ROOT Summer Student Course

ROOT Data Analysis Framework https://root.cern





This course is recorded (slides and audio)

(For the benefit of everybody)

Trainer





Computer Science PhD Student

My research: Portable data structures



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My research: ROOT RDataFrame R&D

Trainer

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My research: ROOT R&D (RDataFrame, RNTuple, Python)





Make sure you can login to SWAN: <u>https://swan.cern.ch</u>

- The Jupyter Notebook service of CERN
- IMPORTANT: first visit <u>https://cernbox.cern.ch</u>



X



Configure Environment

Specify the parameters that will be used to contextualise the container which is created for you. See SWAN service website for more details and contact to administrators.

Select AlmaLinux 9 as Platform to try out our new experimental Alma9 image with JupyterLab as default interface! More information here.

Software stack more ...

5a 🔶

Platform more ...

CentOS 7 (gcc11)

Environment script more...

e.g. \$CERNBOX_HOME/MySWAN/myscript.sh

Number of cores more...

2

Memory more...

3

Start my Session

Use the SWAN default settings





- Go to the <u>github repository</u>
- Click on the SWAN badge

ROOT co	ourse for students
Open in 🔊 SWAN	launch binder 💭 open GH Codespaces

Introduction

A Quick Tour of ROOT



ROOT is an **international collaboration**:

- Large effort contributed by **CERN**
- And also FNAL, GSI, Princeton

ROOT is its user **community**, **contributors** and **developers**

ROOT is **open source software:** contributions are welcome!

What can you do with ROOT?





Link to publication

ROOT can be seen as a collection of building blocks for various activities, like:

- Data analysis: histograms, graphs, functions
- I/O: row-wise, column-wise storage of any C++ object
- **Statistical tools** (RooFit/RooStats): rich modeling and statistical inference
- Math: **non-trivial functions** (e.g. Erf, Bessel), optimised math functions
- C++ interpretation: full language compliance
- Multivariate Analysis (TMVA): e.g. Boosted decision trees, Neural Nets
- Advanced graphics (2D, 3D, event display)
- Declarative Analysis: RDataFrame
- And more: HTTP serving, JavaScript visualisation





ROOT Application Domains



LHC Data in ROOT Format

$\sim 2EB$

(exa = 10¹⁸)

as of 2024

https://root.cern

- ROOT web site: the source of information for ROOT users
 - For beginners and experts
 - Installation instructions
 - Class documentation
 - Manuals, presentations
 - Forum



Resources

- - ROOT Forum: <u>https://root-forum.cern.ch</u>
 - ROOT Website: <u>https://root.cern</u>
 - Further reading: <u>https://root.cern/get_started</u>
 - (includes booklet for beginners: "The ROOT Primer")
 - Documentation: <u>https://root.cern/doc/master/</u>



Scope of this Course

• We have 3 hours:

- Not enough to teach you a HEP analysis
- Instead, introduction to key elements physicists use from ROOT:
 - Histogramming
 - □ Fitting
 - Reading data
 - Data analysis





We now move to the course material on Jupyter Notebooks

Wrap up



- Covered a number of topics today:
 - What is ROOT and how to use it?
 - How to draw histograms, functions and graphs
 - How to fit histograms
 - How to read and write files
 - What is RDataFrame and how to use it

Resources

- - ROOT Forum: <u>https://root-forum.cern.ch</u>
 - ROOT Website: <u>https://root.cern</u>
 - Further reading: <u>https://root.cern/get_started</u>
 - (includes booklet for beginners: "The ROOT Primer")
 - Documentation: <u>https://root.cern/doc/master/</u>





Post-workshop survey

• Thank you for attending the course today!

 At last - we would like to ask you to fill in a **short post-workshop survey** on indico - your opinion matters and we want to make the course even better in the future

Extra material for self study

Foreword

- Most topics (but not all) were already covered in the main part of the course
- Treat the following slides as a good summary of what you've already learned plus some extra information
- Additionally, after every sub-module you are pointed to some extra exercises (in the) where you will practice both using notebooks (as during the course), but you will also attempt writing and executing C++ ROOT macros

The ROOT Prompt and Macros

The ROOT Prompt

- C++ is a compiled language
 - A compiler is used to translate source code into machine instructions
- ROOT provides a C++ interpreter
 - Interactive C++, without the need of a compiler, like Python, Ruby, Haskell ...
 - Code is Just-in-Time compiled!
 - Is started with the command:



• The interactive shell is also called "ROOT prompt" or "ROOT interactive prompt"

ROOT As a Calculator

$$\frac{1}{1-x} = 1 + x + x^2 + x^3 + x^4 + \dots$$
$$= \sum_{n=0}^{\infty} x^n$$

ROOT can be used as a simple calculator, but we let's make a step forward: declare **variables** and use a *for* control structure. root [0] double x=.5
(double) 0.5
root [1] int N=30
(int) 30
root [2] double gs=0;



Special commands which are not C++ can be typed at the prompt, they start with a "."

root [1] .<command>

- ► For example:
 - To quit root use .q
 - To issue a shell command use **.! <OS_command>**
 - .help or .? gives the full list

ROOT Macros

- We have seen how to interactively type lines at the prompt
- The next step is to write "ROOT Macros" lightweight programs
- The general structure for a macro stored in file *MacroName.C* is:



Running a Macro

• A macro is executed at the system prompt by typing:

> root MacroName.C

or executed at the ROOT prompt using .x:

> root
root [0] .x MacroName.C

or it can be loaded into a ROOT session and then be run by typing:

root [0] .L MacroName.C
root [1] MacroName();

Interpretation and Compilation

We have seen how ROOT interprets and "just in time compiles" code. ROOT also allows to compile code "traditionally". At the ROOT prompt:

root [1] .L macro1.C+
root [2] macro1()

Generate shared library and execute function

ROOT libraries can also be used to produce standalone, compiled applications:

Advanced Users

int main() {
 ExampleMacro();
 return 0;

> g++ -o ExampleMacro ExampleMacro.C `root-config --cflags --libs` > ./ExampleMacro



► Go to folder: <u>student-course/exercises/extra/00_C++_Interpreter</u>

Histograms, Graphs and Functions

Histograms

- A simple form of data reduction
 - Can have billions of collisions, the Physics displayed in a few histograms
 - Possible to calculate statistical quantities: mean, rms, skewness, ...
- Collect quantities in bins (discrete categories)
- ROOT provides a rich set of histograms
 - Focus on the class TH1D today: one dimensional histogram filled with doubles
 - but also available:
 - multiple dimensions histogram TH{1,2,3} classes
 - histograms holding different precision types: floats F, integers I, strings S



My First Histogram



Note that in **the SWAN notebooks**: the figure is not shown directly.

You have to:

1. Either call gPad->Draw() at the end:

```
In [1]: TH1D h("myHist", "myTitle", 64, -4, 4);
h.Draw();
gPad->Draw();
```

2. Or you can create a TCanvas and draw it:

```
In [2]: TCanvas cl;
TH1D h("myHist", "myTitle", 64, -4, 4);
h.Draw();
cl.Draw();
```



My First Histogram

root [0] TH1D h("myHist", "myTitle", 64, -4, 4) root [1] h.FillRandom("gaus") root [2] h.Draw()


And now in Python!





See the documentation of the <u>THistPainter</u> class for all possible options on drawing histograms





Functions

- Mathematical functions are represented by the TF1 class
- Functions have names, formulas and line properties
- The formulas can be:
 - Mathematical formulas (written as strings)
 - C++ functions/functors/lambdas (highly performant custom functions)
 - Python functions
- Functions can be written with and without **parameters**
 - Crucial for fits and parameter estimation
- Functions (as well as integrals and derivatives of functions) can be evaluated

ROOT as a Function Plotter



ROOT as a Function Plotter

► The class TF1 represents one-dimensional functions (e.g. *f(x)*):

root [0] TF1 f1("f1","sin(x)/x",0.,10.); //in brackets: name, formula, min, max root [1] f1.Draw();

An extended version of this example is the definition of a function with parameters:

>>> f2 = ROOT.TF1("f2","[0]*sin([1]*x)/x",0.,10.)
>>> f2.SetParameters(1,1)
>>> f2.Draw()

C++

Python

Another Example: Histogram and function drawn together



Drawing - important options

option	description
"SAME"	superimpose on top of existing picture
"L"	connect all computed points with a straight line
"C"	connect all computed points with a smooth curve
"FC"	draw a fill area below a smooth curve

TGraph Painter documentation



See 132nd LHCC Meeting

- Display points and associated errors
- Fundamental to display trends

Graphs

My First Graph



Drawing Options

95%

99%

99.9%

See the documentation of <u>TGraphPainter</u> for the Graph drawing options







Time For Exercises

Go to folder: <u>student-course/exercises/extra/01_Histograms_Graphs_Functions</u>

Parameter Estimation and Fitting

What is Fitting?

- Estimate parameters of a hypothetical distribution from the observed data distribution
 - $y = f(x | \theta)$ is the fit model function
- Find the best estimate of the parameters θ assuming **f**(**x** | θ)
- Both Likelihood and Chi2 fitting are supported in ROOT



Example

Higgs $\rightarrow \gamma\gamma$ spectrum We can fit for:

- the expected number of Higgs events
- the Higgs mass

49

Fitting in ROOT

- Create first a **parametric** function object, **TF1**, which represents our model
 - need to set the initial values of the function parameters
 - or use a pre-defined function
- Fit the data object (Histogram or Graph):
 - Call the **Fit** method passing the function object
 - various options are possible (see the **TH1**::**Fit** documentation)
- **Examine** the result:
 - get parameter values, uncertainties, correlation
 - get fit quality estimation
- **Draw** the fit function:
 - automatically, on top of the Histogram or the Graph when calling
 TH1::Fit or TGraph::Fit

Creating the Fit Function

- Parametric function object (**TF1**):
 - write formula expressions using functions:

TF1 f1("f1","[0]*TMath::Gaus(x,[1],[2])");

- [0],[1],[2] indicate the parameters.
- We could also use meaningful names, like [a],[mean],[sigma]
- Use the available functions in ROOT library
 - Pre-defined functions e.g.: gaus, expo, landau...

TF1("f1","gaus");

- for more complex examples and fitting options see <u>backup slides</u>
- for full list of functions see the documentation of <u>TH1::Fit()</u>, and the <u>TFormula reference doc</u>

Fitting Histograms example

We have a histogram, h1, and we want to fit a function to it:

<pre>root [0] TF1 f1("f1","gaus"); root [1] h1.Fit(&f1);</pre>							
FCN=2	27.2252 FROM	MIGRAD	STATUS=CON	VERGED	60 CALLS	61 TC	JTAL
		EDM=1.1	2393e-07	STRATE	GY= 1 EF	RROR MATRIX ACC	CURATE
EXT	PARAMETER				STEP	FIRST	
NO.	NAME	VALUE	ERRO	OR	SIZE	DERIVATIVE	90
1	Constant	7.98760e+	01 3.2288	82e+00	6.64363e-03	-1.55477e-05	80
2	Mean	-1.12183e-	02 3.1622	23e-02	8.18642e-05	-1.49026e-02	70
3	Sigma	9.73840e-	01 2.4473	38e-02	1.69250e-05	-5.41154e-03	50

For displaying the fit parameters:

gStyle->SetOptFit(1111);



Minimization

- The fit is done by minimizing the least-square or maximizing the likelihood function.
- A direct solution exists only in case of linear fitting
 - it is done automatically in such cases (e.g fitting polynomials).
- Otherwise an **iterative algorithm** is used:
 - Minuit is the minimization algorithm used by default
 - ROOT provides two implementations*: Minuit and Minuit2
 - To change the minimizer:

ROOT::Math::MinimizerOptions::SetDefaultMinimizer("Minuit2");

Other commands are also available to control the minimization, see
 <u>documentation</u>
 *other algorithms exists for example Eumili or

*other algorithms exists, for example, Fumili, or minimizers based on GSL (genetic and simulated annealing algorithms)

Fitting - references for the future

RooFit: ROOT toolkit for complex fitting

- ROOT fitting can handle complicated functions but complex models require many lines of code
- RooFit provides functionality for building complex fitting models
- Fitting often requires Normalization of pdfs
 - not always trivial to perform \rightarrow RooFit does it automatically
- RooFit also provides:
 - MC data generation from model
 - advance **visualization** of fitting results
 - **simultaneous fit** to different data samples
 - full model description for **reusability**
 - **built-in optimization** for optimal computational performances



For more info see the <u>manual</u> or the RooFit <u>courses</u>

TMVA: Machine Learning in ROOT

- ROOT ML tools are provided in **TMVA** (*Toolkit for MultiVariate Analysis*)
- TMVA provides a set of algorithms for standard HEP usage
 - Common interface to different algorithms with consistent evaluation and comparison
 - Capability for classification and regression
 - Embedded in ROOT: direct connection to input data (ROOT I/O)
 - Most popular algorithms are BDT and ANN (also supporting some DL tools)
- Interfaces to external ML library :
 - e.g. to Python tools: scikit-learn, Tensorflow/Keras, PyTorch
- Fast inference system for Deep Learning models (SOFIE) and BDT
 - new tool to generate code and easily evaluate ML models in ROOT that can be trained with other tools (e.g Keras, PyTorch) or xgboost
- ► For more info see the <u>manual</u>

Time For Exercises

- Go to folder: <u>student-course/exercises/extra/02_Fitting</u>
 - plenty of examples start from the easier ones, continue with more complex

- Note on extras how to make nice plots:
 - see the <u>backup</u> slides
 - see extra tutorial module, go to folder: <u>student-course/exercises/extra/05 Graphics</u>

Reading and Writing Data

The ROOT File

- In ROOT, objects are written in files*, represented by TFile instances
- TFiles are *binary* and can be compressed (transparently for the user)

TFiles are self-descriptive:

• The information how to retrieve objects from a file is stored with the objects

* this is an understatement - we'll not go into the details in this course!

TFile in Action

TFile f("myfile.root", "RECREATE");

Option	Description
NEW or CREATE	Create a new file and open it for writing, if the file already exists the file is not opened.
RECREATE	Create a new file, if the file already exists it will be overwritten.
UPDATE	Open an existing file for writing. If no file exists, it is created.
READ	Open an existing file for reading (default).

TFile in Action: Writing

- TFile f("file.root", "RECREATE");
 TH1F h("h", "h", 64, 0, 8);
 h.Write("h");
 f.Close(); ▶ Write to a file
 - Close the file and make sure the operation succeeded

> rootls -l file.root
TH1F Jun 24 15:02 2022 h "h"

C++

TFile in Action: Reading

Python Get the histogram by name! Possible only in Python f.h.Draw() import ROOT f = ROOT.TFile("file.root")

TBrowser interactive tool > root [0] TBrowser t

- *rootls* tool: list content
- **TFile::ls()**: prints content
 - Great for interactive usage







Go to folder: <u>student-course/exercises/extra/03_Working_With_Files</u>

The ROOT Columnar Format

Columns and Rows

- High Energy Physics: many statistically independent collision events
- Create an event class, serialise and write out N instances into a file?
 - \rightarrow No. Very inefficient!
- Organise the dataset in columns

Columnar Representation



Relations Among Columns

Х	у	Z
-1.10228	-1.79939	4.452822
1.867178	-0.59662	3.842313
-0.52418	1.868521	3.766139
-0.38061	0.969128	1 084074
0.55. 74	-0.21231	<mark>/ .</mark> 50281
-0.184	1.187305	.443902
0.20564	-0.7701	0.635417
1.079222	137 /	1.271904
-0.27492	- 1 <u>4</u> 3	3.038899
2.047779	-17 268	4.197329
-0.45868	4 2	2.293266
0.304731	<mark>.</mark> 0.884	0.875442
-0.7127	-0.2223	0.556881
-0.27	1.181767	470484
0.88 .02	-0.65411	3209
-2.03555	0.527648	4.421883
-1.45905	-0.464	2.344113
1.230661	-0.00565	1.514559
		-3 <u>562347</u>





The TTree data format

- A columnar dataset in ROOT is represented by the class **TTree**:
 - Also called *tree*, columns also called *branches*
 - Columns can contain **any arbitrary** C++ type

An entry point to modern ROOT



RDataFrame: quick how-to

- 1. <u>build a data-frame</u> object by specifying your data-set
- 2. apply a series of transformations to your data
 - o <u>filter</u> (e.g. apply some cuts) or
 - define <u>new columns</u>
- 3. apply actions to the transformed data to produce results (e.g. fill a histogram)

Simple Code Example


Filling multiple histograms

h1 = df.Filter("theta > 0").Histo1D("pt") h2 = df.Filter("theta < 0").Histo1D("pt") h1.Draw() // event loop is run Lazily once here h2.Draw("SAME") // no need to run loop again here

Book all your actions upfront. The first time a result is accessed, RDataFrame will fill all booked results.

More on histograms

h = df.Histo1D(("myName", "Title;x", 10, 0., 1.),"x")

You can specify a model histogram with

- a name and a title
- a predefined axis range
- Here, the histogram is created with 10 bins ranging from 0 to 1, and the axis is labelled "x".

Define a new column

`Define` takes the name of the new column and its expression. Later you can use the new column as if it was present in your data.

Working with collections

h = df.Define(
 "good_pt",
 "sqrt(px*px + py*py)[E>100]"
).Histo1D("good_pt")

sqrt(px*px + py*py)[E>100]:

- px, py and E are columns the elements of which are RVecs
- Operations on RVecs like sum, product, sqrt preserve the dimensionality of the array
- [E>100] selects the elements of the array that satisfy the condition
- E > 100: boolean expressions on RVecs such as E > 100 return a mask, that is an array with information on which values pass the selection (e.g. [0, 1, 0, 0] if only the second element satisfies the condition)

Think of your analysis as data-flow

// d2 is a new data-frame, a transformed version of d
auto d2 = d.Filter("x > 0")
.Define("z", "x*x + y*y");
filter
x>0

// make multiple histograms out of it
auto hz = d2.Histo1D("z");
auto hx = d2.Histo1D("x");

You can store transformed data-frames in variables, then use them as you would use an RDataFrame. d2

histo

х

define

histo

Cutflow reports

<pre>// output</pre>				
xcut	:	pass=49	all=100	 49.000 %
ycut	:	pass=22	all=49	 44.898 %

When called on the main RDF object, `Report` prints statistics for all filters *with a name*

Saving data to file

We filter the data, add a new column, and then save everything to file. No boilerplate code at all.

Using callables instead of strings

Expert Feature

// define a c++11 lambda - an inline function - that checks "x>0"
auto IsPos = [](double x) { return x > 0.; };
// pass it to the filter together with a list of branch names
auto h = df.Filter(IsPos, {"theta"}).Histo1D("pt");
h->Draw();

any callable (function, lambda, functor class) can be used as a filter, as long as it returns a boolean

RDataFrame: declarative analyses

- df = ROOT.RDataFrame("t", "f.root")
- df = df.Define("dphi",

"MyDeltaPhi(phi1, phi2)")

- h = df.Histo1D("dphi")
- h.Draw()
 - full control over *the analysis*
 - no boilerplate
 - common tasks are not already implemented?
 - parallelization is not trivial?

RDataFrame: parallelism

- ROOT.EnableImplicitMT()
- df = ROOT.RDataFrame("t", "f.root")
- df = df.Define("dphi",

```
"ROOT::VecOps::DeltaPhi(phi1, phi2)")
```

- h = df.Histo1D("dphi")
- h.Draw()
 - full control over *the analysis*
 - no boilerplate
 - common tasks are already implemented
 - parallelization is trivial



C++ and just-in-time compiled code d.Filter("th > 0").Snapshot("t","f.root","pt*");

PyROOT -- just leave out the `;` d.Filter("th > 0").Snapshot("t","f.root","pt*")





► Go to folder: <u>student-course/exercises/extra/04_RDataFrame</u>

Backup - fitting details

Building More Complex Functions

Any C++ object (functor) implementing double operator() (double *x, double *p)



• also a lambda function (with Cling and C++-11)

TF1 f1("f1",[](double *x, double *p){return p[0]*x[0];},0,10,1);

a lambda can be used also as a string expression, which will be JIT'ed by CLING

TF1 f1("f1","[](double *x, double *p){return p[0]*x[0];}",0,10,1);

Functionality provided by TFormula

TFormula is based on Cling. Additional functionality provided:

- better parameter definition
 - TF1("f1","gaus(x, [Constant],[Mean],[Sigma])");
- function composition by concatenating expressions
 - TF1 fs("sigma","[0]*x+[1]");
 - TF1 f1("f1", "gaus(x, [C], [Mean], sigma(x, [A], [B])");
- normalized sum for component fitting
 - TF1 model("model","NSUM(expo, gaus)"
- convolutions
 - TF1 voigt("voigt", "CONV(breitwiegner, gaus)", xmin, xmax);
- can define vectorized functions for faster fitting and evaluation
 - see <u>vectorizedFit</u> tutorial
- support for auto-differentiation (automatic generation of gradient and Hessian)

Fitting Options

- Likelihood fit for histograms
 - option "L" for count histograms;
 - option "WL" in case of weighted counts.
- Default is chi-square with observed errors (and skipping empty bins)
 - option "P" for Pearson chi-square

expected errors, and including empty bins

- Use integral function of the function in bin
- Compute MINOS errors : option "E"

h1->Fit("gaus","L");

h1->Fit("gaus","LW");

h1->Fit("gaus","P");

h1->Fit("gaus","L I");

h1->Fit("gaus","L E");

Some More Fitting Options

Fitting in a Range

(CC) BY

- h1->Fit("gaus","","",-1.5,1.5);
- For doing several fits
 - h1->Fit("expo","+","",2.,4);
- Quiet / Verbose: option "Q"/"V"
 - h1->Fit("gaus","V");
 - Avoid storing and drawing fit function (useful when fitting many times)

```
h1->Fit("gaus","L N 0");
```

Save result of the fit, option "S"

```
auto result = h1->Fit("gaus","LS");
result->Print("V");
```

All fitting options documented in reference guide or Manual



Parameter Errors

Errors returned by the fit are computed from the second derivatives of the log-likelihood function

- Assume the negative log-likelihood function is a parabola around minimum
- This is true asymptotically and in this case the parameter estimates are also normally distributed.
- The estimated correlation matrix is then:

$$\mathbf{\hat{V}}(\mathbf{\hat{\theta}}) = \left[\left(-\frac{\partial^2 \ln L(\mathbf{x}; \mathbf{\theta})}{\partial^2 \mathbf{\theta}} \right)_{\mathbf{\theta} = \mathbf{\hat{\theta}}} \right]^{-1} = \mathbf{H}^{-1}$$



- A better approximation to estimate the confidence level of the parameter is to use directly the log-likelihood function and look at the difference from the minimum.
 - Method of Minuit/Minos (Fit option "E")
 - obtain a confidence interval which is in general not symmetric around the best parameter estimate

```
auto r = h1->Fit(f1, "E S");
r->LowerError(par_number);
r->UpperError(par_number);
```



Backup - Creating a Nice Plot Survival Kit



The Markers

From the TAttMarker documentation: https://root.cern/doc/master/classTAttMarker.html



kDot=1, kPlus, kStar, kCircle=4, kMultiply=5, kFullDotSmall=6, kFullDotMedium=7, kFullDotLarge=8, kFullCircle=20, kFullSquare=21, kFullTriangleUp=22, kFullTriangleDown=23, kOpenCircle=24, kOpenSquare=25, kOpenTriangleUp=26, kOpenDiamond=27, kOpenCross=28, kFullStar=29, kOpenStar=30, kOpenTriangleDown=32, kFullDiamond=33, kFullCross=34 etc...

Also available through more friendly names 😌

root [3] g.SetMarkerStyle(kFullTriangleUp) c1 File Edit View Options Tools Help 12 0.5 1.5 2 2.5 3 3.5 4

root [3] g.SetMarkerStyle(kFullTriangleUp) root [4] g.SetMarkerSize(3)



root [5] g.SetMarkerColor(kAzure) root [6] g.SetLineColor(kRed - 2) root [7] g.SetLineWidth(2)

root [8] g.SetLineStyle(3)

Question:

How do you find information on line styles?

See TAttLine documentation



The Colors (TColorWheel)









root [13] gPad->SetLogy();

