

Combine & CMS Likelihood Publications

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CMS Combine

RooStats / RooFit - based software tool used for **statistical analysis within the CMS experiment**.

→ Ideally should re-use (benefit) as much as possible the functionality of RooFit/RooStats without the user needing to remember lots of "tricks"/"gotchas" and write scripts

→ Combine mostly provides **"workflows"** for the most **common statistical methods** and uses LHC/CMS statistics committee **best-practices**

General features

- Human readable inputs (datacards)
- Build **binned / unbinned likelihood models**
- Intuitive and powerful models combination
- Statistical tests Bayesian/frequentist/hybrid
- **Diagnostics tools** for fits inspection

Documentation: https://cms-analysis.github.io/HiggsAnalysis-CombinedLimit/latest/

- Summaries of what the tool is doing (brief statistics)
- Detailed examples of tool functionality for common and more advanced methods
- Tutorials designed to get new users up to speed on the basics



From Statistics Committee Questionnaires 2021-2022

CMS Combine Publication

Publication for Combine: https://arxiv.org/abs/2404.06614 (sub. to CSBS)

- Guide on **installation via Docker** (pre-compiled version 9.1.0) other installation strategies described online
- Definition of **statistical model** and how to construct them in combine **Datacards**
 - Examples for counting, template and parameteric models
 - Physics models
- Common statistical routines available
 - Pseudo-data generation
 - Upper limits (frequentist + Bayesian) and significance calculations
 - Maximum likelihood fits and scans
 - Fitting diagnostics (plotting, GoF tests, impacts)

EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH (CERN)
CMS CMS-CAT-23-001
The CMS statistical analysis and combination tool: COMBINE
The CMS Collaboration*
Abstract
This paper describes the COMBINE software package used for statistical analyses by the CMS Collaboration. The package, originally designed to perform searches for a Higgs boson and the combined analysis of those searches, has evolved to become the statistical analysis tool presently used in the majority of measurements and searches performed by the CMS Collaboration. It is not specific to the CMS experiment, and this paper is intended to serve as a reference for users outside of the CMS Collabo- ration, providing an outline of the most salient features and capabilities. Readers are provided with the possibility to run COMBINE and reproduce examples provided in this paper using a publicly available container image. Since the package is constantly evolving to meet the demands of ever-increasing data sets and analysis sophistication, this paper cannot cover all details of COMBINE. However, the online documentation referenced within this paper provides an up-to-date and complete user guide.
Submitted to Computing and Software for Big Science
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Apr 2024

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[physics.data-an]

arXiv:2404.06614v1

Statistical model

- Primary observables \vec{x}
- Parameters of interest $\vec{\mu}$
- Nuisance parameters \vec{v}
- Auxiliary observables \vec{y}

$$p(\vec{x}, \vec{y}; \vec{\Phi}) = p(\vec{x}; \vec{\mu}, \vec{\nu}) \prod_{k} p_k(y_k; \nu_k).$$

Each element of the vector \vec{x} is referred to as a "channel" (each of which is statistically independent) so that

$$p(\vec{x};\vec{\mu},\vec{\nu}) \rightarrow \prod_i p_i(x_i;\vec{\mu},\vec{\nu})$$

Need to define probability distributions *p* to specify statistical model.

Likelihood constructed by
(in Combine –Log(L)= CachingNLL)
$$\mathcal{L}(\vec{\Phi}) = \prod_{d} p(\vec{x}_{d}; \vec{\mu}, \vec{\nu}) \prod_{k} p_{k}(y_{k}; \nu_{k})$$

Extremely basic example – a counting experiment Datacard

					<u> </u>			
1 2 3	imax 1 jmax 2 kmax 3		3.0	50000 ⁻				
4	# A sin	gle cha	nnel -	ch1 -	in whi	ch 0 events are observed in	data	
5	bin		ch1	_				
6	observa	tion	0	0 Observable = Observed number of events				
7	#							
8	bin		ch1	ch1	ch1			
9	process		ppX	WW	tt	Evenested contributions		
10	n process		0	1	2	Expected contributions		
11	rate		1.47	0.64	0.22			
12	#							
13	lumi	lnN	1.11	1.11	1.11			
14	xs	lnN	1.20	-	-	'Systematic" uncertainties		
15	nWW	gmN 4	-	0.16	-	-		

Extremely basic example – a counting experiment Datacard



Statistical model based on Datacard + Object inputs



Statistical model based on Datacard + Object inputs



- Combinations based on datacard combination (always perform combinations at "likelihood level")
- Same statistical model can be used for **multiple statistical routines** in combine!

5

0 110

120

130

x = m (GeV)

140

150

Physics Models

Physics models are the way combine defines a set of **parameters of interest** and uses them to parameterize the **rates of different processes** (usually "signal")



```
\hookrightarrow modelInstance> [--PO <options>]
```

r_{ggH}

Statistical Results

Combine also handles producing statistical results once model is constructed. For the most common statistical routines, the idea is that it should be **1 command line**.

\$ combine datacard-1-counting-experiment.txt -M MarkovChainMC --tries 100

> -- MarkovChainMC --

- > Limit: r < 2.21031 +/- 0.0133576 @ 95% credibility (100 tries)
- > Done in 0.05 min (cpu), 0.05 min (real)

combine datacard-5-multi-signal.root -M MultiDimFit --algo singles --mass 125 \$

```
--- MultiDimFit ---
 best fit parameter values and profile-likelihood uncertainties:
>
               +0.882 -0.749/+0.795 (68%)
    r ggH :
>
    r ggH : +4.683 -2.746/+3.464 (68%)
> Done in 0.00 min (cpu), 0.04 min (real)
```

combine datacard-3-parametric-analysis.txt -M Significance --mass 125 \$

```
-- Significance --
>
```

- > Significance: 2.56729
- > Done in 0.00 min (cpu), 0.00 min (real)

More **complicated workflows + many more options** to tweak runtime, sampling strategies, accuracy etc. exist in the **online docs**.

+ ROOT file output

Branch name	Type	Description
limit	Double_t	Main result of the statistical routine being performed.
limitErr	Double_t	Estimated uncertainty in the result.
mh	Double_t	Value specified withmass command line option.
		The default value is 120.
iToy	Int_t	Pseudo-data set identifier if running withtoys.
iSeed	Int_t	Random seed specified with -s.
t_cpu	Float_t	Estimated processing time.
t_real	Float_t	Elapsed wall-clock time for routine.
quantileExpected	Float_t	Quantile identifier for methods that calculate ex-
		pected and observed results. The meaning is method-
		dependent. Negative values are reserved for entries
		that are not related to quantiles of a calculation. The
		default is set to -1 and specifies that the entry corre-
		sponds to the result obtained from the observed data.
quantileExpected	Float_t	Quantile identifier for methods that calculate expected and observed results. The meaning is method- dependent. Negative values are reserved for entries that are not related to quantiles of a calculation. The default is set to -1 and specifies that the entry corresponds to the result obtained from the observed data.

Published Statistical Models

The **datacard + its inputs** are publishable products from CMS

→ with Combine now available, these can be (re)interpreted using the same software as the original results

First such publication from CMS is the Run-1 Higgs discovery model

CDS Search records Q Communities My dashboard	+D Log in
CMS statistical models	
Published April 15, 2024 Version v1.0 Model 🍙 Open	1K 118
CMS Higgs boson observation statistical model	VIEWS & DOWNLOADS
CMS Collaboration alla	 Show more details
Introduction	Versions
This resource contains the full statistical model from the Higgs Run-1 combination, which led to the Higgs boson discovery, in the format of Combine datacards. The instructions below include a few basic examples on how to extract the significance and signal strength measurements, for more details please consult the Combine documentation.	Version v1.0 Apr 15, 2024 10.17181/c2948-e8875
Datacards Datacards for the combination (and per-decay channel sub-combinations) leading to the Higos-boson discovery at CMS are in the 125.5 folder. The nuisance parameters	Cite all versions? You can cite all versions by using the DOI 10.17181/2cp5k-ggn24. This DOI represents all versions, and will always resolve to the latest one. Read more.
corresponding to different sources of systematic uncertainties are described in the *.html and *.yml files located in that folder.	
For the full combination of decay channels, the relevant datacard is 125.5/comb.txt. The individual datacards for each of the analyses in CMS targeting the main Higgs boson decay modes are also in the 125.5 folder.	Communities
Software instructions	CMS statistical models
General installation instructions for Combine can be found in the Combine documentation.	Details
> container image is provided to ensure reproducible results. The results in this README are obtained using v9.2.1:	
docker runname combine -it gitlab-registry.cern.ch/cms-cloud/combine-standalone:v9.2.1	DOI (Cite this version - v1.0) DOI 10.17181/c2948-e8875
slim version of the container image is also available at gitlab-registry.cern.ch/cms-cloud/combine-standalone:v9.2.1-slim. Versions of packages in the slim container image do not match exactly with the ones in the default container, so small differences in the output of commands with respect to the ones shown below are to be expected.	DOI (Cite all versions) DOI 10.17181/2cp5k-ggn24
You can copy files (such as the datacards and other inputs for combine) using docker cp as documented here.	Resource type
For the commands below, you may require running ulimit -s unlimited; ulimit -u unlimited to avoid memory issues.	Model
https://new-cds.cern.ch/records/c2948-e8875	Publisher CERN

Release includes

- Datacards + inputs
- Recommended container for combine version
- Instructions for
 - Use with example physics models
 - Deriving important results
- html with descriptions of all nuisance parameters in the model



Published Statistical Models

Different results can be produced from the same published inputs

• After all, this is how we operate in CMS ightarrow No surgery of the binary workspaces needed



CMS plans to **regularly release CMS statistical models** with publications

- → Continuous Integration suite being developed to assist CMS users
- → Several workflow managers now being used (eg luigi, snakemake) in CMS to perform statistical calculations themselves
 - → Makes encapsulation of workflow and validations for publication that much easier





Thoughts on future developments

The rest of these slides are my own personal thoughts on development needed going forward. **Not necessarily the opinion of all of CMS!**

These don't include the (obvious?) developments related to improvements in the underlying ROOT/RooFit framework which we benefit from greatly (combine v10 is on its way), or support for different platforms (installation via container, CernVM, CVMFS, standalone, on top of StatAnalysis, conda ...)

1. Scripts here, there and everywhere

Over the years, there have (naturally) been a lot **of useful scripts/tools** that have been added to the package

- Do things with / to the datacards
- Do things with outputs of combine (plots, tables ...)
- Handle larger workflows (Impacts, job submission ...)

							hist many hist
python test/systeme	ematicsAn	alyzer.p	y data/tutorials/	shapes/simple	e-shapes-TH1.txtall -f html > out.html 👘	<pre>veve normalization for process bkg -> n_exp_final_bin Vexpand n_exp_final_binbinl_proc_bkg</pre>	prur"hroc"pxà
						RooProduct::n_exp_final_binbin1_proc_bkg[n_exp_binbin1_proc_bkg * shap	eBkg_bkg_bin1norm] = 521.163
Nuisance	e Rep	ort)		<pre> is a product, which contains n_exp_binbinl_proc_bkg Vexpand n_exp_binbinl_proc_bkg RooRealVar::n exp binbinl proc bkg = 1 C L(-INF - +INF)</pre>	
						default value = 521.163204829	
Nuisance (types)	Range		Processes	Channels		Top-level normalization for process sig -> n_exp_binbin1_p ▼expand n_exp_binbin1_proc_sig	roc_sig
					-	Dumping ProcessNormalization n_exp_binbin1_proc_sig @ 0x96d9690 nominal value: 1	
lumi (InN)	1.000	1.100	background, signal	bin1(1) [+]		log-normals (1): kappa = 1.1, logKappa = 0.0953102, theta = lumi = 0 asymm log-normals (0):	Q qLHC test stat example
alpha (shape)	1 111	1 1 50	background	bin1(1) [+]	-	other terms (1): term r (class RooRealVar), value = 1	
aipira (onapo)			buokground	5(1)[1]		default value = 1.0	expected for sig+bkg expected for ktr-only
bgnorm (InN)	1.000	1.300	background, signal	bin1(1) [+]			10 ⁻¹ observed value
12					-		$p_{\mu} = 0.0768$ 1- $p_{\mu} = 0.5900$
sigma (shape)	1.000	1.000	signal	bin1(1) [+]			10^{-2} $CL_s = 0.1302$
-					-		10-3
							No. And
			py1	thon test/p	olotlestStatCLs.pyinput mygrid.root -	poi rval allmass MASS	
							q _{r,LHC} (r = 1, m _H = 120 GeV)

text2workspace.py data/tutorials/counting/realistic-multi-channel.txt

Process Normalizations

Normalisation Values Evaluated at MH = 125

Channel - bin1

python test/printWorkspaceNormalisations.py data/tutorials/counting/realistic-mult

None of these are described in the paper (purposefully omitted) but some are described in the online docs

1. Scripts here, there and everywhere: combineTool.py

The combineTool.py* script is the most powerful and handles a lot of arduous workflows for users

combineTool.py -M HybridNewGrid ./poi_grid_configuration.json -d toy-hgg-125.root



combineTool.py -M Impacts -d htt_tt.root -m 125 -o impacts.json



- It would be useful if all of these useful scripts became part of the main command line interface
- There are plans to move combineTool over to the Combine package but as a wrapper, it might make more sense that this becomes the main interface for the user ie:

```
combine --M blah ... \rightarrow combineTool(.py) --M blah ...
```

• Could also facilitate IO captures for better integration into (re)interpretation frameworks?

2. Input formats

Combine supports non-ROOT based inputs for template-based models (counting experiments already require no inputs)



- I would like to see more use of these alternative input forms (.json also supported)
- ROOT JSON for serialization would be a natural way to specify inputs to extend to parametric models
 - Note this is different to fully specifying the statistical model in JSON (discuss)
 - Some custom CMS objects (RooParametricHist, RooMultiPdf,...) need to be thought about

2. Input formats – interface?

Datacard mostly acts as a map between objects (eg in a ROOT file), and values to pdfs that should be constructed

It's possible to simply construct the binary workspace directly by skipping the Datacard parsing step

text2workspace.py <datacard.txt>
--dump-datacard > myscript.py

No need to write a .txt Datacard file since one can just fill/edit the python dictionaries/lists in a (re)interpretation workflow

myscript.py

```
Ē
from HiggsAnalysis.CombinedLimit.DatacardParser import *
from HiggsAnalysis.CombinedLimit.ModelTools import *
from HiggsAnalysis.CombinedLimit.ShapeTools import *
from HiggsAnalysis.CombinedLimit.PhysicsModel import *
from sys import exit
from optparse import OptionParser
parser = OptionParser()
addDatacardParserOptions(parser)
options,args = parser.parse_args()
options.bin = True # make a binary workspace
DC = Datacard()
MB = None
DC.bins = ['bin1'] # <type 'list'>
DC.obs = {'bin1': 0.0} # <type 'dict'>
DC.processes = ['ggH', 'qqWW', 'ggWW', 'others'] # <type 'list'>
DC.signals =
             ['ggH'] # <type 'list'>
DC.isSignal = {'qqWW': False, 'ggWW': False, 'ggH': True, 'others': False} # <tyr
DC.keyline = [('bin1', 'ggH', True), ('bin1', 'qqWW', False), ('bin1', 'ggWW', F
DC.exp = {'bin1': {'qqWW': 0.63, 'ggWW': 0.06, 'ggH': 1.47, 'others': 0.22}} # <
DC.systs = [('lumi', False, 'lnN', [], {'bin1': {'qqWW': 0.0, 'ggWW': 1.11, 'ggH'
DC.shapeMap = {} # <type 'dict'>
DC.hasShapes = False # <type 'bool'>
DC.flatParamNuisances = {} # <type 'dict'>
DC.rateParams = {} # <type 'dict'>
DC.extArgs = {} # <type 'dict'>
DC.rateParamsOrder = set([]) # <type 'set'>
DC.frozenNuisances = set([]) # <type 'set'>
DC.systematicsShapeMap = {} # <type 'dict'>
DC.nuisanceEditLines = [] # <type 'list'>
DC.groups = {} # <type 'dict'>
DC.discretes = [] # <type 'list'>
options.out
              = "combine_workspace.root"
                                         # Output workspace name
options.fileName = "./"
                               # Path to input ROOT files
options.verbose = "1"
                               # Verbosity
if DC.hasShapes:
   MB = ShapeBuilder(DC, options)
else:
   MB = CountingModelBuilder(DC, options)
# Set physics models
MB.setPhysics(defaultModel)
MB.doModel()
```



3. Interpretors

Combine provides the implementation of the model and performs the calculations but work on going to support **other tools** to do this (no ROOT dependence) ...

E.G 1: pyHF

- For simple template-based modes, able to translate between Combine Datacard and pyHF JSON formats
- Can use pyHF interpretation tools to calculate limits etc from CMS datacards

E.G 2: combinetf

- Extension to use TensorFlow for computational graph (+autograd functionality) by converting Datacard to hdf5 format
- Performance boost for extremely complicated template models (many bins)
- Restricted to template-based methods only and not documented (or widely used yet) in CMS

	Likelihood	${\sf Likelihood}{+}{\sf Gradient}$	Hessian	
Combine, TR1950X 1 Thread	10ms	830ms	-	
TF, TR1950X 1 Thread	70ms	430ms	165s	
TF, TR1950X 32 Thread	20ms	71ms	32s	
TF, 2x Xeon Silver 4110 32 Thread	17ms	54ms	24s	
TF, GTX1080	7ms	13ms	10s	
TF, V100	4ms	7ms	8s	
<u>J. Bendavid</u>	5 K.			



K. Skovpen

4. Lists of (other) issues

Without going into detail, there are lots of things that need doing

→ Lots of room for improvement and publishing statistical models will help development from wider community

lssues			<u>PRs</u>				
Filters - Q is:issue is:open	© Labels 17 ♀ Milestones 3 Net	wissue Filters • Q is:pris:open		C Labels 17	⇔ Milestones 3	New pull rec	quest
□ ③ 68 Open ✓ 97 Closed Author ▼ Label ▼	Projects • Milestones • Assignee •	Sort - 🚺 39 Open 🗸 763 Closed	Author - Label - Project	ts - Milestones	• Reviews •	Assignee - S	ort 🕶
Warning about long formulas still relevant? #953 opened on Apr 22 by nsmith-		□ \$\$ Create CMakeLists.txt × #967 opened 2 days ago by will-cern					
O Double to int casting can cause precision issues #945 opened on Apr 17 by GlacomoBoldrini		□ 11 Update CI workflows ✓ #965 opened last week by anigamova					
O Consider using CITATION.cff for making citation easier #942 opened on Apr 15 by matthewfeickert		3 11 Fix a bug in src/VerticalInterpPdf.cc × (combine.v10) #964 opened last week by anigamova					
O Poor error reporting from AsymptoticLimits with bad fits #925 opened on Mar 26 by andrzejnovak		Il Update CMakeLists.txt - make path to header file match how it #961 opened 3 weeks ago by will-cern	will be ×				Ç 7
O Local standalone conda installation problems on macOS #898 opened on Feb 7 by ikrommyd		\$1 Updated CMakeLists.txt - new option to modify rootmap to avoi #957 opened last month by will-cern	id conflicts \checkmark				
Obcker instructions for Mac users #896 opened on Jan 9 by glacomoortona		5 In Avoid warnings when building with CMSSW 14_1_X combine.vi<br #955 opened on May 1 by guitargeek	10				
Ocde duplication found (enhancement) (needs work) #884 opened on Dec 16, 2023 by adavidzh		Il Avoid problems with FastVerticalInterpHistPdf2Base initiali #952 opened on Apr 19 by guilargeek	zation ✓ combine.v10				
O Different results with each run (question) #883 opened on Dec 16, 2023 by nucleosynthesis		10 11 Fix copy constructors in RooMultiPdf for ROOT v6.30 × (combine #951 opened on Apr 18 by anigemove	e.v10				
O Version missing #880 opened on Dec 14, 2023 by adavidzh		□ 2 1) Use override keywar were necessary ✓ combine.v10					Ç 7
O Remove AtlasPdfs when they are integrated into ROOT (enhancement) (LHC Comb #872 opened on Nov 20, 2023 by nsmith-		save opened on Apr // by guildingeek □ 11 Avoid using deprecated RooDataSet constructor ✓ combine.v10					Ç 3
G Fix linter error for type comparison #857 opened on Sep 7, 2023 by nsmith-		#947 opened on Apr 17 by guitargeek 11 Add a CMakeLists.txt for compiling with cmake (combine.v10)					Q 4
O Fitting Bernstein in multiple ranges #849 opened on Jul 11, 2023 by Charlotte-Knight		#943 opened on Apr 16 by will-cern #943 opened on Apr 16 by will-cern In Document thefromfile option from combineTool ✓					
O Need to improve toy generation documentation #847 opened on Jul 6, 2023 by adevit		#937 opened on Apr 11 by runtingt □ 11 Don't trigger docs builds from 112x branch ×					
Reporting a vulnerability #835 opened on Apr 10, 2023 by Igibek		2 #935 opened on Apr 8 by kcormi UDdate bin-wise-stats.md					5
Improve fitting routines #823 opened on Eah 27, 2023 by anigamous P 3 tasks		#929 opened on Apr 2 by pfackeldey	into combine de combine da				
Simplify dr		#008 opened on Feb 22 by pkausw					ا لې
#822 opened on Peb 27, 2023 by anigamova ③ Binned bias test		Il WIP: Fixes for EFT combination & RobustHesse parallelisation ∽ #906 opened on Feb 22 by ajglibert	/				
#821 opened on Feb 27. 2023 by anigamova		10 Move combineTool.py and routines needed to create impact plo	ots to combine 🗸 cat-hackathon	combine.v10		1	11 📿

Summary

Combine is more or less THE statistics tool in CMS

- Datacard + inputs → defines statistical model, Combine constructs it and performs statistical calculations
- Counting, template and parametric modes supported, different physics models and different calculations from the same underlying inputs

Future developments ongoing

- Restructuring of the software package in discussion: Less scripts, more consolidation of workflow management
- Input formats: I think Physics model should stay separate from underlying objects but ROOT JSON could replace our typical inputs and could be used to store the constructed workspace too
- Interpretors: Users might not want to use combine, plain RooFit, pyHF, combinetf should be supported looking forward

Plenty of room for improvement

- Combine has evolved over a period >10 years since before the Higgs discovery so naturally there are things to be updated/improved
- I have a long list of issues that irritate me and need fixing (ask me about -t vs -T!)
- However, tool is still a big part of doing CMS analyses and its still (imo) a good tool for statistics

Thanks!



Backup Slides

Timeline for public likelihoods



L. Heinrich

Template based shape analysis





<u>-t vs -T</u>

Never ending source of confusion is the difference between -t and -T in combine

Reason is that there are "levels" of toy generation with combine

-t supports ~all methods

 \rightarrow I want to generate a toy dataset to make plots with/perform a test of a fit ...

 \rightarrow useful as lots of extra diagnostic info can be saved (toys themselves, fit results + propagated yields/bin contents for each toy ...)

-T is used specifically for toy-based methods

 \rightarrow i.e anything using –M HybridNew (limits, p-values, FC intervals)

 \rightarrow DetailedOutput implemented in certain test-statistics only?

The type of toy generation is defaulted differently between the two

-t \rightarrow Hybrid by default, frequentist if you add –toysFreq

-T \rightarrow frequentist by default if using --LHCmode <X> , can use Hybrid if specify –genNuisances

There's even another toy generation for sampling from post-fit covariances for making plots inside FitDiagnostics ତ

Of course, all of this is documented as such but some consolidation