RooStats
Lecture and Tutorials

Outline

- Introduction to RooFit
  - Basic functionality
  - Model building using the workspace
  - Composite models
- Exercises on RooFit:
  - building and fitting models
- Introduction to RooStats
  - Interval estimation tools (Likelihood/Bayesian)
  - Hypothesis tests
  - Frequentist interval/limit calculator (CLs)
- Exercises on interval/limit estimation and discovery significance (hypothesis test)

RooStats Project

- Collaborative project to provide and consolidate advanced statistical tools needed by LHC experiments
- Joint contribution from ATLAS, CMS, ROOT and RooFit
  - developments over-sighted by ATLAS and CMS statistics committees
  - initiated from previous code developed in ATLAS and CMS
  - used by both collaborations

RooStats Goal

- Common framework for statistical calculations
  - work on arbitrary models and datasets
    - factorize modeling from statistical calculations
  - implement most accepted techniques
    - frequentists, Bayesian and likelihood based tools
  - possible to easy compare different statistical methods
  - provide utility for combinations of results
  - using same tools across experiments facilitates the combinations of results

Statistical Applications

- Statistical problems:
  - point estimation (covered by RooFit)
  - estimation of confidence (credible) intervals
  - hypothesis tests
  - goodness of fit (not yet addressed)

RooStats Technology

- Built on top of RooFit
  - generic and convenient description of models (probability density function or likelihood functions)
  - provides *workspace* (RooWorkspace)
    - container for model and data and can be written to disk
    - inputs to all RooStats statistical tools
    - convenient for sharing models (e.g digital publishing of results)
  - easily generation of models (workspace factory and HistFactory tool)
  - tools for combinations of model (e.g. simultaneous pdf)
- Use of ROOT core libraries:
  - minimization (e.g. Minuit), numerical integration, etc...
  - additional tools provided when needed (e.g. Markov-Chain MC)

RooStats Design

- C++ interfaces and classes mapping to real statistical concepts

RooStats Calculator classes

Interval Calculators

- ProfileLikelihoodCalculator
  - interval estimation using asymptotic properties of the likelihood function
- BayesianCalculator
  - interval estimation based on Bayes theorem using adaptive numerical integration
- MCMCCalculator
  - Bayesian calculator using Markov-Chain Monte Carlo

HypoTest Calculators

- HypoTestInverter
  - invert hypothesis test results to estimate an interval
    - CLs limits, FC interval
- NeymanConstruction and FeldmanCousins
  - frequentist interval calculators
- HybridCalculator, FrequentistCalculator
  - frequentist hypothesis test calculators using toy data (difference in treatment of nuisance parameters)
- AsymptoticCalculator
  - hypothesis tests using asymptotic properties of likelihood function

ModelConfig Class

- `ModelConfig` class input to all Roostats calculators
  - contains a reference to the RooFit workspace class
  - provides the workspace meta information needed to run RooStats calculators
    - pdf of the model stored in the workspace
    - what are observables (needed for toy generations)
    - what are the parameters of interest and the nuisance parameters
    - global observables (from auxiliary measurements) for frequentist calculators
    - prior pdf for the Bayesian tools
  - ModelConfig can be imported in workspace for storage and later retrieval

Building ModelConfig Class

- ModelConfig must be built after having the workspace
- Identify all the components which are present in the workspace

```
//specify components of model for statistical tools
ModelConfig  modelConfig("G(xlmu,1)");
modelConfig.SetWorkspace(workspace);
//set components using the name of ws objects
modelConfig.SetPdf( "normal");
modelConfig.SetParameterOfInterest("poi");
modelConfig.SetObservables("obs");
```

- Some tools (Bayesian) require to specify prior pdf

```
//Bayesian tools would also need a prior
modelConfig.SetPriorPdf( "prior");
```

- ModelConfig can be imported in workspace to be then stored in a file

```
//can import modelConfig into workspace too
workspace.import(*modelConfig);
```

Profile Likelihood Calculator

- Method based on properties of the likelihood function
- Profile likelihood function:

$$\lambda(\mu) = \frac{L(x|\mu, \hat{\hat{\nu}})}{L(x|\hat{\mu}, \hat{\nu})}$$

→ maximize w.r.t nuisance parameters ν and fix POI μ

→ maximize w.r.t. all parameters

λ is a function of only the parameter of interest μ

- Uses asymptotic properties of λ based on Wilks' theorem:
- from a Taylor expansion of $\log\lambda$ around the minimum:
  - ➔ $-2\log\lambda$ is a parabola (λ is a gaussian function)
  - ➔ interval on μ from $\log\lambda$ values

- Method of MINUIT/MINOS
  - lower/upper limits for 1D
  - contours for 2 parameters

Using the Profile Likelihood Calculator

```
// create the class using data and model
ProfileLikelihoodCalculator plc(*data, *model);

// set the confidence level
plc.SetConfidenceLevel(0.683);

// compute the interval
LikelihoodInterval* interval = plc.GetInterval();
double lowerLimit = interval->LowerLimit(*mu);
double upperLimit = interval->UpperLimit(*mu);

// plot the interval
LikelihoodIntervalPlot plot(interval);
plot.Draw();
```

- For one-dimensional intervals:
  - 68% CL (1 σ) interval : $\Delta\log\boldsymbol{\lambda} = 0.5$
  - 95% CL interval : $\Delta\log\boldsymbol{\lambda} = 1.96$
- **`LikelihoodIntervalPlot`** can plot the 2D contours

Bayesian Analysis in RooStats

- **RooStats** provides classes for
  - marginalize posterior and estimate credible interval

posterior probability

likelihood function

prior probability

nuisance parameters marginalization

$$P(\mu|x) = \frac{\int L(x|\mu,\nu)\Pi(\mu,\nu)d\nu}{\underbrace{\iint L(x|\mu,\nu)\Pi(\mu,\nu)d\mu d\nu}_{\text{normalisation term}}}$$

POI data

Bayesian Theorem

  - support for different integration algorithms:
    - adaptive (numerical)
    - MC integration
    - Markov-Chain
  - can work with models with many parameters (e.g few hundreds)

Bayesian Classes

- **`BayesianCalculator`** class
  - posterior and interval estimation using numerical integration
  - working only for one parameter of interest but can integrate (marginalize) many nuisance parameters
  - support for different integration algorithms, using **`BayesianCalculator::SetIntegrationType`**
    - adaptive numerical (default type), working only for few nuisances (< 10)
    - Monte Carlo integration (PLAIN, MISER, VEGAS)
    - TOYMC : average from toys where the nuisance parameters are sampled from a given p.d.f. (nuisance pdf), but can work in model with many parameters
  - can compute:
    - central interval
    - one-sided interval (upper limit)
    - a shortest interval
  - provide plot of posterior and interval

Example: 68% CL central interval

```
BayesianCalculator bc(data, model);
bc.SetConfidenceLevel(0.683);
bc.SetLeftSideTailFraction(0.5);
bc.SetIntegrationType("ADAPTIVE");
SimpleInterval* interval = bc.GetInterval();
double lowerLimit = interval->LowerLimit();
double upperLimit = interval->UpperLimit();
RooPlot * plot = bc.GetPosteriorPlot();
plot->Draw();
```

MCMC Calculator

- **`MCMCCalculator`** class
  - integration using Markov-Chain Monte Carlo (Metropolis Hastings algorithm)
  - can deal with more than one parameter of interest
  - can work with many nuisance parameters
    - e.g. used in Higgs combination with more than 300 nuisances
  - possible to specify ProposalFunction
    - multivariate Gaussian from fit result
    - Sequential proposal
  - can visualize posterior and also the chain result

MCMCCalculator

```
MCMCCalculator mc(data, model);
mc.SetConfidenceLevel(0.683);
mc.SetLeftSideTailFraction(0.5);
SequentialProposal sp(0.1);
mc.SetProposalFunction(sp);
mc.SetNumIters(1000000);
mc.SetNumBurnInSteps(50);
MCInterval* interval = bc.GetInterval();
RooRealVar * s = (RooRealVar*)
model.GetParametersOfInterest()->find("s");
double lowerLimit = interval->LowerLimit(*s);
double upperLimit = interval->UpperLimit(*s);
MCMCIntervalPlot plot(*interval);
```

Running RooStats

- RooStats provides standard tutorials taking all as input workspace, ModelConfig and data set names
- StandardProfileLikelihoodDemo.C

```
run ProfileLikelihoodCalculator - get interval and produce plot

root[]StandardProfileLikelihoodDemo("ws.root","w","ModelConfig","data")
```

- StandardBayesianNumericalDemo.C

```
run Bayesiancalculator: get a credible interval and produce plot of posterior function

root[]StandardBayesianNumericalDemo("ws.root","w","ModelConfig","data")
```

- StandardBayesianMCMCDemo.C

```
run bayesian MCMCCalculator: get a credible interval and produce plot of posterior function

root[]StandardBayesianMCMCDemo("ws.root","w","ModelConfig","data")
```

Time For Exercises !

Follow the Twiki page at
https://twiki.cern.ch/twiki/bin/view/RooStats/RooStatsTutorialsMarch2015

RooStats
Part2

- Hypothesis tests in RooStats using toys and asymptotic formulae
- Hypothesis test inversion
  - Limit and interval calculators
    - CLs, Feldman-Cousins

Frequentist Hypothesis Tests

- Ingredients:
  - Null Hypothesis: the hypothesis being tested (e.g. $\theta = \theta_0$), assumed to be true and one tries to reject it
  - Alternate Hypothesis: the competitive hypothesis (e.g. $\theta \neq \theta_0$)
  - w is the critical region, a subspace of all possible data:
    - size of test : $\alpha = P(X \in w \mid H_0)$
    - power of test : $1- \beta = P(X \in w \mid H_1)$
  - Test statistics: a function of the data, t(X) ,used for defining the critical region in multidimensional data: $X \in w \rightarrow t(X) \in w_t$

RooStats Hypothesis Test

- Define null and alternate model using ModelConfig
  - can use ModelConfig::SetSnapshot(const RooArgSet &) to define parameter values for the null in case of a common model (e.g. $\mu = 0$ for the B model)
- Select test statistics to use
- Select calculator
  - Use toys or asymptotic formula to get sampling distribution of test statistics
  - FrequentistCalculator or HybridCalculator have different treatment of nuisance parameters

Test Statistics

- Test statistics maps multidimensional space in one, in a way relevant to the hypothesis being tested

RooStats has the three common test statistics used in the field (and more)

- simple likelihood ratio (used at LEP, nuisance parameters fixed)

$$Q_{LEP} = L_{s+b}(\mu = 1)/L_b(\mu = 0)$$

- ratio of profiled likelihoods (used commonly at Tevatron)

$$Q_{TEV} = L_{s+b}(\mu = 1, \hat{\hat{\nu}})/L_b(\mu = 0, \hat{\hat{\nu}}')$$

- profile likelihood ratio (related to Wilks's theorem)

$$\lambda(\mu) = L_{s+b}(\mu, \hat{\hat{\nu}})/L_{s+b}(\hat{\mu}, \hat{\nu})$$

- preferred choice is profile likelihood ratio which has known asymptotic distribution

FrequentistCalculator

- Generate toys using nuisance parameter at their conditional ML estimate ($\hat{\theta} = \theta_\mu$) by fitting them to the observed data
- Treat constraint terms in the likelihood (e.g. systematic errors) as auxiliary measurements
  - introduce global observables which will be varied (tossed) for each pseudo-experiment
  - $L = \text{Poisson}(n_{obs} \mid \mu + b)\ \text{Gaussian}(b_0 \mid b, \sigma_b)$
    - b_0 is a global observables, varied for each toys but it needs to be considered constant when fitting
    - n_{obs} is the observable which is part of the data set
    - μ is the parameter of interest (poi)
    - b is the nuisance parameter

HybridCalculator

- Nuisance parameters are integrated using their pdf (the constraint term) which is interpreted as a Bayesian prior
  - integration is done by generating for each toys different nuisance parameters values
  - need to have a pdf for the nuisance parameters (often it can be derived automatically from the model)

$$L = \text{Poisson}(\, n_{obs} \mid \mu + b)\ \text{Gaussian}(\, b \mid b_0, \sigma_b)$$

$$L = \int \text{Poisson}(\, n_{obs} \mid \mu + b)\ \text{Gaussian}(\, b \mid b_0, \sigma_b)\, db$$

Example: FrequentistCalculator

- Define the models
  - N.B for discovery significance null is B model and alt is S+B

```
// create first HypoTest calculator (data, alt model , null model)
FrequentistCalculator fcalc(*data, *sbModel, *bModel);

// create the test statistics
ProfileLikelihoodTestStat profll(*sbModel->GetPdf());
// use one-sided profile likelihood for discovery tests
profll.SetOneSidedDiscovery(true);

// configure  ToyMCSampler and set the test statistics
ToyMCSampler *toymcs = (ToyMCSampler*)fcalc.GetTestStatSampler();
toymcs->SetTestStatistic(&profll);

fcalc.SetToys(1000,1000);  // set number of toys for (null, alt)

// run the test
HypoTestResult * r = fcalc.GetHypoTest();
r->Print();

// plot test statistic distributions
HypoTestPlot * plot = new HypoTestPlot(*r);
plot->Draw();
```

```
Results HypoTestCalculator_result:
 - Null p-value = 0.034 +/- 0.00573097
 - Significance = 1.82501 sigma
 - Number of Alt toys: 1000
 - Number of Null toys: 1000
```

AsymptoticCalculator

- Use the asymptotic formula for the test statistic distributions
- one-sided profile likelihood test statistic:
  - null model ($\mu = \mu_{TEST}$)
    - half X^2 distribution
  - alt model ($\mu \neq \mu_{TEST}$)
    - non-central X^2
    - use Asimov data to get the non centrality parameter $\Lambda = (\mu - \mu_{TEST})/\sigma$
- p-values for null and alternate can be obtained without generating toys

$$\lambda(\mu) = \frac{L(x|\mu, \hat{\hat{\nu}})}{L(x|\hat{\mu}, \hat{\nu})}$$

$\lambda(\mu) = 0$ for
$\hat{\mu} < 0$ (discovery)
$\hat{\mu} < \mu_{TEST}$ (limits)

➡ see Cowan, Cranmer, Gross, Vitells, arXiv:1007.1727, EPJC 71 (2011) 1-1

Example: Discovery Significance

- Performing the tests for different mass hypotheses (*i.e* different signal models):

Inversion of Hypothesis Tests

- one-to-one mapping between hypothesis tests and confidence intervals

Table 20.1 Relationships between hypothesis testing and interval estimation

Property of test	Property of corresponding confidence interval
Size $= \alpha$	Confidence coefficient $= 1 - \alpha$
Power = probability of rejecting a false value of $\theta = 1 - \beta$	Probability of not covering a false value of $\theta = 1 - \beta$
Most powerful	Uniformly most accurate
$\longleftarrow$	$\left\{ \begin{array}{c} \textit{Unbiased} \\ 1 - \beta \geq \alpha \end{array} \right\}$ $\longrightarrow$
Equal-tails test $\alpha_1 = \alpha_2 = \frac{1}{2}\alpha$	Central interval

from G. Feldman visiting Harvard statistics department

They explained that in statistical theory there is a one-to-one correspondence between a hypothesis test and a confidence interval. (The confidence interval is a hypothesis test for each value in the interval.) The Neyman-Pearson Theorem states that the likelihood ratio gives the most powerful hypothesis test. Therefore, it must be the standard method of constructing a confidence interval.

Hypothesis Test Inversion

- Performing an hypothesis test at each value of the parameter
- Interval can be derived by inverting the p-value curve, function of the parameter of interest (μ)
  - value of μ which has p-value α (e.g. 0.05), is the upper limit of 1-α confidence interval (e.g. 95%)

Hypothesis Test Inversion

- use one-sided test for upper limits (e.g. one-side profile likelihood test statistics)
- use two-sided test for a 2-sided interval

Example: 1-σ interval for a Gaussian measurement

HypoTestInverter class

- Input is an Hypothesis Test calculator:
  - Frequentist/Hybrid/AsymptoticCalculator
  - possible to customize test statistic, number of toys, etc..
    - N.B: null model is S+B, alternate is B only model
- Compute an Interval (result is a **`ConfInterval`** object):
  - scan given interval of μ and perform hypothesis tests
  - compute upper/lower limit from scan result
    - can use $CL_s = CL_{s+b} \ / \ CL_b$ for the p-value
  - result (**`HypoTestInverterResult`**) contains all the hypothesis test results for each scanned μ value
  - can compute expected limits and bands

HypoTestInverter

- **HypoTestInverter** class in RooStats

```
// create first HypoTest calculator (N.B null is s+b model)
FrequentistCalculator fc(*data, *bModel, *sbModel);

HypoTestInverter calc(*fc);
calc.UseCLs(true);

// configure  ToyMCSampler and set the test statistics
ToyMCSampler *toymcs = (ToyMCSampler*)fc.GetTestStatSampler();

ProfileLikelihoodTestStat profll(*sbModel->GetPdf());
// for CLs (bounded intervals) use one-sided profile likelihood
profll.SetOneSided(true);
toymcs->SetTestStatistic(&profll);

// configure and run the scan
calc.SetFixedScan(npoints,poimin,poimax);
HypoTestInverterResult * r = calc.GetInterval();

// get result and plot it
double upperLimit = r->UpperLimit();
double expectedLimit = r->GetExpectedUpperLimit(0);

HypoTestInverterPlot *plot = new HypoTestInverterPlot("hi","",r);
plot->Draw();
```

Running the HypoTestInverter

Hypothesis test results for each scanned point

Scan result

How expected limit and bands are obtained ?

- compute p-value for quantiles (median, +/1,2 sigma) of the B model test statistic distribution (*i.e.* use quantile as the observed value)

p-value, CL_{s+b} (or CL_b) is integral of S+B (or B) test statistic distribution from data value

Asymptotic Limits

- **AsymptoticCalculator** class for HypoTestInverter
  - use the asymptotic formula for the test statistic distributions
    - χ^2 approximation for the profile likelihood ratio
      - see G. Cowan *et al.*, arXiv:1007.1727,EPJC 71 (2011) 1-1
  - p-values CL_{s+b} (null) and CL_b (alt) obtained without generating toys
  - also expected limits from the alt distribution

```
// create first HypoTest calculator (N.B null is s+b model)
AsymptoticCalculator ac(*data, *bModel, *sbModel);

HypoTestInverter calc(*ac);
// run inverter same as using other calculators
........
```

Example of Scan

- 95% CL limit on a Gaussian measurement:
  - Gauss(x,μ,1), with μ≥0

deficit, observation x = -1.5

excess, observation x = 1.5

use CL_s as p-value to avoid setting limits which are too good

Example: Computing Limits

- By computing limits for different mass hypothesis:

Limits on bounded measurements

from Bob Cousins:

Downward fluctuations in searches for excesses

Classic example: Upper limit on mean μ of Gaussian based on measurement *x* (in units of σ).

If $\mu \geq 0$ in model, as measured x becomes increasingly negative, standard classical upper limit becomes small and then null.

Issue acute 15-25 years ago in expts to measure ν_e mass in (tritium β decay): several measured $m_\nu^2 < 0$.

Frequentist 1-sided 95% C.L. Upper Limits, based on α = 1 – C.L. = 5% (called CL_{sb} at LEP).

For *x* < –1.64 σ the confidence interval is the *null* set!

Bob Cousins, CMSDAS, 1/2012

Feldman-Cousins intervals

- HypoTestInverter class can compute also a Feldman-Cousins interval
  - need to use FrequentistCalculator and CL_{s+b} as p-value
  - use the 2-sided profile likelihood test statistic

$$\lambda(\mu) = \frac{L(x|\mu, \hat{\hat{\nu}})}{L(x|\hat{\mu}, \hat{\nu})}$$

observation x = -1.5

observation x = 1.5

Feldman-Cousins Interval

from Kyle Cranmer:

A different way to picture Feldman-Cousins

CENTER FOR COSMOLOGY AND PARTICLE PHYSICS

Most people think of plot on left when thinking of Feldman-Cousins

- bars are regions "ordered by" $R = P(n|\mu)/P(n|\mu_{\rm best})$, with $\int_{x_1}^{x_2} P(x|\mu)dx = \alpha.$

But this picture doesn't generalize well to many measured quantities.

- Instead, just use R as the test statistic... and R is λ(μ)

Kyle Cranmer (NYU) CERN School HEP, Romania, Sept. 2011 134

Example: Feldman-Cousins interval

- Same RooStats code but with different configuration can compute also a Feldman-Cousins interval

StandardHypoTestInvDemo.C

- Standard ROOT macro to run the Hypothesis Test inversion.
- Inputs to the macro:
  - workspace file, workspace name
  - name of S+B model (null) and for B model (alt)
    - if no B model is given, use S+B model with poi = 0
  - data set name
  - calculator type: frequentist (= 0), hybrid (=1), or asymptotic (=2)
  - test statistics
- options:
  - use CL_s or CL_{s+b} for computing limit
  - number of points to scan and min, max of interval

```
load the macro after having created the workspace and saved in file SPlusBExpoModel.root
root[] .L StandardHypoTestInvDemo.C

run for CLs (with  frequentist calculator (type = 0) and one-side PL test statistics (type = 3) scan 10 points in [0,100]

root[] StandardHypoTestInvDemo("SPlusBExpoModel.root","w","ModelConfig","","data",0,3, true, 10, 0, 100)

run for Asymptotic CLs (scan 20 points in [0,100])

root[] StandardHypoTestInvDemo(SPlusBExpoModel.root","w","ModelConfig","","data",2,3, true, 20, 0, 100)

run for Feldman-Cousins  ( scan 10 points in [0,100])

root[] StandardHypoTestInvDemo(SPlusBExpoModel.root","w","ModelConfig","","data",0,2, false, 10, 0, 100)
```

HistFactory – a new class of pdfs

- Focus of RooFit traditionally on analytical models
  - Assumes you can formulate signal/background in an analytical form
  - Often possible in e+e- experiments,
    shapes for hadron colliders cumbersome → **rely on MC simulation**

Analytical form:
Gaussian+Polynomial

Template form:
Histogram (discrete)

K. Cranmer, G. Lewis, L. Moneta, A. Shibata, and W. Verkerke, *HistFactory: A tool for creating statistical models for use with RooFit and RooStats*, CERN-OPEN-2012-016 (2012). `http://cdsweb.cern.ch/record/1456844`.

Model Building with HistFactory

- Tool to build models from input histograms

RooFit
Workspace

RooFit/RooStats at LHC (Higgs analysis)

Class RooWorkspace

Simplify packaging and sharing of models

RooStats toolkit

Statistical tests based on likelihoods from RooFit models

HistFactory package

Constructing models from Monte Carlo templates

How well does it scale?

Graph of the full ATLAS Higgs combination model

Model has ~23.000 function objects, ~1600 parameters

Reading/writing of full model takes ~4 seconds

ROOT file with workspace is ~6 Mb

Summary

- RooFit/RooStats allow you to perform advanced statistical data/analysis
  - LHC results (*e.g.* Higgs observation)
- Capable of using different tools and interpretations (Frequentist/Bayesian) on the same model
- Generic tools capable to deal with large variety of models
  - based on histograms or un-binned data
  - multi-dimensional observations
- Provide tools to facilitate complex model building
  - HistFactory for histogram based analysis

Documentation

- RooStats TWiki: https://twiki.cern.ch/twiki/bin/view/RooStats/WebHome
- RooStats users guide (not really completed)
  - http://root.cern.ch/viewcvs/branches/dev/roostats/roofit/roostats/doc/usersguide/RooStats_UsersGuide.pdf
- For reference and citation: ACAT 2010 proceedings papers: http://arxiv.org/abs/1009.1003
- RooStats tutorial macros: http://root.cern.ch/root/html534/tutorials/roostats/index.html
- HistFactory document: https://cdsweb.cern.ch/record/1456844/files/CERN-OPEN-2012-016.pdf
- RooStats user support:
  - Request support via ROOT talk forum: http://root.cern.ch/phpBB2/viewforum.php?f=15 (questions on statistical concepts accepted)
  - contact me directly (email: Lorenzo.Moneta at cern.ch)
- Contacts for statistical questions:
  - ATLAS statistics forum:
    - TWiki: https://twiki.cern.ch/twiki/bin/view/AtlasProtected/StatisticsTools
  - CMS statistics committee:
    - TWiki: https://twiki.cern.ch/twiki/bin/view/CMS/StatisticsCommittee

Time For Exercises !

Follow the Twiki page at
https://twiki.cern.ch/twiki/bin/view/RooStats/RooStatsTutorialsMarch2015