MaCh3 Framework

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What is MaCh3?

Bayesian analysis framework, using Markov Chain Monte Carlo (MCMC) to measure constraints on oscillation parameters

Developed for analyses on T2K:

- Has been used to construct 3 sigma credible intervals
- Analyses use **complex systematic models**
- Large number of parameters (~800 in total)
- Can fit **many different samples at both near and far**
  - ➔ e.g. 22 near + 6 far samples for T2K

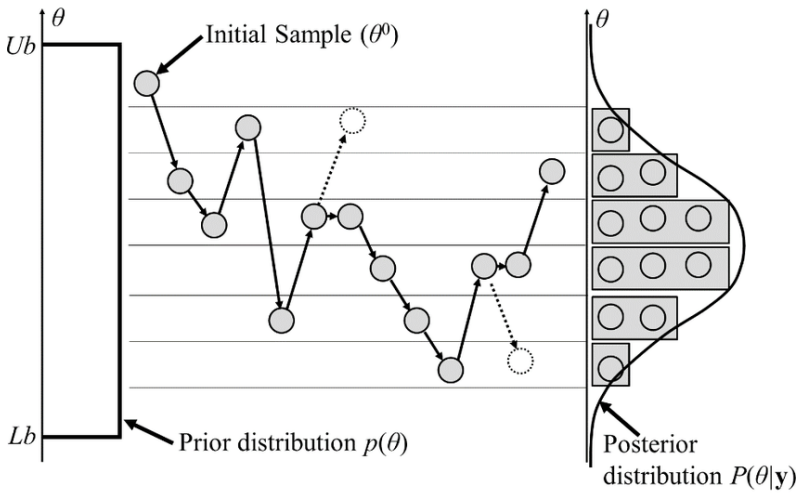
Also used for T2K+NOvA joint-fit, T2K+SK atmospherics and being developed for Hyper-K and DUNE

- Code under-going **refactor** to support many experiments more easily (see slide 10)
- Lots of expertise from other oscillation experiments and analyses
- Approximately 20 people in MaCh3 group across all experiments
  - Work of many people no longer active in the group as well!

Reminder: Markov Chains

- Like any Bayesian analysis, founded on Bayesian inference.
- Want to understand the joint-distribution; likelihood of parameters to data and prior knowledge of parameters

$$P(\theta|D) = \frac{P(\theta)P(D|\theta)}{\int P(\theta)P(D|\theta)d\theta}$$



- Markov chains sample this joint-distribution to build up a posterior distribution
- MaCh3 uses Metropolis-Hastings MCMC (no reason it can't use another algorithm)
- **MCMC / Bayesian results are not unheard of in neutrino physics!!**
  - T2K: 10.5281/zenodo.6683821
  - NovA: https://indico.fnal.gov/event/55483/
  - IceCube: https://arxiv.org/pdf/2011.03545.pdf
  - KATRIN: 10.1038/s41567-021-01463-1

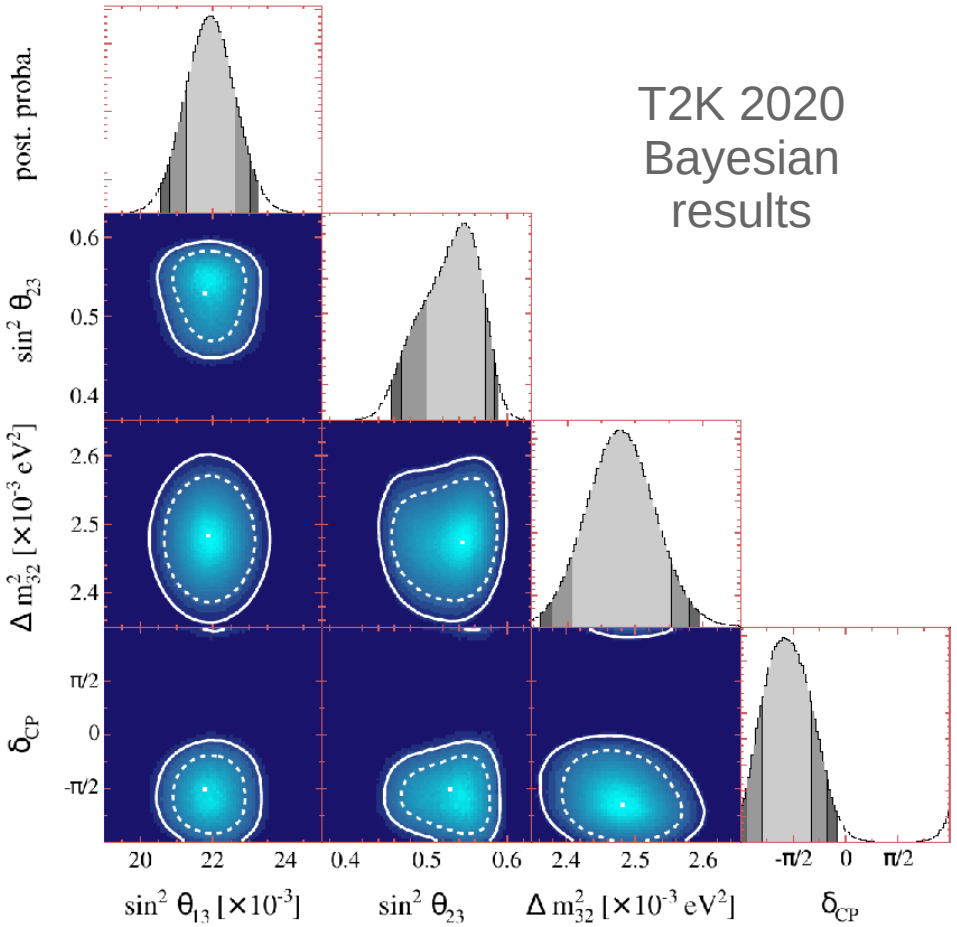
What do you get out?

- **Each chain gives N-dimensional posterior distribution**

- **Marginalise** out into 1D or 2D posteriors
  - Marginalising across parameters as easy as:

    TH1D::Fill(double dCP_at_five_sigma)
  - **Construct credible intervals** containing X fraction of posterior density
  - Require “enough” steps to get stable credible intervals

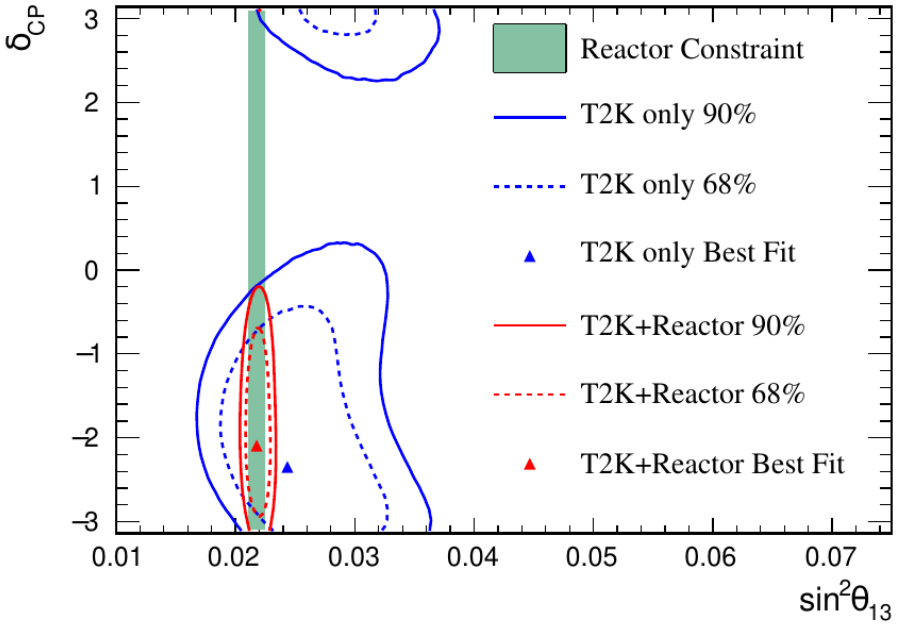
- Detailed view of systematics as have all dimensions of parameter space:
  - Can make 1D/2D intervals in any of the parameters (systematic or signal) without rerunning

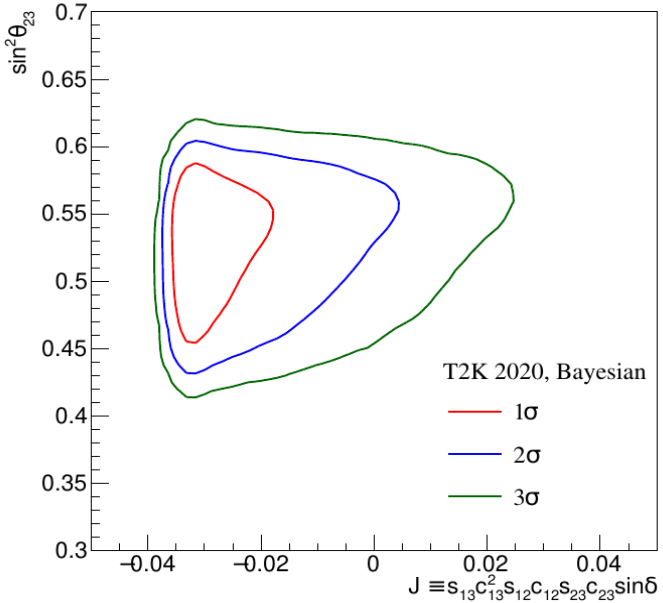


T2K 2020 Bayesian results

Some cool tricks of MCMC

- Because of properties of of markov chains (irreducibility) can **(h)add many chains ran in parallel**
- Can **reweight chains** to investigate impact of prior. Usually just reweight one parameter at a time.
- **Simultaneously does NH and IH** as chains can “flip” across hierarchies
- **No need to Feldman-Cousins** as we don’t use Wilk’s theorem
- Metropolis-Hastings doesn’t require a continuous likelihood so **event-migration not a problem**
- **Can make intervals on any function of parameters in fit** e.g. don’t re-run fits for Jarlskog invariant





Back to MaCh3

What do we need/want to run a fit?

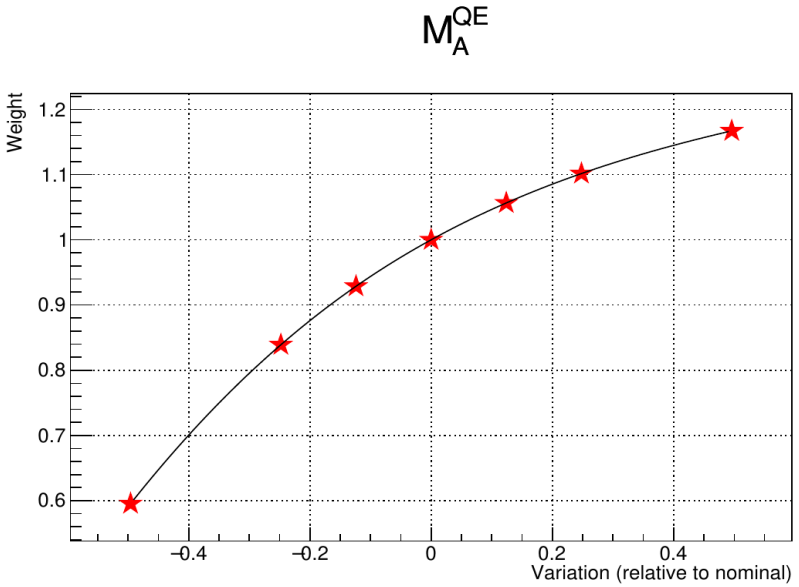
- CAF files!
  - CAF files with all the events you want to include in an analysis
  - If you want event migration in or out of sample cuts then include these in the CAFs!
  - If you want to apply shifts or smears in a kinematic variable then it has to be in the CAFs!
- Systematics:
  - Pre-fit covariance matrices. What’s the prior uncertainty and relationship between parameters?
  - Systematic model is defined in configurable format in MaCh3
  - **Four types of systematics: splines, normalisations, shifts and functional parameters**

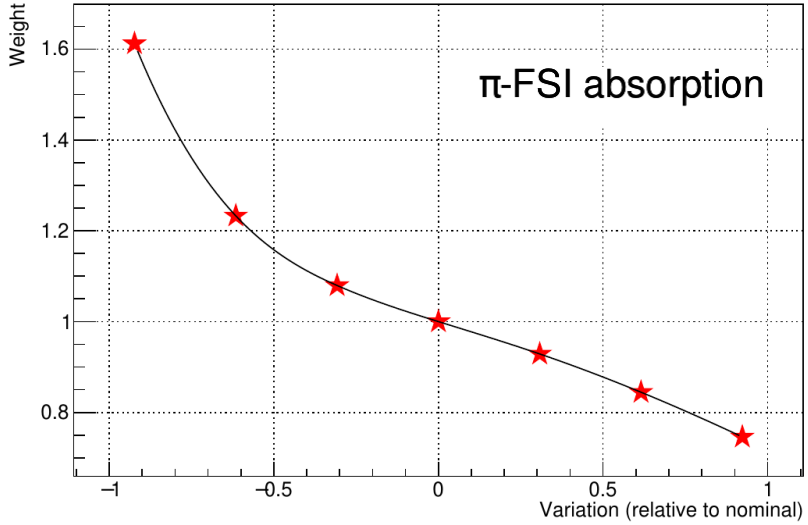
Splined responses

- Interpolate the response of a parameter using cubic splines
  - Continuous 1D response for variations of parameters without interfacing to generator directly. Event-by-event or binned.

- **Binned**:
  - Average the response of events in particular bins of kinematics
  - **Bin in oscillation channel, interaction mode in MaCh3 and have a binned spline per systematic**
  - **Binned in true-neutrino energy and 1 or 2 extra dimensions**
    e.g. on T2K True E_{nu} + lepton momentum + lepton angle
- **Event-by-event**:
  - No gaussian assumptions in binned response
  - Down-side is can be quite RAM heavy
  - GPU accelerated evaluation of the splines!

- **Read splines in from spline input file**. Don't remake splines at start of each fit simply load them in.
  - Liban has written the code for NuSystematics to produce weights for different values of systematics and then to produce splines





Normalisation parameters

- Any function which just changes normalistion
  - e.g. uncertainty on total xsec
- Can be applied to:
  - specific nuclear targets
  - neutrino flavours
  - in kinematic regions
- Configurable
  - Extremely easy to add normalisation parameters into MaCh3
  - Human readable and “friendly”

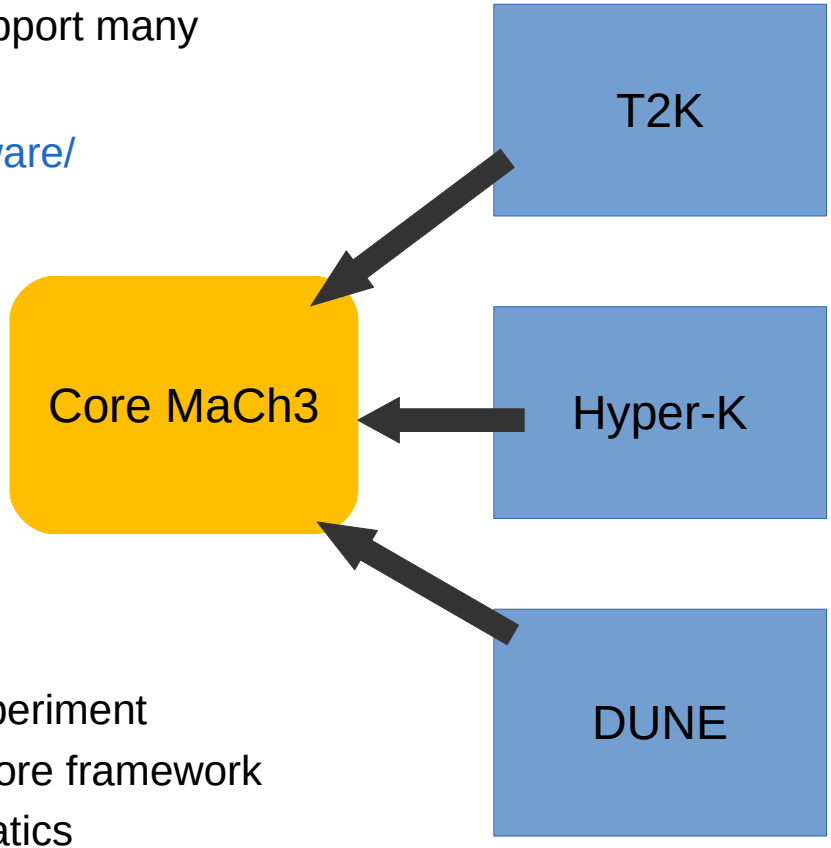
```
-
  name: CC_norm_nu
  generated: 1
  prior: 1
  lowerbound: 0
  upperbound: 9999
  error: 0.02
  renorm: 0
  type: norm
  detid: 985
  stepscale: 4.0
  mode: 0 1 2 3 4 9 11 14
  element: 12 16
  nupdg: 12 14 16
  etru_range: 0.3 0.6
  correlation:
    CC_norm_nubar: -0.999999
```

Kinematic shifts and functional parameters

- Apply event-by-events shifts in analysis
- Best example of this is the binding energy parameter in T2K analyses
  - Directly shift events reconstructed energy
  - Shift is given by a set of input histograms which code interfaces to
- Functional parameters:
  - If response of a parameter is given by some function of kinematic variables then we can apply this event-by-event
  - E.g. T2K used to use Bernstein Polynomials for uncertainty on RPA effect for CCQE interactions (BeRPA)
- Shift and functional parameters are “natural” candidates for nuclear effects and detector systematics which might directly effect reconstructed variables
  - Again, Metropolis-Hastings doesn’t mind about the likelihood being discontinuous!

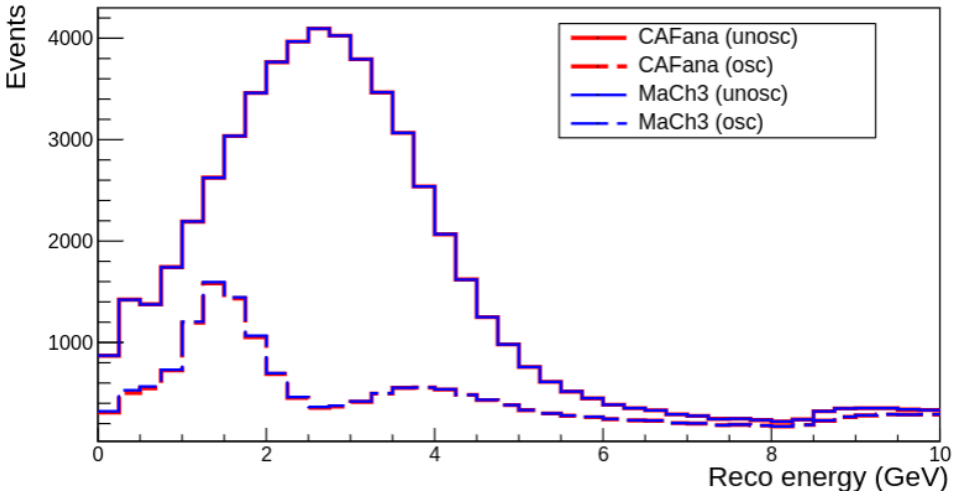
Code Maintenance

- MaCh3 is currently under-going a makeover to more easily support many experiments
- **New repo to host core code:** https://github.com/mach3-software/
- **Core code** contains the “heavy” lifting:
  - setting systematics, systematic evaluation
  - reweighting MC histograms
  - likelihood calculation
  - oscillation probability calculation
  - MCMC (Metropolis-Hastings)
- Experiment specific code will then be in separate repositories and will checkout core code and build against it
- Experiment specific code only contains information for that experiment
  - Mainly just reading in MC and spline files and passing it to core framework
  - Some experiment specific implementations of some systematics
- Should make code easier to maintain and read
- Any speed or ease of life improvements in the core code go to all experiments.



Reminder: Current status of MaCh3 DUNE

- Liban has been validated MaCh3 event rates, spectra and variations of systematics against TDR inputs
- Moving code to build against new refactor core code
  - Will result in getting all the speed improvements from T2K
- Ready to run some fits to check against TDR
- **Liban Warsame and Tom Holvey are both hoping to work with ND inputs soon!!**



Summary

- Hopefully now have a clearer understanding of what MaCh3 can do and what it needs!
- MCMC provides complimentary info to “traditional” frequentist fits
- MaCh3 is trying to be as flexible as possible with including many samples and many systematics
  - Emphasis on configurable systs and sample cuts
  - Saves analysers time!
- Large group of expertise from T2K and joint-fits
- Have several post-docs and students to support DUNE and also the MaCh3 framework in general
- If more features or functionality are desired then talk to us!

BACKUPS

Metropolis-Hastings algorithm

Markov chains semi-randomly step around parameter space and give you the probability of each point in this space.

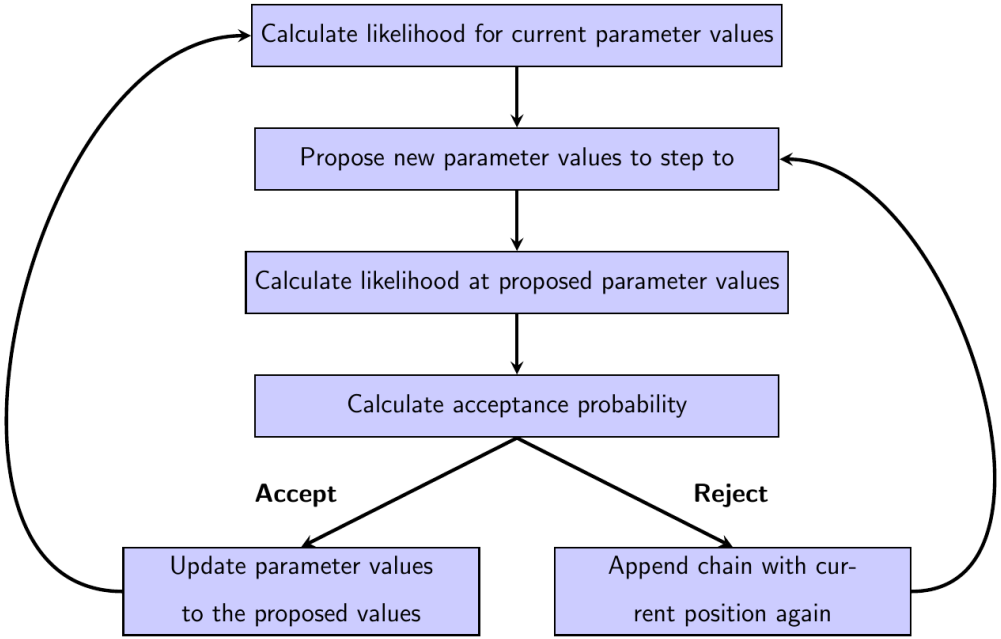
We use the Metropolis-Hastings algorithm. Acceptance ratio:

$$\alpha(\vec{x}_n, \vec{y}_n) = \min\left(1, \frac{P(\vec{y}_n|D)}{P(\vec{x}_n|D)}\right)$$

Generate number between 0-1 if acceptance ratio greater than this then step!

i.e. always **accept a step if probability higher**. Sometimes step to lower probability.

Unlike other fitters in T2K we jointly sample ND280 + SK data



Back to MaCh3

Sample interface

- Read in the MC file and specify the binning of the sample
- Binning, kinematic cuts for each sample are configurable in xml file
- Reweight MC from systematic parameter values
- Passes binned samples to MCMC to calculate likelihood etc.

Covariance

- Specifies prior uncertainty on parameters and correlation with others
- Passes prior penalty term to likelihood
- Upper and lower bounds of parameters
- All configurable in xml file (we'll probably move to YAML in the future)

Other features:

- PCA of covariance matrices
- MC stat uncertainty
- Chain diagnostic tools

Oscillation calculation

- Can be done event-by-event or binned
- Currently use Prob3++ and GPU accelerated version
- Moving towards CUDAProb (CPU and GPU).
- Can support other oscillation calculators e.g. SQUIDS for non-PMNS physics in the future

Systematics!

- **Splines, Normalisations, Kinematic shifts, Functional responses**
- **Will describe these in detail in the next slides!**
- **If there are ideas for systematics that aren't covered here then please say**!

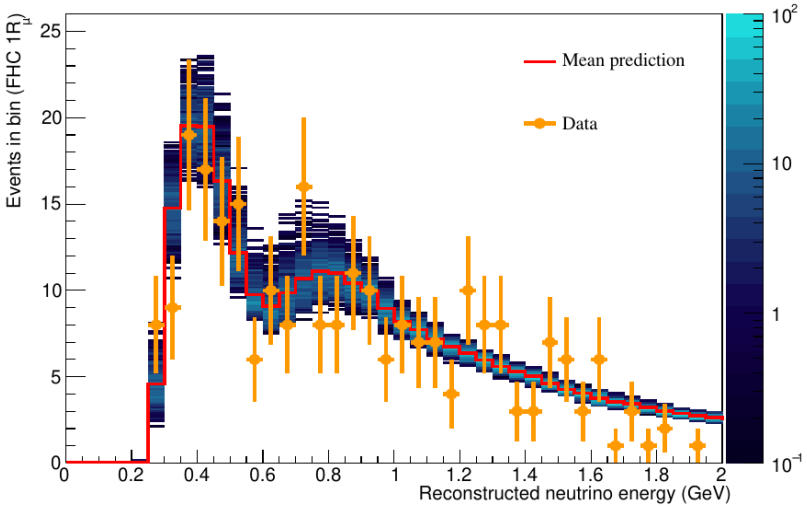
Posterior predictive checks

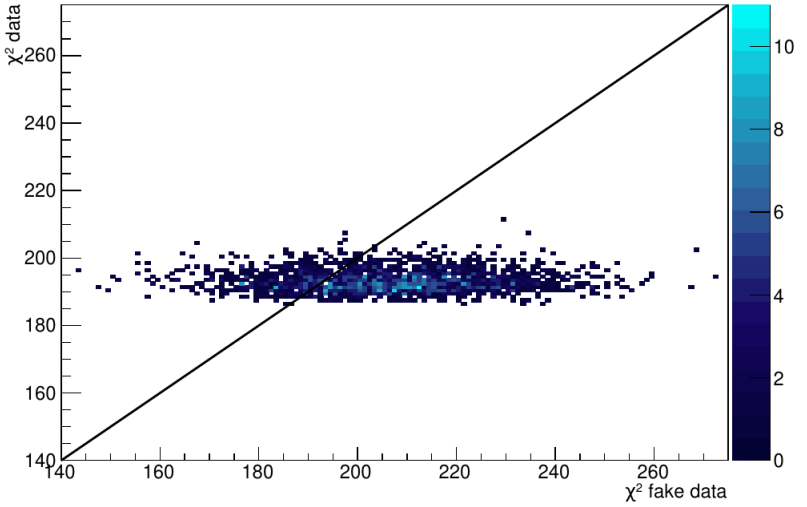
Don't get quite the same p-value that frequentist fits get.

A common tool for MCMC analyses are posterior predictive p-values where syst + stat throws are compared to the MC prediction and the data.

Fraction of throws with better fit to data compared to throw gives you p-value.

Prior-predictive p-values can also be a useful tool for bayesian analyses where you look at compatability of your model and the data pre-fit.





Significance tests

- Bayes factors!
- Ratio of the number of steps in one hypothesis/model compared to another
- Mass hierarchy and octant are the obvious ones for LBL analyses
- Use Jeffrey’s scale
  - No direct mapping to “5 sigma” in chi2

Computational needs / speed

- For ND280+SK fit on T2K:
  - Typically see step times of 0.15s/step
  - ~8GB of RAM
- Require GPUs for osc calc
- CPU-only osc calc. Currently very slow but this will be improved in the future