Signal Extraction and Parameter Estimation via Density Ratios

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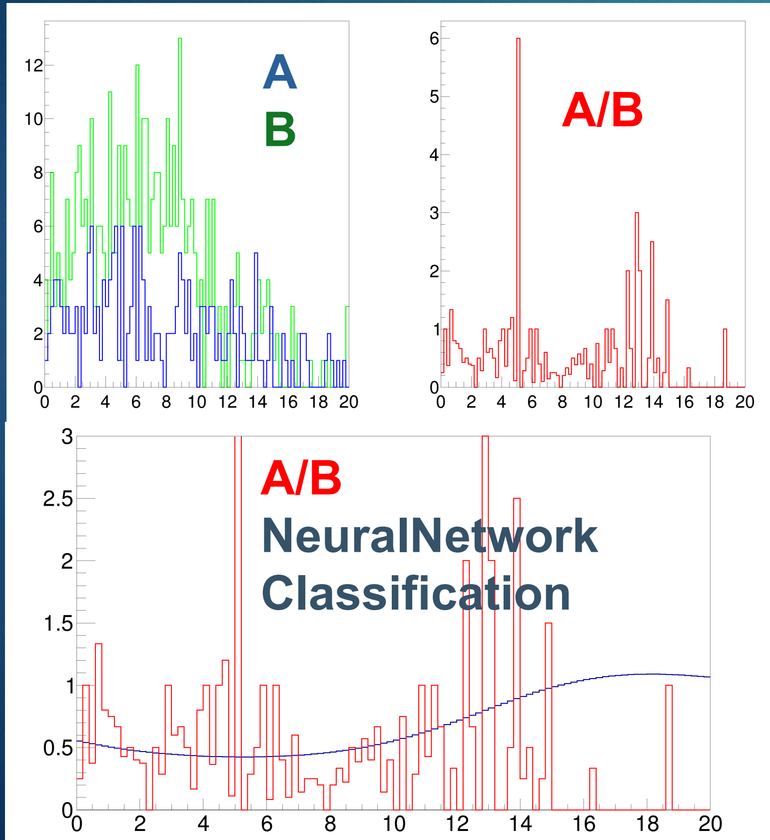
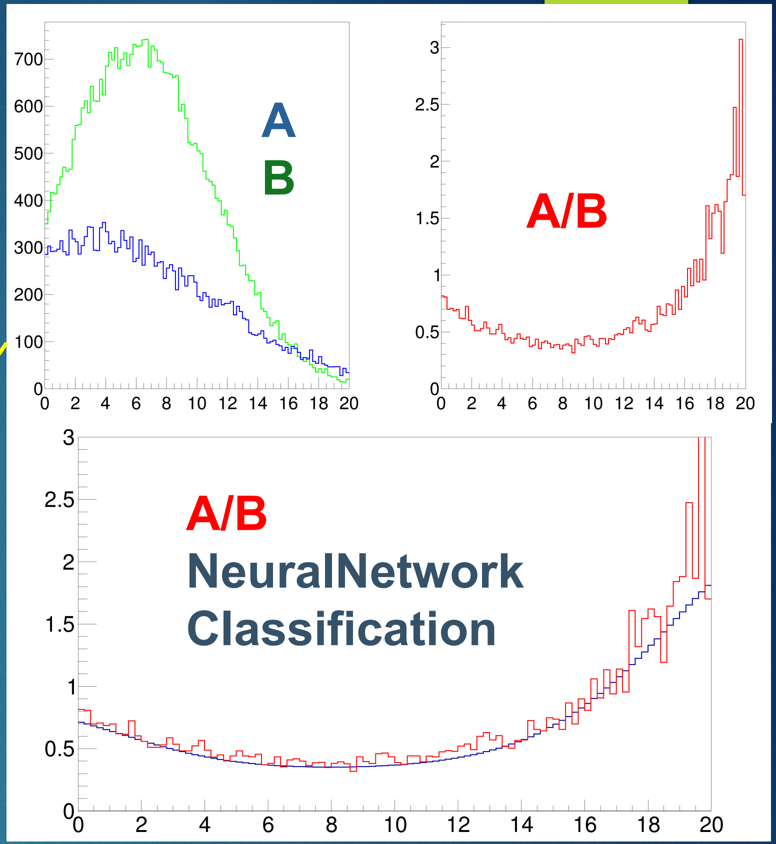
Density Ratios

- Often we require the ratio of 2 different distributions :
  Density Ratio

- In 1D we may just use 2 histograms and create a 3rd which is their ratio



100x less events



- But in many dimensions this become infeasible
- Similar to having very low statistics
- Alternatively we can use Machine Learning classification tasks which are suited to such problems

Previous Work with Density Ratios

arXiv > physics > arXiv:2207.11254

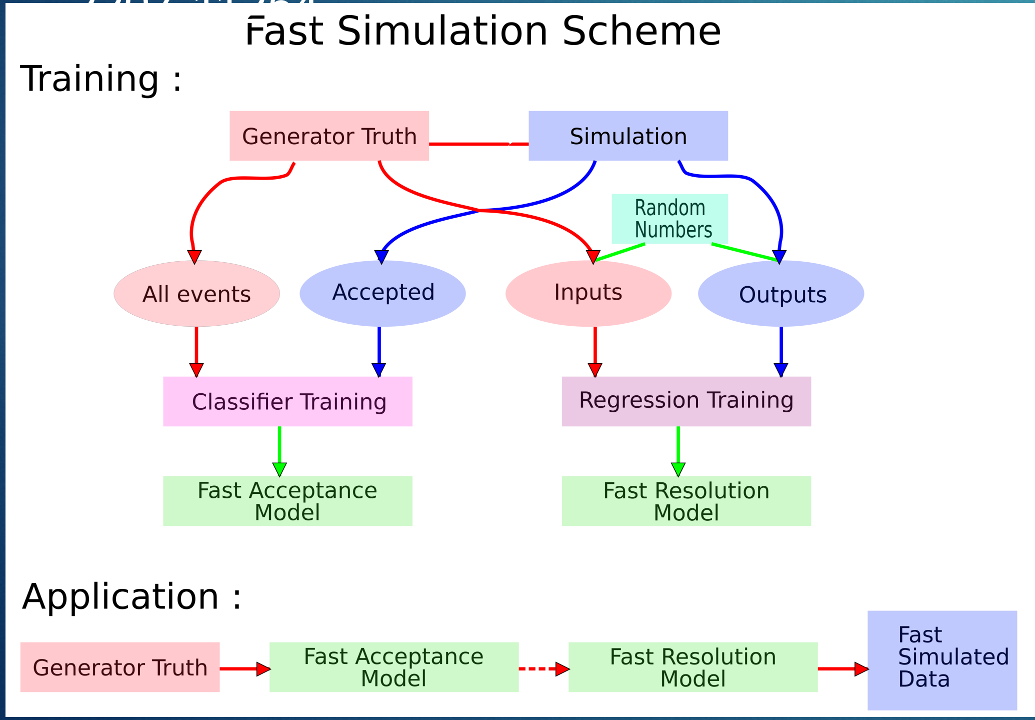
Physics > Data Analysis, Statistics and Probability

[Submitted on 22 Jul 2022]

Machine Learned Particle Detector Simulations

D. Darulis, R. Tyson, D. G. Ireland, D. I. Glazier, B. McKinnon, P. Pauli

https://arxiv.org/abs/2207.11254



Excellent tool for mapping acceptance probabilities in multi-dimensions

i.e. probability a particle is detected at particular point

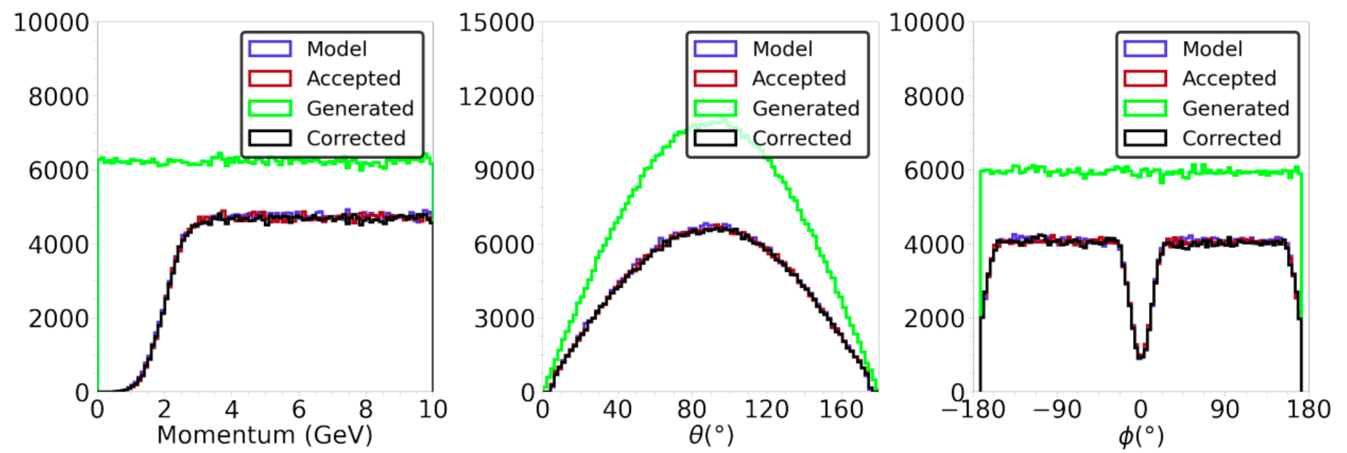


Figure 11: Results of applying a neural network with a Gaussian transform for acceptance modelling with a BDT correction. The BDT used 100 weak learners with a maximum depth of 10 and a learning rate of 0.1. The network used is the higher capacity model with 4 hidden layers of 512, 256, 128, and 16 neurons respectively. The improvement in the 3-vector component distributions is smaller than in the case of the low capacity network.

- Optimised algorithm using combination of Neural
- Networks and BDT for multi-dimensional correlations and accuracy

Full Reaction Simulations

Momentum resolutions / correlations Toy Simulation

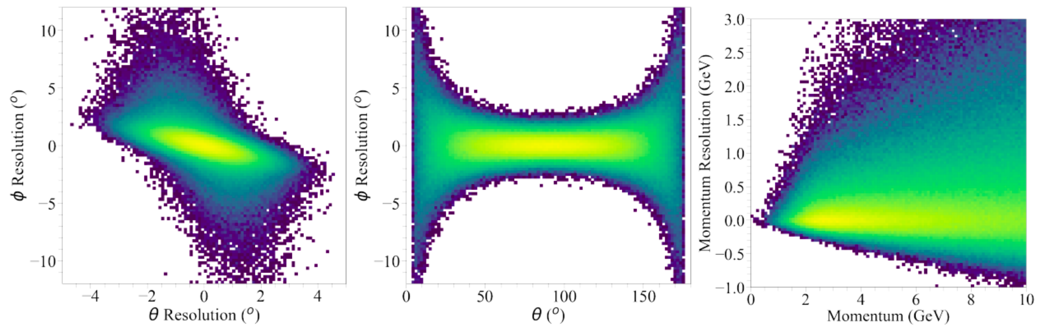
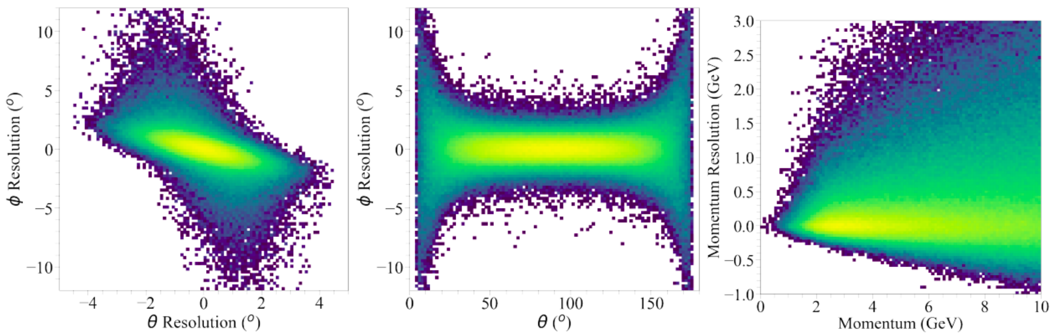


Figure 3: Some of the multidimensional correlations in the toy detector reconstruction. It is important that the machine learned simulation can reproduce these features.

Momentum resolutions / correlations ML Simulation



- Resolutions mapped with Decision Tree inference

Kinematic distributions : invariant masses decay angles

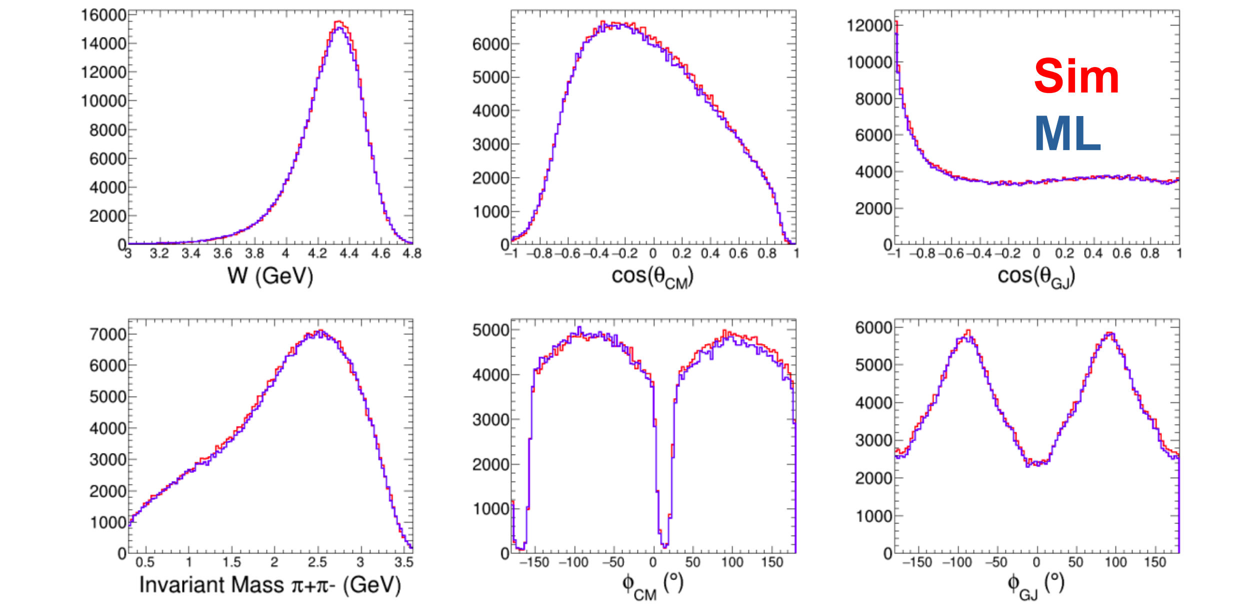


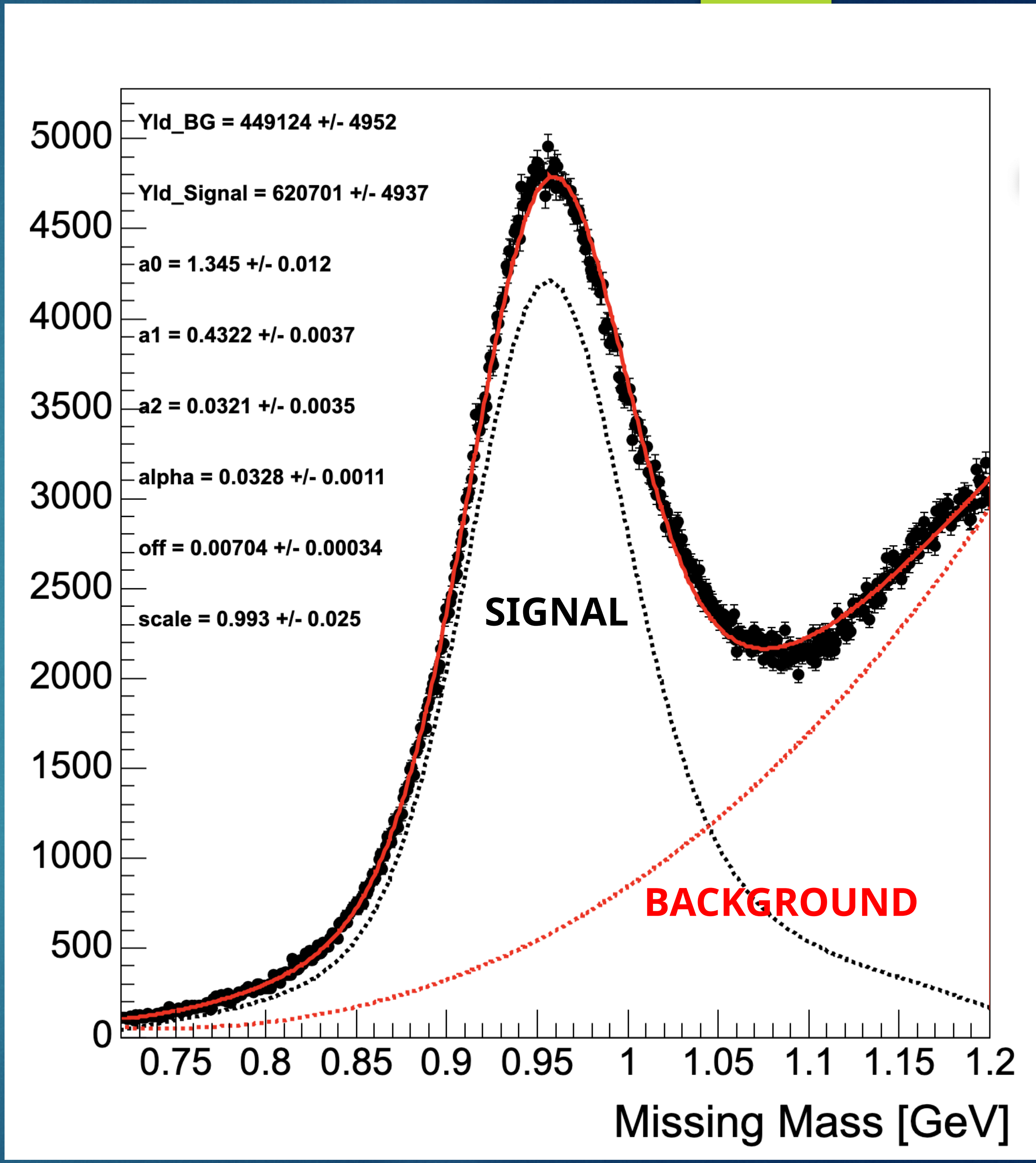
Figure 26: Accepted and reconstructed physics variables for the Fast (blue) and Toy (red) simulations of the 2 pion photoproduction reaction. The distributions show: the invariant mass of the three final state particles, W; the invariant mass of the two pions, $M(2\pi)$; the production angles in the centre-of-mass system ($\cos(\theta_{CM}), \phi_{CM}$); and the decay angles of the two pions.

Machine Learning With Experimental Data

- Often train ML with simulated data – requires excellent agreement between simulation and experimental data.

- Instead we can train ML with experimental data – this relies on being able to separate contributions from different event sources in the data.

- In the example plot, we would need to separate the background and neutron signal to use the neutron data in training.

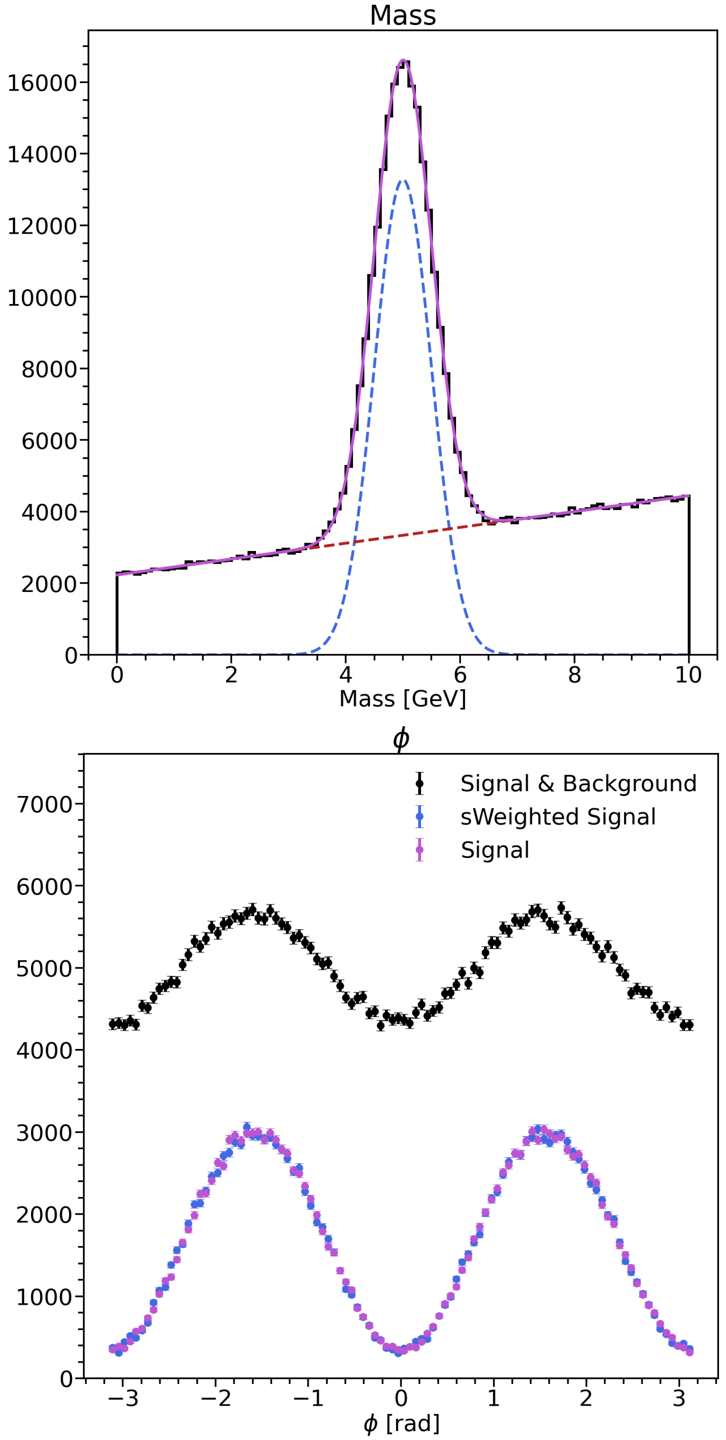


Based on work with R.Tyson:
To be published
[arXiv:2409.08183 (2024)]

sPlot and sWeights

- The sPlot formalism aims to unfold the contributions of different event sources to the experimental data.
- sPlot generalises side-band subtraction weights to where there is no clear isolated background to subtract from the total event sample.
- The data is assumed to have:
  - discriminating variables where distribution of event sources are known
  - control variables where distributions of event sources are unknown.
- Fit expected pdf to discriminating variables to obtain sWeights that allow to reconstruct distribution of control variables.
- Requires that the discriminatory variable and control variables are independent of each other.

M. Pivk, F. R. Le Diberder. SPlot : A Statistical tool to unfold data distributions. *Nucl. Instrum*

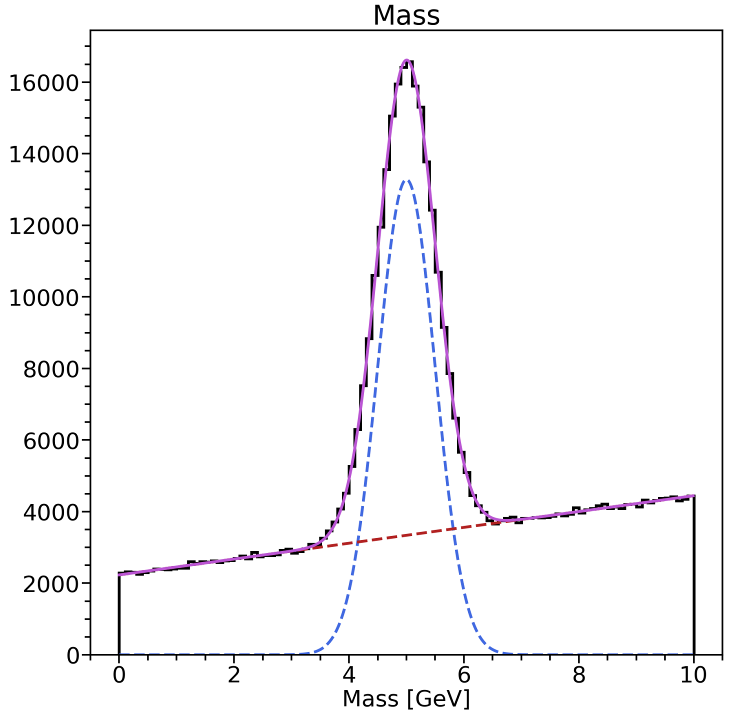


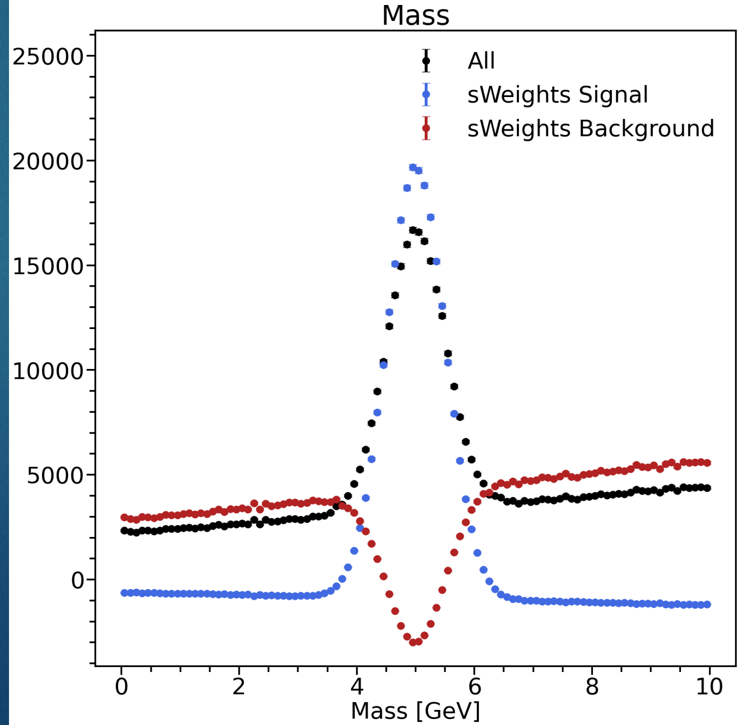
Negative sWeights

- Essential characteristic of sWeights is that they can be negative.
- Necessary to preserves the statistical properties of the dataset eg correct uncertainties and normalisation.
- Creates issues for ML training : -ve weights in general allow loss to become arbitrarily negative
- Circumvent this issue starting with sample weighted binary cross entropy loss

$$L(f(x_i)) = -\sum_i w_i(y_i \log f(x_i) - (1-y_i)\log(1-f(x_i)))$$

- And convert sWeights to positive definite probabilities through density ratio classification task.





Density Ratio Weights (drWeights)

- For this we can use density ratio estimation:
  - Summing the sWeights for a given species recovers the yield of that species.
  - Define weights for a given species equivalent to the ratio of its probability density over the sum of probability densities of all species in the data ie

$$W_{dr}(x_i) = \frac{D_S(x_i)}{D_S(x_i) + D_B(x_i)} = \frac{D_S(x_i)}{D_{all}(x_i)} \,.$$

- To convert the signal weights we create a training sample with "all events weighted by signal sWeights" as class 1 and "all events weighted by 1" as class 0.

- Avoids the issues due to negative weights as all events in class 0 are contained in class 1

  Requires : $\sum w_i < N$ (number of events). True by definition of signal sWeights

- ML classifier with this training sample will have output for signal $f(x_i)$:

$$f(x_i) = \frac{D_S(x_i)}{D_S(x_i) + D_{all}(x_i)}$$

  Then transform to probability W_{dr}

$$\Rightarrow W_{dr}(x_i) = \frac{f(x_i)}{1 - f(x_i)} \,.$$

See also Nachman/ThalerNeural : resampler for monte carlo reweighting with preserved uncertainties. Phys. Rev. D, 102:076004, Oct 2020

Density Ratio Weights (drWeights)

- The solution to this is to convert sWeights to positive definite probabilities
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Create the training sample with all events weighted by signal sWeights as class 1 and all events weighted by 1 as class 0.

Two key takeaways are:

Creating the training sample in such a way allows to use the binary cross-entropy loss function even in the presence of negative sWeights.

Creating the training sample in such a way allows a binary classification model to convert the signal sWeights to positive definite probabilities.

Couple of Notes

- sPlot requires that the discriminatory variable and control variables are independent of each other.

⇒ conversion should only be made with the control variables

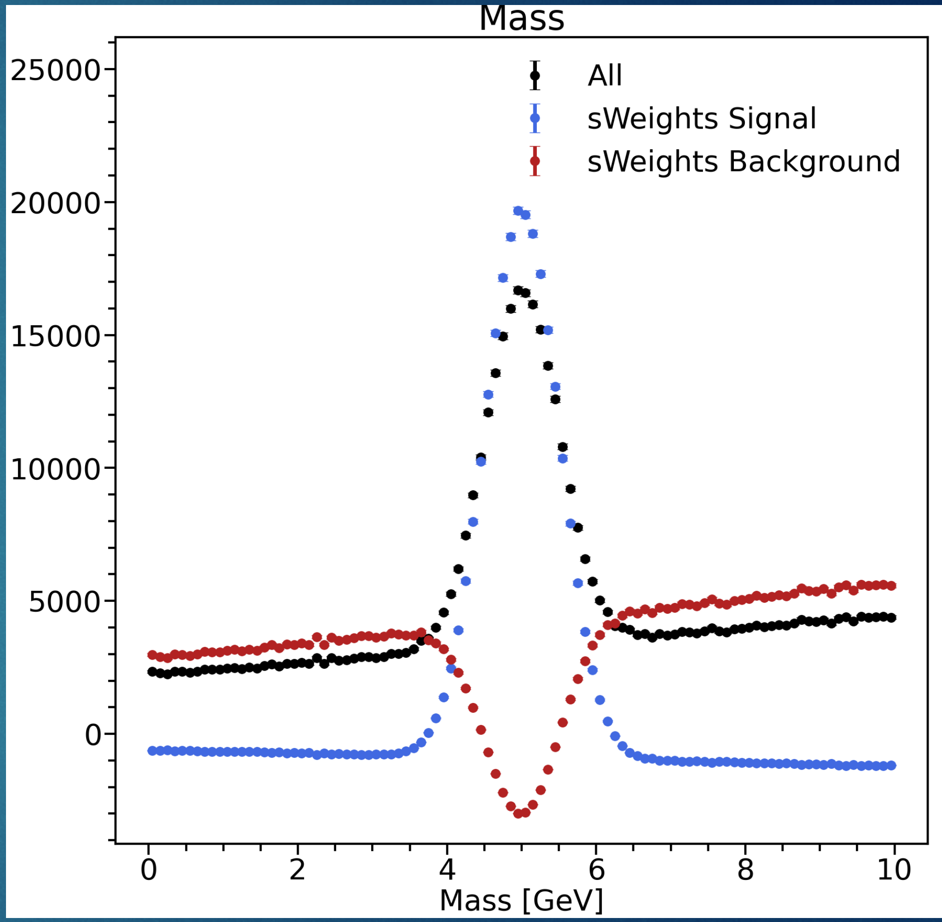
- sPlot unfolds the control variable distributions

⇒ conversion works only at the distribution level and not on an event by event basis.

- sWeighted uncertainty is calculated by taking the sum of the squared sWeights.

⇒ This doesn't work with converted weights W_{dr}.
But we can just propagate sWeight sum of squared weights

- We can apply the method twice, or more, ie correct the drWeights for better results.



Toy Example

- Create toy event generator to produce three dimensional events:
  - mass such as an invariant mass as discriminatory variable
  - azimuthal (ϕ) angular distribution
  - z = cos θ.

- Signal events were generated with a Gaussian distribution in mass and a cos 2ϕ distribution of amplitude 0.8.

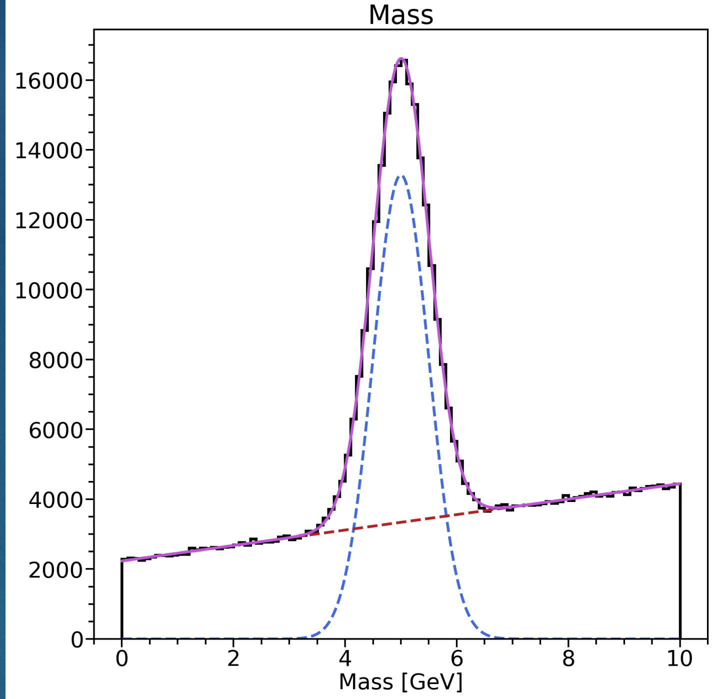
- Background events were generated with a Chebyshev polynomial distribution in mass and a cos 2ϕ distribution of amplitude -0.2.

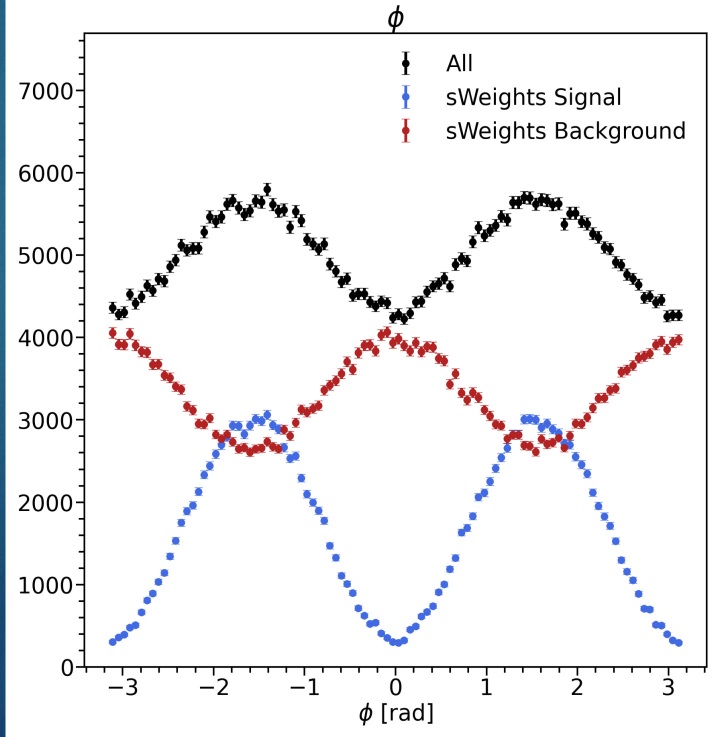
- The aim is to measure the signal asymmetry in ϕ by unfolding the signal distribution in the control variable ϕ .

Fit of signal and background PDFs allows us to determine sWeights

Applying sWeights To Φ distributions gives our signal cos(2Φ)
Fit to this (blue) to get back our amplitude of 0.8

See github repo





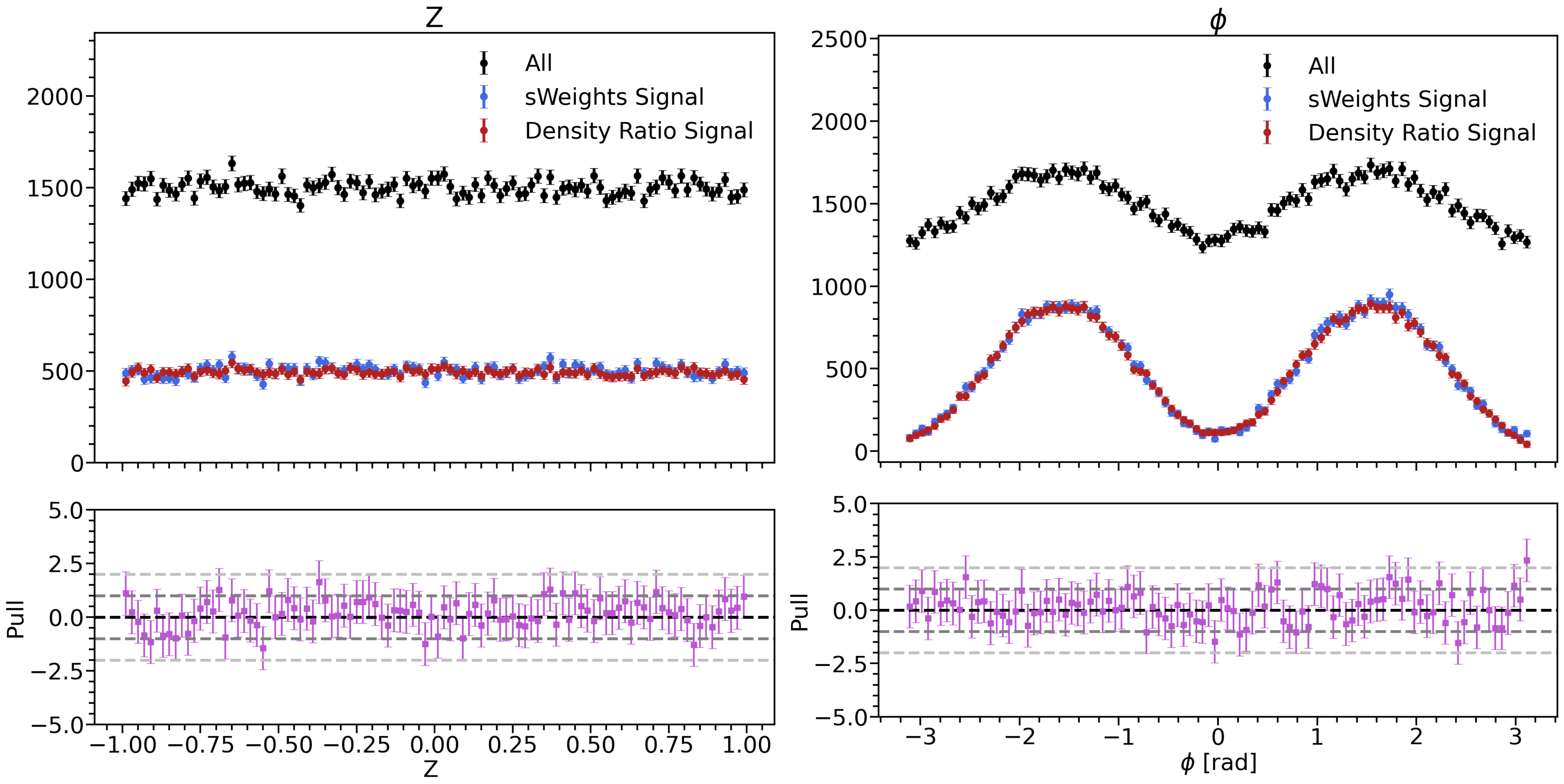
Apply two consecutive Gradient Boosted Decision Trees to convert sWeights.

→ Second acts as reweighter fine-tuning results

→ Measurably improves results

Several other learning models tested, generally good performance.

Training rate ~2 kHz, prediction rate ~500 kHz on 5 cores of a AMD EPYC 9554 64-Core Processor at 3.1GHz.



Excellent agreement Between blue sWeights and red drWeights

Deviations not statistically significant

Quantifying how well it works

- Want to reproduce signal ϕ asymmetry amplitude of 0.8.
- Repeat training the density ratio model and fitting ϕ asymmetry for 2000 independent toy datasets of 100k events
- Use Signal to Background ratio of (1:9).
- Obtain mean amplitude and uncertainty along with the standard deviation of the amplitude over the 2000 datasets
- Fit performed via binned χ2
- The expectations are:
  - mean should be consistent with the nominal value of 0.8
  - mean uncertainty and standard deviation should be numerically similar i.e. the fluctuation of results is consistent with the calculated uncertainty
  - i.e. **σrms /σfit** ~ 1.0

Weights	Amp. Mean	$\hat{\sigma}_{rms}$	$\bar{\sigma}_{fit}$	$\frac{\hat{\sigma}_{rms}}{\bar{\sigma}_{fit}}$	$\frac{\chi^2}{N}$	$\bar{g_{fit}}$	$\bar{\sigma}_{g_{fit}}$
$sWeights$	0.801	0.027	0.027	1.01	0.94	0.02	0.97
$drWeights$	0.792	0.031	0.027	1.15	0.66	0.01	0.81

Table 1: Comparison of the ϕ amplitude measured with the signal distribution generated with a ϕ amplitude of 0.8 for 10^5 events with a signal to background ratio of 1:9. The data generation and training were repeated 2000 times. The mean and standard deviation ($\hat{\sigma}_{rms}$) of the measured amplitudes are reported, along with the mean fit uncertainty. We also show the mean reduced χ^2 of the 2000 fits and the average of the pull (g_{fit}) means and standard deviations of the histogram to the fit result, with each mean and standard deviation constructed from the 100 bins of the test histogram.

Quantifying how well it works

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Start with large background sample
Reproduce correct asymmetry to systematic deviation of 1% (0.3σ)
Fit uncertainties underestimated by 15%
-i.e we get 15% more spread of results
$\chi^2/N < 1$ => Smoothing of distribution
Pull distributions of histograms to fit results also have width (σ_{gfit}) < 1
but no bias mean $g_{fit}=0$
=>smoothing of distribution

$\frac{\chi^2}{N}$	$\bar{g_{fit}}$	$\bar{\sigma}_{g_{fit}}$
0.94	0.02	0.97
0.66	0.01	0.81

e signal distribution generated
background ratio of 1:9. The
mean and standard deviation
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More complex distributions

- Increase frequency of cos terms
- Observe systematic drop-off in measured amplitude with frequency
- Effect of smoothing/averaging of distributions over data structures
- Similar to resolution effects from detector

- Note sPlot results also drop – presumably due to histogram binning effects

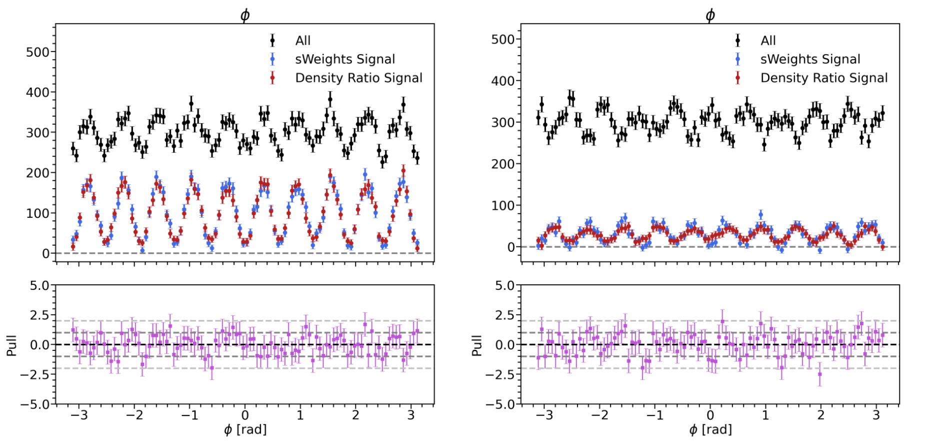


Figure 4: A comparison of all events, *sWeights* signal events (blue) and *drWeights* red for a cosine of frequency = 10, a for 1:2 (left) and 1:9 (right) signal-to-background ratio.

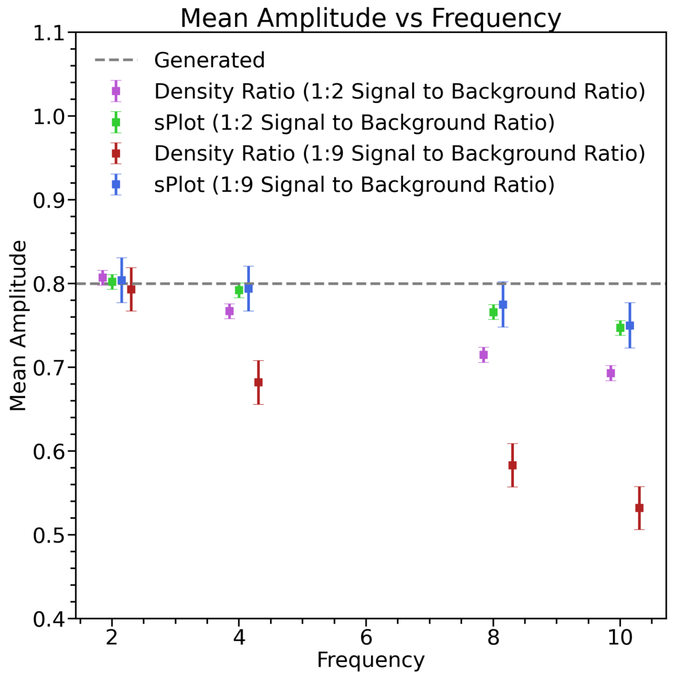


Figure 5: Effect on the fitted cosine amplitude from increasing its frequency. We compare the *sWeight* and *drWeight* cases for different signal-to-background ratios.

Correcting for averaging effects

- We can iterate our GBDT correction reweighters
- Get increasingly better agreement with number of interations
- Standard deviation of Toy results increases
- Eventually match sPlot amplitude

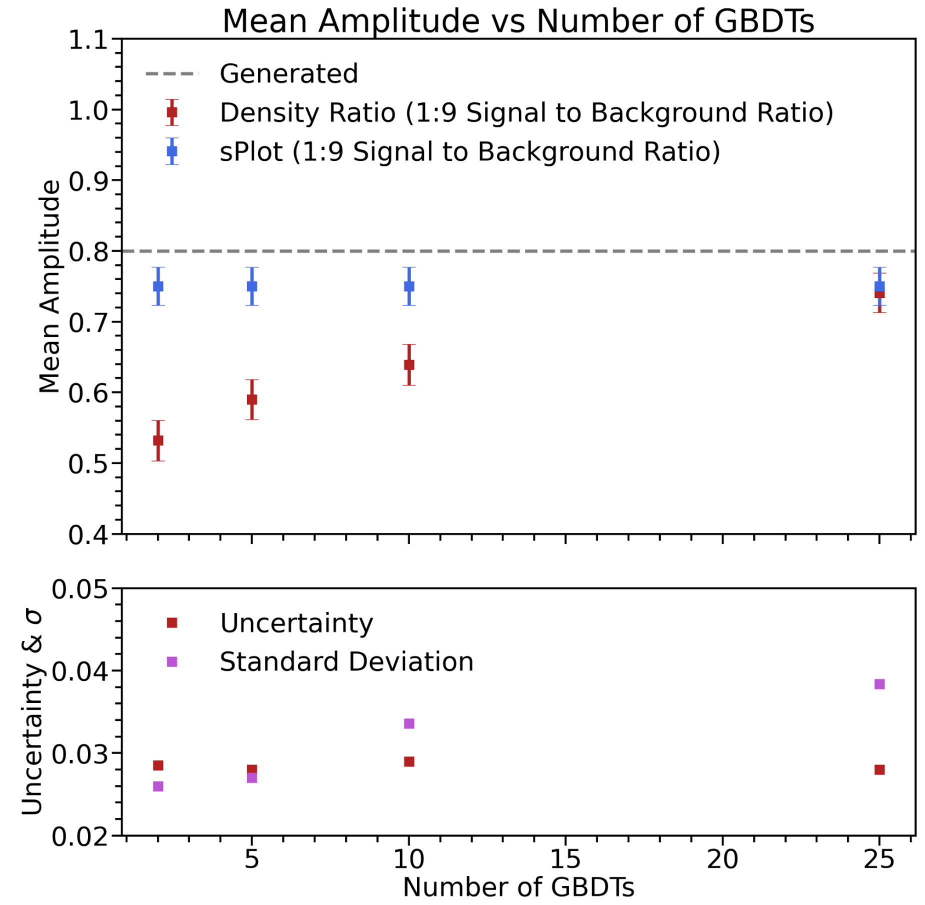
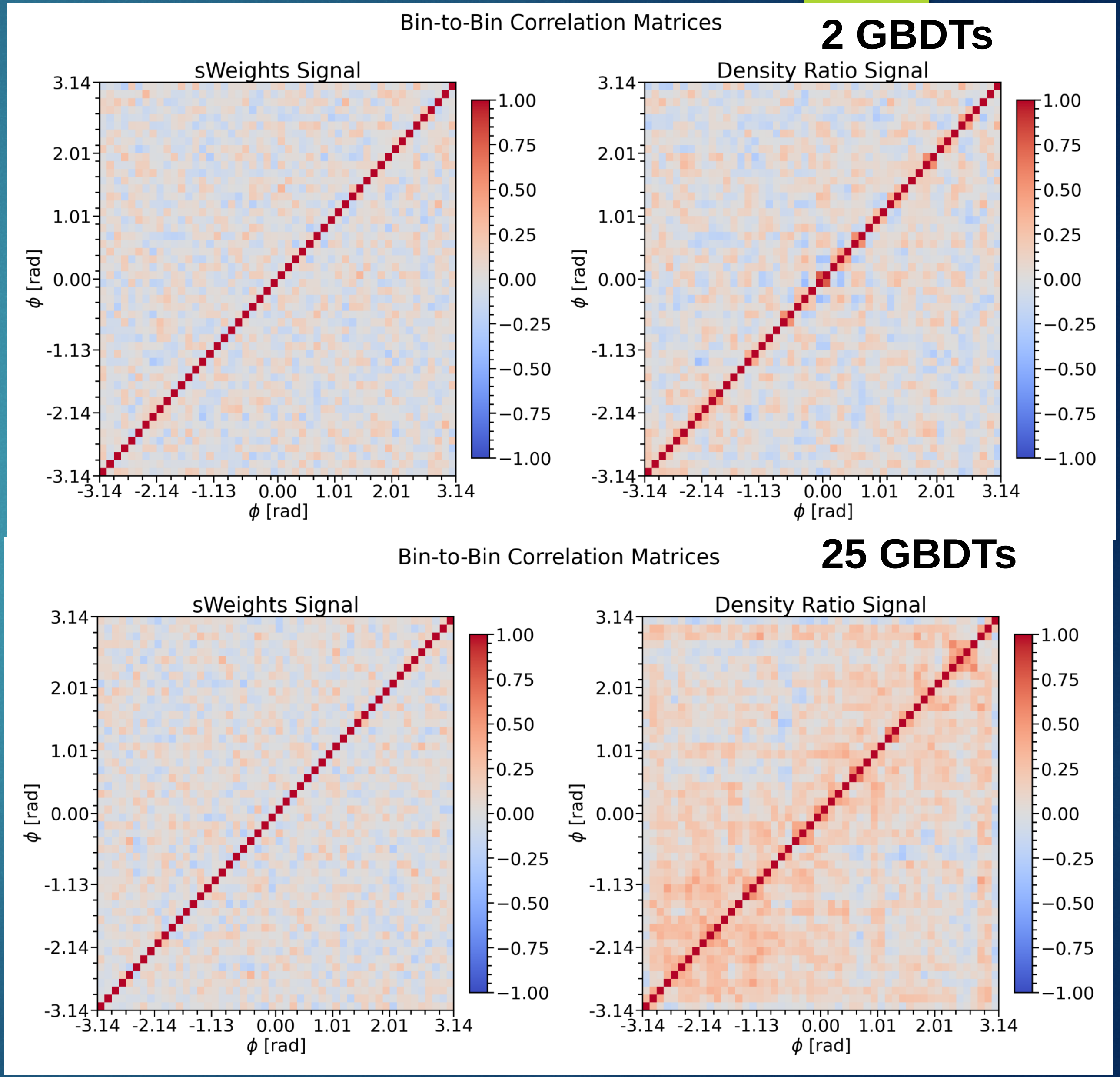


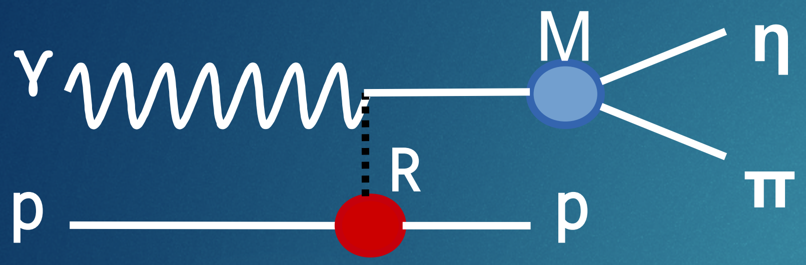
Figure 6: Effect on the fitted cosine amplitude from increasing the number of GBDTs, for a cosine frequency of 10. We compare the *sWeight* and *drWeight* cases and the uncertainty and standard deviations of the *drWeights*.

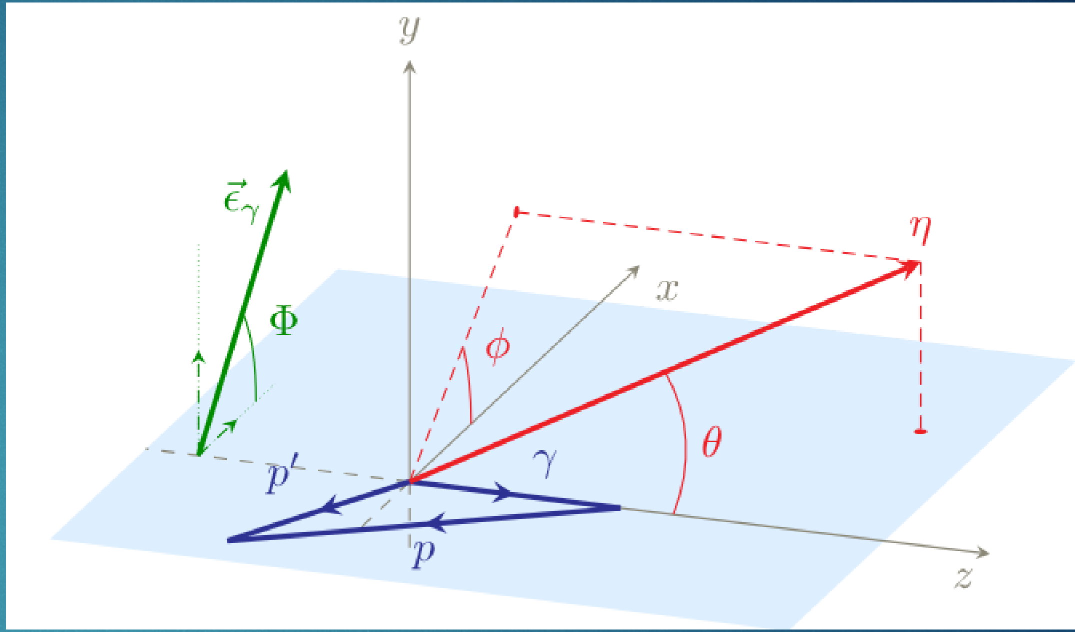
Correlations induced by procedure

- We can examine the correlation matrix of our resulting distributions
- Consider correlations between all bins in histograms
- Splot histograms are uncorrelated
- If with 2 GBTs we observe correlation effects
- With 25 GBTs these increase
- This has implications for particular applications of this technique
- Smoothing/correlations may need unfolded from distributions



Extracting Physics Parameters Via Density Ratios





- Consider physics reaction of 2 meson photoproduction
- Production and decay of M described by 3 angles (θ,ϕ,Φ) at fixed s, t and Mass(ηπ)
- Experimentally measurable as Spherical Harmonics (θ,ϕ) modulated further by cos(2Φ) term
- Decompose distributions into moments of Spherical Harmonics (Fourier Analysis)

Toy Experiments

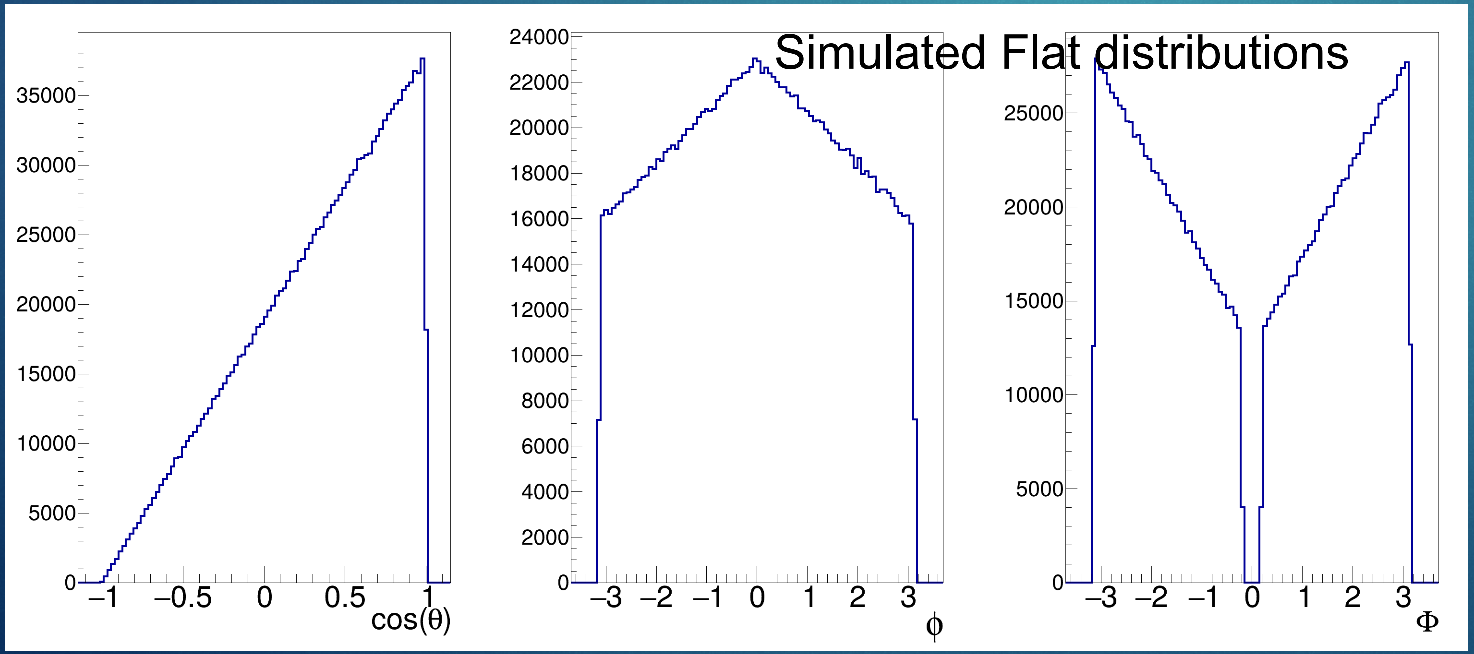
- Generate data $\Omega=(\theta,\phi),\Phi$
  $N = 100\text{k}$ events

$$I(\Omega,\Phi) = I^0(\Omega) - P_\gamma I^1(\Omega)\cos 2\Phi - P_\gamma I^2(\Omega)\sin 2\Phi,$$

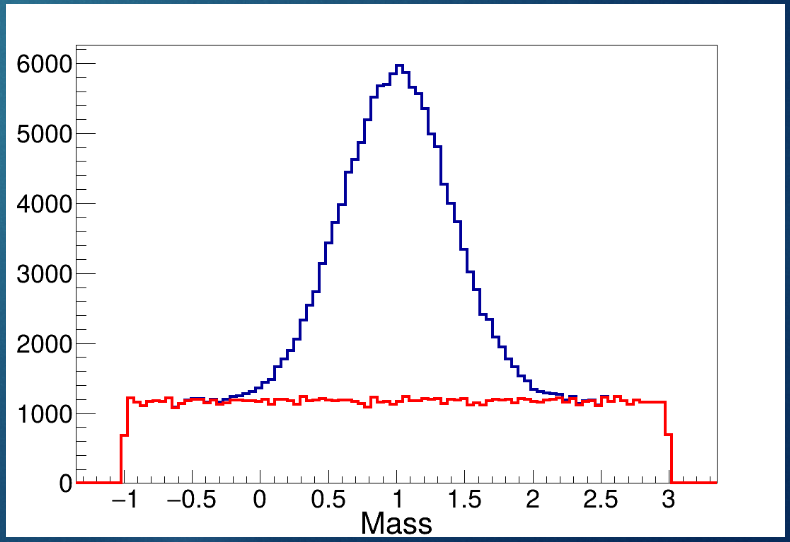
$$\mathcal{I}^0(\Omega) = \kappa \sum_{L,M} H^0(LM) Y_L^M(\Omega)$$

$$\mathcal{I}^{1,2}(\Omega) = -\kappa \sum_{L,M} H^{1,2}(LM) Y_L^M(\Omega)$$

- Where $H^{0,1,2}(LM)$ are moment parameters used to generate the data
- These are then the parameters we wish to then extract
- Fold in Toy detector acceptance effects

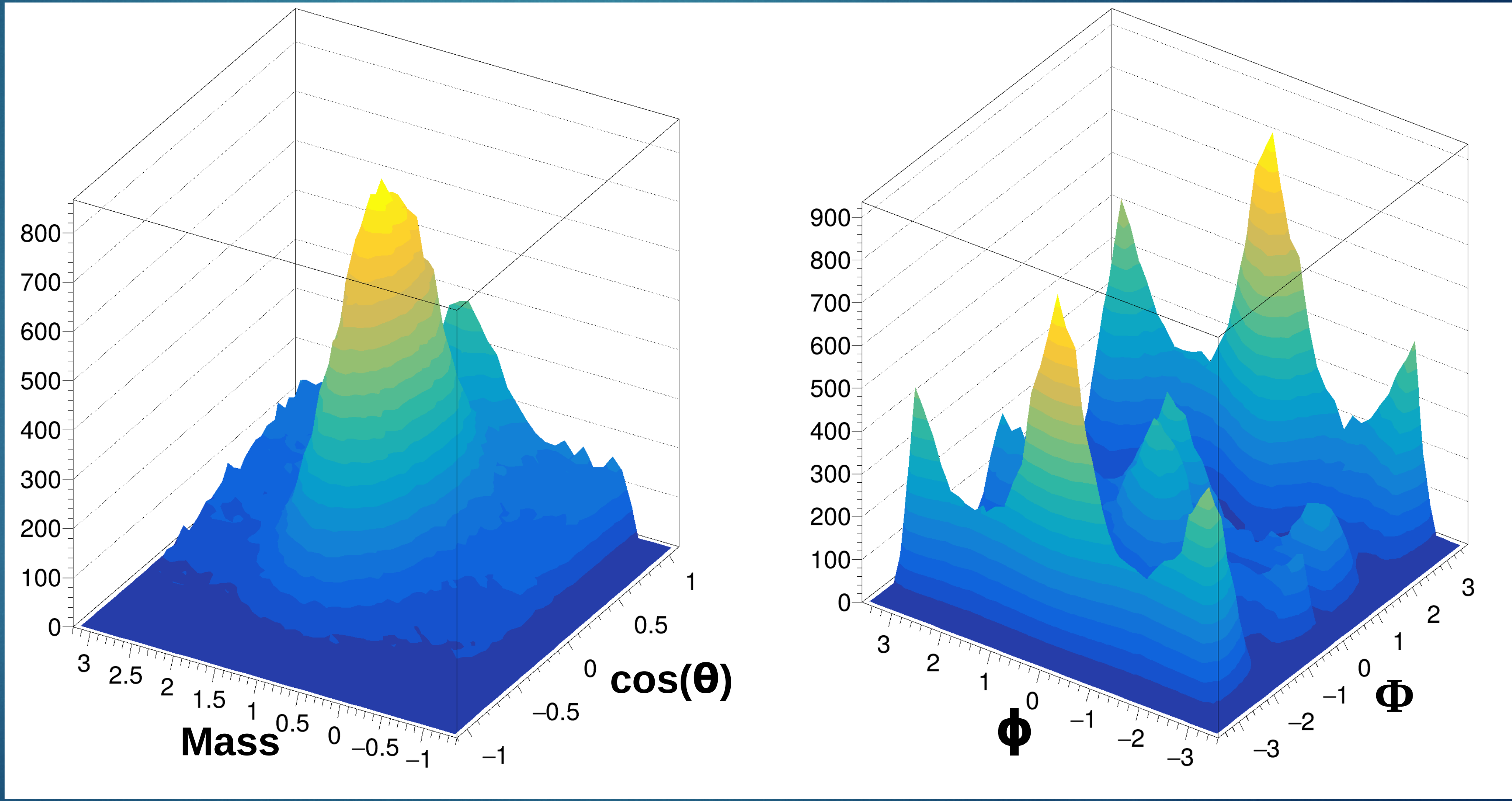


And add background



Generated Toy Dataset Distributions

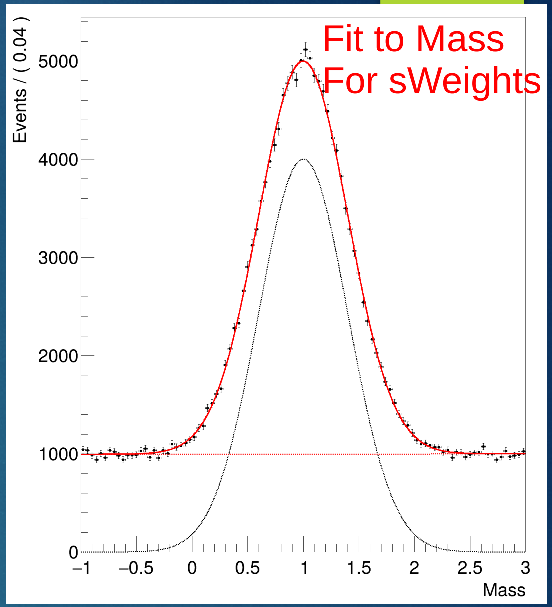
- 2D histrograms of Background + Acceptance Toy Data

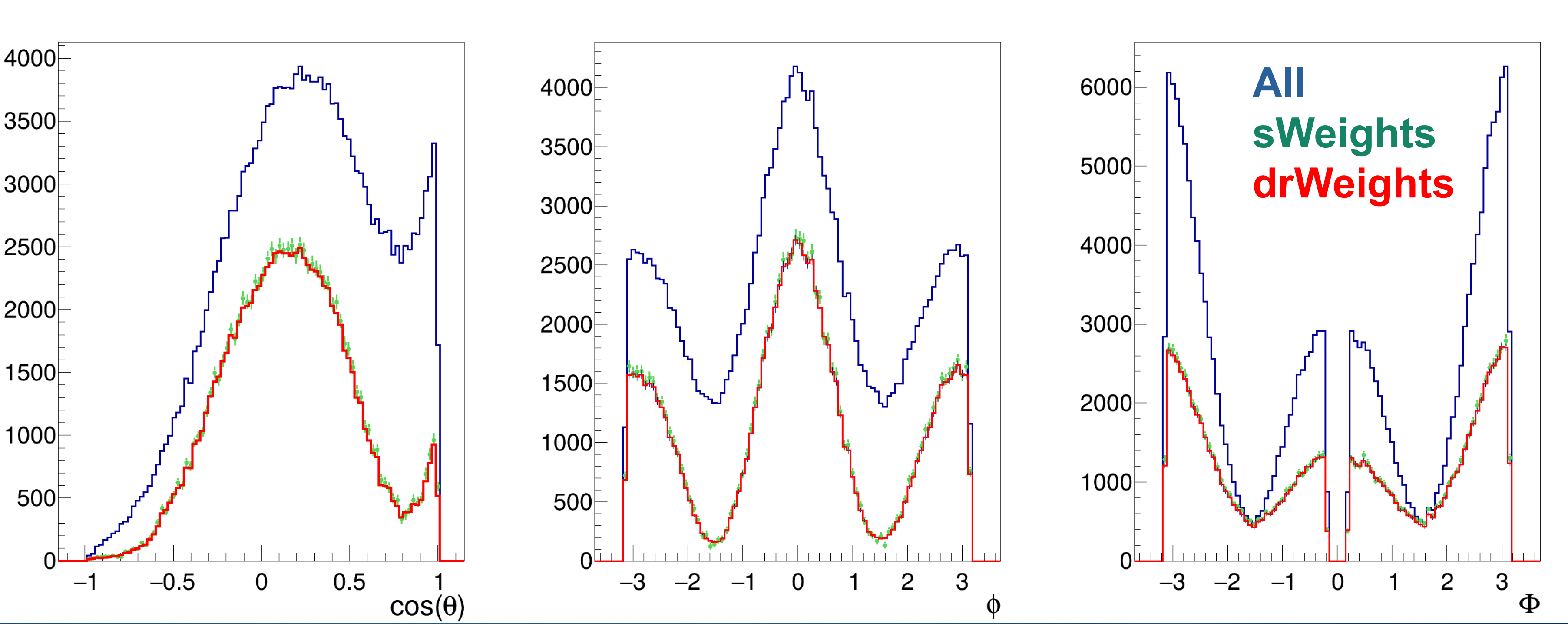


Background removal weights

- Perform fit to Mass distribution → sWeights
- Use Density Ratio to convert to drWeights

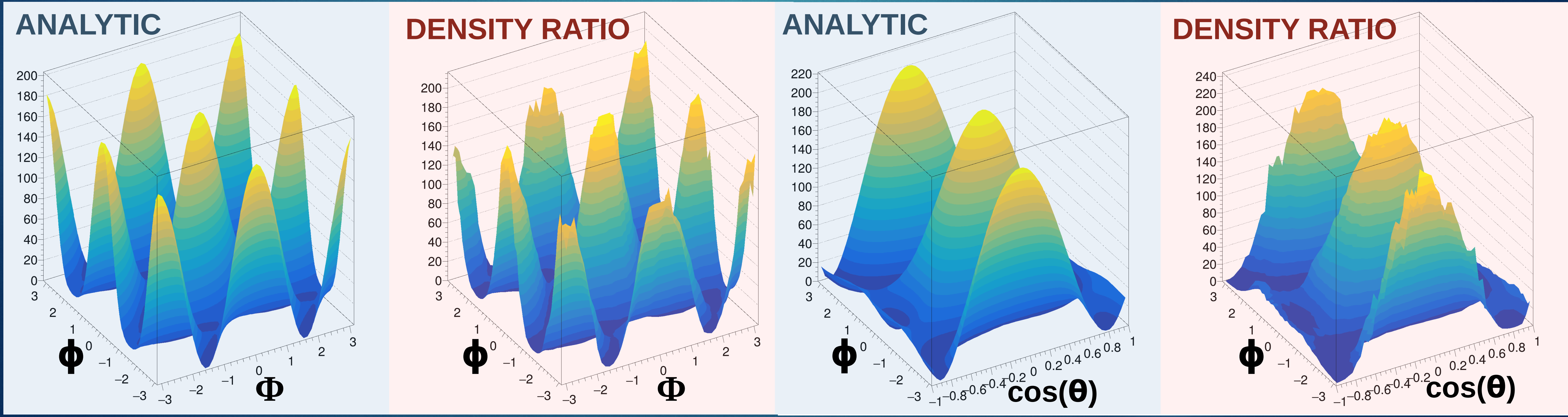
- Plot Signal distribution via weights :





Producing Acceptance Corrected Model

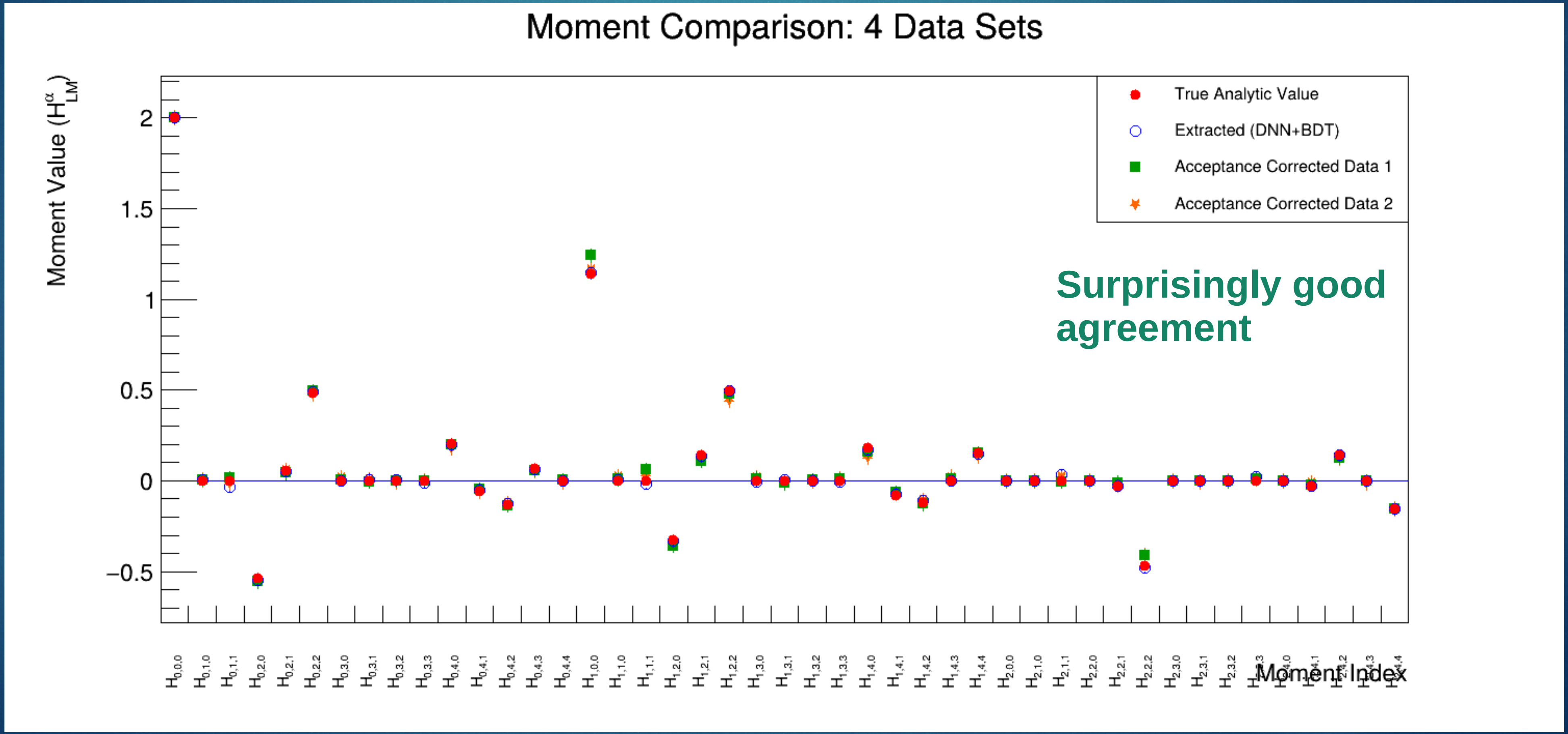
- Perform Classification between Simulated Flat data And drWeighted data
- Use primary DNN with Gradient Boosted Decision Tree reweighter => Background subtracted, acceptance corrected model
- Can’t really extrapolate, but can interpolate over holes if distribution not varying too fast



Extracting Sperhical Harmonic Moments

- We now have 3D numerically integrable functions (use Vegas)

  => Extract moments by integrating over spherical harmonic terms



That's nice but we really want the amplitudes

- Spherical harmonic moments relate to underlying partial wave amplitudes which are produced by mesonic resonance decays
- Equations relating moments to partial waves are non-linear and complex

$$H^0(2,0) = 2\left(\frac{2\sqrt{5}}{5}|S_0^+||D_0^+|\cos(\phi_{D_0}^+) + \frac{2}{7}|D_0^+|^2 + \frac{1}{7}|D_{+1}^+|^2 + \frac{1}{7}|D_{-1}^+|^2\right)$$

$$H^1(2,0) = 2\left(\frac{2\sqrt{5}}{5}|S_0^+||D_0^+|\cos(\phi_{D_0}^+) + \frac{1}{7}|D_0^+|^2 - \frac{1}{7}|D_{+1}^+||D_{-1}^+|\cos(\phi_{D_{+1}}^+ - \phi_{D_{-1}}^+)\right)$$

$$\begin{aligned} H^0(2,1) = 2\Bigg(&\frac{\sqrt{5}}{5}\left(|S_0^+||D_{+1}^+|\cos(\phi_{D_{+1}}^+) - |S_0^+||D_{-1}^+|\cos(\phi_{D_{-1}}^+)\right) \\ &+\frac{1}{7}\left(|D_{+1}^+||D_0^+|\cos(\phi_{D_{+1}}^+ - \phi_{D_0}^+) - |D_0^+||D_{-1}^+|\cos(\phi_{D_0}^+ - \phi_{D_{-1}}^+)\right)\Bigg) \end{aligned}$$

$$\begin{aligned} H^1(2,1) = 2\Bigg(&\frac{\sqrt{5}}{5}\left(|S_0^+||D_{+1}^+|\cos(\phi_{D_{+1}}^+) - |S_0^+||D_{-1}^+|\cos(\phi_{D_{-1}}^+)\right) \\ &-\frac{1}{7}\left(|D_{+1}^+||D_0^+|\cos(\phi_{D_{+1}}^+ - \phi_{D_0}^+) - |D_0^+||D_{-1}^+|\cos(\phi_{D_0}^+ - \phi_{D_{-1}}^+)\right)\Bigg) \end{aligned}$$

$$\begin{aligned} \frac{H^2(2,1)}{i} = 2\Bigg(&-\frac{\sqrt{5}}{5}\left(|S_0^+||D_{+1}^+|\cos(\phi_{D_{+1}}^+) + |S_0^+||D_{-1}^+|\cos(\phi_{D_{-1}}^+)\right) \\ &-\frac{1}{7}\left(|D_{+1}^+||D_0^+|\cos(\phi_{D_{+1}}^+ - \phi_{D_0}^+) + |D_0^+||D_{-1}^+|\cos(\phi_{D_0}^+ - \phi_{D_{-1}}^+)\right)\Bigg) \end{aligned}$$

$$\begin{aligned} \frac{H^3(2,1)}{i} = 2\Bigg(&\frac{\sqrt{5}}{5}\left(|S_0^+||D_{+1}^+|\sin(\phi_{D_{+1}}^+) - |S_0^+||D_{-1}^+|\sin(\phi_{D_{-1}}^+)\right) \\ &+\frac{1}{7}\left(|D_{+1}^+||D_0^+|\sin(\phi_{D_{+1}}^+ - \phi_{D_0}^+) - |D_0^+||D_{-1}^+|\sin(\phi_{D_0}^+ - \phi_{D_{-1}}^+)\right)\Bigg) \end{aligned}$$

$$H^0(0,0) = 2\left(|S_0^+|^2 + |D_{+1}^+|^2 + |D_0^+|^2 + |D_{-1}^+|^2\right)$$

$$H^1(0,0) = 2\left(|S_0^+|^2 + |D_0^+|^2 - 2|D_{+1}^+||D_{-1}^+|\cos(\phi_{D_{+1}}^+ - \phi_{D_{-1}}^+)\right)$$

$$H^1(4,1) = \frac{2\sqrt{30}}{21}\left(-|D_{+1}^+||D_0^+|\cos(\phi_{D_{+1}}^+ - \phi_{D_0}^+) + |D_0^+||D_{-1}^+|\cos(\phi_{D_0}^+ - \phi_{D_{-1}}^+)\right)$$

$$\frac{H^2(4,1)}{i} = \frac{2\sqrt{30}}{21}\left(-|D_{+1}^+||D_0^+|\cos(\phi_{D_{+1}}^+ - \phi_{D_0}^+) - |D_0^+||D_{-1}^+|\cos(\phi_{D_0}^+ - \phi_{D_{-1}}^+)\right)$$

$$\frac{H^3(4,1)}{i} = \frac{2\sqrt{30}}{21}\left(|D_{+1}^+||D_0^+|\sin(\phi_{D_{+1}}^+ - \phi_{D_0}^+) - |D_0^+||D_{-1}^+|\sin(\phi_{D_0}^+ - \phi_{D_{-1}}^+)\right)$$

$$H^0(4,2) = -\frac{4\sqrt{10}}{21}|D_{+1}^+||D_{-1}^+|\cos(\phi_{D_{+1}}^+ - \phi_{D_{-1}}^+)$$

$$H^1(4,2) = \frac{2\sqrt{10}}{21}\left(\sqrt{2}|D_{+1}^+|^2 + \sqrt{2}|D_{-1}^+|^2\right)$$

$$\frac{H^2(4,2)}{i} = \frac{2\sqrt{10}}{21}\left(-\sqrt{2}|D_{+1}^+|^2 + \sqrt{2}|D_{-1}^+|^2\right)$$

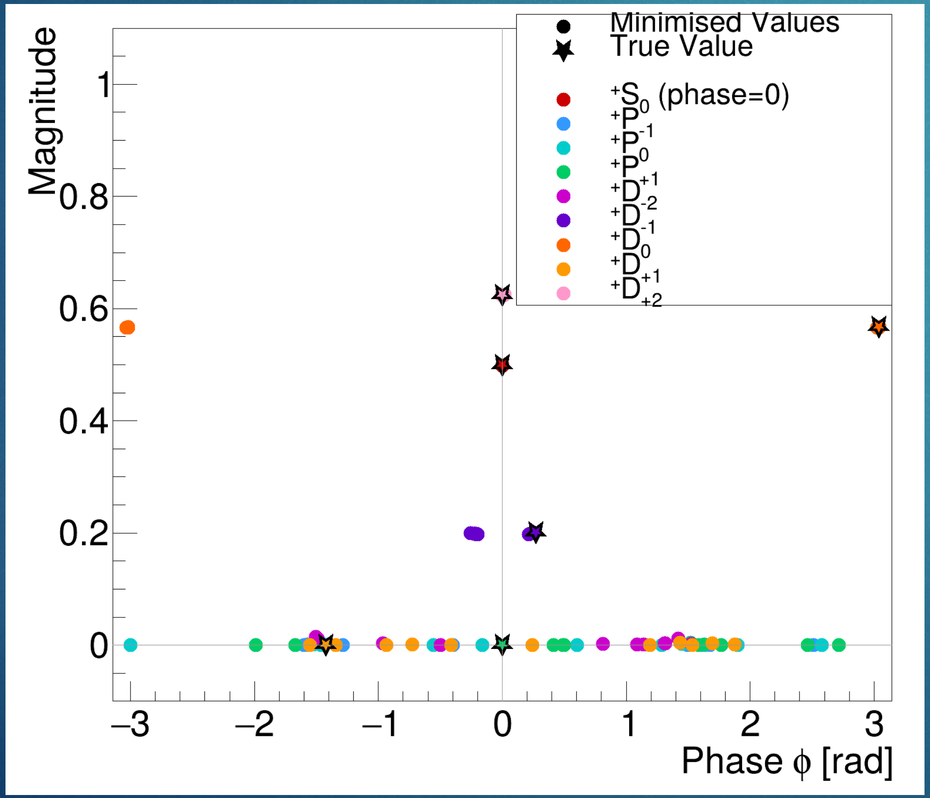
$$\frac{H^3(4,2)}{i} = -\frac{4\sqrt{10}}{21}|D_{+1}^+||D_{-1}^+|\sin(\phi_{D_{+1}}^+ - \phi_{D_{-1}}^+)$$

This is a very difficult numerical problem – lots of local maxima in likelihood space

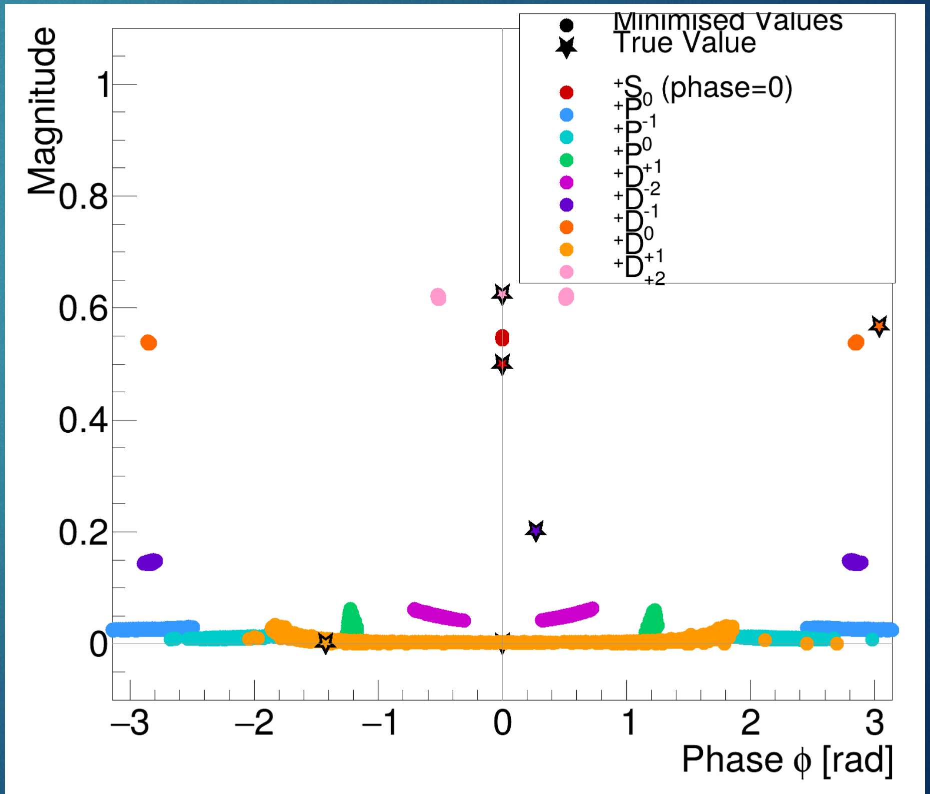
Brute Force : χ^2 mimimisation

- Solve simultaneous equations through minimising χ^2
- This can work, but need to perform a lot of minimisations to get the true minima
- Are there more efficient ML methods for this ?

With True Moments



With DensityRatio Moments



Summary

- Relatively basic machine learning methods may be used to construct reliable density ratios between different distributions
- These density ratios have a number of applications in nuclear/particle physics analysis
- Here we mentioned
  - Fast simulation
  - Calculating probability weights for background subtraction
  - Constructing ND non-parameteric functions for acceptance corrected data
- In the latter case it was shown how these functions can be used to extract experimental observables which can then be used to extract the underlying physics
- But not tested with real experiments, unlikely to give accurate results, but may be useful for initiating other methods such as likelihood fits.

Number of Events

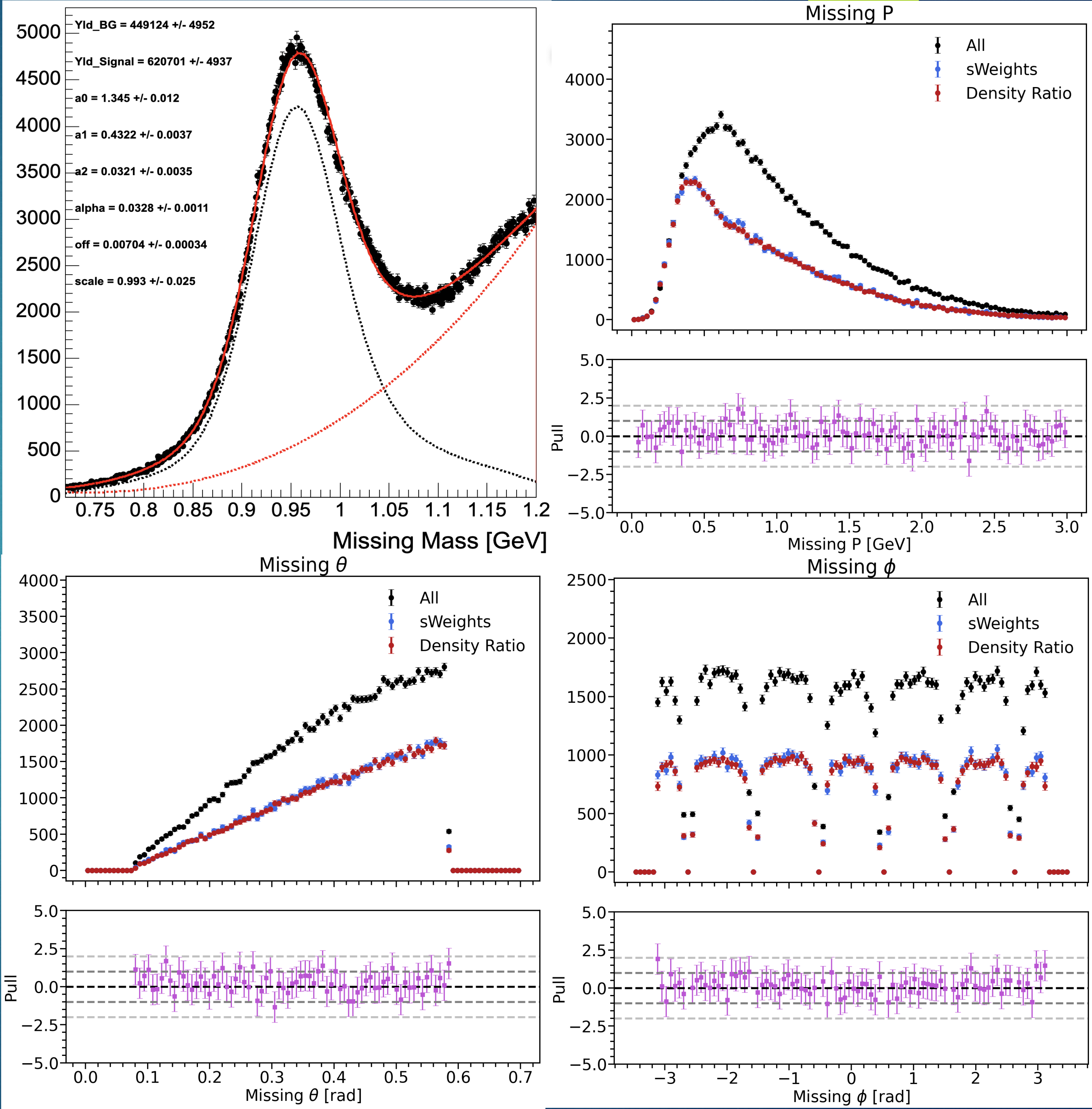
- Same test as before, vary number of events.
- Use signal to background ratio of (1:9).
- At 1000 events we have only 100 signal events.
- drWeights are robust and function well with large backgrounds and limited statistics.
- Issues with sWeights at low event number due to -ve bin contents in binned $\chi 2$
- Expected behaviour when use event based maximum likelihood instead

# Events Weights	Mean	σ	σ Uncertainty
1000 sWeights drWeights	17.94 ± 14.67 0.679 ± 0.5902	84.81 0.2710	5.78 0.46
10,000 sWeights drWeights	0.870 ± 0.0953 0.778 ± 0.1038	0.1090 0.0929	1.14 0.89
100,000 sWeights drWeights	0.804 ± 0.0274 0.793 ± 0.0285	0.0244 0.0260	0.089 0.91
1,000,000 sWeights drWeights	0.799 ± 0.0090 0.792 ± 0.0092	0.0104 0.0110	1.16 1.20

Testing with real data

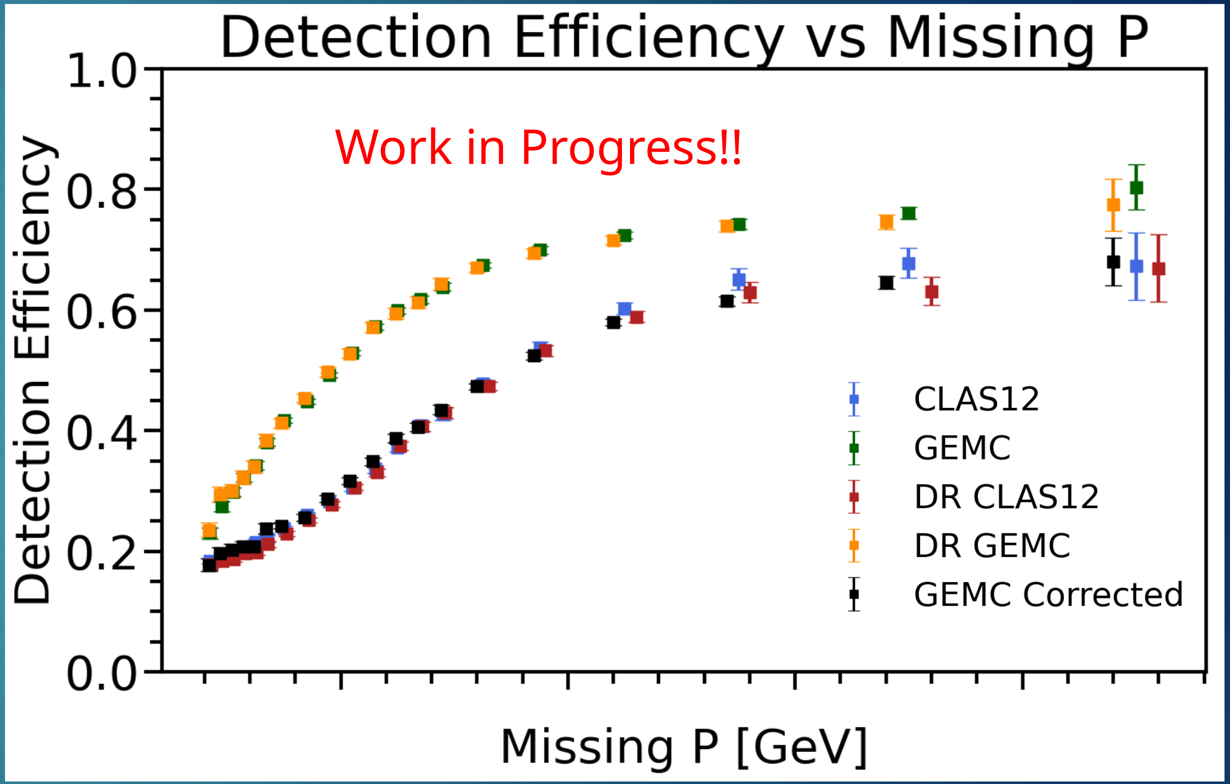
$$ep \rightarrow e'\pi^{+}(n)$$

- Apply this technique to CLAS12 neutron detection.
- Fit neutron missing mass using simulated template.
- Produce drWeights over the reconstructed neutron spherical momentum components.
- Show results for neutron momentum using sWeights and drWeights



Example Application

- We can estimate the neutron detection efficiency by comparing the reconstructed to detected neutron.
- We can also use density ratios to obtain a multi-dimensional model of the neutron detection efficiency (see Slide 3,14 & arxiv:2207.11254).
- Neutron detection is hard to simulate as it relies on detecting the various reaction products produced in scattering between the neutron and calorimeter material.
- To obtain an accurate multidimensional model of neutron detection efficiency we should use experimental data, this relies on being able to convert sWeights to probabilities.



Possible GEANTless Simulations

- Use exclusive reactions to train acceptance algorithm
  e.g. $\gamma + p \rightarrow \pi^+ + \pi^- + p'$
- Filter all events with $\pi+\pi-$ and calculate missing proton momentum $\mathbf{p'}_{\mathbf{calc}}$
- If proton also detected flag (acceptance=1), if not (acceptance=0)
- Train classifier with $\mathbf{p}_{\mathbf{calc}}$ components on acceptance=0 and 1 events
  - Equivalent to Slide 16 analysis

  => proton acceptance as function of **calculated** variables.

  - Equivalent to fast sim parameterisation Slide 3

- Issues : We want as a function of **truth** variables
  There will be background under the mass peak so need drWeights

Signal to Background Ratio