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# RooFit in ATLAS Top group

Tomas Dado (CERN)

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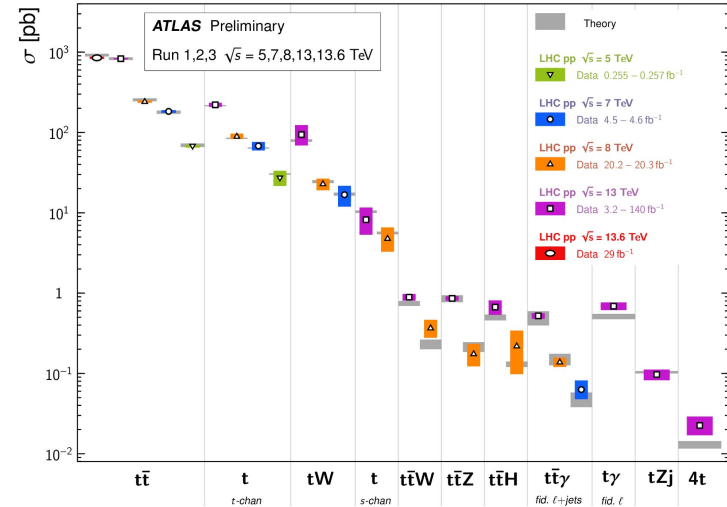
RooFit workshop, April 2024

# Introduction

- ATLAS top group has diverse physics programme
  - High stat. SM properties measurements
    - Top mass measurements
    - Inclusive/differential  $t\bar{t}$  cross-section
    - Yukawa coupling
    - Charge asymmetry
    - ....
  - Low stat. SM measurements
    - $T(t\bar{t})+X$  ( $X=Z,W,t\bar{t}$ , ...) cross-sections
  - Searches
    - FCNC searches with top quarks
- Many analyses require “fitting”
  - I.e. parameter extraction from data

Top Quark Production Cross Section Measurements

Status: November 2023

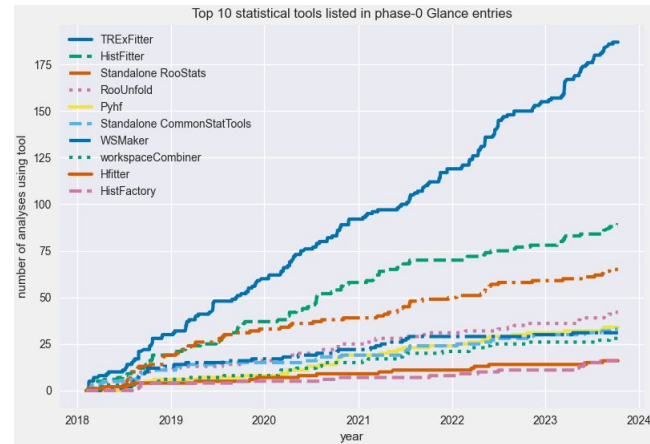


# Different statistical approaches in the top group

- Most common approach: binned-likelihoods
  - One notable exception - top mass measurements (unbinned-likelihood)
- **Unfolding**
  - **IBU** commonly used for inclusive  $t\bar{t}$ bar(+jets)
    - RooUnfold implementation
  - **FBU (Fully Bayesian Unfolding)** used in a handful of measurements
    - Does not use ROOT
  - **Profile-likelihood unfolding**
    - RooFit/HistFactory-like implementation
- **Non-unfolding measurements**
  - Profile-likelihood fits - HistFactory-like
    - Pure HistFactory
    - HistFactory with “extensions” - more details in the next slides
  - Pseudo-experiment approaches
    - Often custom code

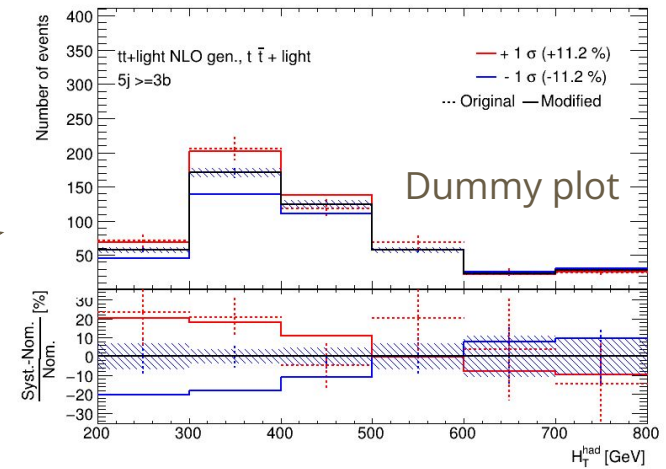
# TRExFitter

- Most commonly used tool for binned profile-likelihood fits
- A convenient tool to run HistFactory-like fits
- The tool:
  - Human readable text config (custom, yaml-like format)
    - No code needs to be written
  - Can read ntuples (very inefficient, uses ttree->Draw) or ROOT histograms
  - Can produce plots for the inputs - +- 1 sigma variations
  - Can produce the WS (HistoFactory-like)
  - Can run the fit (minimisation)
  - Can produce pre/post-fit plots (including variables/regions not used in the fit)
  - Can run significance/limit estimate (using xRooFit)
  - Can produce systematic breakdown
    - “Ranking” of each NP
    - “Grouped impact” for a set of NPs
  - Can produce “likelihood scan” (including 2D scan)



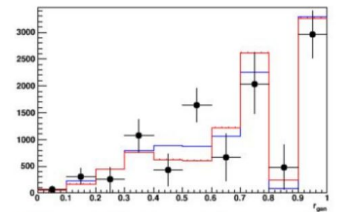
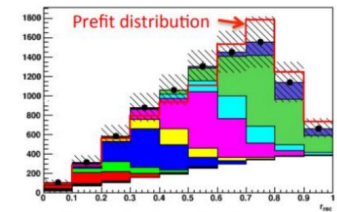
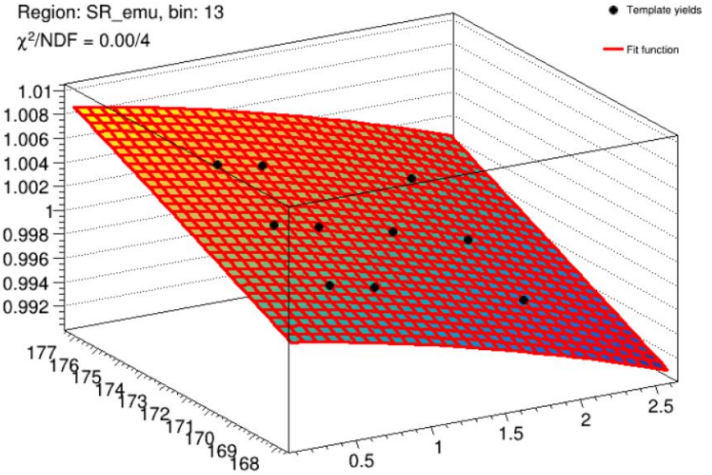
# TRExFitter as HistFactory wrapper

- Preprocessing of histograms
  - Smoothing (reduce MC stat impact)
  - Pruning (remove noise, speed up)
  - Symmetrisation
  - ...
- Pass histograms to HistFactory to build the model/WS
- In some setups: heavily leveraged **“AddPreprocessFunction()”**
  - Allows huge flexibility
    - Fit charge asymmetry instead of cross-section
    - Template fits (e.g. top quark mass, CP-odd Higgs, ...)
    - EFT limit extraction!
  - Really changed the fit from “cross-section” to “almost any parameter that you can get from the cross-section”

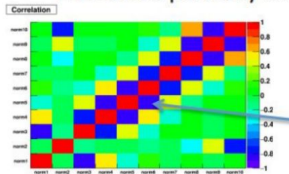


# TRExFitter as not only HistFactory wrapper

- Sometimes the HistFactory model is too limiting
  - **Reparametrisation of ShapeFactors** is needed
    - Template parametrisation per bin →
    - Replace ShapeFactors with the formulae
  - **Additional likelihood terms** are needed
    - E.g. regularisation in the unfolding



Fit worked perfectly ....



Strong anti-correlations to neighbour bins

From W. Buttinger

- Can include **regularization** as additional **likelihood term**:
  - Entropy- based term
  - Derivative-based term : Tikhonov  $e^{-\frac{1}{2}\chi^2} = e^{-\frac{1}{2}r^2 \sum (x_i - x_i^{ref})^2}$

- Done by RooFit workspace manipulations
  - Not calling HistFactory methods

# Usage of RooStats in TRexFitter

- Using **RooStats** to build the WS
  - HistFactory methods
- Using **ModelConfig** in multiple places for metadata bookkeeping
- **Limits/significance calculation with toys** (not-asymptotics)
  - Using RooStats methods/classes for the limit estimate
    - FrequentistCalculator
    - ProfileLikelihoodTestStat
    - ToyMCSampler
    - HypoTestInverter
    - HypoTestInverterResult
  - Using xRooFit for the asymptotic estimate

# Some observations

- **Reasons I have heard why people prefer/like TRexFitter**
  - Simple configuration - no code needed to make paper-quality plots/results
  - Good support if things do not work (mattermost and mailing list - fast turnaround)
    - Something to consider for ROOT (e.g. mattermost support channel)?
  - Can do many things
    - Not just results, but validation plots, pre-processing etc
  - Allows extensions - i.e. not “just” HistFactory model
    - Opportunities to use a known tool for new types of measurements
  - Relatively decent documentation (for HEP standards)
- **What people do not like about TRexFitter**
  - The code is huge (50k+ lines of c++) and often not so nice
  - Sometimes we break things, sometimes changes in ROOT break things (e.g. fit no longer converges when it converged in the previous version)
- **Relatively long turnaround time for ROOT releases**
  - Issues are often fixed fast, but releases can take many months
    - Often build our own untagged versions which is not great
- **We often get questions about statistics** and not related to TRexFitter or Roofit



# Possible future improvements (RooFit)

- **Performance improvements**
  - Parallelisation, GPU support, autodiff, ...
  - Often multiple fit runs that are close (e.g. limits, LH scan)
    - Possible speed up as the minima should not be far apart?
- **Minuit2/minimisation improvements?**
  - E.g. recent strategy 3 addition helped to solve a lot of numerical problems
    - More improvements possible on numerical precision?
  - Lacking documentation for the strategy descriptions (or hard to find)
- **Better support for toys?**
  - E.g. LEE estimate? More-dimensional LEE estimate?
  - Toys for postfit yield estimate per bin?
    - Using bootstrap sampling
  - Should be kept outside of RooFit e.g. in xRooFit?
- **General**
  - Often running EFT fits - non-quadratic NLL - problematic?
  - Documentation for less-common RooFit functions/methods

# What can we (ATLAS) do to help?

- Would making our code (TRExFitter) **public** be helpful/useful?
- Do you need **more realistic WSs**?
  - Only problematic ones?
  - Or also “standard” WS that have no obvious issues?
- Are you interested in some **performance numbers**?
  - E.g. running time/memory consumption?
  
- **We are willing and happy to help!**