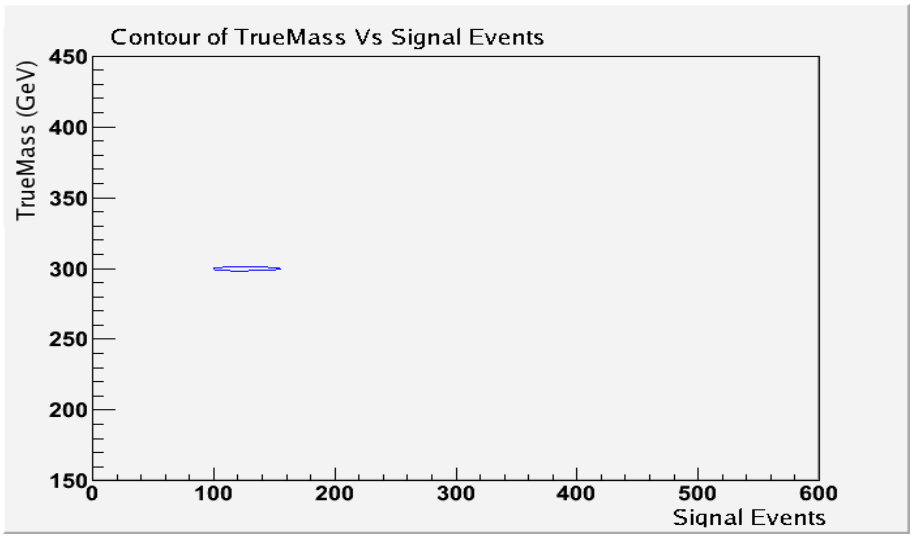

Figure 27: Three Tests, however only the 2D Profile Likelihood Test was successful, shown is the 90% confidence interval

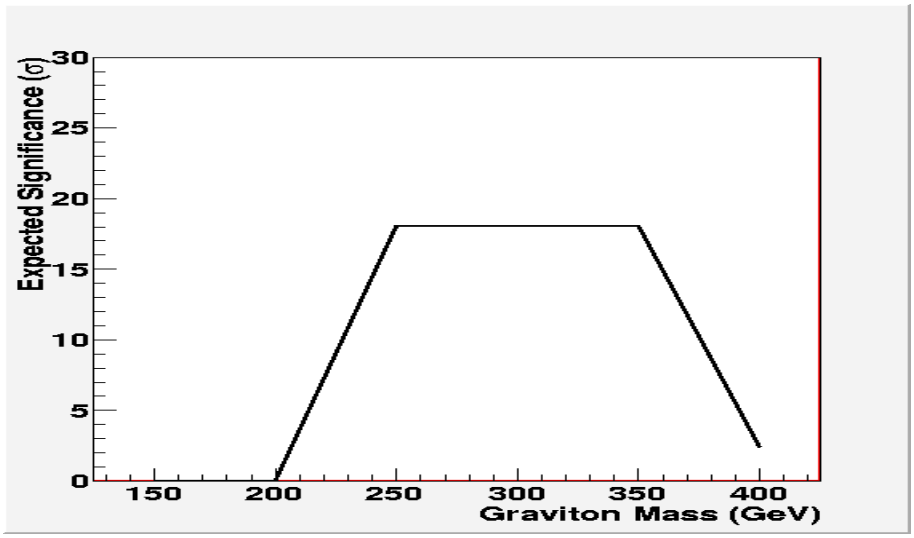

Figure 28: Combination of WorkSpaces to give model significance with varying Model Graviton Mass, when a 300 GeV TrueMass Graviton exists

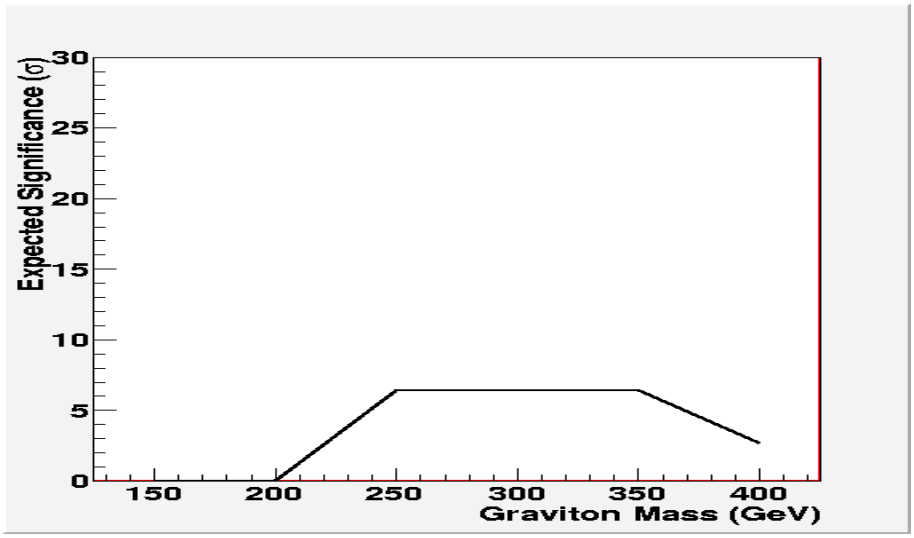

Figure 29: Combination of WorkSpaces to give model significance with varying Model Graviton Mass, when a 300 GeV TrueMass Graviton exists but with 25% of the expected number of events

D Model Range

In this last appendix you will find then model & data stored in each of the WorkSpace's used to compute the significances for the Combination Run macro.

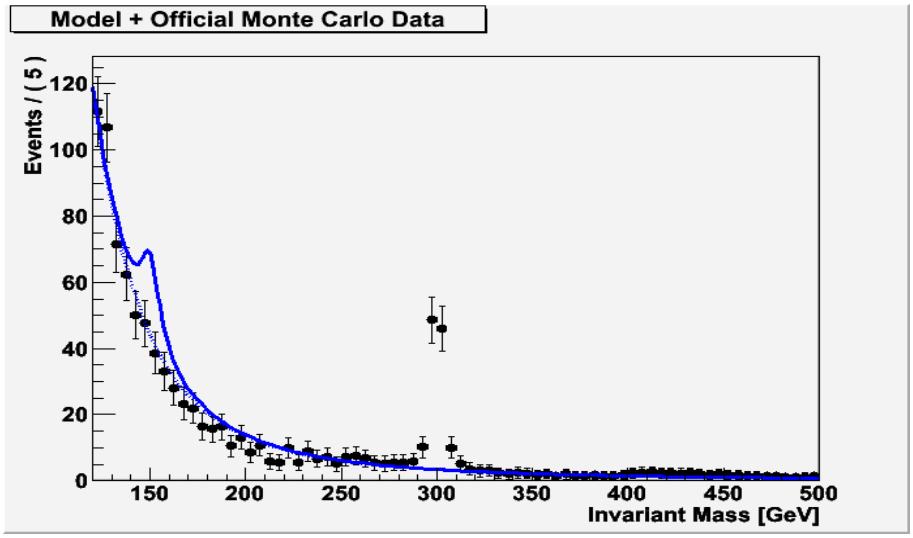

Figure 30: Model for 150 GeV Graviton with Official 300 GeV Graviton dataset

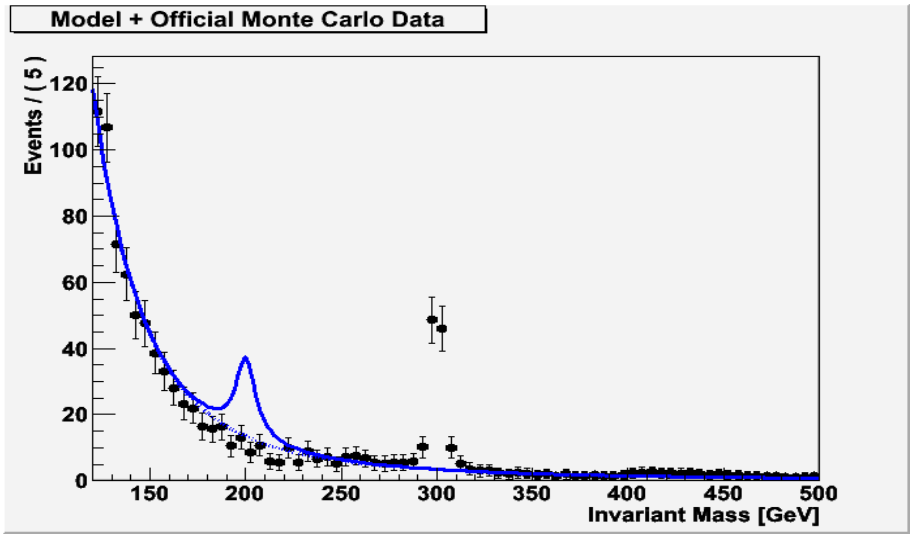

Figure 31: Model for 200 GeV Graviton with Official 300 GeV Graviton dataset

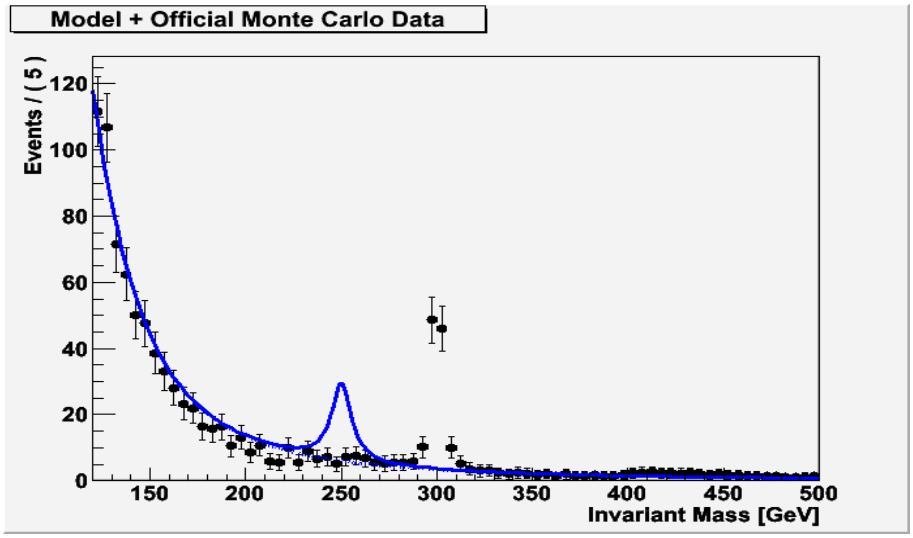

Figure 32: Model for 250 GeV Graviton with Official 300 GeV Graviton dataset

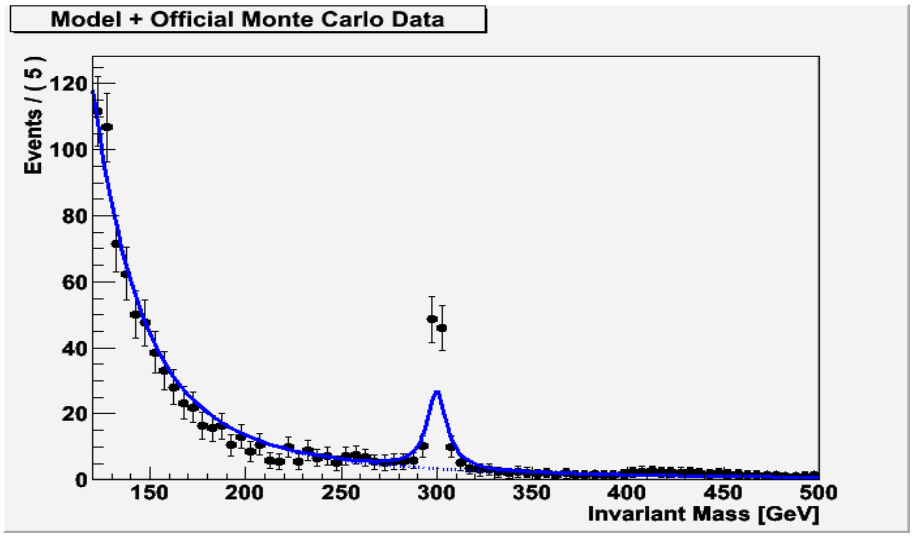

Figure 33: Model for 300 GeV Graviton with Official 300 GeV Graviton dataset

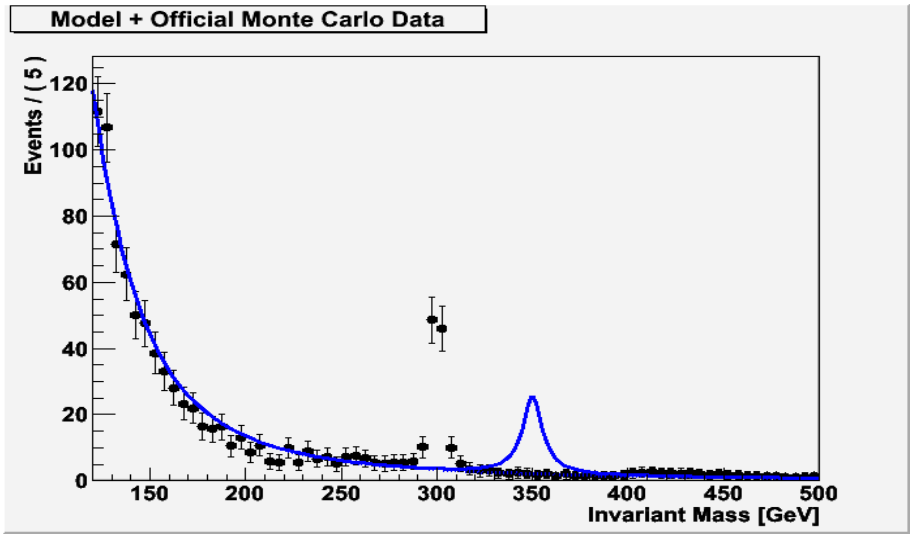

Figure 34: Model for 350 GeV Graviton with Official 300 GeV Graviton dataset

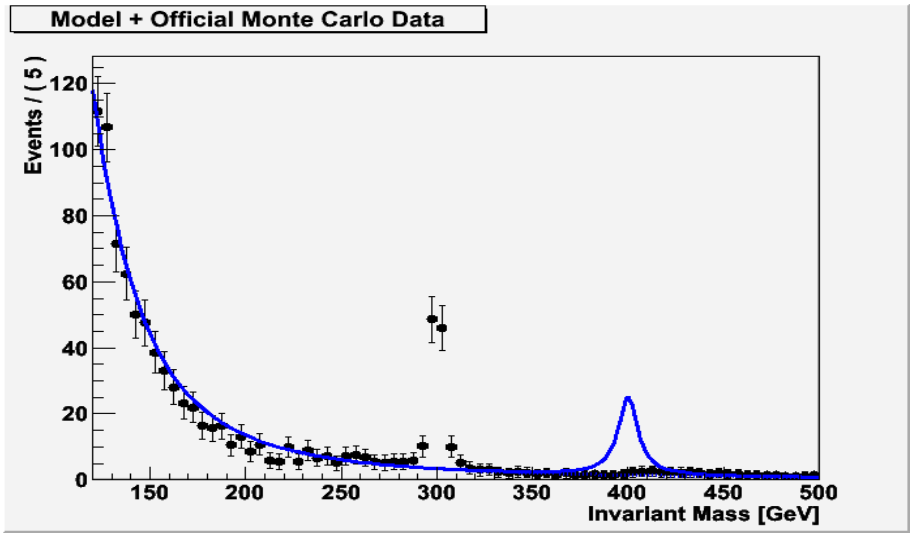

Figure 35: Model for 400 GeV Graviton with Official 300 GeV Graviton dataset

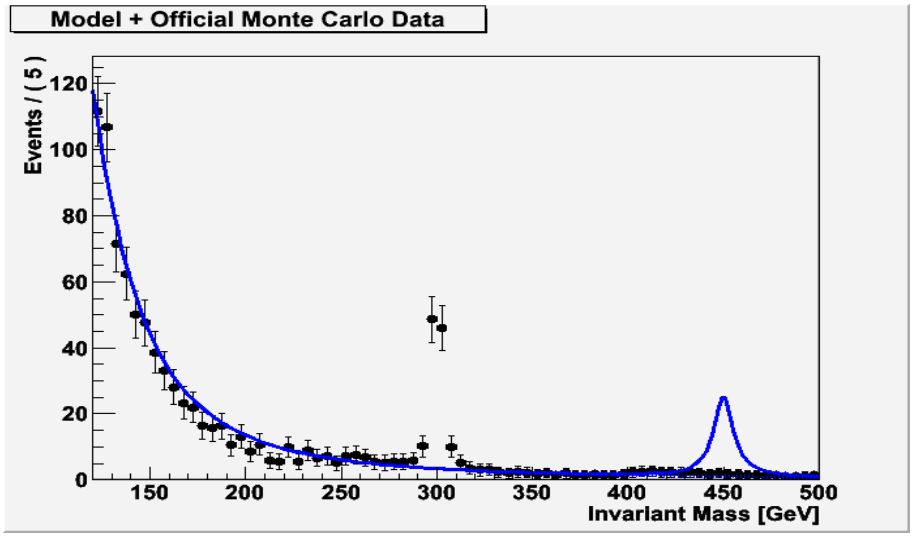

Figure 36: Model for 450 GeV Graviton with Official 300 GeV Graviton dataset

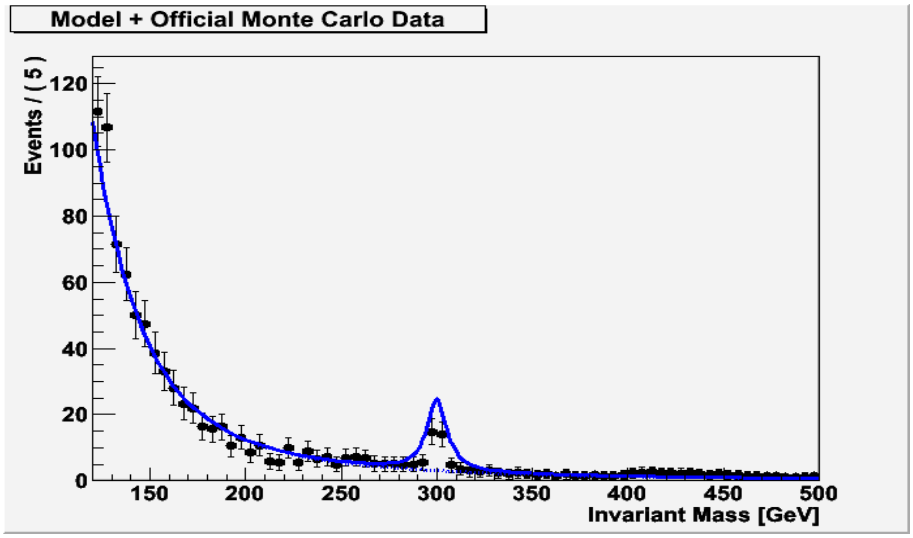

Figure 37: Model for 300 GeV Graviton with Official 300 GeV Graviton dataset but 25% the expected number of signal events