The RooStats Project

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RooStats is a project to create advanced statistical tools required for the analysis of LHC data, with emphasis on discoveries, confidence intervals, and combined measurements. The idea is to provide the major statistical techniques as a set of C++ classes with coherent interfaces, which can be used on arbitrary model and datasets in a common way. The classes are built on top of RooFit, which provides a very convenient functionality for modeling the probability density functions or the likelihood functions, required as inputs for any statistical technique. Furthermore, RooFit provides the functionality for easily creating models, for analysis combination and for digital publication of the likelihood function and the data. We will present in detail the design and the implementation of the different statistical methods of RooStats. These include various classes for interval estimation and for hypothesis test depending on different statistical techniques such as those based on the likelihood function, or on frequentists or bayesian statistics. These methods can be applied in complex problems, including cases with multiple parameters of interest and various nuisance parameters.

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1. Introduction

The Large Hadron Collider (LHC), which started to take data at the end of 2009 is expected to produce an unprecedented amount of data to be analyzed. These data offer a tremendous potential for the discovery of new physics and pose many challenges to the statistical techniques used in High Energy Physics. Different statistical approaches are used for statistical inference and results from different methods will be needed since they proceed through different treatment of systematic uncertainties and they answer different questions. Furthermore, statistical combinations of analyses of different search channels will be required and combinations of results obtained by different experiments will be performed. Up to now, in the past experiments like those at LEP or at the Tevatron, dedicated code specific to the statistical method and to the analysis has been used to produce a result (e.g. an exclusion limit) and to perform the combinations. Therefore, there has been a need to develop generic and versatile software for implementing these required statistical tools. The code should provide a unified framework in order to be used for different statistical techniques. Three major types of statistical inference have been identified:

- **Classical / Frequentist**: this “school” of statistics restricts itself to making statements of the form “probability of the data given the hypothesis”. The definition of probability in this context is based on a limit of frequencies of various outcomes. In that sense it is objective.

- **Bayesian**: this “school” of statistics allows one to make statements of the form "probability of the hypothesis given the data", which requires a prior probability of the hypothesis. Often the definition of probability in this context is a “degree of belief”.

- **Likelihood-based**: this intermediate approach also uses a frequentist notion of probability (ie. does not require a prior for the hypothesis), but also it is not guaranteed to pose the properties (ie. coverage) that frequentists methods aim to achieve (or achieve by construction). These approaches do “obey the likelihood principle” (as do Bayesian methods), while frequentist methods do not.

The goal is to be able to use for the same input model different statistical methods. These methods differ also in the way the incorporate the nuisance parameters for producing the results and they answer different statistical questions, so there is a need to have all three results. The software needs also to be versatile in order to be able to cope with both simple analyses, such as those based on number counting, and complex ones which use the parametrization of experimental distributions.

A new project, RooStats, was initiated at the end of 2008 with the aim to deliver this unified statistical framework. It started from merging previous code developed by Kyle Cranmer for Phystat 2008 [1] and from a CMS project, RooStatsCms [2]. RooStats is organized as a joint collaboration between ATLAS and CMS and it is based on ROOT and RooFit. The developments are over-sighted by the ATLAS and CMS statistical committees. It has been built on top of ROOT [3], since ROOT is the most widely used tool in HEP for data analysis and it provides the needed basic software (mathematical libraries, graphics libraries for plotting, I/O and dictionary libraries). RooStats is also based on the classes of the RooFit toolkit [4], which allows a convenient description of the data model and it is a well-established software within the HEP community.
statistical tools require as input model a probability density function and/or a likelihood function. RooFit provides classes facilitating the building of the model and a way to re-use it for multiple statistical methods. This is possible, since RooFit has no statistical notion of parameters and observables, so it can work naturally with both frequentist and bayesian techniques. RooStats can then be seen as providing high-level statistical tools, while RooFit provides the core data modeling language as well as many low-level aspects of the functionality.

1.1 Type of Statistical Questions

One of the first steps in any statistical analysis is to carefully pose the question that one wishes to answer. Most of these questions can be classified as follows:

- **Parameter Estimation**: find the most likely (‘best fit’) values of the parameters of a model given data.

- **Hypothesis Testing**: based on the data accept or reject a given hypothesis. Often one tests a null hypothesis against an alternative. When the hypothesis has no free parameters it is called ‘simple’ and when it has free parameters it is called ‘composite’.

- **Confidence intervals**: find a region in the parameter space that is consistent with the data. In the frequentist setting, one desires for this interval or region to ‘cover’ the true parameter point with a specified probability (or confidence). In the Bayesian setting, one wishes for the interval or region to contain some fixed amount of the posterior probability.

- **Goodness of Fit**: quantify how well a model fits the data, without reference to an alternative.

RooFit provides the functionality for point estimation while RooStats provides tools for confidence interval estimations and hypothesis testing in addition to some miscellaneous utilities. Classes for goodness of fit are currently provided in the core ROOT mathematical libraries.\(^1\).

2. RooStats Interfaces

One of the fundamental design philosophies behind RooStats is a conceptually clear mapping between mathematics and software. We have tried to identify fundamental concepts in statistics and assign corresponding C++ classes or interfaces. The interfaces have been designed to reflect the types of statistical questions shown above and they are implemented as C++ classes according on the type of statistical technique.

As shown in figure 1, RooStats provides a common interface for confidence interval calculations, `IntervalCalculator`, and another interface for performing the hypothesis tests, `HypoTestCalculator`.

The `IntervalCalculator` produces as result a confidence interval, which is represented by the RooStats `ConfInterval` interface. The resulting type of `ConfInterval` will depend on the implementation used for the interval calculator. There are many types of intervals, they can be simple one dimensional intervals or disconnected regions in multiple dimensions. The common

\(^1\)see the ROOT functions `TH1::Chi2Test` and `TMath::KolmogorovTest`
interface provides a method, `ConfInterval::IsInInterval(p)`, to ask the interval if a given point is inside. The `IntervalCalculator` interface allows the user to pass the model, the data set, the parameters of interest, the nuisance parameters and the confidence level or size of the test. After configuring the calculator, a `ConfInterval` pointer is returned via the method `IntervalCalculator::GetInterval()`.

The `HypoTestCalculator` is the interface for performing hypothesis tests. After configuring the class, by passing the model, the data set and the parameter sets specifying the null and the alternate hypothesis, it returns, via `HypoTestCalculator::GetHypoTest()`, a pointer to the `HypoTestResult` interface, which holds the result of the test and can be used to obtain the p values of the null and alternate hypothesis, the confidence level values and the corresponding significance, defined in terms of 1-sided Gaussian standard deviations.

3. RooStats Calculators

Using the different statistical techniques, frequentists, bayesian or likelihood based, RooStats provides implementation classes for the interfaces described above. We will give below a brief description of the methods; for a detailed description of the statistical techniques, see for example [5]. For a full description of the RooStats classes, see the RooStats reference documentation.

3.1 ProfileLikelihood Calculator

The `ProfileLikelihoodCalculator` class is a combined calculator implementing both the `IntervalCalculator` and the `HypoTestCalculator` interfaces. It is based on the asymptotic property of the likelihood function, which can be used to estimate a parameter, its confidence level and to perform an hypothesis test for a given parameter value.

The likelihood function is defined, for example, by the equation:

$$L(x, \theta) = \prod_{i=1}^{N} f(x_i, \theta).$$  \hspace{1cm} (3.1)

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2 see http://root.cern.ch/root/htmldoc/ROOFIT_ROOSTATS_Index.html
where \( \mathbf{x} = (x_a, x_b, x_c, \ldots) \) is a set of \( N \) measured quantities, whose distributions are described by a joint probability density function, \( f(\mathbf{x}, \theta) \), where \( \theta = (\theta_1, \theta_2, \theta_3, \ldots) \) is a set of \( K \) parameters. For simplicity, let’s focus on one dimensional case where we have a parameter of interest, \( \theta_0 \) and \( K - 1 \) nuisance parameters. The profile likelihood is a function of \( \theta_0 \) and it is defined as

\[
\lambda(\theta_0) = \frac{L(\theta_0, \hat{\theta}_{\neq 0})}{L(\hat{\theta}_0, \hat{\theta}_{\neq 0})}.
\]

The denominator, \( L(\hat{\theta}_0) \) is the maximum likelihood value, obtained from the best fit to the data, while the numerator is the maximum value obtained by fixing \( \theta_0 \) and varying the remaining \( K - 1 \) parameters. It can be shown (Wilks’s theorem) that asymptotically \(-2 \ln \lambda(\theta_0)\) is distributed as a \( \chi^2(1) \) distribution (\( \chi^2(n) \) in the case of \( n \) parameter of interest). This is not surprising since in the asymptotic limit the Likelihood function becomes a Gaussian centered around the maximum likelihood estimator \( \hat{\theta}_0 \), and the profile likelihood curve has a parabolic shape:

\[
-2 \ln \lambda(\theta_0) = -2(\ln L(\theta_0) - \ln L(\hat{\theta}_0)) = n_\sigma^2, \quad \text{with} \quad n_\sigma = \frac{\theta_0 - \hat{\theta}_0}{\sigma}.
\]

where \( \sigma \) represent the Gaussian standard deviations of the parameter \( \theta_0 \). From this construction, it is possible to obtained the one- or two-sided confidence interval we are interested in (see for example figure 2). Even in case of non parabolic log-likelihood functions, it can be shown, due to the invariance property of the likelihood ratios, that this approach is still valid. This method has been also called in the physics community as the of MINOS method since it has been implemented by the MINOS algorithm of the Minuit program [6].

![Figure 2: Plot of the log profile likelihood curve (−log λ) as function of the parameter of interest S. The one \( \sigma \) interval (66.8% CL) is obtained from the intersect with the horizontal dashed line (−log λ = 0.5).](image)
ProfileLikelihoodCalculator returns as result a LikelihoodInterval, which can represents a multi dimensional contour in the case of \( n \) parameters of interest. A class exists, LikelihoodIntervalPlot, to visualize the likelihood interval in the case of one or two dimension (figure 2 shows the obtained plot in one dimensional problem).

Given the fact that asymptotically \( -2 \ln \lambda \) is distributed as a \( \chi^2 \) distribution, an hypothesis tests can be performed for the null hypothesis \( H_0 \), corresponding to \( \theta = \theta' \), and the alternate hypothesis \( H_1 \) for \( \theta \neq \theta' \).

3.2 Bayesian Calculators

RooStats provide two different types of Bayesian calculators, the BayesianCalculator class and MCMCCalculator. Both are based on the Bayes theorem to estimate the posterior probability for the desired parameters of interest. From the posterior probability distribution the Bayesian credible interval can then be obtained. Both classes need to be configured by passing, in addition to the model and the data sets, also the prior distributions of the parameters of interest and of the nuisance parameters, if those are present.

The BayesianCalculator class works only for one single parameter of interest and it uses analytical or numerical integration to compute the posterior probability. The result of the class is a one dimensional interval (class SimpleInterval), which is obtained from the cumulative posterior distribution.

The MCMCCalculator uses the Markov-Chain Monte Carlo to perform the integration. It runs the Metropolis-Hastings algorithm to construct the Markov Chain. The class allows to configure the Metropolis-Hastings algorithm, via number of iterations and burn-in-steps. Moreover, it is possible to replace the default uniform proposal function with any other distribution function. The result of the MCMCCalculator is a MCMCInterval, which can compute the confidence interval on a desired parameter of interest from the obtained Markov Chain. MCMCInterval integrates the posterior where it is the tallest until it finds the correct cut-off height \( C \) to give the target confidence level \( 1 - \alpha \). That is, to find

\[
\int_{f(x) \geq C} f(x) \, dx = 1 - \alpha
\]

To do the integration, the posterior can be represented using an histogram in one or multi-dimensions or using a kernel estimator. The class MCMCIntervalPlot class can be used to visualize the interval and the Markov chain.

As an alternative, a class interfacing the RooStats model to the Bayesian Analysis Toolkit [7], which uses Markov Chain Monte Carlo, is available.

3.3 Neyman Construction

The Neyman construction is a pure frequentist method to construct an interval at a given confidence level value, \( 1 - \alpha \), in order that if we repeat the experiment many times the interval will contain the true value a fraction \( 1 - \alpha \) of the time. A detailed description of the method is given in [5]. RooStats provides a class, NeymanConstruction implementing this technique. The class derives from IntervalCalculator and returns as result a PointSetInterval, a
concrete implementation of ConfInterval. The Neyman Construction is not a uniquely defined statistical technique, it requires that one specifies an ordering rule or ordering principle, which is usually encoded by choosing a specific test statistic and limits of integration (corresponding to upper/lower/central limits). As a result, the RooStats class must be configured with the corresponding information before it can produce an interval. These have been generalized with the interfaces TestStatistic, TestStatSampler, and SamplingDistribution. Common configurations, such as the unified Feldman-Cousins approach, where the ordering is based on the profile likelihood ratio as test statistics and it is described in their paper [8], can be enforced by using the FeldmanCousins class.

The Neyman construction considers every point in the parameter space independently, no assumptions are made that the interval is connected or of a particular shape. The result consists then of a set of scanned points with the information if they are inside or outside the interval (PointSetInterval class). The user indicates which points in the parameter space to perform the construction or provides a range with the number of points which will be scanned uniformly in a grid. For each scanned point, the calculator will obtain the sampling distribution of the chosen test statistics. This is typically obtained by toy Monte Carlo sampling, but other techniques exist and they can be in principle used, although there are not yet implemented in RooStats. The tool also implements a generalization of the Feldman-Cousins procedure when nuisance parameters are present as described in [1, 9]

### 3.4 Hybrid Calculator

The RooStats HybridCalculator class for hypothesis testing implements a traditional frequentist toy Monte Carlo method, like in the Neyman construction, but with a Bayesian marginalization of nuisance parameters [10] Hence the technique is often referred to as a “Bayesian-Frequentist Hybrid”. For example, we define the null hypothesis, $H_0$, that no signal is present over the background and $H_{sb}$ the alternate hypothesis that signal is also present. In order to quantify the degree in which each hypotheses are favored or excluded by the experimental observation, one chooses a test-statistics which ranks the possible experimental outcomes. A commonly used test statistics consists as the ratio of the likelihood function in both hypotheses: $Q = \frac{L_{sb}}{L_b}$ and the quantity $-2\ln Q$ may also be used instead of $Q$. The HybridCalculator class provides alternative choices for the test statistics such as the number of events or the profiled likelihood ratio (see equation 3.2).

A comparison of $Q_{obs}$ for the data being tested to the probability distribution of the test statistics expected in both hypotheses allows to compute the confidence levels, $CL_{ab}$ and $CL_b$. Since the functional form of the test statistic distribution is not always known a priori, a large amount of toy Monte Carlo experiments are performed in order to determine it for two families of pseudo datasets: the ones in the signal+background and the ones in the background-only hypothesis. Figure 3 provides an example of the obtained distributions.

Systematics uncertainties are taken into account using Bayesian Monte Carlo sampling. For each toy Monte Carlo experiment, the effective value of the nuisance parameters is varied before generating the toy sample. The whole phase space of the nuisance parameters is thus sampled through Monte Carlo integration. The final net effect consists in a broadening of the test statistic
Figure 3: Result from the hybrid calculator, the distributions of $-2\ln Q$ in the background-only (red, on the right) and signal+background (blue, on the left) hypotheses. The black line represents the value of $-2\ln Q$ on the tested data. The shaded areas represent $1 - CL_b$ (red) and $CL_{sb}$ (blue).

distribution and thus, as expected in presence of systematic uncertainties, a degraded separation of the hypotheses.

Moreover, by varying the parameter of interest representing the hypothesis being tested (for example varying the signal cross-section) one can obtain a one sided confidence interval (i.e. an exclusion limit). RooStats provides a class, HypoTestInverter, which implements the interface IntervalCalculator and it performs the scanning of the hypothesis test results of the hybrid calculator for various values of one parameter of interest. By looking where the confidence level curve of the result intersects the desired confidence level, an upper limit can be derived, assuming the interval is connected.

4. Combination of Results

Combining results from multiple experiments in order to enhance sensitivity of a measurement or improve the power of a hypothesis test is common. The challenge of combining results is primarily logistical, since a proper combination requires low-level information from each experiment be brought together to form one large statistical test. Again, this is hindered by the fact that the ingredients to the combination are heterogeneous (e.g. different formats, technologies, and conventions). A major advancement that was made by the RooStats project is the concept of the workspace. The power of the workspace is that it allows one to save data and an arbitrarily complicated model to disk in a ROOT file. These files can then be shared or archived, and they provide all the low-level
ingredients necessary for a proper combination in a unified framework. This allows then a digital publishing of the results.

The RooWorkspace class of RooFit provides the low-level functionality for storing the full model and the data and, in addition, it provides a convenient functionality to create easily the model via a string interface (workspace factory).

5. RooStats Utilities

In addition to the previously described methods, RooStats provides also some statistical utilities. These include functions to calculate the p-value or Z-value (e.g. significance in 1-sided Gaussian standard deviations) for a number counting experiments.

Another utility is the class RooStats::SPlot, which implements the SPlot technique \[11\] to disentangle signal from background via an extended maximum likelihood fit and with a tool to access the quality and validity of the fit by producing distributions for the control variables. RooStats::SPlot complements the ROOT TSPlot class with the possibility to use arbitrary models created with RooFit’s data modeling language.

The BernsteinCorrection is another utility class to augment a nominal probability density function with a polynomial correction term. This is useful for incorporating systematic variations to the nominal probability density function. The Bernstein basis polynomials are particularly appropriate because they are positive definite.

The HLFactory is a user friendly wrapper around the RooFit workspace class to build the input model for RooStats from a text file. Other high level factory tools are planned and will available in future versions of RooStats.

6. Conclusions

RooStats is a new software package providing the major statistical tools required for the LHC data analysis. These tools are implemented by using common interfaces, so they can be re-used with the same input model and they can be applied both in simple number counting problems and in complex ones, with multi parameter of interests and various nuisance parameters.

RooStats is distributed together with ROOT and its latest production version, released in December 2009, is 5.26.00. Examples of usage are provided in the tutorials/roostats directory of the ROOT distribution. These examples macro exist for each of the RooStats calculator. In addition to numbers (interval limits, significance, etc..) they produce also statistical plots of the result (confidence level contours or test statistics distributions like in figure 3). The examples are based on models with Poisson statistics (number counting experiments) or gaussian signal model with flat background and they take into account systematic uncertainties in the nuisance parameters. Furthermore, a tutorial of the FeldmanCousins class is provided, which uses the same model of the neutrino oscillation search described in \[8\].

RooStats is starting now to be used by both ATLAS and CMS for producing the results of their data analysis and it is then planned to be used in the future for their analysis combinations.

\[3\] see http://root.cern.ch/root/html/TSPlot.html
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