Data Combination - In Practice -



Jan Kieseler 29.3.2022





• Full likelihood combinations (only some pointers)

General common pitfalls and challenges when performing combinations

• Example of likelihood approximation

Method validation based on toys



 Combined hands-on/hands-off examples using <u>Convino</u> (<u>https://github.com/jkiesele/Convino</u>)

Outline







Convino Setup

- Please check **now** if you can 'ssh **-X** to' <u>lxplus.cern.ch</u>
- Make sure to use X forwarding if you can

```
> bash
> cd /afs/cern.ch/user/j/jkiesele/public/Convino/latest
> source lxplus_env.sh
> cd
> mkdir convino_tutorial
> cd convino_tutorial
```

- > convino /afs/cern.ch/user/j/jkiesele/public/Convino/latest/examples/exampleconfig.txt
- If you don't have access or anything does not work, you can still follow this lecture fully
- There is no need to spend the whole lecture trying to get it to work if it does not work out of the box



Please indicate if you can run the example by adding a "1_C " in front of your name



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Rename



Combining full likelihoods: Combine and HistFactory

- "Cleanest way" of performing the combination: works for limits and measurements
- Standard tools used for likelihood fits and full likelihood combinations in CMS and ATLAS
- Build on top of ROOT and RooFit
- Likelihood is persisted in RooFit workspace
- Inputs of different human readable sorts (text files+ROOT histograms, JSON)

Combine

- 3-day tutorial (CMS only): <u>https://indico.cern.ch/event/976099/timetable/?view=standard</u>
- Public documentation: <u>https://cms-analysis.github.io/HiggsAnalysis-CombinedLimit/</u>

HistFactory-based, e.g. TRExFitter:

- Original Histfactory document: <u>https://cds.cern.ch/record/1456844?In=en</u>
- Tutorial/docs: <u>https://trexfitter-docs.web.cern.ch/trexfitter-docs/</u>

Other pythonic approaches using automatic differentiation

> Combine-tensorflow <u>Github</u>



am not an expert here!



https://cds.cern.ch/record/2752552?In=en



- Modelling of the likelihood
- Template morphing
- Analytic functional forms
- Uncertainties due to limited statistics in the nominal MC samples

• Different result representations

- Limit setting (asymptotic+toy based)
- Significance / p-value determination
- Confidence intervals
- Discrete profiling
- Unfolding (combine)

• Diagnostics

- Uncertainty impacts
- nuisance parameter constraints and pulls
- Goodness of fit tests
- Checks on toy / Asimov data



• Very powerful tools are available: impossible to cover them here

Introduce Correlation Assumptions

- Consider two measurements from two different experiments
- one or more parameters of interest
- nuisance parameters, representing sources of systematic uncertainties or analysis repeated for each variation
- $-2\ln L^{\alpha}(\mu,\theta^{\alpha}) = -2\ln P(y^{\alpha}|\mu,\theta^{\alpha}) + \sum_{i} \frac{\theta^{\alpha_{i}^{2}}}{\sigma_{i}^{\alpha_{i}}} \quad \text{or} \quad -2\ln L^{\alpha}(\mu,\lambda^{\alpha}) = -2\ln P(y^{\alpha}|\mu,\lambda^{\alpha}) + \sum_{i} \lambda^{\alpha_{i}^{2}}$
- Correlations between uncertainty sources for different experiments

"Different parameter settings and strategies are used to evaluate the systematic uncertainties due to initial and final state radiation. Preliminary investigations indicate that the methodologies used are approximately equivalent, and describe to a large extent the same physics aspects. Moreover, different baseline Monte Carlo programs and hadronisation models are used for the evaluation of the MC modelling systematics. In the presence of these underlying differences, we opt to reduce the assumed correlations across experiments for the MC and Rad categories from 100% to 50%."

CMS-PAS-TOP-12-001

• Express as
$$\sum_{i} \lambda^{\alpha 2}_{i} \rightarrow \lambda^{T} (C^{\alpha})^{-1} \lambda$$

Then when combining the likelihoods this becomes





Pitfalls in practice: Ill-defined Assumptions

- Assumed strong correlations between
- $\rightarrow \lambda_0$ and λ_1
- λ_1 and λ_2

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- This is equivalent to stating:
- λ_0 and λ_1 describe (almost) the same uncertainty
- λ_1 and λ_2 describe (almost) the same uncertainty
- λ_0 and λ_2 have no correlation whatsoever
- In practice, similar situations can occur quite frequently when assigning correlations
- These can easily lead to C being not positive definite and/or not invertible
 - If this occurs, and the fit fails, this is not an issue of the program but a result of ill defined assumptions

Even if C is invertible and p.d. (e.g. smaller correlations), it might still be worth thinking about the assumption again

"Different parameter settings and strategies are used to evaluate the systematic uncertainties due to initial and final state radiation. Preliminary investigations indicate that the methodologies used are approximately equivalent, and describe to a large extent the same physics aspects. Moreover, different baseline Monte Carlo programs and hadronisation models are used for the evaluation of the MC modelling systematics. In the presence of these underlying differences, we opt to reduce the assumed correlations across experiments for the MC and Rad categories from 100% to 50%."

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Pitfalls in practice: Cause and Effect

*Uncertainty A is correlated with uncertainty B"What does it really (not) mean?



- The variation of sources of uncertainties having a similar effect on a measurement (or limit) does not imply anything w.r.t. the correlations of the sources
- The measured distribution cannot tell us anything about the correlations between uncertainty sources





Ancillary Measurements



- judge correlations between the sources A and B







Pitfalls in Practice: Grouped Correlations

- Estimating the correlations between individual sources often challenging
- Often used fall-back: correlations between groups of uncertainties "The modelling uncertainty sources of the measurements performed by ATLAS and CMS should be somewhat correlated"
- Often right from a physics perspective, but also ill defined
- Impact on different measurements
- Signs are lost
- Impossible to treat fully consistently if correlations between sources in the same group exist

'Quasi-solutions'

- Try to avoid assigning correlations to groups in the first place and try to do it source-by-source
- Possibly try to infer source-by-source correlations from group correlations
- Make sure to check robustness of combined result against these assumptions





Approximate Likelihood Combinations of Measurements

- Consider a measurement of an observable that results in a value X and and total uncertainty σ
 - Performed by repeating the measurement for each uncertainty source
 - (From here on fully Gaussian)
- Can be easily expressed as an approximate likelihood (/chi2) $-2\ln \tilde{L}(\mu,\theta) = (x - (\mu + \theta))^2 / \sigma_{\text{stat}}^2 + \sum_{i} \frac{\theta_i^2}{\sigma_{\theta_i}^2}$

$$-2\ln \tilde{L}(\mu,\theta) = \chi_s^2(\mu,\theta) + \chi_P^2(\theta)$$

- Can be used for the combination directly
- For more complex measurements: Taylor expansion around maximum
 - The first term is constant \rightarrow does not affect the result
 - The second term (first derivatives) are zero, since we maximised the likelihood to perform the measurement
 - The third term (second derivatives) does not vanish ~ Hessian
- **Example** of approximate likelihood: try to express as 3 terms (convino method)

$$-2\ln \tilde{L} = \chi^2 = \chi_s^2(\mu,\theta) + \chi_u^2(?) + \chi_P^2(\theta)$$

"Everything more complex": nuisance parameter constraints, correlations







Syst. A 5 Syst. B 3 Stat 2.		rel. unc. [%]	
syst. B 3 dat 2.	Syst. A	5	
dat 2.	syst. B	3	
3	stat.	2	





Convino Approach

$$-2\ln \tilde{L} = \chi^2 = \chi_s^2(\mu, \theta) + \chi_u^2(?) + \chi_P^2(\theta) \qquad \lambda = \theta/\sigma_\theta \rightarrow$$

- Assume
- $\star \chi^2_{\mu}(?) = \chi^2_{\mu}(\lambda) = \lambda^T D \lambda$ $\chi_P^2(\lambda) = \lambda^T \mathbf{1}\lambda = \sum P_i(\lambda)$

Correlations between nuisance parameters and additional constraints on them "Original" penalty terms

- Assume the covariance of the inputs measurements to be known (minimum requirement, more in the next lecture)
- Re-organise Hessian of measurement α in the following form

$$H_{\rm in}^{\alpha} = \begin{pmatrix} \tilde{C} & \kappa^T \\ \kappa & M \end{pmatrix}^{\alpha}$$

• Derive parameters of the approximate likelihood by comparing analytical Hessian and input Hessian

$-2 \ln \tilde{L} = \chi^2 = \chi_s^2(\mu, \lambda) + \chi_{\mu}^2(?) + \chi_P^2(\lambda)$

(Will help introduce correlation assumptions later)



$$-2\ln(L^{\alpha}) = \chi_{\alpha}^{2} = \sum_{\mu\nu} \tilde{M}_{\mu\nu}^{\alpha} \frac{\xi_{\mu}^{\alpha}\xi_{\nu}^{\alpha}}{\tau_{\mu}^{\alpha}\tau_{\nu}^{\alpha}} + \sum_{ij}\lambda_{i} D_{ij}^{\alpha}\lambda_{j} + \sum_{i} P_{i}^{2}(\lambda_{i}), \text{ with}$$
$$\xi_{\mu}^{\alpha} = x_{\mu}^{\alpha} - \left(\bar{x}_{\mu} \prod_{i} (\lambda_{i} \overline{K_{\mu i}^{\alpha}} / x_{\mu}^{\alpha} + 1) + \sum_{i} \lambda_{i} k_{\mu i}^{\alpha}\right), \quad \tau_{\mu}^{\alpha} = \frac{\bar{x}_{\mu}}{x_{\mu}^{\alpha}}$$

$$H_{\rm in}^{\alpha} = \begin{pmatrix} \tilde{C} & \kappa^T \\ \kappa & M \end{pmatrix}^{\alpha}$$

$$\begin{split} \tilde{H}^{\alpha}_{\mu\nu}(0) &= \frac{1}{2} \left(\frac{\partial^2}{\partial \Delta x^{\alpha}_{\mu} \partial \Delta x^{\alpha}_{\nu}} \chi^2_{\alpha} \right) \Big|_{\lambda_i = 0, \ \Delta x^{\alpha}_{\mu} = 0 \ \forall \ i, \ \mu} &= \tilde{M}_{\mu\nu}, \quad \Leftrightarrow \quad M \\ \tilde{H}^{\alpha}_{\mu i}(0) &= \frac{1}{2} \left(\frac{\partial^2}{\partial \Delta x^{\alpha}_{\mu} \partial \lambda_i} \chi^2_{\alpha} \right) \Big|_{\lambda_i = 0, \ \Delta x^{\alpha}_{\mu} = 0 \ \forall \ i, \ \mu} &= \sum_{\nu} \tilde{M}_{\mu\nu}(-\tilde{k}^{\alpha}_{\nu i}), \\ \Leftrightarrow \quad \left| \tilde{k}^{\alpha}_{\nu i} \right|_{\mu\nu} = -\sum_{\mu} ((M^{\alpha})^{-1})_{\mu\nu} \ \kappa^{\alpha}_{\mu i}. \end{split}$$

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Identify χ_s^2



$$-2\ln(L^{\alpha}) = \chi_{\alpha}^{2} = \sum_{\mu\nu} \tilde{M}_{\mu\nu}^{\alpha} \frac{\xi_{\mu}^{\alpha}\xi_{\nu}^{\alpha}}{\tau_{\mu}^{\alpha}\tau_{\nu}^{\alpha}} + \sum_{ij}\lambda_{i}D_{ij}^{\alpha}\lambda_{j} + \sum_{i}P_{i}^{2}(\lambda_{i}), \text{ with}$$
$$\xi_{\mu}^{\alpha} = x_{\mu}^{\alpha} - \left(\bar{x}_{\mu}\prod_{i}(\lambda_{i}K_{\mu i}^{\alpha}/x_{\mu}^{\alpha}+1) + \sum_{i}\lambda_{i}k_{\mu i}^{\alpha}\right), \quad \tau_{\mu}^{\alpha} = \frac{\bar{x}_{\mu}}{x_{\mu}^{\alpha}}$$

$$\begin{split} \tilde{H}_{ij}^{\alpha}(0) &= \frac{1}{2} \left(\frac{\partial^2}{\partial \lambda_i \partial \lambda_j} \chi_{\alpha}^2 \right) \Big|_{\lambda_i = 0, \ \Delta x_{\mu}^{\alpha} = 0 \ \forall \ i, \ \mu} \\ &= \left| D_{ij}^{\alpha} + \delta_{ij} \frac{1}{2} \frac{\partial^2}{\partial \lambda_i^2} P_i^2 \right|_{\lambda_i = 0} + \sum_{\mu\nu} M_{\mu\nu}^{\alpha} \tilde{k}_{\nu i}^{\alpha} \tilde{k}_{\mu j}^{\alpha}. \end{split}$$
$$&\Leftrightarrow \left| D_{ij}^{\alpha} \right| = \tilde{C}_{ij}^{\alpha} - \delta_{ij} - \sum_{\mu\nu} M_{\mu\nu}^{\alpha} \tilde{k}_{\nu i}^{\alpha} \tilde{k}_{\mu j}^{\alpha}. \end{split}$$

→All parameters identified, combination can be performed

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Identify χ_{μ}^2

$$H_{\rm in}^{\alpha} = \begin{pmatrix} \tilde{C} & \kappa^T \\ \kappa & M \end{pmatrix}^{\alpha}$$

 $\chi_P^2(\lambda) = \lambda^T 1 \lambda = \sum P_i(\lambda)$ by definition, can use same method to introduce correlations discussed before ($\sum \lambda_i^{\alpha 2} \to \lambda^T (C^{\alpha})^{-1} \lambda$)









- Ultimate test of a model: toy experiments with known 'true' reference value
- E.g. generate independent bins, given an expectation value for each bin
- ► X_{t,i} can also be chosen randomly



- The toy needs to include all possible variations that are expected to occur in practice

 - Systematic dependencies in each bin, for each x

Validation workflow





Interpretation of the validation results



Validate the combination of measurements w.r.t. a combined measurement

- How much does the (approximate) combination method bias the central result
- How well is the uncertainty (possibly asymmetric) modelled by the combination method

➡In either case, performing toy-based validation is usually very valuable

➡Can be used to validate even models that are not generally correct, but might still work for the specific case







Validate the model fit to the data

- Does the model have a bias
- Does the model describe the fluctuations correctly and assigns the uncertainty correctly





In practice: Convino Validation

- Combine pseudo 'cross section' measurements
 - Binned distributions
 - The measured value scales with N
- No systematic uncertainties

$$egin{array}{rcl} x^a&=&s\cdot 100,\ x^b&=&x^a+10\sqrt{x^a}, \end{array}$$

• Bias as expected from a chi2 approach



 For other combinations, the statistical uncertainty of the measurements might not scale with the number of events
 Choice needs to be adapted to the observable





Systematic uncertainties

- Reduce the relative impact from statistical uncertainties to 0.5%
- Introduce 2 systematic uncertainties per pseudo measurement
- Limit contribution per uncertainty to t
- Correlate one uncertainty of one with one of the other



➡Also validated using toys for many other scenarios







COMBINED HANDS-ON/ HANDS-OFF COMBINATION EXAMPLES

- > bash
- > cd /afs/cern.ch/user/j/jkiesele/public/Convino/latest
- > source lxplus_env.sh
- > cd

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- > mkdir convino_tutorial
- > cd convino tutorial
- > cp -r /afs/cern.ch/user/j/jkiesele/public/Convino/tutorial/* .

> convino /afs/cern.ch/user/j/jkiesele/public/Convino/latest/examples/exampleconfig.txt



The Convino Inputs

>	cd ~/convino_tutorial/1
	<pre># This is the 'base file' for example 1 # The header can and should contain some description</pre>
	[global] #information mostly for extra options in differential measurements. Can be left empty in most case
	[end global]
	[inputs]
	nFiles = 2
	<pre>file0 = measurement_1.txt file1 = measurement_2.txt</pre>
	[end inputs]
	[observables]
	<pre># This block defines which estimates should be combined. # The combined name of the observable can be chosen freely.</pre>
	<pre>combined_a = estimate_a1 + estimate_a2</pre>
	[end observables]
	[correlations]
	<pre># define correlations with the following syntax # lumi_a1 = (0.3) lumi_a2 # this line assigns a correlation of 0.3 between lumi_a1 and lumi_a2</pre>
	<pre># if there were more uncertainties, one can define multiple correlations in one line, e.g. # lumi_a1 = (0.3) lumi_a2 + (0.4) JES_a2</pre>
	[end correlations]
	[uncertainty impacts]
	<pre># this is optional to evaluate uncertainty impacts (can take longer) # example (commented out) # lumi_total = lumi_a1 + lumi_a2</pre>
	[end uncertainty impacts]

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(🔴 🔴 🔴 measurement_1.txt [not fitted] # the uncertainties listed here describe orthogonal uncertainties, # e.g. when repeating the measurement after varying different sources of uncertainties. # the "stat" keyword is reserved and must be given last lumi_a1 stat estimate_a1 4. 0.1 [end not fitted] [systematics] # can be used to define whether an uncertainty is absolute or relative.
the default is absolute; example (commented out): # lumi_a1 = relative [end systematics] [estimates] # The central value of each estimates is defined here n_estimates = 1 name_0 = estimate_a1 value_0 = 100; [end estimates] measurement_2.txt

[end estimates]





Example 1

result.txt

[pre-combine systematics correlations] lumi_a1 1.0000000 0.0000000 lumi_a2 0.0000000 1.0000000 [end pre-combine systematics correlations]

[post-combine systematics correlations] multiplied by: 1000 lumi_a1 1000.0000 998.74870 lumi_a2 998.74870 1000.0000 [end post-combine systematics correlations]

[pre-combine estimate correlations]

[end pre-combine estimate correlations]

[post-combine result correlations] combined_a 1.0000000 [end post-combine result correlations]

[post-combine result covariance] combined_a 8.0050000 [end post-combine result covariance]

combined (minimum chi^2=0): combined_a: 100 +2.82931 -2.82931 [full correlation matrix] multiplied by: 1000 lumi a1 1000.0000 998.74870 999.37415 998.74870 1000.0000 999.37415 lumi a2 combined_a 999.37415 999.37415 1000.0000 [end full correlation matrix]

[full covariance matrix] lumi a1 0.4991720 0.4985479 1.9954389 lumi a2 0.4985479 0.4991720 1.9954389 combined_a 1.9954389 1.9954389 7.9867499 [end full covariance matrix]

Name	pull	constrai	nt	
lumi_a1	0.000	0.706		
lumi_a2	0.000	0.706		
Simple i	impact ta	able: name,	impact	[%]
		combined_a		
lumi_a1		2.82754018	868783	
lumi_a2		2.82754018	868783	

merged impacts

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No correlations assumed

Post combination: large correlations

One result with large correlation with itself;)

Central result and total uncertainty: how large is the reduction?

Full covariance (nuisance parameters and combined value)

Pulls and constraints

Simple impacts (calculated from correlation coefficients)

 Introduce a correlation between the luminosity uncertainties of experiments A and B:

base_file.txt

```
[correlations]
```

```
# define correlations with t
# lumi_a1 = (0.3) lumi_a2
# this line assigns a correl
```



- Run convino with convino --prefix withcorr base file.txt to create withcorr result.txt
- How does the combined result change?
- Printout
- Result file







Correlation Scan

• Use the scan option of convino, adapt base_file.txt

lumi_a1 = (0 & -0.99 : 0.99) lumi_a2

scans the correlation coefficient from -0.99 to 0.99, and assumes a correlation of zero as the central value



> convino -sp base_file.txt
> mupdf scan_results/combined_a_lumi_a1_lumi_a2_0.pdf

• What do we see? [scan_results/combined_a_lumi_a1_lumi_a2_0.pdf]





Correlation Scan

• Use the scan option of convino, adapt base_file.txt

lumi_a1 = (0 & -0.99 : 0.99) lumi_a2

scans the correlation coefficient from -0.99 to 0.99, and assumes a correlation of zero as the central value



- With larger correlation coefficient, the uncertainty increases.
- This is not true in general. Large correlation != conservative



Example 2: Correlations Reduce Uncertainty

- NB: Of course, if the impacts have opposite sign, the combined result gets more precise with larger correlation
- But, also in other cases... assume measurements with very different impact of uncertainties (example 2)

measurement_1.txt			e e e measurement_2.txt				
[not fitted]			[not fitted]				
estimate_a1	sys_b1 0.5	stat 0.1	estimate_a2	lumi_a2 1	syst_a2 3.	stat 0.1	
[end not fitted]			[end not fitted]				



cd ../2
convino -sp base_file.txt
mupdf scan_results/combined_a_syst_a2_sys_b1_0.pdf

• What do we see?

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Results Example 2



Large correlations does not equal conservative
 Assume correlations carefully, and check the dependence (e.g. through scans)

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Example 3: Ill-defined assumptions

🔴 🕘 📄 me	asuremen	nt_1.txt		🌔 😑 🛑 📄 meas	surement	_2.
[not fitted]				[not fitted]		
estimate_a1	syst_a1 3.	syst_b1 2.	stat 0.1	estimate_a2	lumi_a2 1	sy 3.
[end not fitted]				[end not fitted]		

- Run the example
- What is the problem?
- Does removing the line syst_b1 = ... help?

txt — Edited st_a2 stat 0.1 [correlations]
 syst_a1 = (0.99) lumi_a2 + (0.99) syst_a2
 syst_b1 = (0.99) lumi_a2

[end correlations]



Example 4: Correlated Nuisances



- More complex example
 - Main contribution from sys c2
 - Moderate correlations between the nuisance parameters of measurement 1
- (e.g. BLUE)
- Compare the correlation scan and central results when including or ignoring these correlations (do a scan)
 - For convenience, the correlation matrix without correlations between nuisance parameters is in the same file
 - To create distinct outputs you can use the 'prefix' option: convino -sp --prefix ignorecorr base_file.txt

• Often these moderate correlations are considered as removable to apply methods and tools that cannot treat these correlations







Results Example 4



- Dependence and results differ quite significantly
- Here, ignoring the correlations gives a larger uncertainty
- This is not true in general
- These correlations can be more important than they seem at first glance







Ignoring Correlations: Toy Example



- Generate pseudo measurements with different contributions of systematic uncertainties
- Compare to combined likelihood
- In particular uncertainties can be largely over- or underestimated.



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Back to grouped uncertainties

🔴 🕘 📄 me	asuremer	nt_1.txt		🌔 😑 🛑 mea	surement _.	_2
[not fitted]				[not fitted]		
estimate_a1	syst_a1 3.	syst_b1 2.	stat 0.1	estimate_a2	lumi_a2 1	1.1 10
[end not fitted]				[end not fitted]		

- Despite it not being fully well defined, orthogonal uncertainties can be grouped by summing them up quadratically
- In practice, if the measurements to be combined have a similar split into sub contributions, this might be ok

[correlation mag	atrix]				
sys_a2 sys_b2 sys_c2 sys_d2 estimate_a1	(1) (1) (0.1) (0.9) (10.6)	1 0.3 0.4 0.3 0.2026484018	1 0.3 0.2 0.2652968037	1 0.6 0.8479452055	1 0.105936073
[end correlati	on matr	ix]			

- The concept breaks down entirely when there are correlations between the nuisance parameters of one individual measurement → any attempt results in information loss
- We should help avoid this grouping in the future





Common pitfalls are often related to (consistency of) correlation assumptions

It is instrumental to precisely distinguish between cause and effect

All methods rely on having sufficient information accessible and being able to make use of it

Summary

Well designed toy experiments are incredibly helpful for combinations as well as measurements and limits

For the combination of measurements approximate likelihood methods can be instructive and fully sufficient

