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Data Science Applications in Physics, Balkan School in Tirana 2024

The replica method application using the ROOT framework

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Outlook

Introduction

recall of the concept of confidence interval

The replica method

generation of pseudodata, study of uncertainties and correlations, building uncertainty bands

Implementation in ROOT

basics of ROOT, hands-on session (using a proposed program)

 \Box Suppose we are interested in estimating the physical quantity θ from the measurement of x_1, x_2, \ldots, x_n indipendent random variables

 \rightarrow introduce an estimator $t(x_1, x_2, \ldots, x_n)$ such that $E[t] = \theta_0$ $θ$ ₀ the true value of the physical quantity θ

 \rightarrow thus evaluating t on the measured sample (x_1, x_2, \ldots, x_n) gives an estimate of θ \rightarrow a second measurement $(x'_1, x'_2, ..., x_n')$ would however give another estimate of θ

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\Box To quantify these fluctuations \rightarrow Confidence Interval (CI) found as follows

i. chose a Confidence Level (CL) γ ($\gamma = 0.68$ or $\gamma = 0.90$ or $\gamma = 0.95$) ii. Find t_a and t_b such that $P(t_a < t < t_b) \equiv \int_{t_a}^{t_b} dt f(t) = γ$ iii. Since it is $P(t_a < t < t_b) = P(\theta_a < \theta < \theta_b)$, find the CI $[\theta_a, \theta_b]$ such that $P(\theta_a < \theta < \theta_b) = \gamma$

ex: Confidence Interval with CL 68% ($\gamma = 0.68$ *)* \rightarrow *interval such that the probability to find there the physical quantity is 68%*

example

Q Example: we measure a sample x_1, x_2, \ldots, x_n of n independent random variables each distributed according to the gaussian distribution $N(\mu, \sigma)$ mean value $\mu \rightarrow$ unknown physical quantity standard deviation $\sigma \rightarrow$ known

Introduce the estimator

 $t(x_1, x_2, ..., x_n) = \frac{1}{n} \sum_{i=1}^n x_i \equiv \overline{x} \rightarrow$ gives an estimate of μ

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To find the CI at 68% CL

we know that the distribution of \bar{x} is N(μ , σ/\sqrt{n}) thus introduce $z = \frac{\bar{x} - \mu}{\sigma/\sqrt{n}} \rightarrow$ distributed as $N(0,1)$

$$
P(-1 < z < 1) \approx 0.68
$$
\n
$$
\rightarrow P\left(-1 < \frac{\overline{x} - \mu}{\frac{\sigma}{\sqrt{n}}} < 1\right) \approx 0.68
$$

n]

The CI at 68%CL is $\left[\overline{x} - \frac{\sigma}{\sqrt{x}}\right]$ $\frac{1}{n}$, \overline{x} + σ

example

Q Example: we measure a sample x_1, x_2, \ldots, x_n of n independent random variables each distributed according to the gaussian distribution $N(\mu, \sigma)$ mean value $\mu \rightarrow$ unknown physical quantity standard deviation $\sigma \rightarrow$ known

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we must know the distribution $f(t)$ of the estimator t!

In general $f(t)$ not known \rightarrow must rely e.g. on MC methods, like the replica method **-> this presentation!** not for one point but for many -> «confidence region» or «confidence band»

Fit of data

Now we consider a more complicated exercise the fit of a data sample!

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To fit the data points we use the function

 $x h_1^q(x) = a x^b (1 - x)^4 \equiv y(x)$ a, b free parameters

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To fit the data points we use the function

 $x h_1^q(x) = a x^b (1 - x)^4 \equiv y(x)$ a, b free parameters

i. Consider a data point $y_i^{meas.}$ with statistical uncertainty σ_i ii. Generate a new point y_i («pseudo-data») according to the gaussian distribution $N(y_i; y_i^{meas.}, \sigma_i) = \exp\left[-\frac{(y_i - y_i^{meas.})^2}{2\sigma_i^2}\right]$ $\left[\frac{y_i^{(1)}(x_i, y_j^{(2)})}{2\sigma_i^2}\right]$ / $\sqrt{2\pi\sigma_i^2}$ iii. iterate for each data point \rightarrow one «replica»

i. Consider a data point $y_i^{meas.}$ with statistical uncertainty σ_i ii. Generate a new point y_i («pseudo-data») according to the gaussian distribution

 $N(y_i; y_i^{meas.}, \sigma_i) = \exp \left[-\frac{(y_i - y_i^{meas.})^2}{2\sigma_i^2}\right]$ $\left[\frac{y_i^{(1)} - y_j^{(2)}}{2\sigma_i^2}\right] / \sqrt{2\pi \sigma_i^2}$

iii. iterate for each data point \rightarrow one «replica» iv. Fit of replica

Generate a second replica and fit again..

10 replica

1000 replica

with real data applications it is difficult to generate more than 100-200 replica, due to the fact that a single fit could take hours..

Control step: distributions of the generated pseudodata

By construction, at each value of x the pseudodata should have a Gaussian distribution with

mean value μ equal to the value of the data point

rms equal to the corresponding stat. uncertainty

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Distribution of fit parameters

Now we have the distributions of the parameters and their uncertainties

Distribution of \hat{a} quite wide, as expected from the fit

the fit Distribution of \hat{b} narrower, as expected from

Distribution of fit parameters

Entries 1000 200 *counts* 200 *counts* $\begin{array}{|c|c|}\n\hline\n\text{Entries} & 1000 \\
\hline\n\end{array}$ Mean 1.323 Std Dev 0.2096 Std Dev 0.2096 \overline{v} Distribution of \hat{b} narrower, as expected from 50 \vdash \vdash historia
Bibliografia Mean 1.323 Std Dev 0.2096 \sim 0 Entries 1000Mean 1.323 Std Dev 0.2096 histB 0 1 2 3 4 5 *b* 0 50 100 150 \hat{b}

Now we have the distributions of the parameters and their uncertainties

Distribution of fit parameters

Now we have all replica.. How can we construct the uncertainty bands at a given confidence level (CL)? here 68% and 90% CL

Look at the distribution of the value of the fit function in several x intervals

For the moment, forget the data points and the fit function.. Concentrate on replica

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and look at the distribution of the value of the fit function in each point

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and look at the distribution of the value of the fit function in each point

Repeat for the other points..

Join the points with lines.. and fill area in between the lines \rightarrow now we have (uncertainty) bands!!

Finally, remove all the fit functions of the replica and draw the data points! Now we are done!

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Constructing the uncertainty bands

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They represent a "property" of quarks in a proton..

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carried by quark (parton) q (known as the «Bjorken variable»)

They represent a "property" of quarks in a proton..

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Now that the steps for implementing the replica method are known, let's see the tools for the implementation

The ROOT framework

 \Box "An open-source data analysis framework used by high energy physics and others.» quote taken from the website of the project «https://root.cern» born at CERN

 \Box Heavily relies on the programming language C/C++ object-oriented here assumed to be known [there is plenty of nice tutorials online..]

- \Box Available for different platforms (Linux, MacOS, Windows) here assumed linux
- \Box The first step, install ROOT following the instructions at https://root.cern/install/ should already be installed in the lab's computers
- \Box Run ROOT by the «root» command «root -l» if you'd like not to display the logo to quit root use unstead «.q»

ROOT interpreter

\Box After running «root», the ROOT interactive shell is opened

commmands → gathered in a «**macro**»

A simple macro

- \Box A macro is essentially a function implementing the commands that constitute the analysis
- \Box Here is an example of the implementation of the sum of first N integers in a macro

```
Users > albikerbizi > Desktop > ScuolaTirana > \mathsf{C} ExampleMacro.C
  1 // This is a simple ROOT macro.
  2 #include "TROOT.h" // ROOT header file.
  3 #include <iostream> // Standard input/output stream of C++
  4<sup>1</sup>using namespace std; // This allows to use commands like cout, endl, cin..
       int main()\overline{\mathbf{S}}5 -6
  \overline{7}int N = 10;
  8
          double sum = 0.0:
  \mathbf{Q}for(int i =0; i<N; i++) sum += i;
 10
          cout << "The result of the sum is " << sum << endl;
 11\text{cut} \ll \text{''End} of macro. \n":
 1213<sup>°</sup>return 0;
 14
```
- \Box Can be loaded in the ROOT interpreter by . L ExampleMacro.C \Box And executed calling the function «main» main()
-
- [.L root [0] .L ExampleMacro.C [root [1] main $\mathbf O$ The result of the sum is 45 End of macro. $(int) $0$$ root $[2]$
- \Box Alternatively can be compiled as a C++ program using the comands g++ ExampleMacro.C -o ExampleMacro.o `root-config --cflags --libs` ./ExampleMacro.o

[albikerbizi@cli-10-106-4-193 ScuolaTirana % g++ ExampleMacro.C -o ExampleMacro.o `root-config --cflags --libs` (albikerbizi@cli-10-106-4-193 ScuolaTirana % ./ExampleMacro.o The result of the sum is 45 End of macro.

Note: When compiling the macro as a C++ program, treat it as a C++ code, e.g. include lines like 3 and 4 above..

Graphics: TCanvas class

 \Box The TCanvas class allows to visualize graphics

 \Box A TCanvas object can be declared and visualized by the following lines

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- \Box There are different classes that represent histograms, all inheriting from the class TH1 for the complete guide see TH1 Class Reference
- \Box Here we focus on 1D and 2D histograms with entries being floating points (prec. 7 digits) TH1F TH1F Class Reference TH2F TH2F Class Reference

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- \Box Here we focus on 1D and 2D histograms with entries being floating points (prec. 7 digits) TH1F TH1F Class Reference \bullet This is a canvas TH2F TH2[F Class Reference](https://root.cern.ch/doc/master/classTColor.html) Eile Edit View Options Tools xmin xmax Title of the histogral \Box 1 D histograms y -title
80 TH1F $*h = new TH1F("h", "Title of the histogram", 40, -3, 3);$ h->GetXaxis()->SetTitle("x-title"); 70 h->GetYaxis()->SetTitle("y-title"); 60 h->SetLineColor(kBlue); # bins 50 h->SetLineColor(kBlue): h->SetLineWidth(1); 40 cosmetics h->SetLineStyle(1); 30 h->SetMarkerColor(kBlue); 20 //h->SetMarkerStyle(20); h->FillRandom("gaus",1000); Fill with a std gaussian $10⁵$ h->Draw("HIST,E"); Draw «h» with boxes («HIST») and errorbars («E») οĒ LineStyle Color table, more in the TColor Class Reference 10 O 8 40 41 $\bf{42}$ $\bf 43$ 44 47 48 49 10 LineV 7 9 $30₁$ 31 32 34 39 33 $35\,$ 37 38 6 8 5 ${\bf 20}$ $\mathbf{21}$ ${\bf 22}$ $\bf 23$ ${\bf 24}$ 25 27 ${\bf 28}$ ${\bf 29}$ $\overline{7}$ see 4 6 10 11 13 14 $15\,$ ${\bf 16}$ 17 18 ${\bf 19}$ 3 **TAttLine** 5 $\overline{\mathbf{2}}$ $\pmb{\mathsf{o}}$ 4 1 3 January 23, 2024 **Albi Kerbizi (Trieste University and INFN)** 2

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\Box 1 D histograms

Costumized binning can be provided in the declaration

```
const int Nbins = 6;
double xbins [Nbins+1] = \{-3, -2, -1, 0, 1, 2, 3\};
TH1F *h = new TH1F("h", "Title of the histogram", Nbins, xbins);
```
Other useful methods

```
for(int ibin=1; ibin<=h->GetNbinsX(); ibin++)For cycle running on all bins
 double bin_content = h->GetBinContent(ibin);
                                                                          Bin 0 underflow
 double bin_error = h->GetBinError(ibin);
                                                                           Bin Nbins+1 overflow
 double bin center = h\rightarrow GetBinCenter(ibin);1/\ldotsdouble counts = \ldots;
 h->SetBinContent(counts);
 h->SetBinError( sqrt(counts) );
ł
TH1F * h2 = (TH1F*) h->Clone("h2"); +\rightarrow h2 is a copy of h, with name «h2»
h2 \rightarrow Divide(h);\rightarrow h2 is divided by h (division of bin contents, for
h2 - > Add(h, 0.2);
                                                       \rightarrow h is multiplied by 0.2 and added to h2 (bin-pe
```
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 \Box The TGraph and TGraphErrors classes allow to construct graphs with

only points TGraph points and errors TGraphError

\Box The constructors are similar

TGraph *gr1 = new TGraph(int nPts, double xPts, double yPts); TGraphErrors *gr2 = new TGraphErrors(int nPts, double xPts, double yPts, double xErr, double yErr);

> nPts = number of points xPts = array of dimension nPts with x-values yPts = array of dimension nPts with y-values xErr / yErr = array of dimension nPts with uncertainties on x / y

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```
nPts = number of points
#include "TGraph.h" // Header with TGraph class
#include "TGraphErrors.h" // Header with TGraphErrors class.
                                                                xPts = array of dimension nPts with x-values
                                                                yPts = array of dimension nPts with y-values
int \text{main}()xErr / yErr = array of dimension nPts with uncertainties on x / yconst int nPts = 10;
 double xPts[nPts], yPts[nPts];
 double xErr[nPts], yErr[nPts];
 double xPts 2 [nPts]:
 TRandom2 *rnd = new <b>TRandom2()</b>;for(int i=0; i<nPts; i++){
   xPts[i] = 0.1 + i*(1.0 - 0.1)/nPts; // Example of x-pointsyErr[i] = 0.04; xErr[i] = 0.03; // Uncertainties on y and x.
   yPts[i] = 1.0*xPts[i]+rnd->Gaus()*yErr[i]; // Example of y points.xPts 2[i] = xPts[i]+0.02; // Small shift for the second graph.
 \mathcal{F}TGraph *gr1 = new TGraph(nPts, xPts, yPts);gr1->SetMarkerColor(kBlue);
                                                      cosmetics
 gr1->SetMarkerStyle(20);
 gr1->SetMarkerSize(0.8);
 TGraphErrors *gr2 = new TGraphErrors(nPts, xPts_2, yPts, xErr, yErr);
 gr2->SetMarkerColor(kRed);
 gr2->SetMarkerStyle(24);
                                                     cosmeticsgr2->SetMarkerSize(0.8);
```
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 \Box The constructors are similar

TGraph *gr1 = new TGraph(int nPts, double xPts, double yPts);

TGraphErrors *gr2 = new TGraphErrors(int nPts, double xPts, double yPts, double xErr, double y

 \Box The TF1 class allows to represent functions

How to draw the function?

\Box The TF1 class allows to represent functions

\Box The general way of defining a TF1 object is the following

- \Box ROOT offers an automatic way of fitting histograms (here 1D) and graphs
- \Box The objects that we need are

 \Box Fit to a TH1F

Fit operation

"R" fit in the range of f "0" do not draw f automatically each time h is drawn Default fit procedure $\rightarrow \chi^2$ minimization

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- \Box ROOT offers an automatic way of fitting histograms (here 1D) and graphs
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```
Default fit procedure \rightarrow \chi^2 minimization
```
- \Box ROOT offers an automatic way of fitting histograms (here 1D) and graphs
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\Box Fit to a TH1F

```
double Gaussian(double *x, double*par){
12
       double N = par[0];
13
       double mu = par[1];
14
15
       double sigma = par[2];
16
       double X = x[0];
17
       return N * TMath::Exp(-TMath::Power((X-mu)/sigma, 2)/2.0);
18
     ŀ
19
     int main() {
20
       TH1F *h = new TH1F("h", "Gaussian distribution", 40, -5.0, 5.0);21
       h->GetXaxis()->SetTitle("x");
22
23
       h->GetYaxis()->SetTitle("counts");
       h->FillRandom("gaus");
24
25
       TF1 *f = new TF1("f", Gaussian, -3.0, 3.0, 3);26
       f->SetParNames("N","mu","sigma");
27
       f->SetParameters(100,0.0,1.0);
28
29
       f->SetLineColor(kBlue);
       h->Fit(f,'R0");
30
31
       TCanvas *c = new TCanvas("c", "This is a canvas", 500, 500);32
       c->SetLeftMargin(0.15); c->SetBottomMargin(0.15); c->cd();
33
                                                                            Draw the histogram 
       gstyle->set0ptFit(1111); To show the fit results in the \overline{a} and function
34
       h\rightarrowDraw("HIST, E");
35
                                  stat box of the histogramf->Draw("l,R,same");
36
37
38
        return <math>0;
39
```
- \Box ROOT offers an automatic way of fitting histograms (here 1D) and graphs
- The objects that we need are

\Box Fit to a TH1F

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TH1F or TGraphErrors already seen TF1 already seen rules for the fitting this slide

- \Box Fit to a TH1F
- \Box Fit to a TGraphErrors

as for TH1F, using the gr->Fit(f,"opt") gr being the pointer to a TGraphErrors

f pointer to the fit function opt options, e.g. opt = R0

default minimizing techinque X2, can be changed as for TH1F

- \Box ROOT offers an automatic way of fitting histograms (here 1D) and graphs
- \Box The objects that we need are

TH1F or TGraphErrors already seen TF1 already seen rules for the fitting this slide

- \Box Fit to a TH1F
- \Box Fit to a TGraphErrors

as for TH1F, using the gr->Fit(f,"opt")

```
1112<sup>2</sup>double myFunction(double *x, double*par){
13
       return par[0] + par[1] * x[0];
14
     \mathcal{F}15
16
     int \text{main}()17
18
       const int nPts = 10;
19
       double xPts[nPts], yPts[nPts], yErr[nPts];
20
       TRandom2 *rnd = new TRandom2();
21
       for(int i=0; i<nPts; i++){
22
         xPts[i] = 0.1+i*(1.0-0.1)/nPts; // Example of x-points23
         yErr[i] = 0.04;
                                        // Uncertainties on y.
24
         yPts[i] = 1.0*xPts[i]+rnd->Gaus() *yErr[i]; // Example of y points.25
       \mathcal{F}26
       TGraphErrors *gr = new TGraphErrors(nPts, xPts, yPts, NULL, yErr);
27
28
       gr->SetMarkerColor(kRed); gr->SetMarkerStyle(24); gr->SetMarkerSize(0.8);
29
30
       TF1 *f = new TF1("f", myFunction, 0.0, 1.0, 2);31
       32
       gr->Fit(f,''R0'');Fit operation
33
       TCanvas *c = new TCanvas("c", "This is a canvas", 500, 500);34
35
       c->SetLeftMargin(0.15); c->SetBottomMargin(0.15); c->cd();
36
       TH2F *h = new TH2F("h", "Title", 10,-0.02,1.15,10,-0.05,1.15);
37
       h->GetXaxis()->SetTitle("x-title"); h->GetYaxis()->SetTitle("y-title");
38
       h->SetStats(kFALSE); h->Draw("");
39
       qStyle->SetOptFit(1111);
40
       gr->Draw('P, same");
41
       f->Draw("l, R, same");
42
       return 0;
43
       \mathcal{F}
```


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[Important to](https://root.cern.ch/doc/master/classTBrowser.html)ols not presented

 \Box There are many other tools offered by ROOT not presented here very important for real data analyses

 \Box ROOT files (TFile Class Reference) used for the storage and reading of ROOT objects like TH1F, TH2F, TGraph, TGraphE TF1, TTree etc..

Q ROOT Trees (TTree) used to store and read data very efficient for drawing and comparing histograms using the ROOT interpreter..

Q ROOT TBrowser (TBrowser Class Reference) to quickly visualize object saved in a ROOT file from the ROOT interpreter

see ROOT documentation and many resources that can be found online..

Conclusions

The replica method is an interesting and powerful tool to explore statistical correlations and construct uncertainty bands

playing with the replica requires the knowledge of different tools for data analysis equivalently, it can be used to better understand the tools

A framework for the implementation of the replica method is offered by ROOT

not simple.. yes, but good practice allows to become familiar with it! *let's start with an exercise!*

For any question, feel free to contact me: albi.kerbizi@ts.infn.it

□ Distribution of the «tensor charge» and evaluation of the CI corresponding at 68% and 90% CL

«tensor charge» fundamental property of the nucleon can be evaluated in lattice $QCD \rightarrow$ important contact point between phenomenological extractions of transversity and the lattice

□ Distribution of the «tensor charge» and evaluation of the CI corresponding at 68% and 90% CL

the (contribution of u-quarks to the) tensor charge g_T^u is given by

$$
g_T^u = \int_{x_{\text{min}}}^{x_{\text{max}}} h(x) \, dx
$$

the range of integration should be between 0 and 1 here data range limited \rightarrow truncated contribution to the tensor charge, in the range $x_{\text{min}} = 0.008, x_{\text{max}} = 0.21$

 \Box Distribution of the «tensor charge» and evaluation of the CI corresponding at 68% and 90% CL

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the range of integration should be between 0 and 1 here data range limited \rightarrow truncated contribution to the tensor charge, in the range $x_{\text{min}} = 0.008, x_{\text{max}} = 0.21$

 \Box Using the file «ReplicaMethod HandsOn.C» (see indico), divide the exercise into steps 1.a. Construct a TF1 representing $h(x)$ for each replica 1.b. Construct a TH1F and will with the values of g_T^u note: to evaluate the integral of f, with f being a TF1, use double gTu = f->Integral(xmin, xmax); 2. Find the CI corresponding to 68% CL and 90%CL either use the class ConfidenceInterval defined at the beginning of the ReplicaMethod_HandsOn.C file

or construct a loop over the histogram's bins your way..

 \Box Distribution of the «tensor charge» and evaluation of the CI corresponding at 68% and 90% CL the (contribution **hxRep** $M_{\rm H}$ \mathbb{R} : the rang here dat \overline{C} and \overline{C} are the tensor contribution to the tensor charge in the range $\mathcal{H} \cup \mathcal{W}$. The original state $\mathcal{H} \cup \mathcal{W}$ q Using the file «ReplicaMethod_HandsOn.C» (see indico), divide the exercise into steps 1.a. Cons $1.b.$ Cons note: the integral of \mathbb{R} integral of \mathbb{R} integral of \mathbb{R} double gradient control \mathbb{F}_p and \mathbb{F}_p and 2. Find either at confidence the confidence of the continuum of the beginning of the beginning of the beginning of the Re (Requilication 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5 or $\overline{\bigcup_{\text{col}}$ construction over the histogram's bins your way. u $g_{_{\sf T}}^{\sf u}$ 0 10 20 30 40 50 60 70 80 counts Entries 1000 Mean 0.2054 Std Dev 0.03156 Tensor charge CI at 68% CL [0.175, 0.235] CI at 90% CL [0.150, 0.255]

Backup

−0.05

−0.05