09/06/22

Unfolding and Regularisation Experiences from neutrino cross-section measurements

Stephen Dolan

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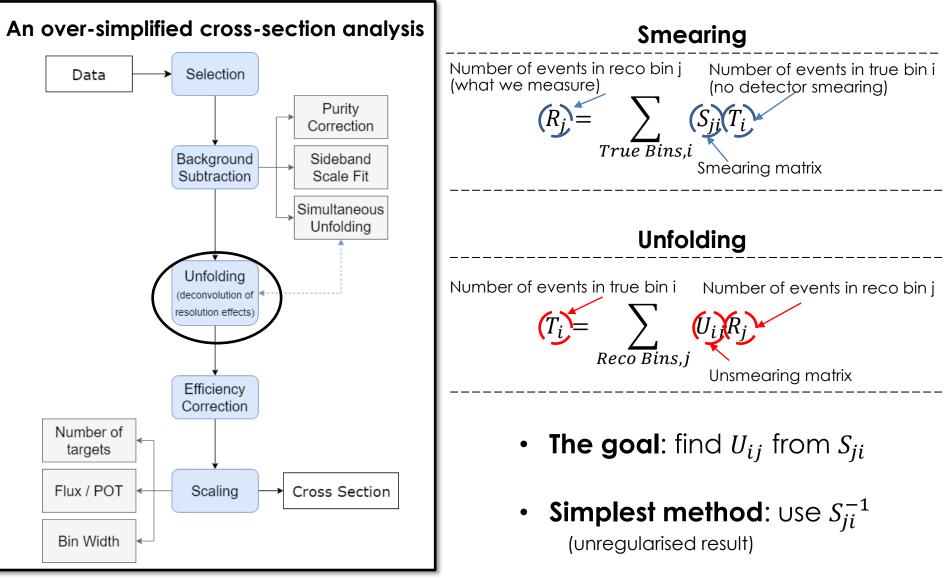
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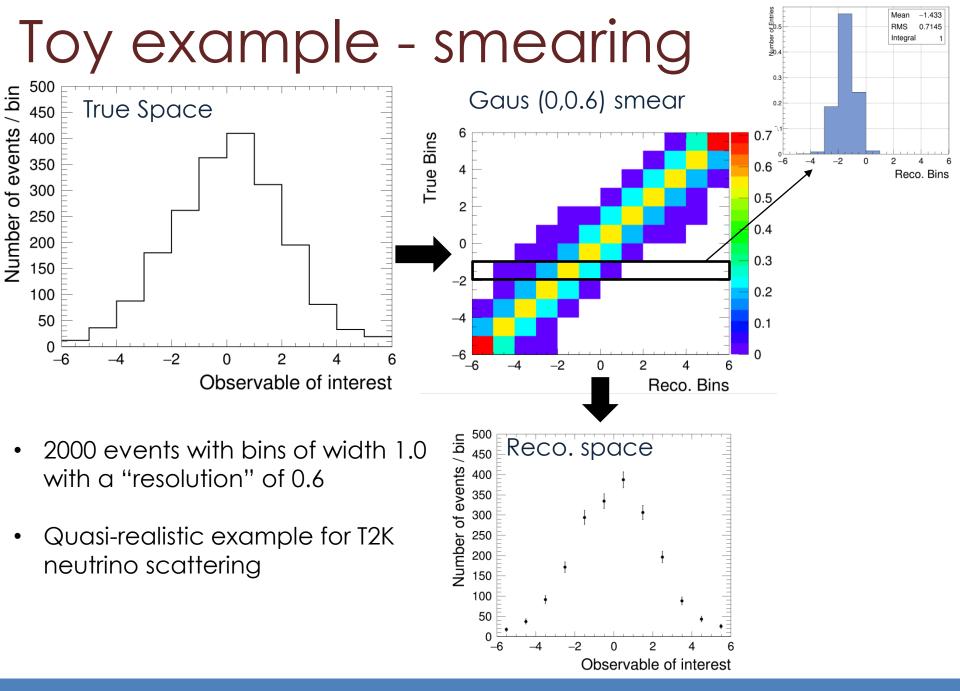


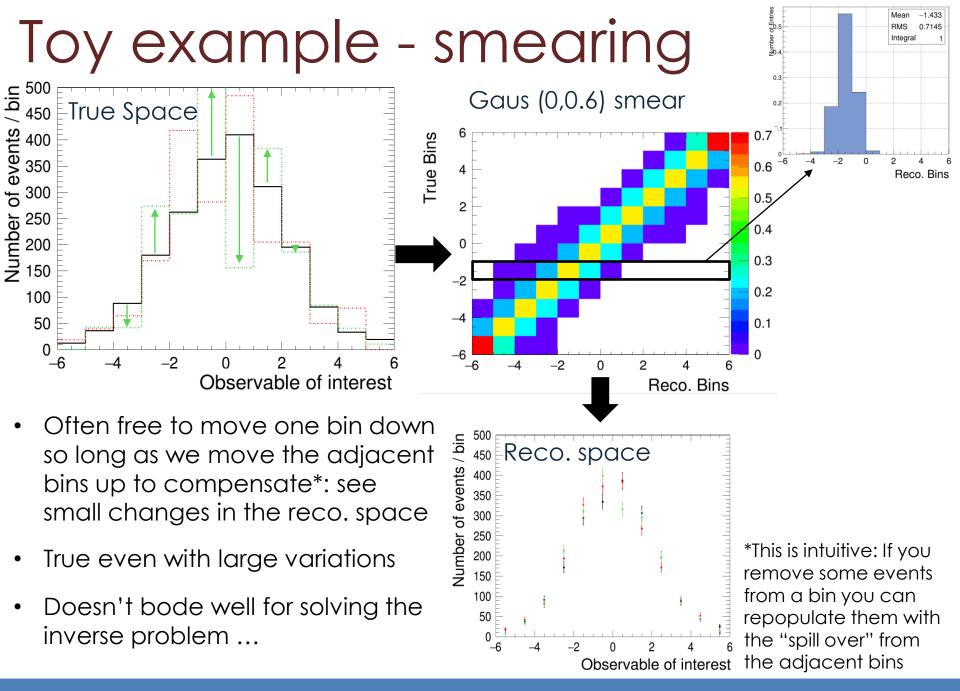
Overview

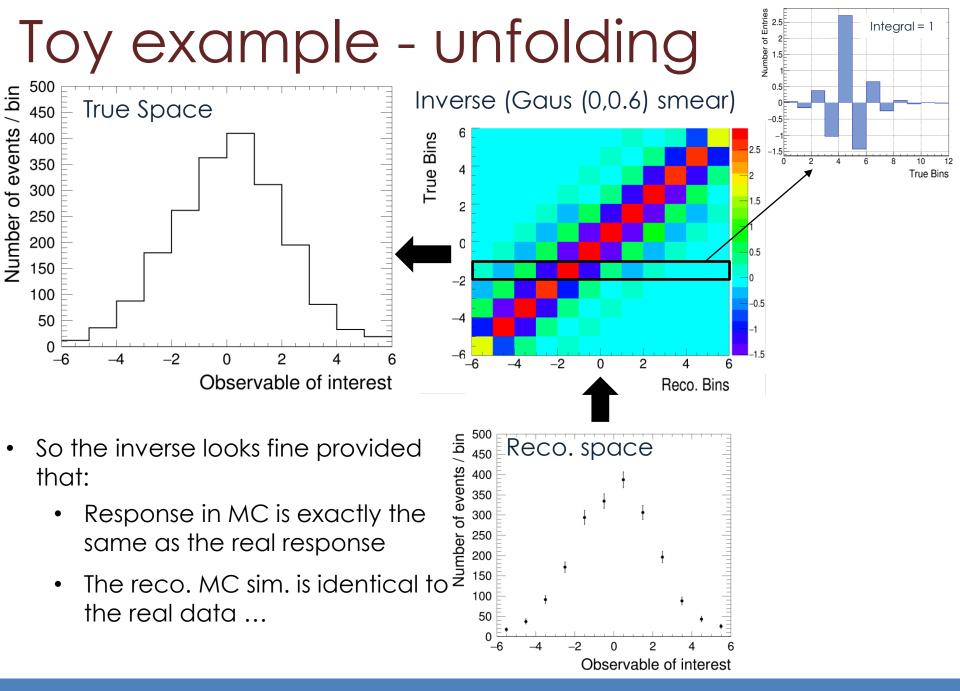
- This talk is meant to be an overview of some experiences with unfolding and regularisation for neutrino cross-section measurements
- This is heavily based on talks I gave at <u>NuInt</u> and <u>PhyStat-nu</u>
- It is very likely that the difference in the expected statistics in ProtoDUNE measurements means that not all the examples are directly applicable
- However, hopefully some of the general considerations and concerns regarding unfolding are transferable

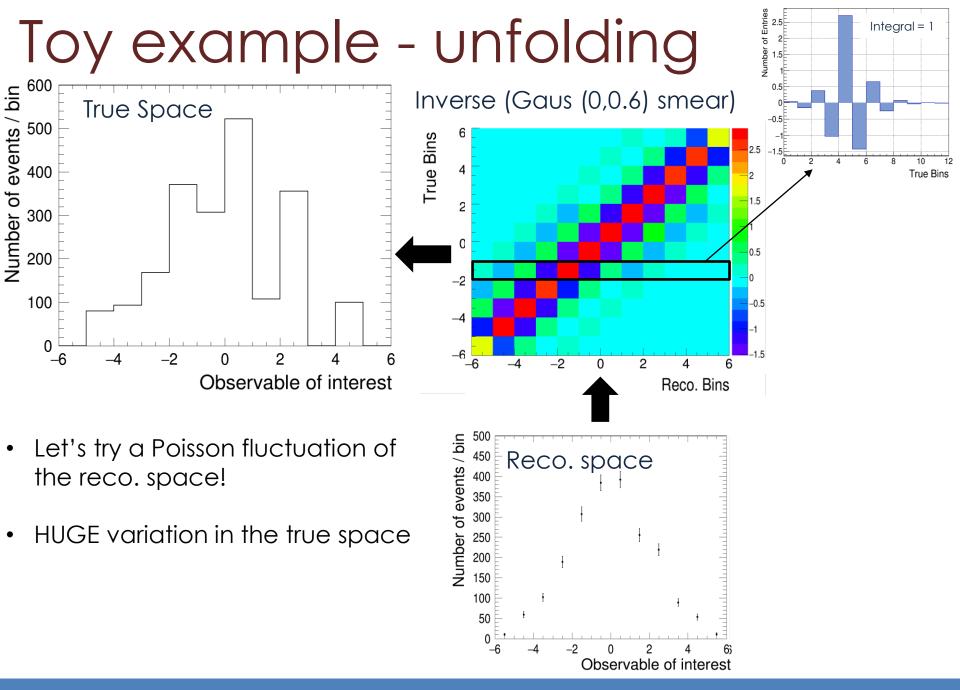
Unfolding



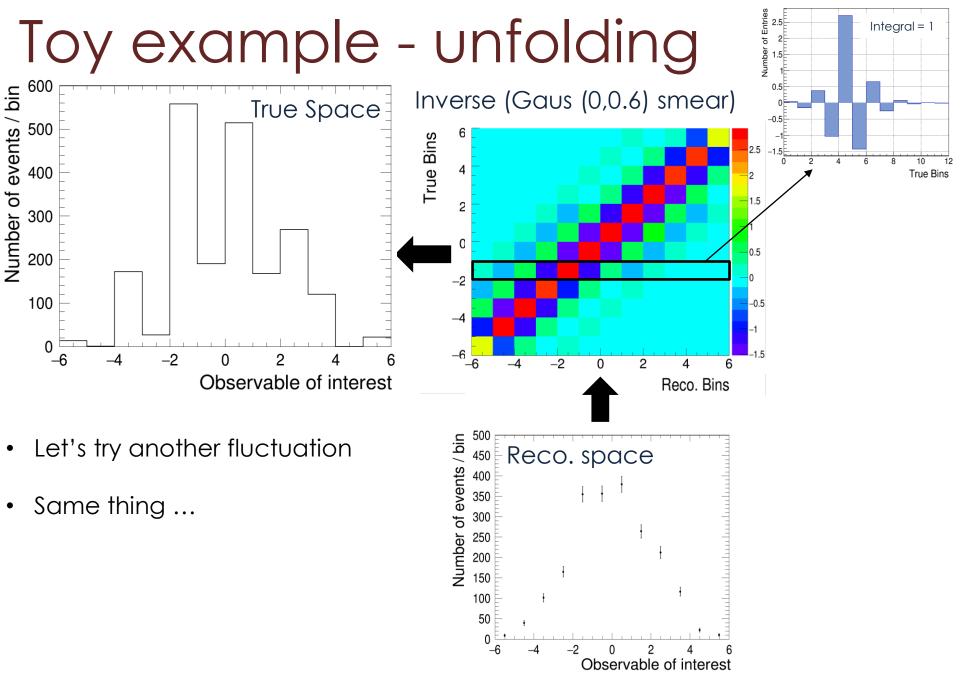






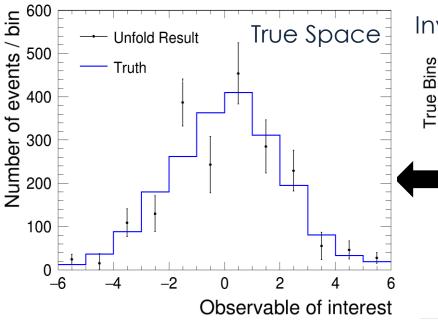


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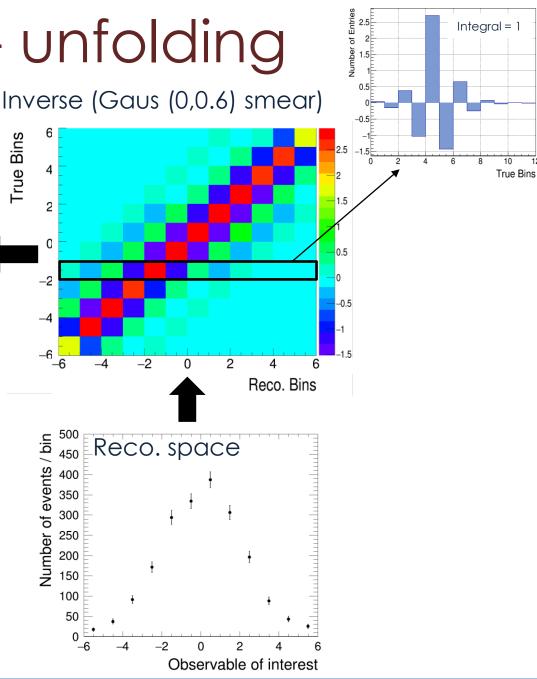


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Toy example - unfolding

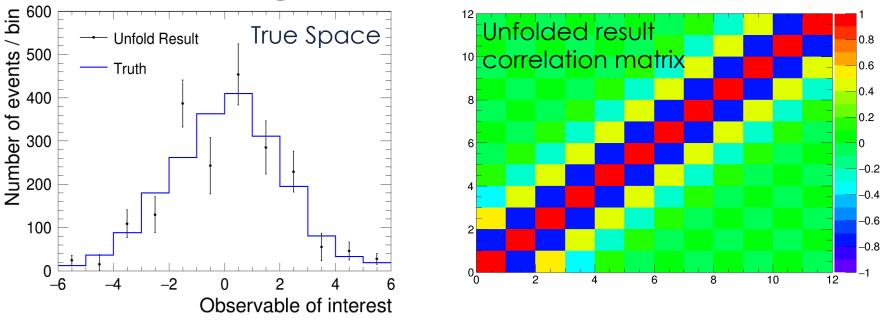


- Many fluctuations allow us to build a result with errors
- In most realistic circumstances we get a result which oscillates around the truth
- It doesn't look great



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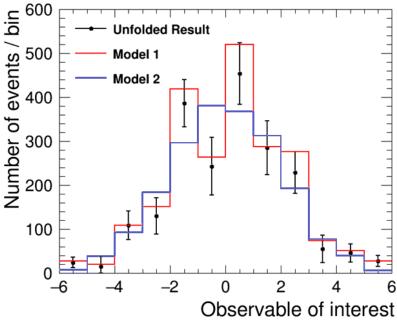
The unregularised result



- The unregularised result typically oscillates around the truth
 - Small variations in reco. space cause large ones in truth space
- Although the agreement between the truth and result looks poor, the result is accompanied by large bin-to-bin anti-correlations
- A quantitative goodness of fit finds: $\frac{\chi^2}{NDOF} = 0.44$, pretty good!
- If we want to minimise bias this is probably the best thing we can do

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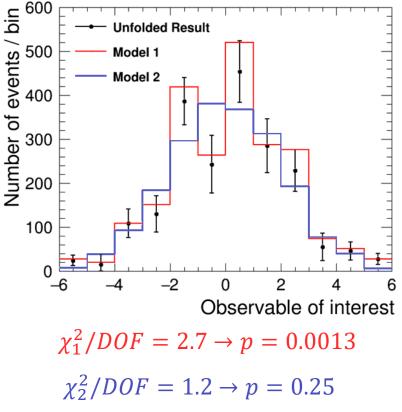
The unregularised result



- Although the result is absolutely correct, it can be almost meaningless without the accompanying covariance matrix.
- Can you judge which of the models on the left fits the result best?

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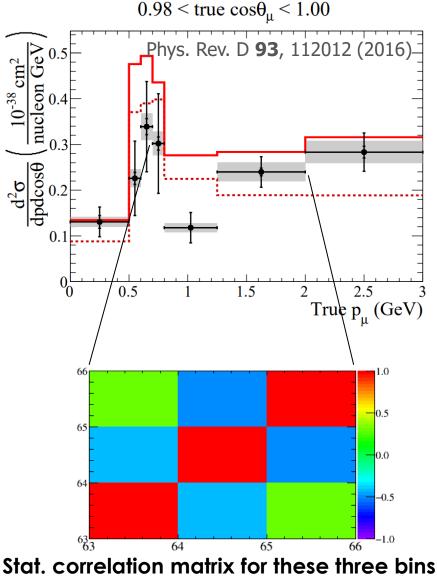
The unregularised result



- Although the result is absolutely correct, it can be almost meaningless without the accompanying covariance matrix.
- Can you judge which of the models on the left fits the result best?
- Even when we have the covariance matrix "chi-by-eye" is not very reliable ...

• The unregularised result is **good for calculating** χ^2 , but potentially very misleading for "by-eye" comparisons.

Case study: $CC0\pi$ analysis



- Our unregularised ND280 $v_{\mu}CC0\pi$ analysis shows a dip in the momentum distribution for forward going muons at about 1 GeV
- Looks interesting! There has been some discussion about what this large "dip" could be
- But in reality the **large anti-correlations** between the pertinent bins make this result compatible with no dip.
- The "dip" may just be a statistical effect from the unregularised unfolding

The case for regularisation

Unregularised results with large anti-correlations are the best option for making χ^2 comparisons, but:

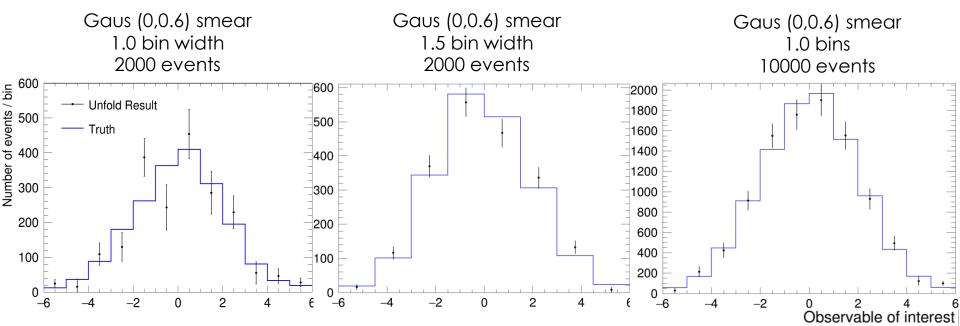
- We might want to have an idea of the result's shape or to compare the model in a specific region of phase-space
- We can't accurately estimate the χ^2 from a plot in a paper or conference

Perhaps producing a result which can be better interpreted by eye could be useful too ...

Can we just re-bin it?

The oscillatory unfolded results are caused by a combination of:

- Fine binning compared to the detector resolution
- Large statistical uncertainty in the reco. data

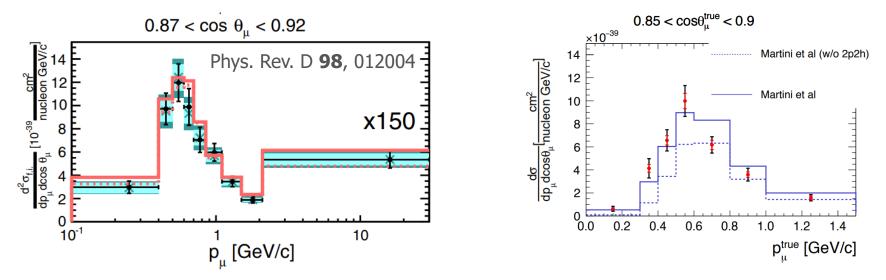


Can we just widen our bins or add more reco. bins for a fixed number of true bins until we get a smooth result?

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Can we just re-bin it?

- Yes! Many of T2K's recent results do this
- This is largely unbiased unfolding where the resolution of the detector is clearly shown by the width of the bins
- Potential issues*:
 - Bin widths optimised on simulation, not on data
 - Coarser binning can give greater model dependencies



* Although these could be mitigated by first extracting a result in fine bins and then combining adjacent bins until the result is smooth

Direct regularisation

- Additional regularisation is often applied when there is insufficient constraints available from the data alone to reliably infer the desired result
 - E.g. if you have as many reco bins as true bins and a significant smearing
- It works by injecting some prior knowledge about the signal you are trying to measure into the cross section extraction with some strength
 - It can be "cross sections are usually smoothly changing"
 - It can also be "cross sections look like GEANT" ...
- In the D'Agostini method, regularisation is gradually weakened by repeated iterations. For the likelyhood fitting method there is no built in regularisation.
- Too strong regularisation can cause both bias and under-coverage
- All this can sometimes avoided by just having more reco bins than true bins
- But if you really insist on using it there are options ...

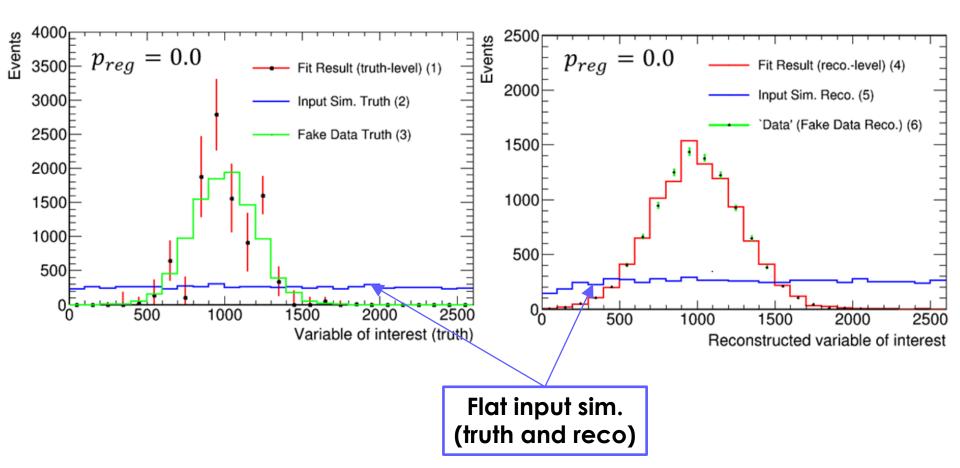
Tikhonov regularisation

 Rather than combining bins completely, another option is to loosely tie them together with a penalty term (to be used in the likelihood fitting method of cross-section extraction – see backups)

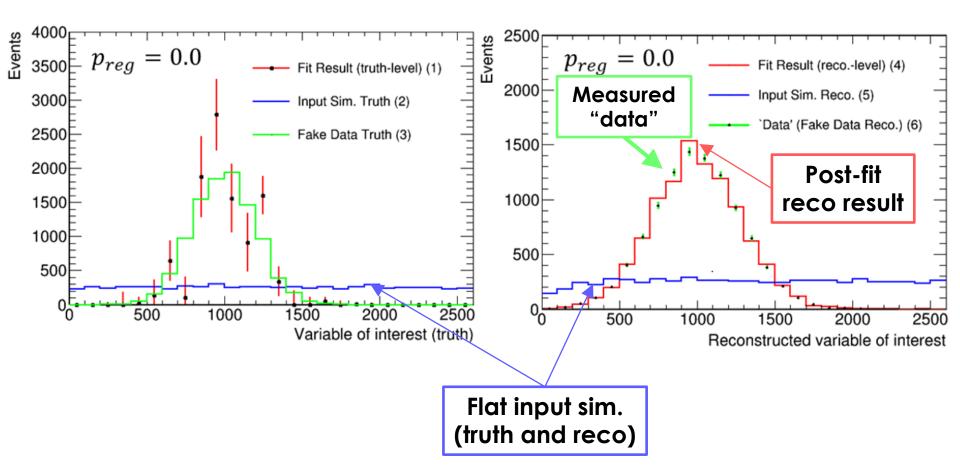
$$\chi^2_{reg} = p_{reg} \sum_i (bin_i - bin_{i-1})^2$$

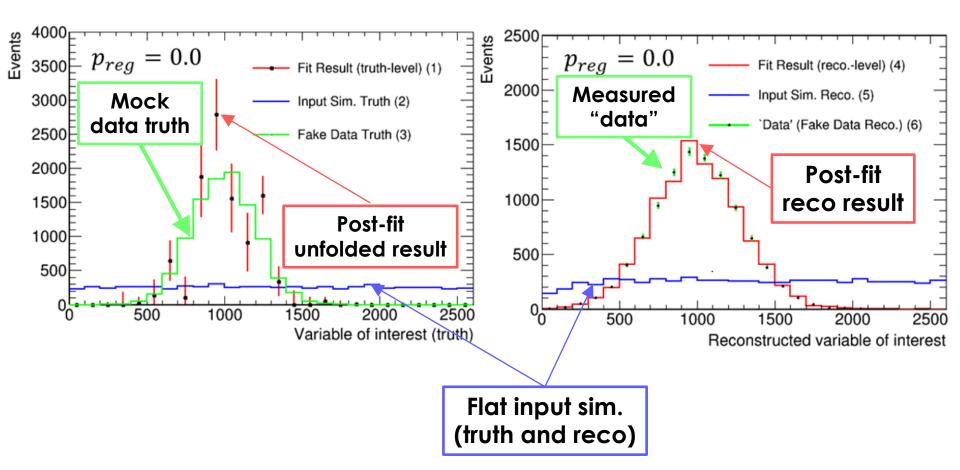
(this is just one potential penalty term, others are possible depending on how exactly you want to smooth your result)

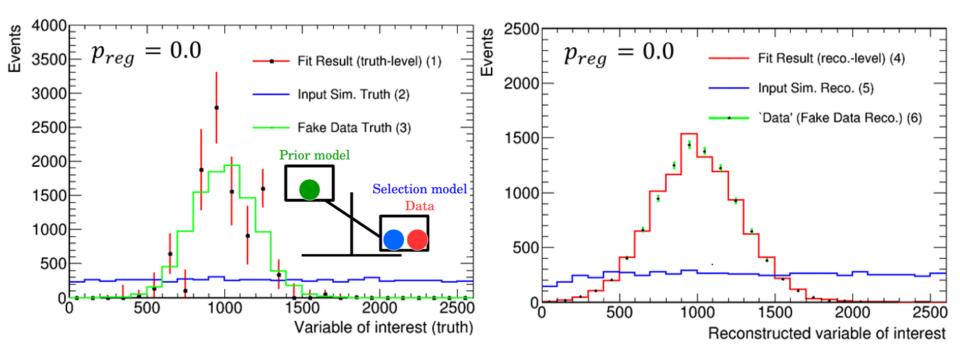
- If p_{reg} is very large then this is equivalent to combining bins
- The inclusion of a penalty term means that the result moves away from the maximum likelihood solution and is therefore **at least a little biased**.
- How can we choose p_{reg} to give us a result we can better compare to by-eye but avoid excessive bias?



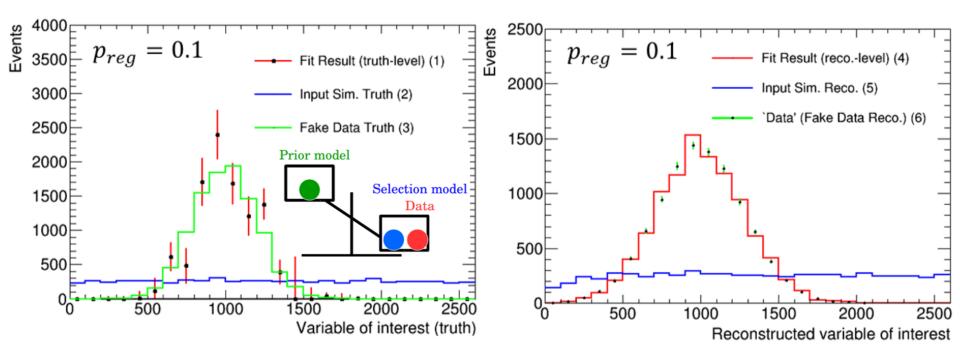
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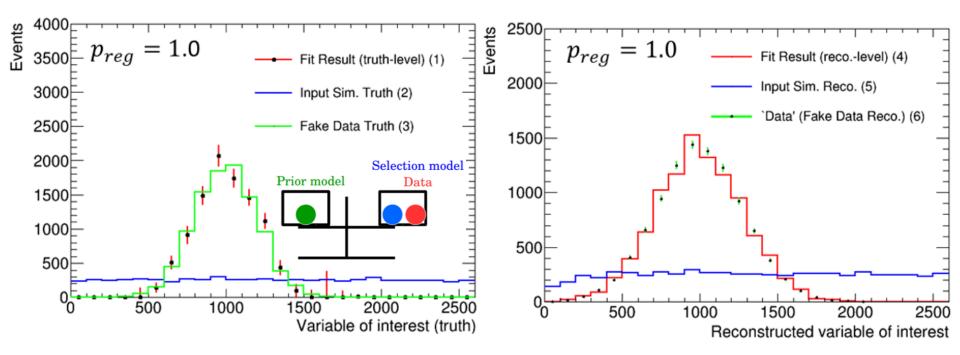




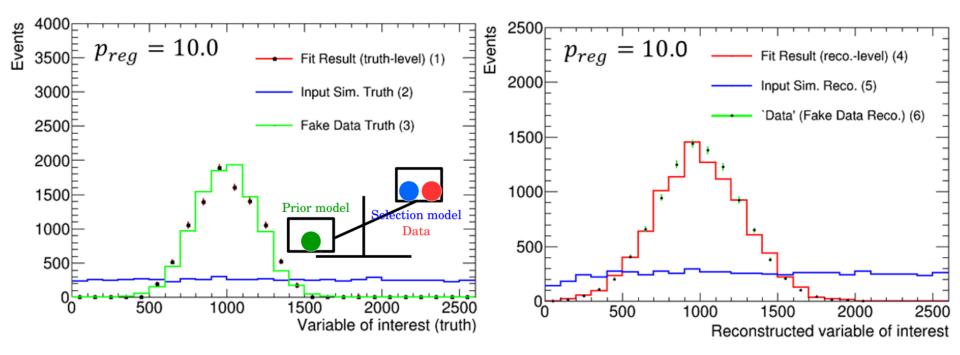
Read p_{reg} as regularisation strength



Read
$$p_{reg}$$
 as regularisation strength

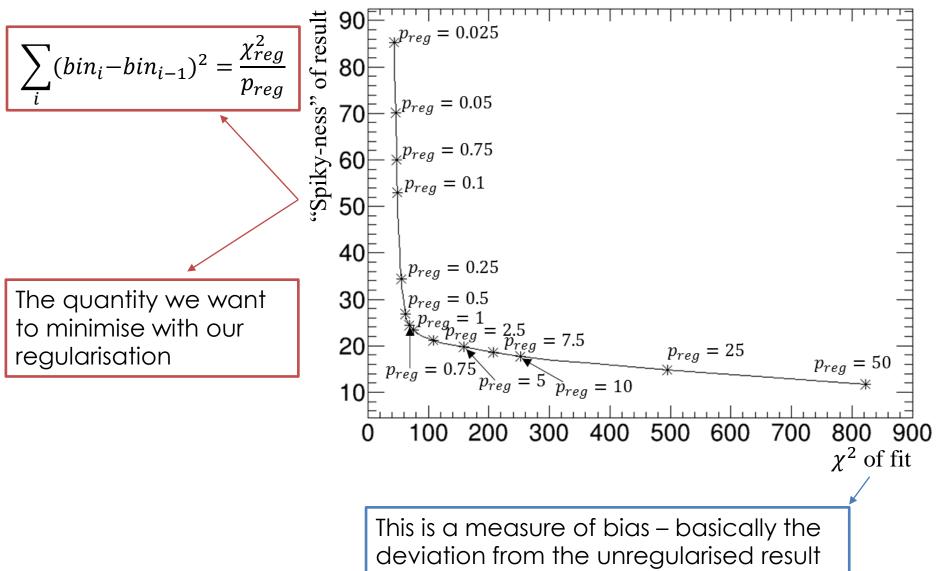


Read
$$p_{reg}$$
 as regularisation strength



Read p_{reg} as regularisation strength

Regularisation optimisation: The L-curve

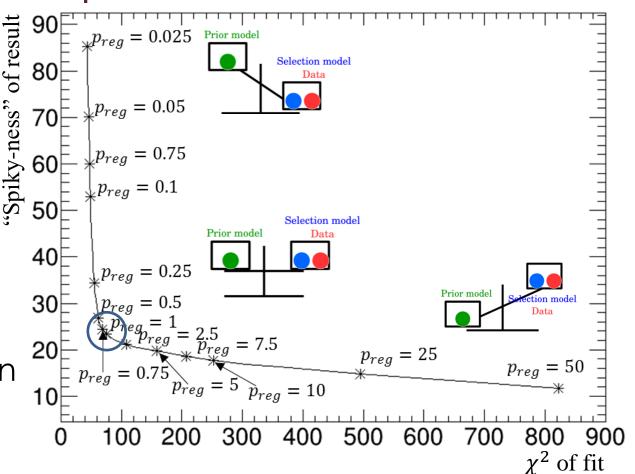


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Regularisation optimisation: The L-curve

Balance
 regulation with
 bias by choosing
 the "kink" in the
 curve

 L-curve can be formed on real data – data driven regularisation



 Well established method to select the smoothest of many almost degenerate solutions:

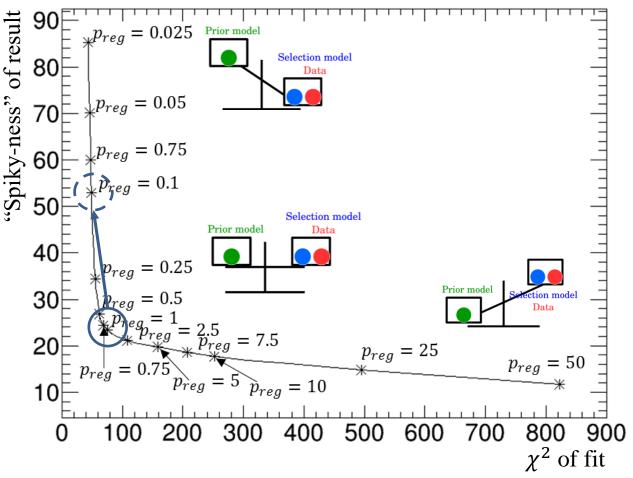
<u>http://epubs.siam.org/doi/abs/10.1137/1034115</u> <u>http://epubs.siam.org/doi/abs/10.1137/0914086</u> <u>http://arxiv.org/pdf/1205.6201v4.pdf</u> - use in TUnfold

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Regularisation optimisation: The L-curve

Caveat: regularisation can lead to undercoverage

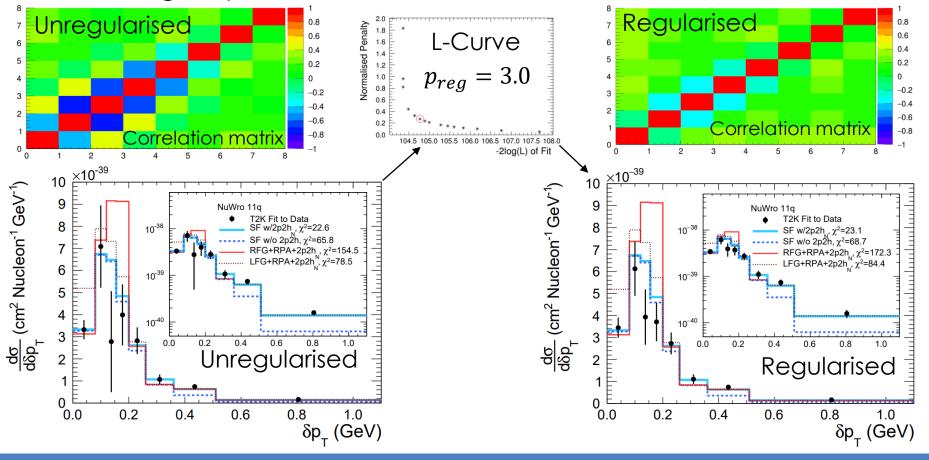
Simple solution: provide the unregularised result.



• **Better solution:** consider providing "undersmoothed" result [Kussela, 2016] – effectively move up the L-Curve to ensure good coverage.

Case study: CC0 π in δp_T

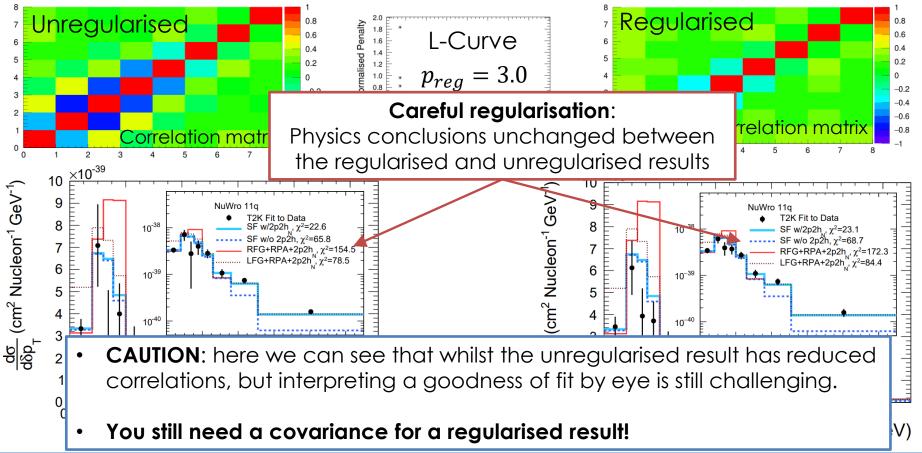
- Measure CC0 π +protons cross section in missing transverse momentum (δp_T) Phys. Rev. D **98**, 032003 (2018)
- Unregularised best for χ^2 , regularised best for actually showing anywhere



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Case study: CC0 π in δp_T

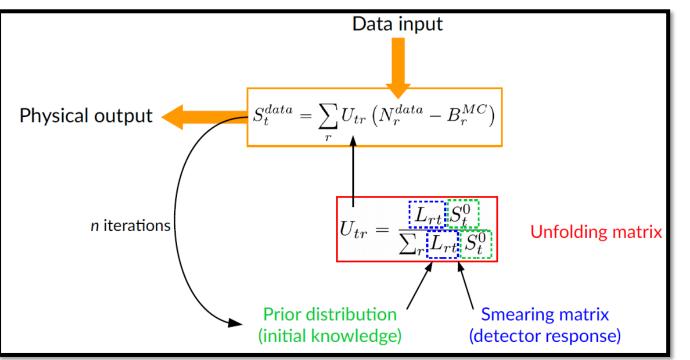
- Measure CC0 π +protons cross section in missing transverse momentum (δp_T) Phys. Rev. D **98**, 032003 (2018)
- Unregularised best for χ^2 , regularised best for actually showing anywhere



D'Agostini's method

*Although this method uses Bayes' theorem, **it is not a Bayesian technique** (in fact it's equivalent to the widelyused "Expectation-maximisation algorithm") [<u>M.Kuusela</u>]

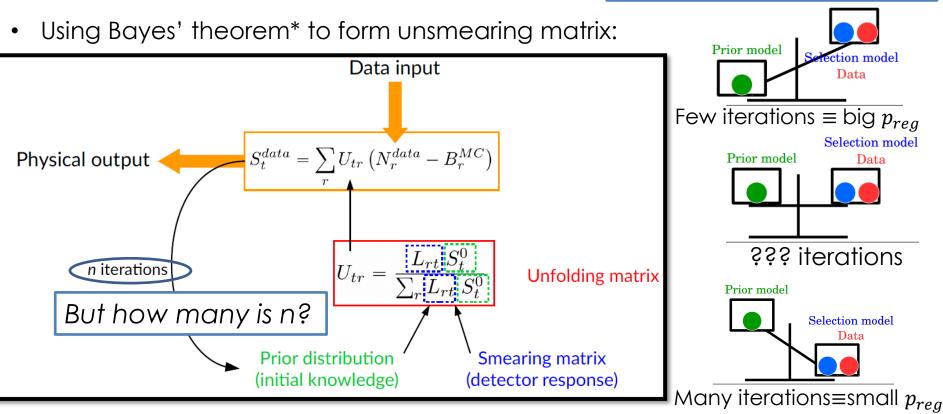
• Using Bayes' theorem* to form unsmearing matrix:



- Most commonly used method (MINERvA, MiniBooNE, T2K)
- If prior formed from MC model dependence is explicit
- Mitigate by updating **prior** with unfolded result and iterating
- Many iterations (problem dependent, typically >>4) \rightarrow unregularised result

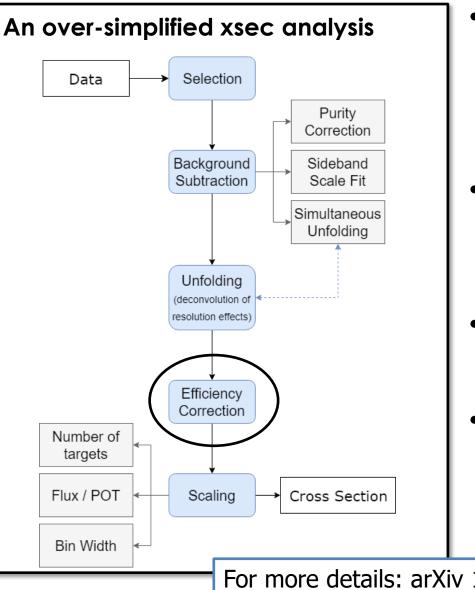
D'Agostini's method

*Although this method uses Bayes' theorem, **it is not a Bayesian technique** (in fact it's equivalent to the widelyused "Expectation-maximisation algorithm") [<u>M.Kuusela</u>]



- Changing the number of iterations can change physics conclusions
- Typically select number of iterations based on mock-data studies
- If real data looks different, can select "wrong" number (toy example in backups)

Efficiency corrections

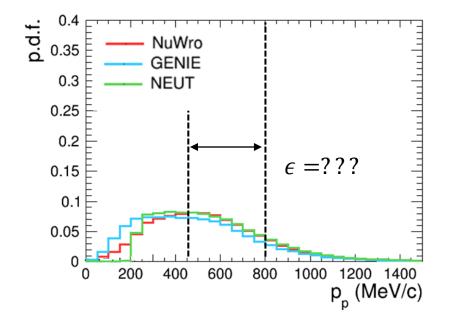


- After unfolding we have the a measure of the true number of *selected* signal events
- To get to a cross section, we need to correct for our detectors acceptance
- It's also easy to add bias here ...
- Not entirely separate from unfolding
 - Unfolding in too few variables can give bias here

For more details: arXiv 1805.07378 (TENSIONS Workshop 2016)

Toy example

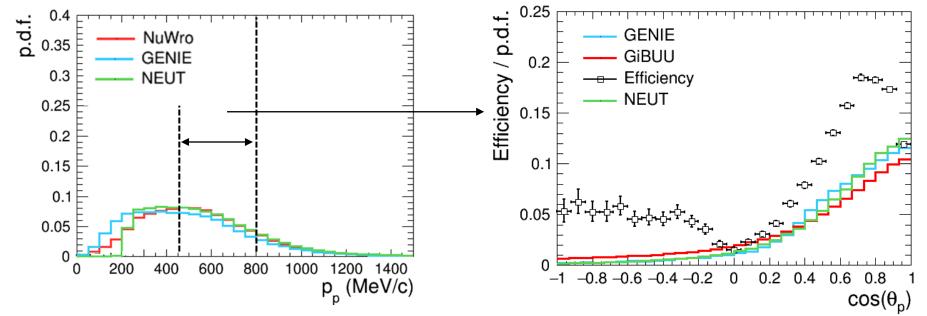
• I want to measure a cross section in some range of proton momentum



- But my detection efficiency depends on both proton momentum and angle (and on other particles, but let's focus on the angle for the moment!)
- I can't know the efficiency (ϵ) without knowing the distribution of proton angle within the bin

Toy example

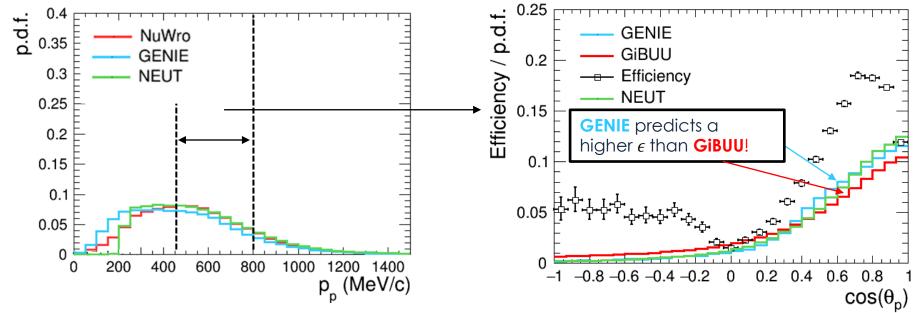
• I want to measure a cross section in some range of proton momentum



 The efficiency in the momentum bin a convolution of the efficiency and the predicted cross section in proton angle

Toy example

• I want to measure a cross section in some range of proton momentum

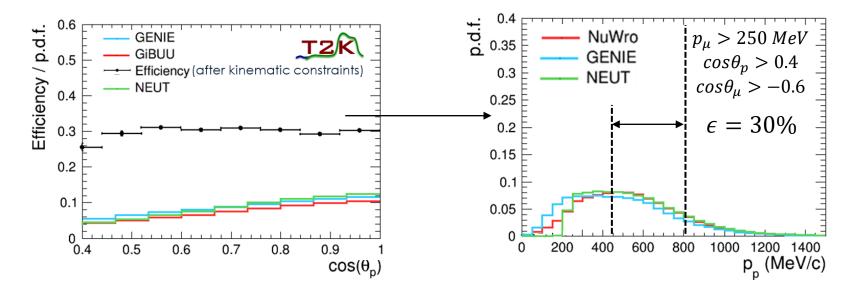


- The efficiency in the momentum bin a convolution of the efficiency **and the predicted cross section** in proton angle
- Compared to GiBUU, GENIE predicts a higher cross section in the high efficiency region → GENIE predicts a higher (~5-10%) efficiency
- Efficiency depends on the input model \rightarrow Bias

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Kinematic constraints

• Placing kinematic constraints on outgoing particles $(p_{\mu,p}, \theta_{\mu,p})$ can leave us with a relatively flat efficiency in a specific region of $\cos \theta_p$



- In this case the shape of the input model doesn't alter the efficiency → model independent correction!
- Analyses should try to ensure integration only over flat-efficiencies in observables where simulations have poor predictive power (Example in backups)

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Summary

- Unfolding / efficiency correcting without bias is hard but there are a variety of ways to try and mitigate this
- All methods give results with important correlations between bins
 - χ^2 (or similar) is usually essential to validate physics conclusions

Unregularised Result

- ✓ Gives correct χ^2 with no unfolding bias
- X Sometimes not for anything other than χ^2 , can't trust "chi-by-eye". • However can still get a smooth result by rebinning (or more reco bins than true bins)
- Useful part of data release and as a reference to check bias of regularised results

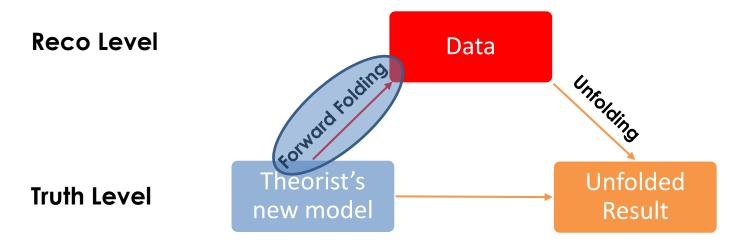
Direct Regularisation

- \checkmark Smoother results, easier to interpret
- X Adds at least some bias worse for getting reliable χ^2
- ➤ Not easy to choose a regularisation strength that suits data based on simulation → Use data-driven methods

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Just don't unfold!

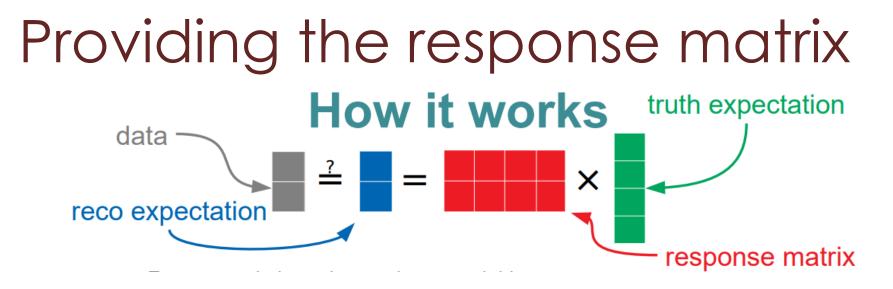
• Producing a good *unfolded* result that can be interpreted by-eye with is **hard**! But maybe there's another way ...



- No inherent bias
- No data point correlations: much easier to judge model comparisons "by eye"
- Best model separation is in the reco. space (Cousins, May, Sun arXiv:1607.07038)

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Thank you for listening



- The challenge for the analyser is building and quantifying uncertainties on the response matrix
- Easy to just supply a reco to truth mapping in some interesting physics variable(s): but this may be highly model-dependent – defeats the purpose of not unfolding
- Ideally response matrix should contain all truth dimensions that effect reconstruction

Example: Gas Interactions analysis

- Reco. binning: 16 bins
 - 4 samples (main + 3 control samples). In each:
 - 2 bins in primary track angle
 - 2 bins in particle multiplicity (1 track vs. n tracks)
 - Truth. binning: 11,760 bins (limited by simulation stats.)
 - 7 in momentum
 - 7 in angle
 - 5 in forward separation of track
 - 6 in backward separation of track
 - 8 bins to categorise events (4 FV, 4 OOFV)

T2K Work in Progress

 θ_{bwd}

 θ_{fwd}

Response Matrix Utils (Lukas Koch)

- A tool for forward folding analyses
 - Builds response matrix
 - Tests model dependence
 - Evaluates uncertainties

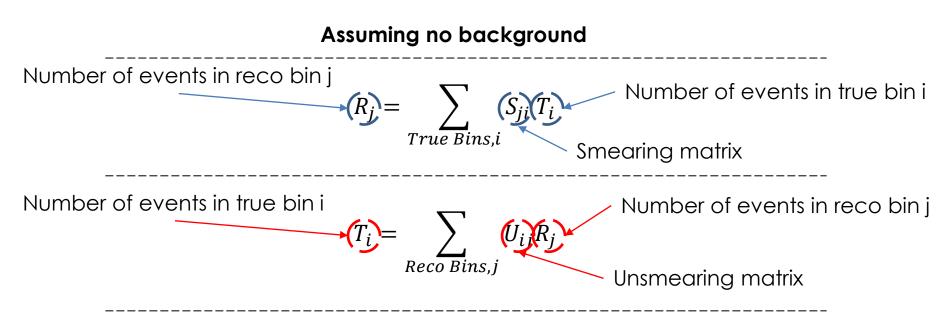


- Compare model to data (likelihoods, p-values, MCMC)
- More information: <u>https://remu.readthedocs.io/</u>



Unfolding

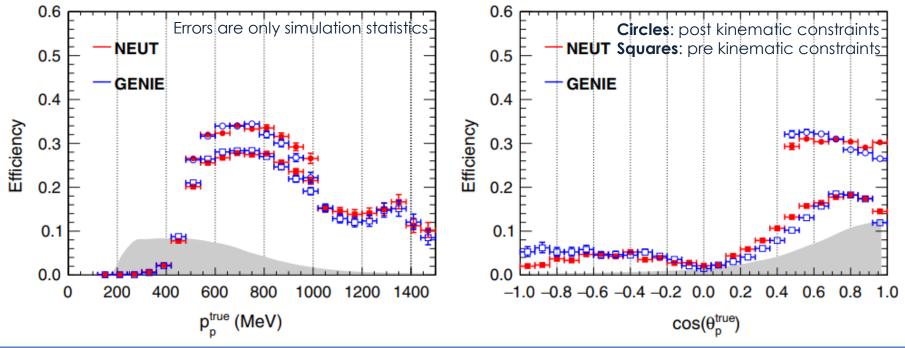
- Measure selected number of events in bins of a reconstructed quantity
 Efficiency correct
 Measure selected number of events in bins of a reconstructed quantity
 Measure selected number of events in bins of a reconstructed quantity
- Want the total number of signal events in bins of a true quantity



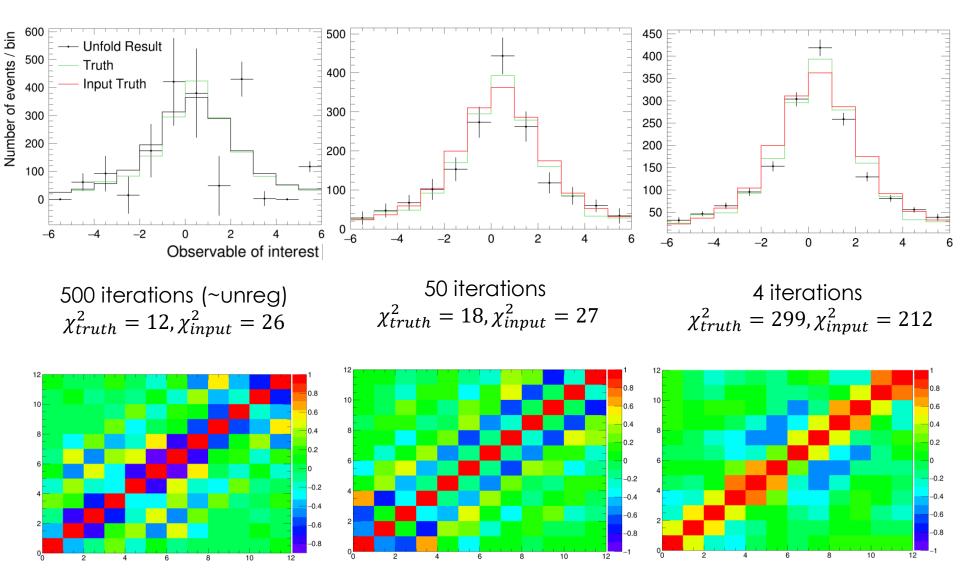
- Unfolding is finding U_{ij} from S_{ji} .
 - Simplest method: use S_{ji}^{-1}

Efficiency correction example

- Phys. Rev. D **98**, 032003
- Measuring δp_T relies on integrating the efficiency over $p_{\mu,p}, \theta_{\mu,p}$
- We set kinematic constraints in each to keep efficiency relatively flat, especially in regions of phase space where models have low predictive power (proton kinematics)
- Still not perfect, ideally should efficiency correct in all relevant kinematics

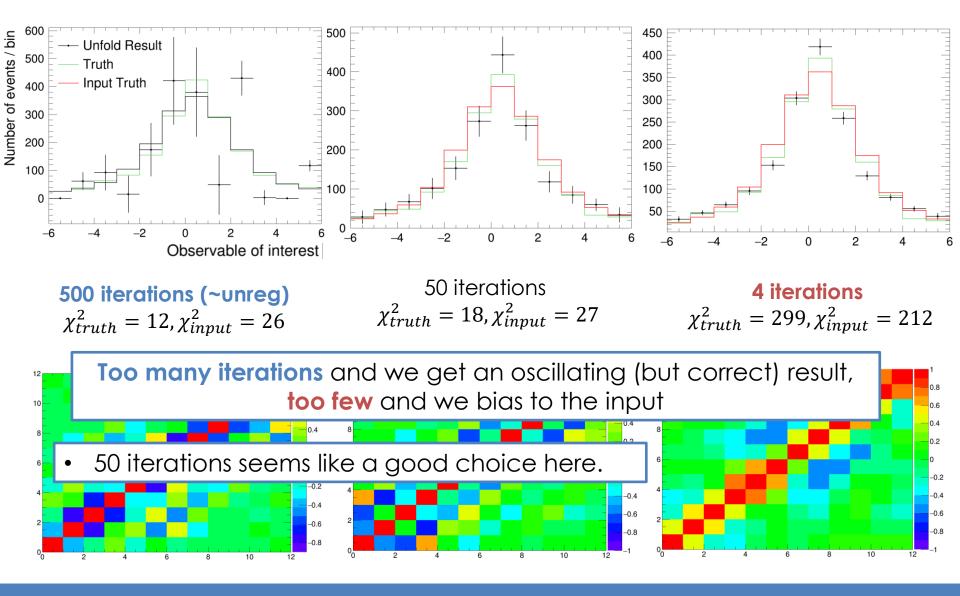


Gaus (0.1,1.0) smear, 1.0 bin width, 2000 events, Truth is a BW(0.4,3.0), Input is a BW(0.3,2.5)



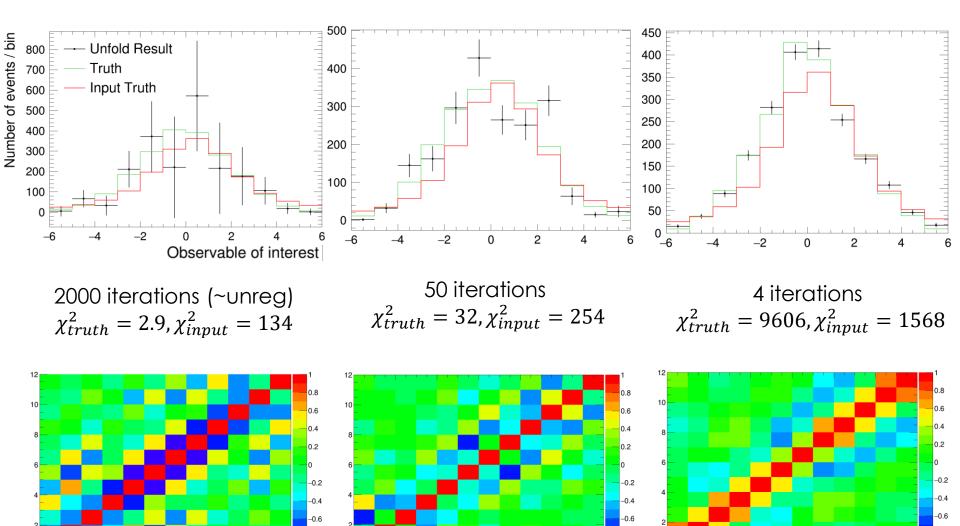
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Gaus (0.1,1.0) smear, 1.0 bin width, 2000 events, Truth is a Gaus (0,2.0), Input is a BW (0.3,2.5)



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ProtoDUNE Hadron Analysis Meeting, 09/06/22

-0.8

12

10

-0.8

12

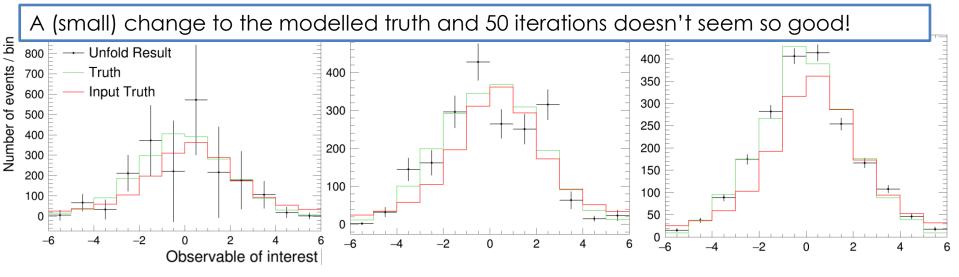
10

-0.8

12

10

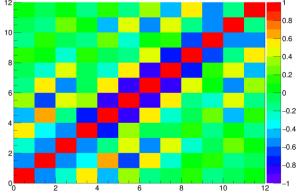
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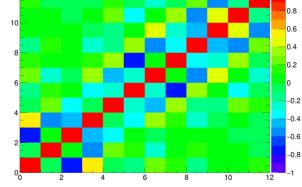


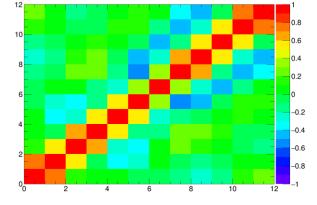
2000 iterations (~unreg) $\chi^2_{truth} = 2.9, \chi^2_{input} = 134$

50 iterations $\chi^2_{truth} = 32, \chi^2_{input} = 254$

4 iterations $\chi^2_{truth} = 9606, \chi^2_{input} = 1568$

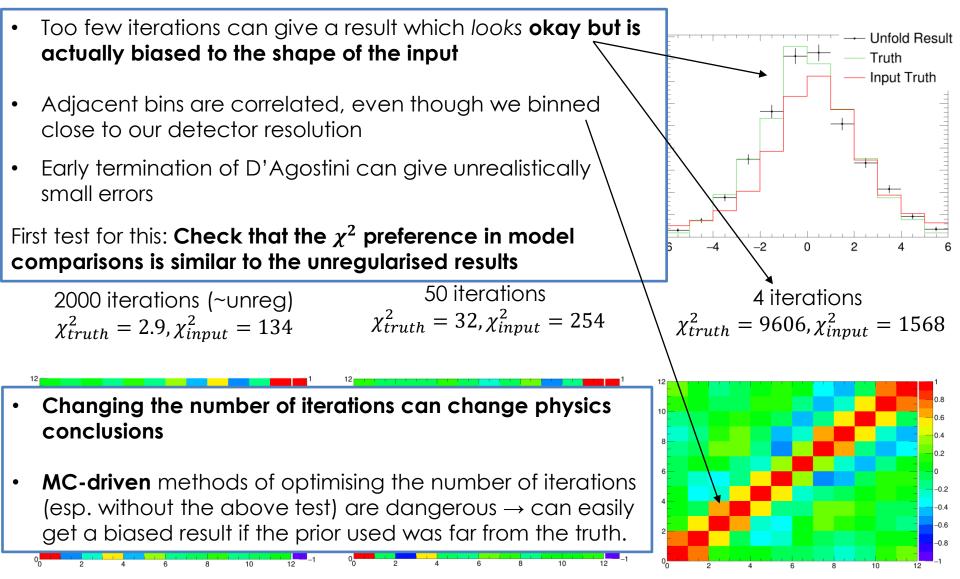




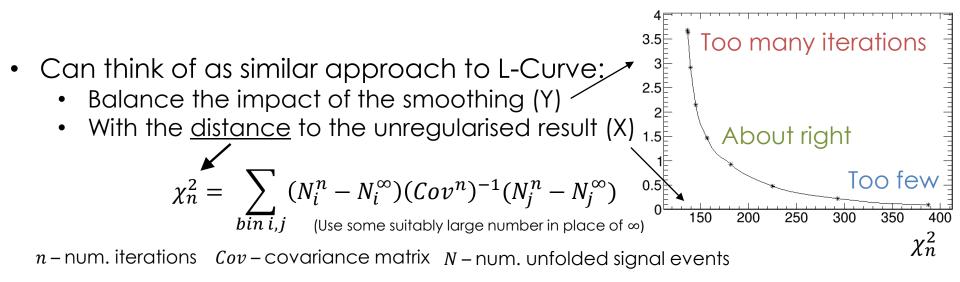


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Gaus (0.1,1.0) smear,1.0 bin width, 2000 events, Truth is a Gaus(0,2.0), Input is a BW(0.3,2.5)



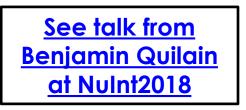
 To mitigate this issue two recent T2K analyses utilising D'Agostini's method employ a data-driven regularisation



• Actual implementation is a little different (see main slides)

Case Study: On-axis CC1 π measurement

- Number of iterations chosen via fake data: 3 7
- Number of interactions chosen via data: 16



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What if my L-curve isn't L-shaped?

Is the condition on the Yaxis reasonable?

• If the form of the penalty pushes the result somewhere that is incompatible with the no regularisation case, the drop on the y-axis can be limited to very small values of p_{reg}

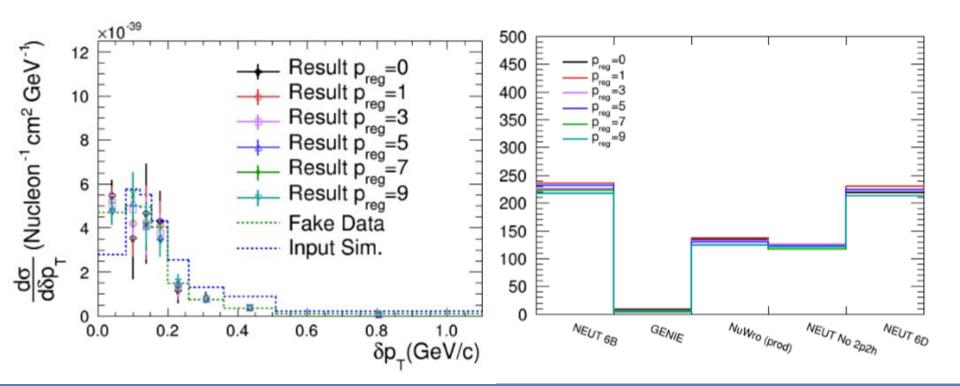
of result 90 $p_{reg} = 0.025$ 80 $p_{reg} = 0.05$ 'Spiky-ness" 70 $_{\bigstar}p_{reg}=0.75$ 60 $p_{reg} = 0.1$ 50 40 = 0.25 p_{rea} $p_{rea} = 0.5$ 30 $p_{reg}^{2.5} = 7.5$ 20 $p_{reg}=25$ $p_{reg} = 50$ $p_{reg} = 0.75$ = 10 \dot{p}_{rea} 10 100 200 300 500 600 800 400 700 900 χ^2 of fit

How did you form the x-axis?
This needs to be a measure of bias.

- What is the first value on the x-axis?
- How does this compare with the x-axis value of the unregulairsed result? If they're very different consider smaller p_{reg}

Aesthetic regularisation

 A result with a carefully chosen regularisation strength shouldn't significantly alter the physics conclusions with respect to the unregularised case – it's just aesthetic.



Unregularised result as a reference for regularised result bias

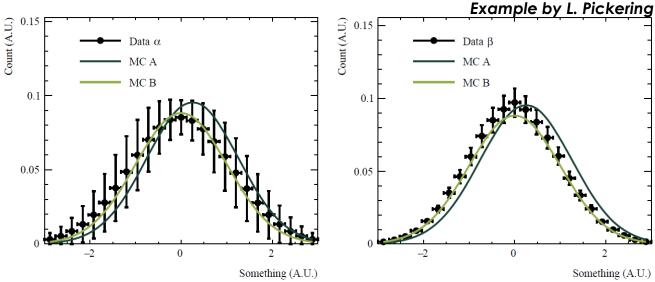
TABLE IX. The full and shape-only χ^2 comparisons to the δp_T result with nominal and no regularization. The table is ordered by the size of the no-regularization shape-only χ^2 . More details of these models can be found in Sec. IVA.

Generator	Full		Shape Only	
	No Reg.	Nom. Reg.	No Reg.	Nom. Reg.
NEUT 5.4.0 (LFG _N + $2p2h_N$)	31.6	30.4	3.38	2.60
NEUT 5.3.2.2 (SF + $2p2h_N$ + 2 × FSI)	15.9	14.8	11.0	10.1
NEUT 5.3.2.2 (SF + $2p2h_N$)	31.9	30.3	16.6	15.5
NuWro 11q (SF + $2p2h_N$)	22.6	23.1	16.8	15.6
NuWro 11q (LFG + $2p2h_N$)	81.5	81.7	39.0	15.6
NuWro 11q (LFG + RPA + $2p2h_N$)	78.5	84.4	39.9	36.3
NEUT 5.3.2.2 (SF + $2p2h_N$ + No FSI)	114	112	42.9	41.4
GENIE 2.12.4 (RFG + $2p2h_E$)	92.9	92.4	47.9	47.7
NuWro 11q (SF w/o 2p2h)	65.8	68.7	55.4	54.8
NEUT 5.3.2.2 (SF w/o 2p2h)	93.3	91.5	61.2	59.6
GiBUU 2016 (LFG + $2p2h_G$)	77.0	78.9	66.1	59.6
NuWro 11q (RFG + $2p2h_N$)	150	155	67.2	69.0
NuWro 11q (RFG + RPA + $2p2h_N$)	155	172	68.6	70.4
GENIE 2.12.4 (RFG w/o 2p2h)	94.6	97.8	74.1	76.2

These numbers are very similar → No change of physics conclusions form regularisation. Important test.

Do I really need a covariance?

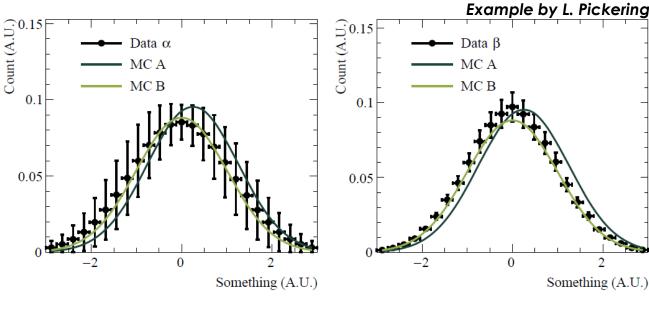
Guess which MC fits each data better better?

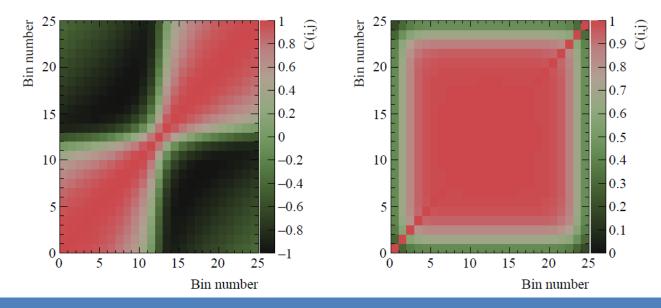


Do I really need a covariance?

How about now?

Can you do chiby-eye?





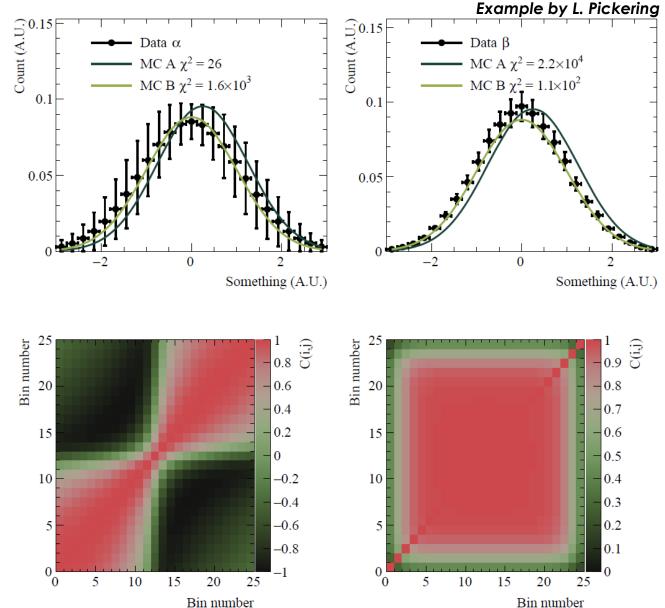
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Chi-by-eye?

Interpreting any result-simulation comparison without a covariance matrix and a goodness of fit is dangerous.

If you really must, then the regularised result is better, but may still be misleading.

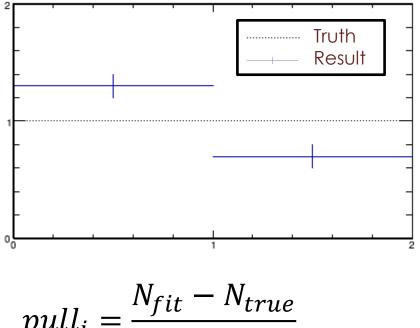
If you make a conclusion by eye, check the χ^2 tell the same story.



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But the result looks awful!?

• Consider a two bin result:



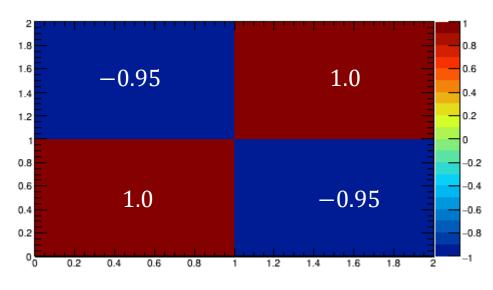
$$pull_{i} = \frac{Aflt}{Error}$$

$$pull_{0} = 3$$

$$pull_{1} = 3$$

$$Fairly awful$$

$$pull_{1} = 3$$



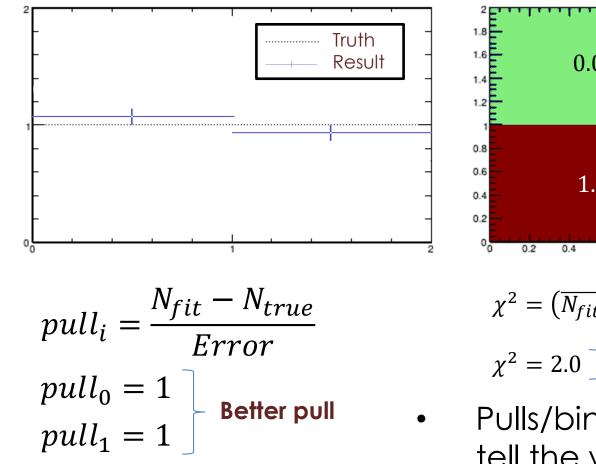
$$\chi^{2} = \left(\overline{N_{fit}} - \overline{N_{true}}\right)(V_{cov})^{-1}\left(\overline{N_{fit}} - \overline{N_{true}}\right)$$

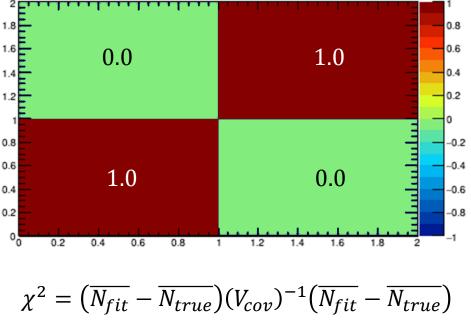
$$\chi^2 = 1.69$$
 Good χ^2

Need to see the correlation matrix to tell whether the result is good or not.

But the result looks awful!?

• Consider a two bin result:



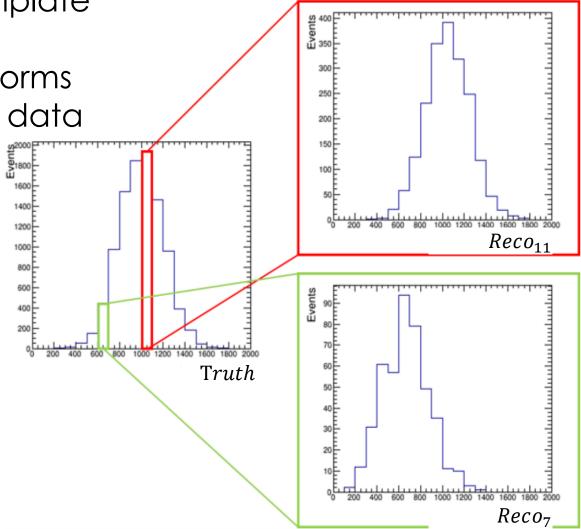


$$\chi^2 = 2.0$$
 Worse χ^2

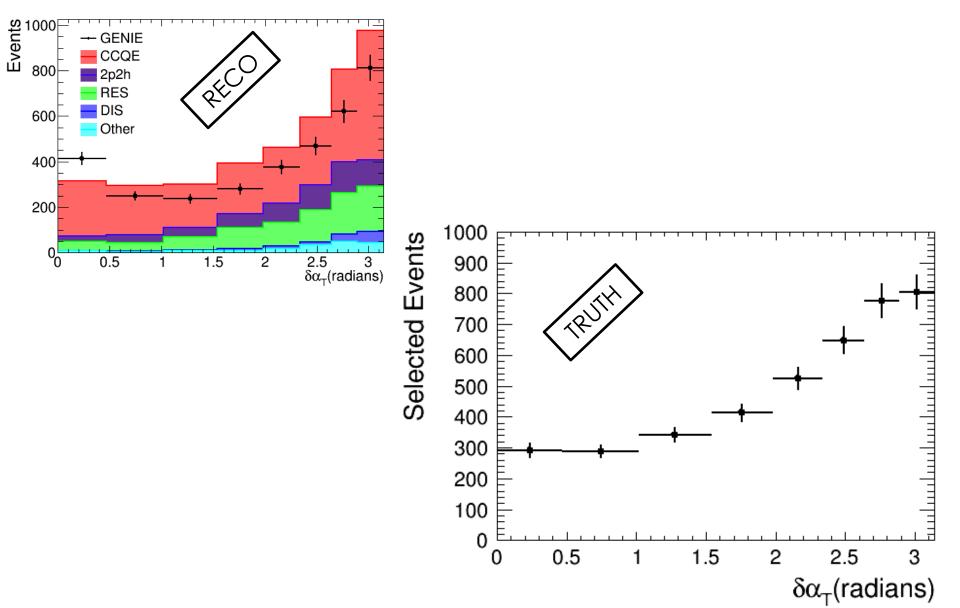
Pulls/bin-to-bin bias doesn't tell the whole story

Unfolding at T2K: likelihood fitting

- True bin \rightarrow Reco. template
- Vary MC template norms
 (c_i) and compare to data
- Maximise Poisson likelihood + syst. penalty term (using max. gradient decent)

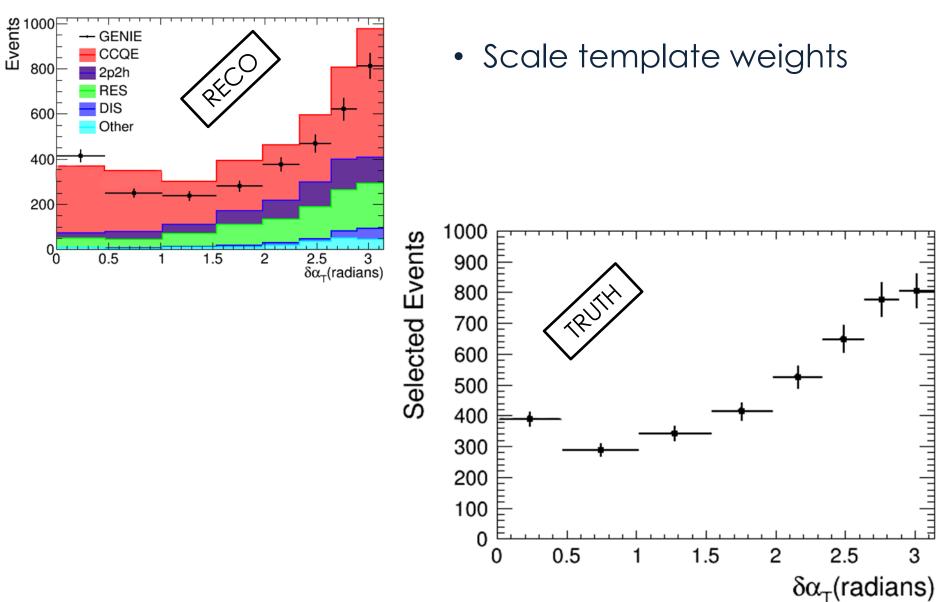


How does it work?



Stephen Dolan

How does it work?



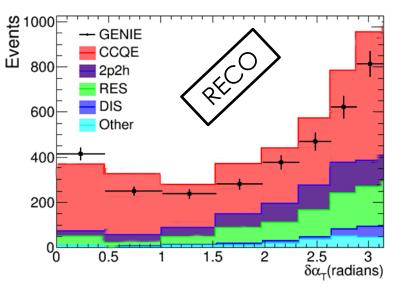
Stephen Dolan

ProtoDUNE Hadron Analysis Meeting, 09/06/22

mhuhuhuhuhu

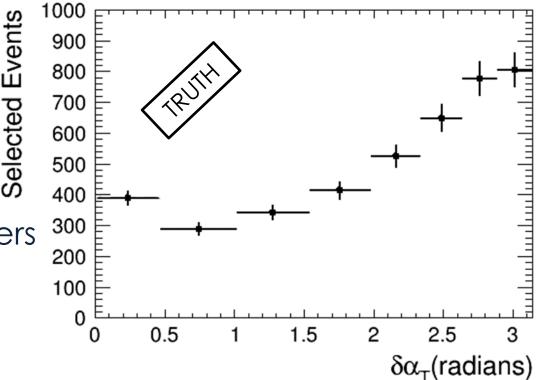
3

How does it work?

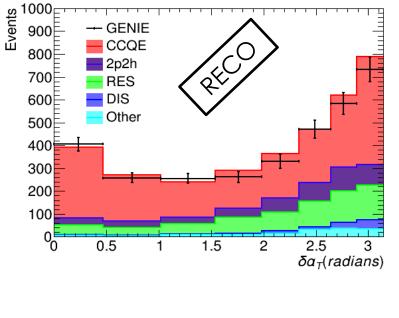


- Overall can alter:
 - Template weights
 - BG Model parameters
 - Flux
 - Detector response

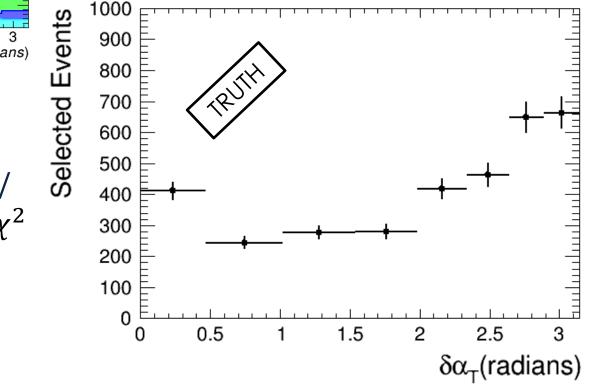
- Alter background systematic parameters
- These should ideally be constrainable by control regions



How does it work?



• Keep iterating to maximize the likelihood



• Maximise likelihood / minimise $-2\ln(L) \approx \chi^2$

Regularisation in the likelihood fitter

• The best fit parameters are those that minimise the following:

$$\chi^2 = \chi^2_{stat(fit\,goodness)} + \chi^2_{syst(penalty)} + \chi^2_{re}$$

$$\chi^2_{stat} = \sum_{j}^{recobins} 2(N_j^{MC} - N_j^{obs} + N_j^{obs} ln \frac{N_j^{obs}}{N_j^{MC}})$$

$$\chi^2_{syst} = (\vec{a}^{syst} - \vec{a}^{syst}_{prior})(V^{syst}_{cov})^{-1}(\vec{a}^{syst} - \vec{a}^{syst}_{prior})$$

 With an optional regularisation term (other terms are possible, exact choice of term is beyond the scope of this talk):

$$\chi^2_{reg} = p_{reg} \sum_{i} (c_i - c_{i-1})^2 = p_{reg} (\boldsymbol{c} - \boldsymbol{c}_{prior}) V^{reg}_{cov} (\boldsymbol{c} - \boldsymbol{c}_{prior})$$