PWA Model building with Parametric and Nonparametric Components

← Lawrence Ng
Florian Kaspar →
PWA Athos 2024

Mass Independent Fits

Pros:

- Minimize model dependence

Cons:

- Prone to instabilities from:
  - Ambiguities
  - Numerical (lower stats)

Mass Dependent Fits

Pros:

- Smooth results by construction
- Assume some physics (i.e. extract resonance parameters)

Cons:

- Biased results / heuristics

Largely unexplored

Maybe we can draw knowledge from other fields?

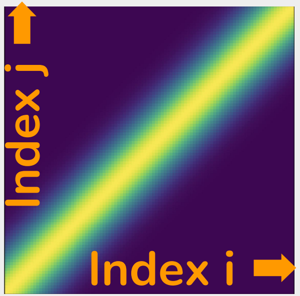
But first, we need some core concepts

Base Knowledge 1/2: **Gaussian Processes**

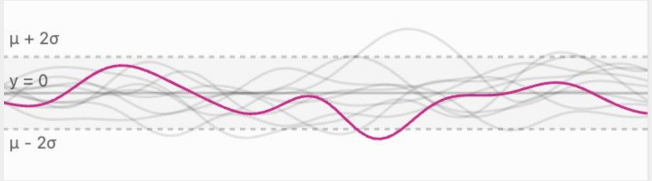
- Generalization of Multivariate Gaussian to infinite dimensions
- At the core: **Kernel Function**
  - $\kappa(x_i, x_j) = Cov(X, X') = \Sigma$
  - Similarity measure / covariance between two points

Radial Basis Function Kernel

$$\sigma^2 \exp\left(-\frac{||t-t'||^2}{2l^2}\right)$$

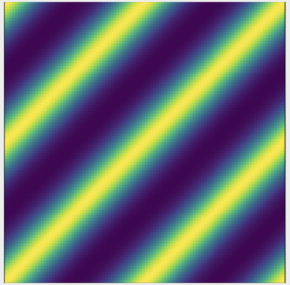


Samples drawn from Kernel

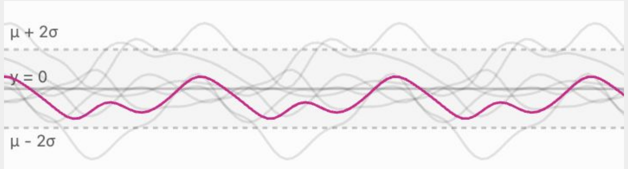


Periodic Kernel

$$\sigma^2 \exp\left(-\frac{2\sin^2(\pi|t-t'|/p)}{l^2}\right)$$



Samples drawn from Kernel



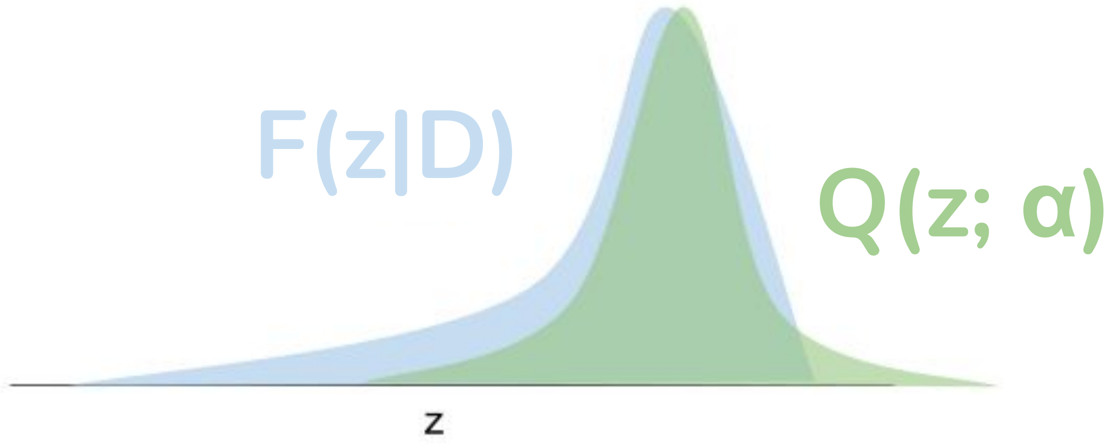
Specific Kernels are chosen based on domain knowledge

*But! We **can** also learn the kernel from data!*

[Distill.pub: A Visual Exploration of Gaussian Processes]

Base Knowledge 2/2: **Variational Inference**

F(z|D) = Complicated Posterior Function
Q(z; α) = Simple function
Vary α such that Q(z; α) ≈ F around some point



Numerical Information Field Theory

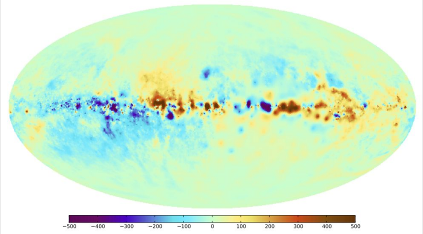
Inference Framework developed for astrophysics at Max Planck Institute for Astrophysics

G. Edenhofer, P. Frank, J. Roth, R. H. Leike, M. Guerdi, L. I. Scheel-Platz, M. Guardiani, V. Eberle, M. Westerkamp, and T. A. Enßlin. Re-Envisioning Numerical Information Field Theory (NIFTy.re): A Library for Gaussian Processes and Variational Inference, 2024.

Mainly working with:
Philipp Frank, Torsten Enßlin, Jakob Knollmüller

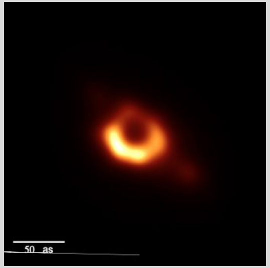
Description

NIFTy, "**N**umerical **I**nformation **F**ield **T**heory", is a Bayesian ~~imaging~~ library.
It is designed to infer the million to billion dimensional posterior distribution ~~in the image space~~ from noisy input data. At the core of NIFTy lies a set of powerful Gaussian Process (GP) models and accurate Variational Inference (VI) algorithms.



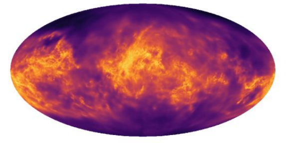
An improved map of the Galactic Faraday sky

N. Oppermann*[1], H. Junklewitz[1], G. Robbers[1], M.R. Bell[1], T.A. Enßlin[1], A. Bonafede[2], R. Braun[3], J.C. Brown[4], T.E. Clarke[5], I.J. Feain[3], B.M. Gaensler[6], A. Hammond[6], L. Harvey-Smith[3], G. Heald[7], M. Johnston-Hollitt[8], U. Klein[9], P.P. Kronberg[10,11], S.A. Mao[3,12], N.M. McClure-Griffiths[3], S.P. O'Sullivan[3], L. Pratley[8], T. Robishaw[13], S. Roy[14], D.H.F.M. Schnitzeler[3,15], C. Sotomayor-Beltran[16], J. Stevens[3], J.M. Stil[4], C. Sunstrum[4], A. Tanna[17], A.R. Taylor[4], and C.L. Van Eck[4]



Variable structures in M87* from space, time and frequency resolved interferometry

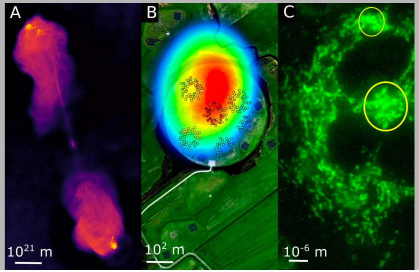
Philipp Arras[1,2], Philipp Frank[1,3], Philipp Haim[1], Jakob Knollmüller[1,2], Reimar Leike[1], Martin Reinecke[1], and Torsten Enßlin[1]



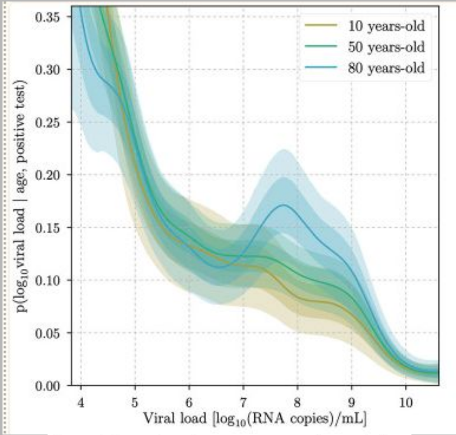
Resolving nearby dust clouds*

R. H. Leike[1,2], M. Glatzle[1,3], and T. A. Enßlin[1,2]

Astrophysics



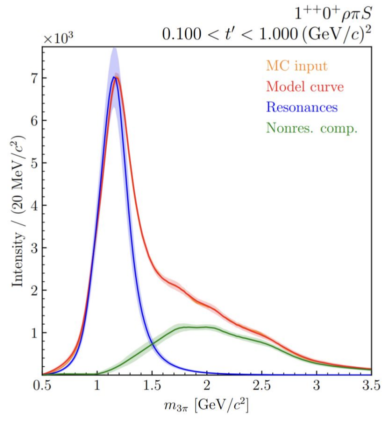
Radiation biology, radio astronomy and cosmic rays using information field theory



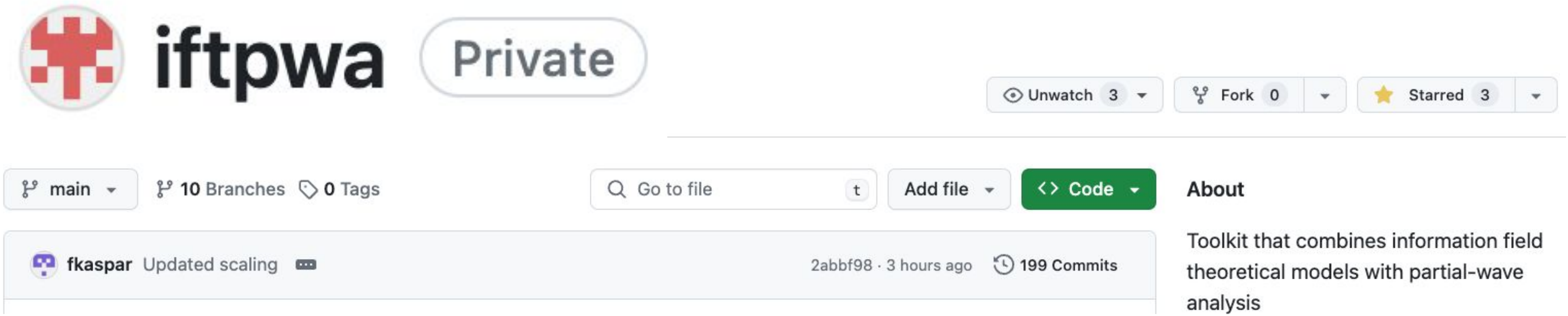
Causal, Bayesian, & non-parametric modeling of the SARS-CoV-2 viral load distribution vs. patient's age

Matteo Guardiani[1,2,*], Philipp Frank[1,2], Andrija Kostić[1,2], Gordian Edenhofer[1,2], Jakob Roth[1,2], Berit Uhlmann[4], Torsten Enßlin[1,2,3]

Biology



Hadron Physics?



- Application of **N**umerical **I**nformation **F**ield **T**heory (NIFTy)
  - Adapted by **COMPASS** **[Florian Kaspar, Stephen Paul, Stephen Wallner, ODSL, ...]** for Hadron Physics
    - **see below:** **EPJ Web Conf. 291 (2024), 02014**
  - **GlueX** exploring use case + contributing to project
- **Modular model building framework** mixing **parametric** (i.e. Breit-Wigner, K-matrices, ...) and **non-parametric** contributions (Gaussian Process)

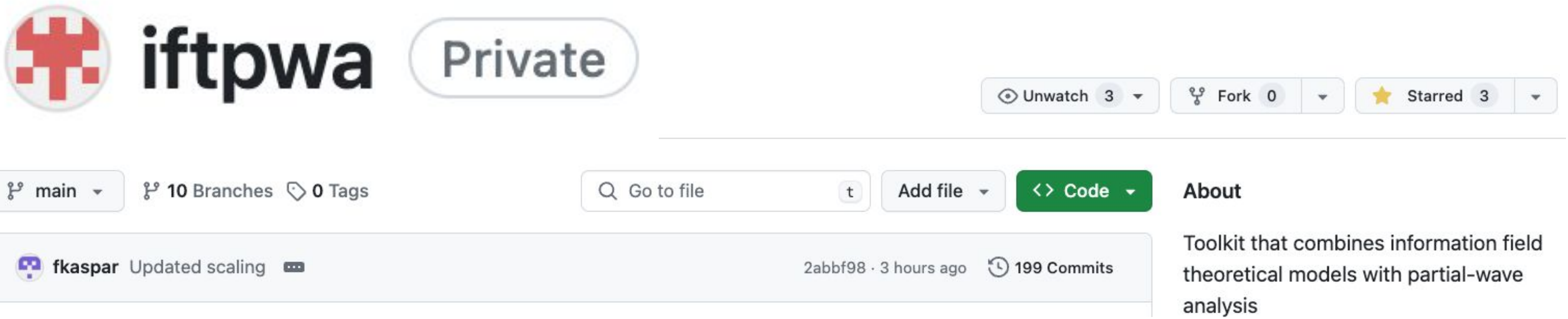
ep-ph] 6 Nov 2023

Progress in the Partial-Wave Analysis Methods at COMPASS

Florian Markus Kaspar[1,2,*], *Julien* Beckers[1,**], and *Jakob* Knollmüller[1,2,***]
for the COMPASS Collaboration

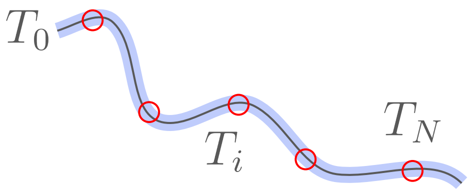
[1]Technische Universität München, Physik Department, James-Franck-Straße 1, 85748 Garching bei München
[2]Excellence Cluster Origins, Boltzmannstraße 2, 85748 Garching bei München

Abstract. We study the excitation spectrum of light and strange mesons in diffractive scattering. We identify different hadron resonances through partial



How does it work?

- Kinematically bin the data like typical Mass Indep. Fit $\rightarrow D_i$
- Each bin described by a set of partial wave amplitudes $\rightarrow T_i$
- `iftpwa` will model the Fields $\{T_0, .., T_N\}$ enforce smoothness across kinematics
    - increasing fit stability (ambiguities / numerical)



Mass bins
NIFTy Latent Posterior Model
Amplitudes at mass bin

Inference Problem

Bayes Theorem

NIFTy ***Posterior***

PWA
Likelihoods

Gaussian Process Prior
(More on this later)

$$P(X|D) \propto P(D|X;\Omega)\, P(X)$$

D = Data

Ω = KNOWN : Decay angular variables, etc

X = UNKNOWN : Dynamics (i.e. mass and -t)

Inference Problem

Bayes Theorem

Any other physics cases?
Please reach out!

NIFTy ***Posterior***

PWA
Likelihoods

Gaussian Process Prior

$$P(F(X)|D) \propto P(D|F(X);\Omega)\ P(F(X))$$

D = Data

Ω = KNOWN : Decay angular variables, etc

X = UNKNOWN : Dynamics (i.e. mass and -t)

F = Arbitrary non-linearity (i.e. thresholding high spin waves, ...)

Inference Problem
Bayes Theorem

NIFTy ***Posterior***

PWA
Likelihoods

Gaussian Process Prior

$$P(X|D) \propto P(D|X;\Omega)\,P(X)$$

Variationally approximated posterior
Allowing inference over large fields
(complex kinematically-binned amplitudes)

Gaussian Process Prior

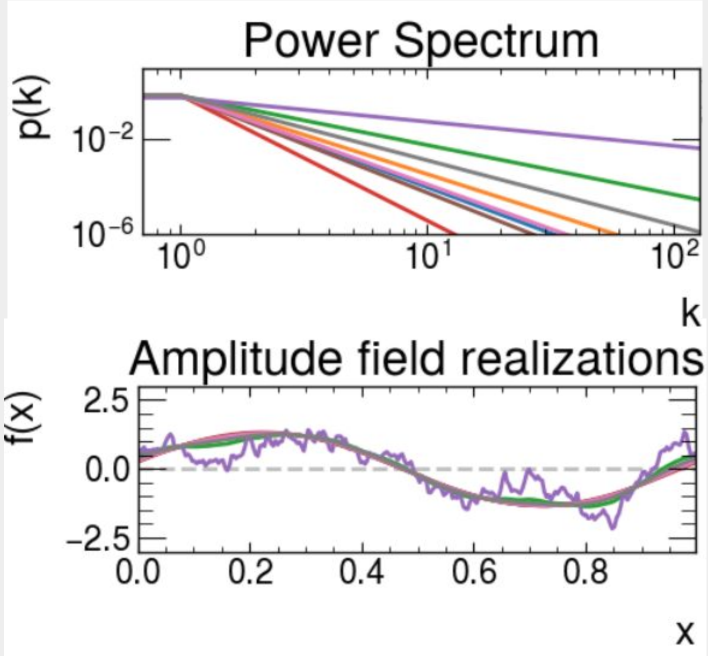
- **Kernels** are defined in **Fourier Space** whose parameters **(~5 of them)** are **Log-Normally Distributed**

Example:

Power spectrum slope parameter ~ LogNormal(-6, 3)

Draw 8 samples

[NIFTy Correlated Field Demo]



Other knobs:

Constant offsets

Deform spectrum beyond simple power law

YAML Configuration

Common/shared PWA framework?

```yaml
GENERAL:
    pwa_manager: GLUEX

# Parameters of partial-wave manager class -> t
PWA_MANAGER:
    cfgfiles: ???
    min_mass: ???
    ...

IFT_MODEL:
    scale: 18000 # Intensity ~ 1e-4 for scale =
    positiveScale: true
    useLogNormalPriorSlope: false
    loglogavgslope: [-4.0, 1.0] # (mean, std)
    ...

LIKELIHOOD:
    approximation: false # no not approximate
    metric_type: normazl #[[2, 'normal'], [18,
    ...

# Parameters of optimization procedure
OPTIMIZATION:
    nSamples: 50 # [[5, 0], [10, 5], [15, 10],
    nIterGlobal: 22
    algoOptKL: LBFGS
    ...
```

ROOTPWA Public

PyAmpTools Public

Define GP Prior Model

Likelihood approx.

Optimizer specs

+

Parametric model Cfg

```python
def etapi_a2a2p():

    m_a2_1320 = LogNormal(sigma=0.0013 * 30, mean=1.3186)
    w_a2_1320 = LogNormal(sigma=0.002 * 30, mean=0.105)

    m_a2_1700 = LogNormal(sigma=0.05, mean=1.700)
    w_a2_1700 = LogNormal(sigma=0.05, mean=0.300)

    resonances = {
        "a2_1320": {
            "name": "$a_2(1320)$",
            "fun": breitwigner_normed,
            "paras": {"mass": m_a2_1320, "width": w_a2_1320},
            "waves": [
                'reaction_000::NegIm::Dm2-',
                'reaction_000::NegIm::Dm1-',
            ],
        },
        "a2_1700": {
            "name": "$a_2(1700)$",
            "fun": breitwigner_normed,
            "preScale": 0.25,
            "paras": {"mass": m_a2_1700, "width": w_a2_1700},
            "waves": [
                'reaction_000::NegIm::Dm2-',
                'reaction_000::NegIm::Dm1-',
            ],
        },
    }

    smoothScales = False
    return resonances, smoothScales
```

Resonance parameter priors

Resonance specs as a dictionary

Input / Output Tests

Gaussian Process Prior

$$P(X|D) \propto P(D|X;\Omega)\, P(X)$$

$P(X)$ describes a distribution of potential functions

- Draw a sample from the prior
- Generate events with the sampled functional form of the amplitude
- Fit the events using
  1) Binned maximum likelihood
  2) ift framework

I/O Study 1

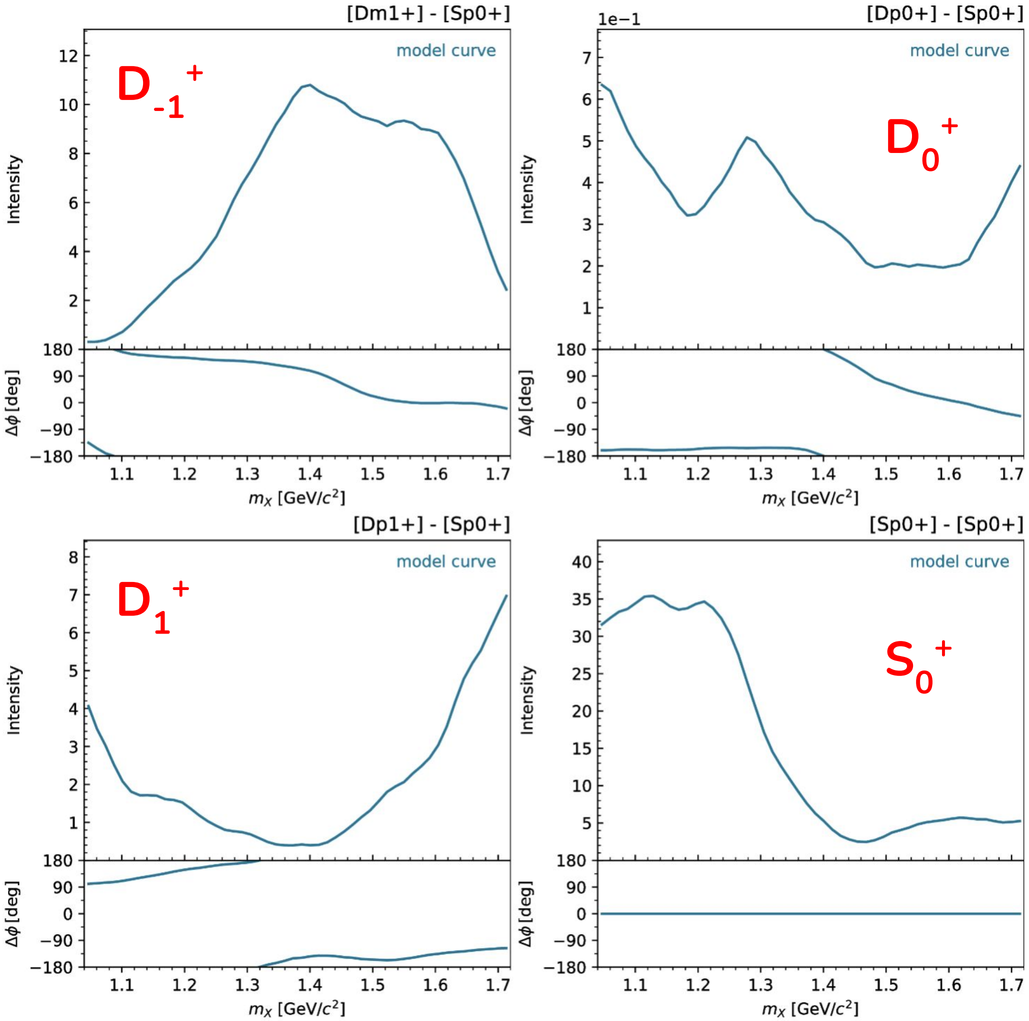
spin

reflectivity

l_m^{ε}

spin-projection

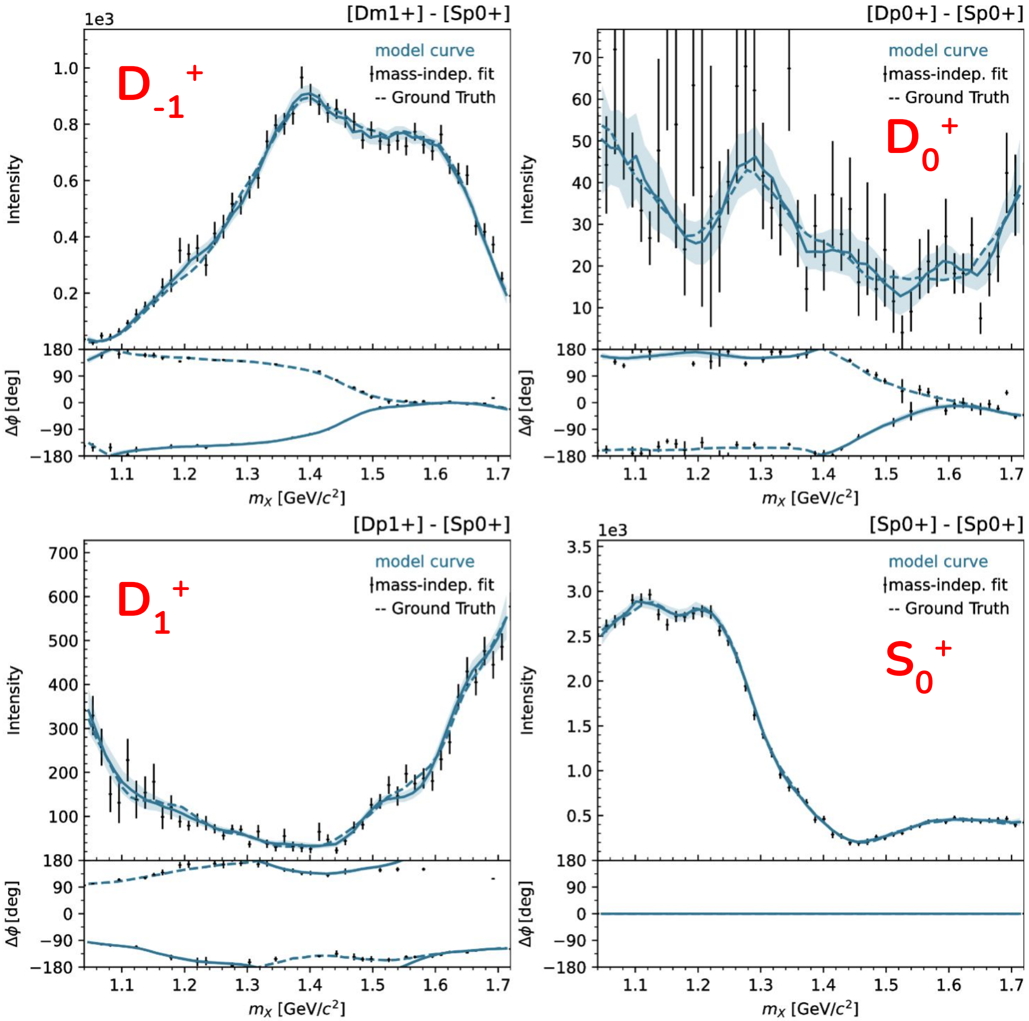
- Polarized photoproduction of two pseudoscalar : **$\gamma p \rightarrow \eta\pi^0 p \rightarrow 4\gamma p$**
  - Amplitudes described in:
    [V.Mathieu et.al. (JPAC), Phys.Rev.D 100 (2019) 5, 054017]
- **No physics, no resonances, arbitrary but smooth amplitudes**
- **Positive reflectivity Waveset: $D_{-1}^{+} D_{0}^{+} D_{1}^{+} S_{0}^{+}$**



Single Prior Sample

Intensity

ΔPhase



Dashed blue line := ground truth

Blue line := ift mean
Blue fill := ift standard deviation

Black error bars := Mass indep. fits

- Both methods perform well
- Binned fits have more scatter
- ift results:
  - captures truth within uncertainties
  - finds the trivial ambiguity

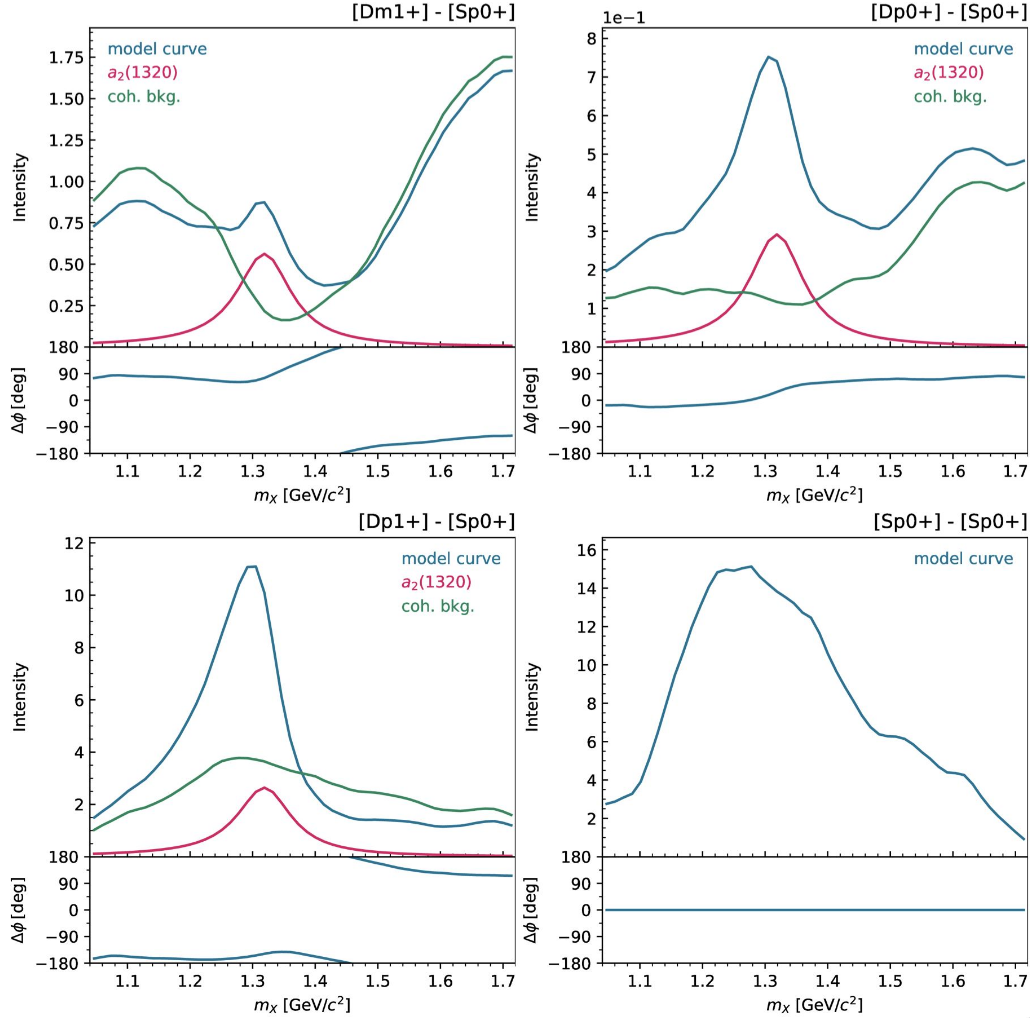
I/O Study 2

Same as Study 1 but with

a_2(1320) Breit-Wigner resonance

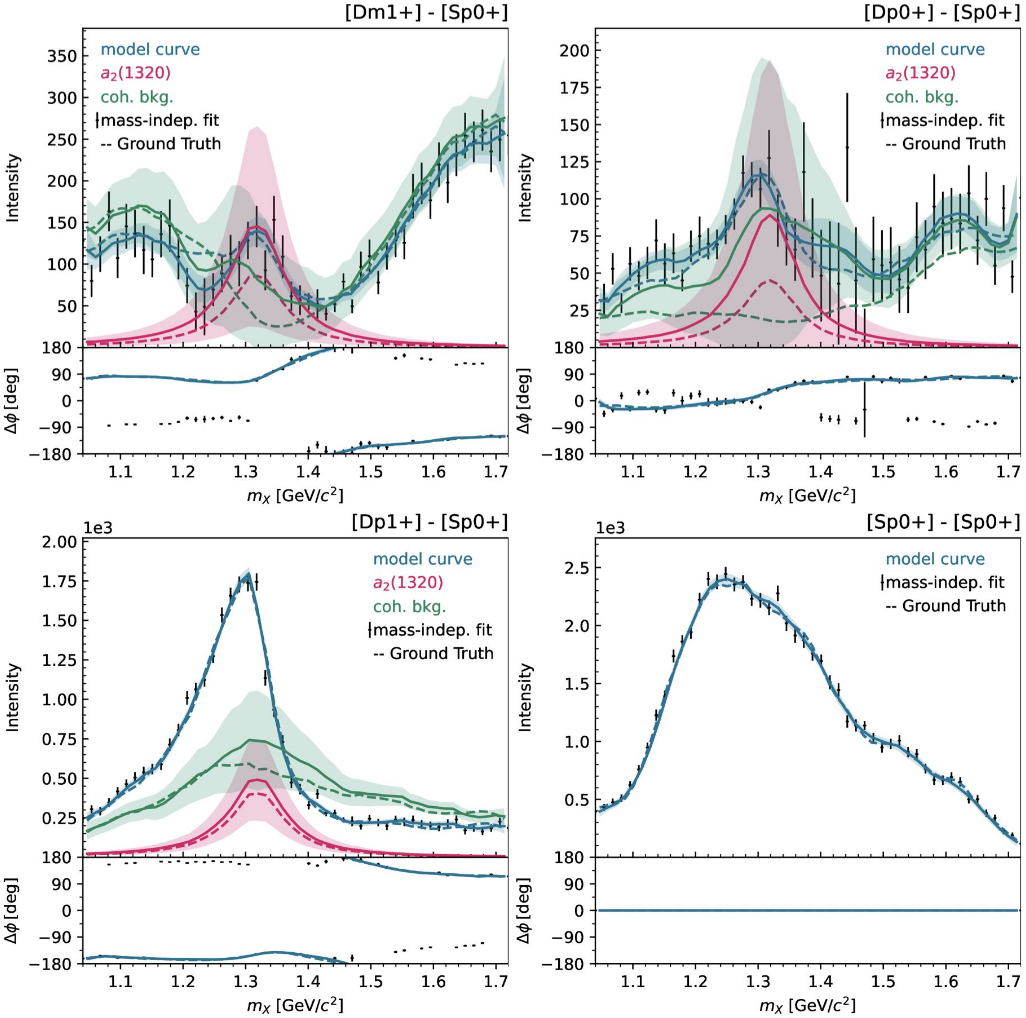
+

Coherent non-parametric background



Single Prior Sample

model curve
$a_2(1320)$
coh. bkg.



model curve

$a_2(1320)$

coh. bkg.

Individual components are mostly recovered (within uncertainties)

Recap | Bayesian Approach:

Self-consistent Model Generation / Fitting

Easily generate models with complex (but also interpretable) dynamics

Fit data under assumption that the data could ≈ be one of these complex models

GlueX Data:
$\gamma p \rightarrow \eta\pi^0 p \rightarrow 4\gamma p$

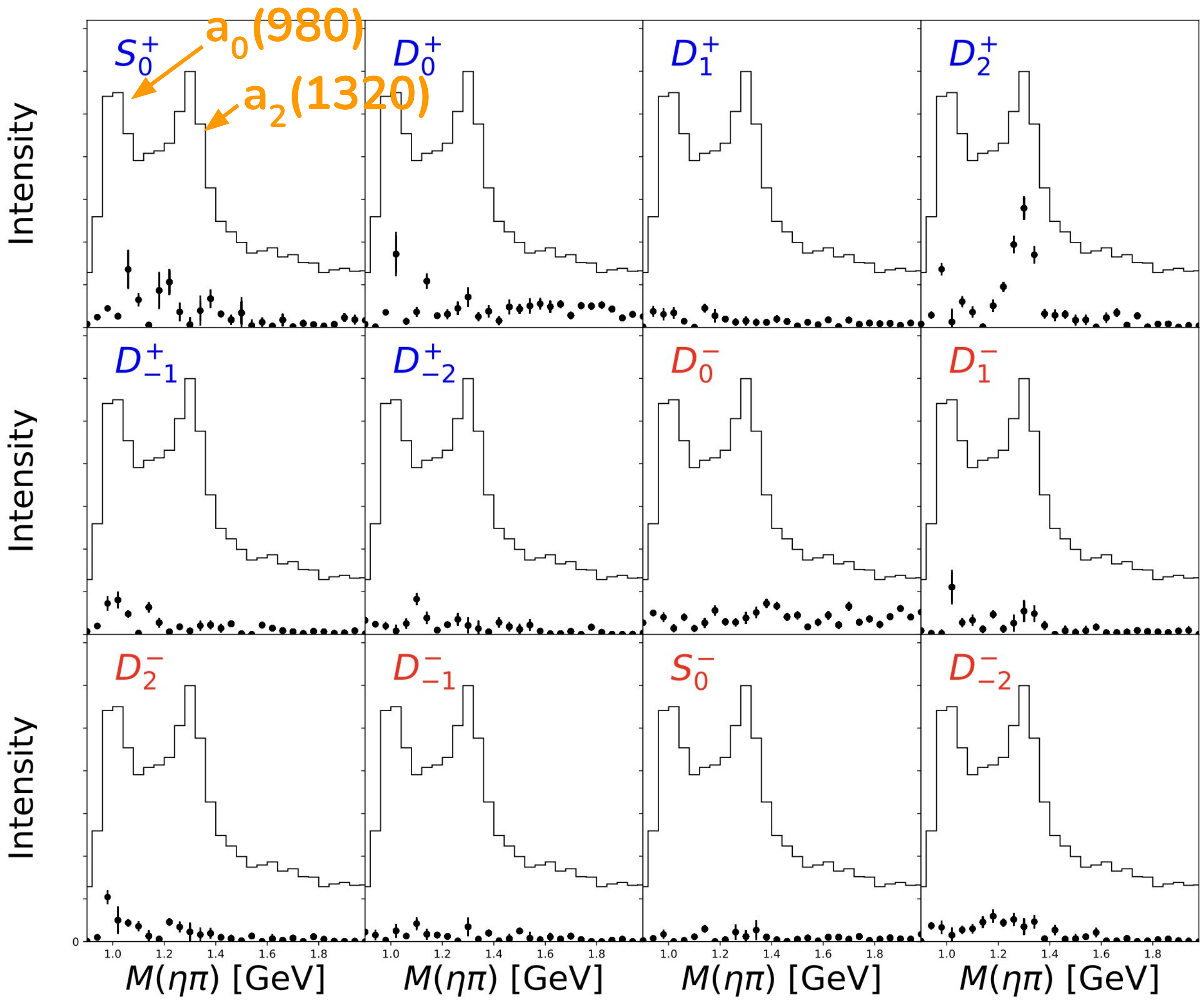
$0.88 < M(\eta\pi) < 2.0$ GeV
$0.1 < -t < 0.2$ GeV^2
GlueX Phase-I **Data** in coherent peak
All S, D waves (both reflectivities)

More Information: Refer to Malte's talk on Tuesday:
Search for Exotic Hadrons in ηπ and η'π at GlueX

Much more complex fit!

Run `ift` analysis with:

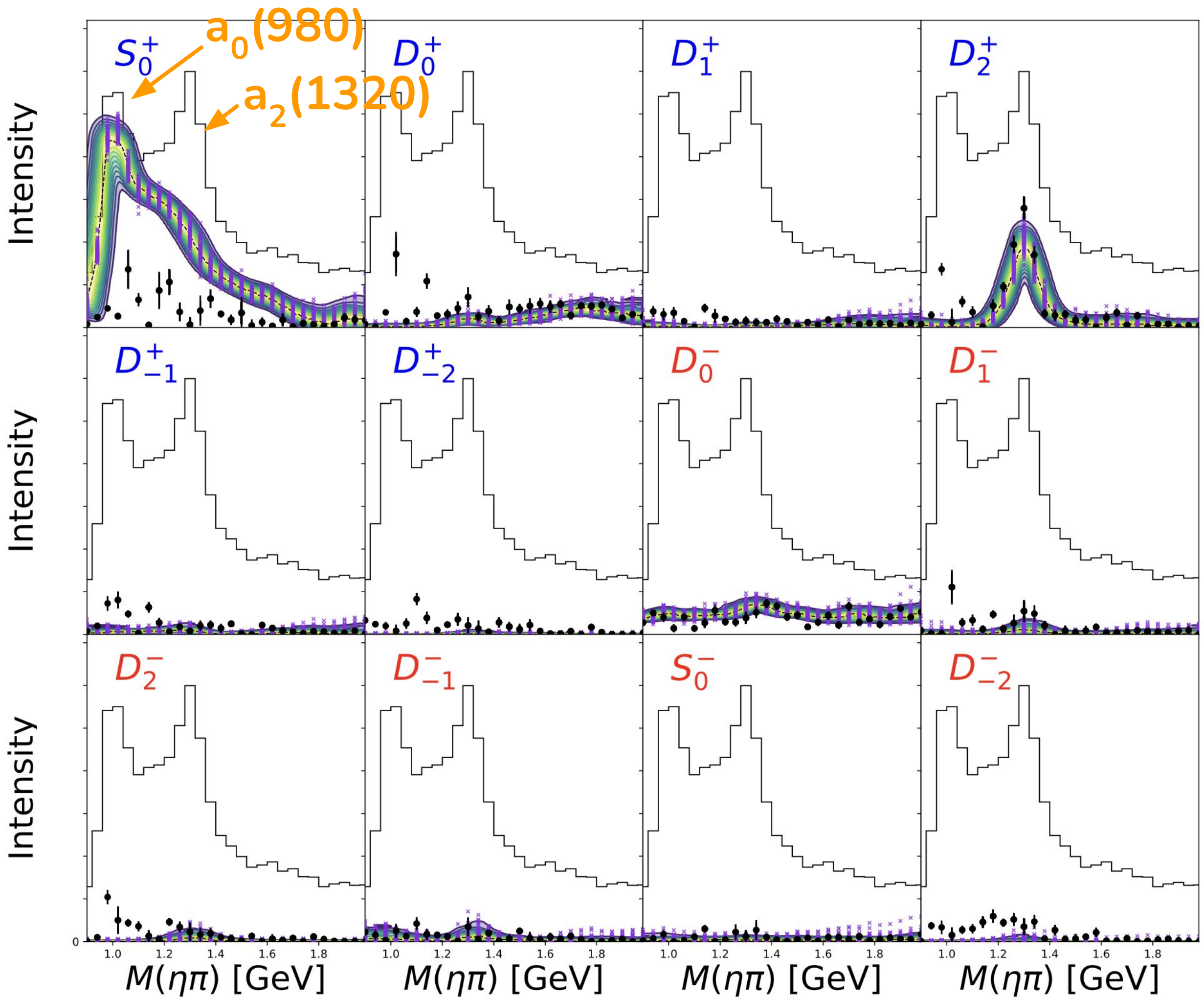
- Breit-Wigner for $a_2(1320)$ and **$a_2(1700)$**
- Coherent Gaussian Process background



GlueX Data: $\gamma p \rightarrow \eta\pi^0 p \rightarrow 4\gamma p$

ɸ : Best / 20 MLE mass-indep fits with random starting parameters

Massive leakage out of the S-wave!



GlueX Data: $\gamma p \rightarrow \eta\pi^0 p \rightarrow 4\gamma p$

ɸ : Best / 20 MLE mass-indep fits with random starting parameters

x : IFT posterior samples

Contours are from a density estimate of x

Conclusion

- `iftpwa` is a model building framework allowing mixing of **parametric** and **non-parametric** components

Florian's end of summer plan? (No guarantees of course!)

- **Publication** on the method
- **Release** of the framework

GlueX Acknowledgements:
http://gluex.org/thanks.html

Backup

Gaussian Process Prior

Power Spectrum

Gaussian Excitation Field

Position (amplitude space) offset

```
GP = HT( A * zero_mode * xi ) + offset
```

Harmonic Transform
Frequency → Position (Amplitude) Space

Power Field Offset

Prior distributions defined by some set of hyperparameters

About 8 of them

Can generate **arbitrarily complex dynamics** with **arbitrary levels of interference** for I/O studies!

IF

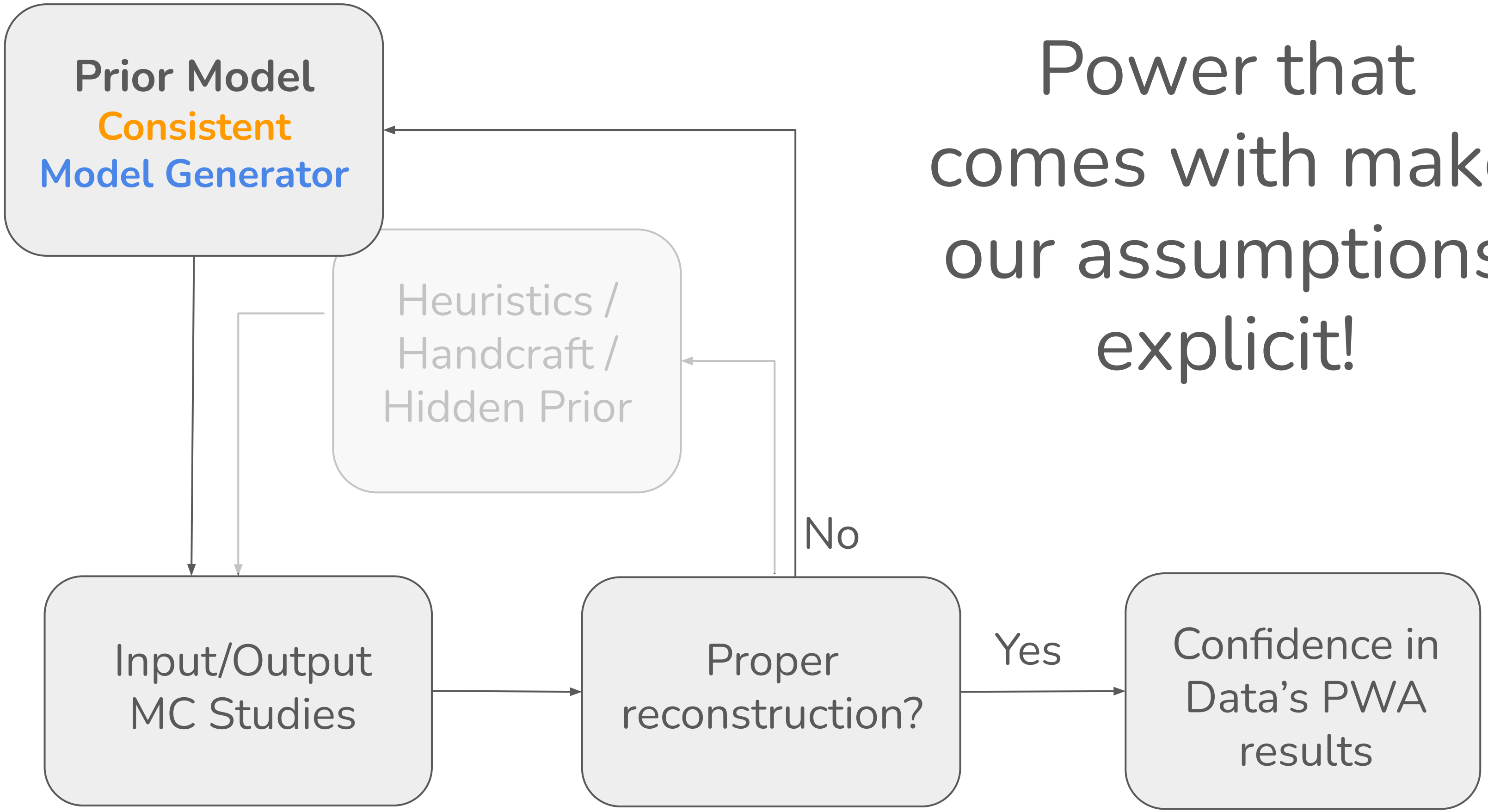
ensemble of I/O studies successfully recovers input

IF

we believe Prior can describe the Data

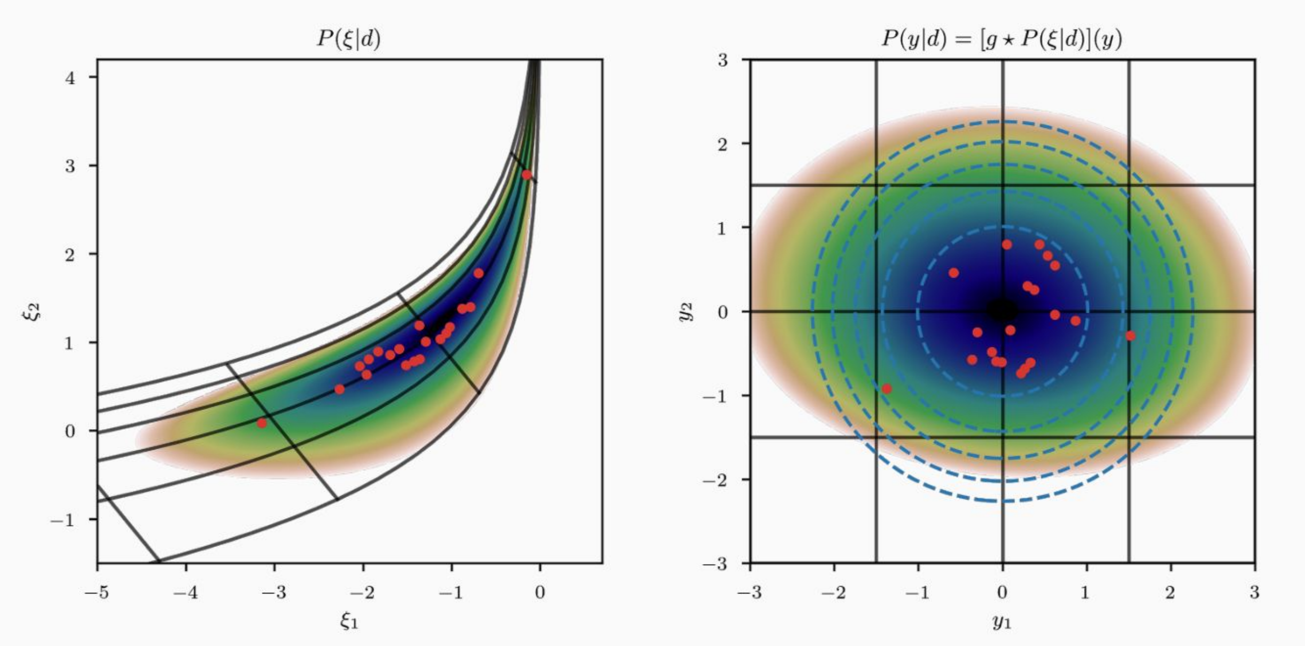
THEN

High confidence in Data’s PWA results



Power that comes with make our assumptions explicit!

Geometric Variational Inference (geoVI) [?]



From Phillip Frank's backup slides on GeoVI

Information Hamiltonian $\mathcal{H}(\xi|d)$:	$-\log(\mathcal{P}(\xi|d))$
Posterior metric $\mathcal{M}(\xi)$:	$\mathcal{M}_{\mathrm{lh}}(\xi) + \mathbb{1}$
Fisher information metric $\mathcal{M}_{\mathrm{lh}}(\xi)$:	$\left\langle \frac{\partial^2 \mathcal{H}(d|\xi)}{\partial \xi \partial \xi'} \right\rangle_{\mathcal{P}(d|\xi)}$

Ecosystem?

Top 6 by ⭐ Starred

awkward Public
Manipulate JSON-like data with NumPy-like idioms.
Python · ☆ 797 · BSD-3-Clause · 80 · 100 (5 issues need help) · 13 · Updated 2 days ago

iminuit Public
Jupyter-friendly Python interface for C++ MINUIT2
Python · ☆ 273 · 70 · 14 · 0 · Updated 2 days ago

pyhf Public
pure-Python HistFactory implementation with tensors and autodiff
Python · ☆ 273 · Apache-2.0 · 78 · 385 (27 issues need help) · 39 · Updated 3 days ago

uproot5 Public
ROOT I/O in pure Python and NumPy.
Python · ☆ 221 · BSD-3-Clause · 67 · 44 · 6 · Updated 2 days ago

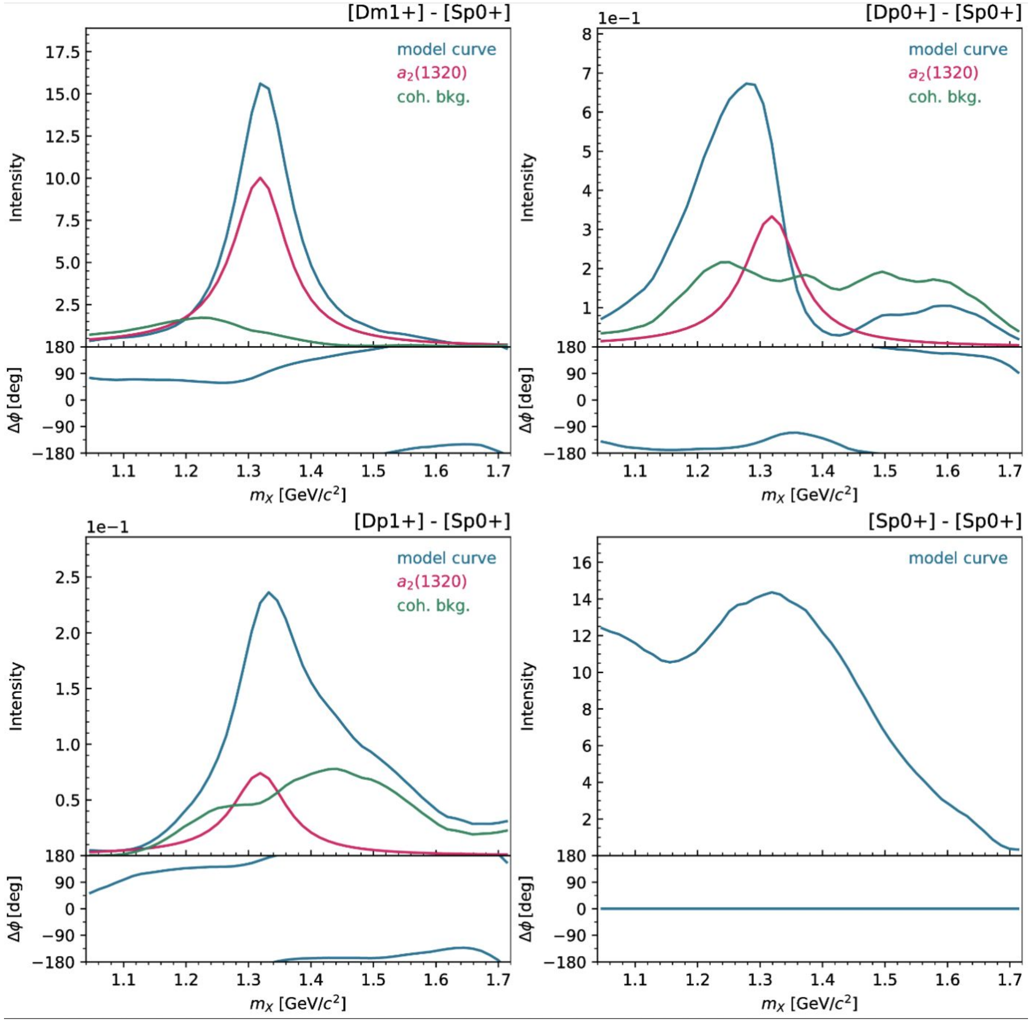
mplhep Public
Extended histogram plotting on top of matplotlib and HEP collaboration compatible styling
Python · ☆ 177 · MIT · 60 · 23 (1 issue needs help) · 4 · Updated last week

particle Public
Package to deal with particles, the PDG particle data table, PDGIDs, etc.
Python · ☆ 145 · BSD-3-Clause · 23 · 8 · 1 · Updated last week

Scikit HEP

scikit-hep

Overview | Repositories 46

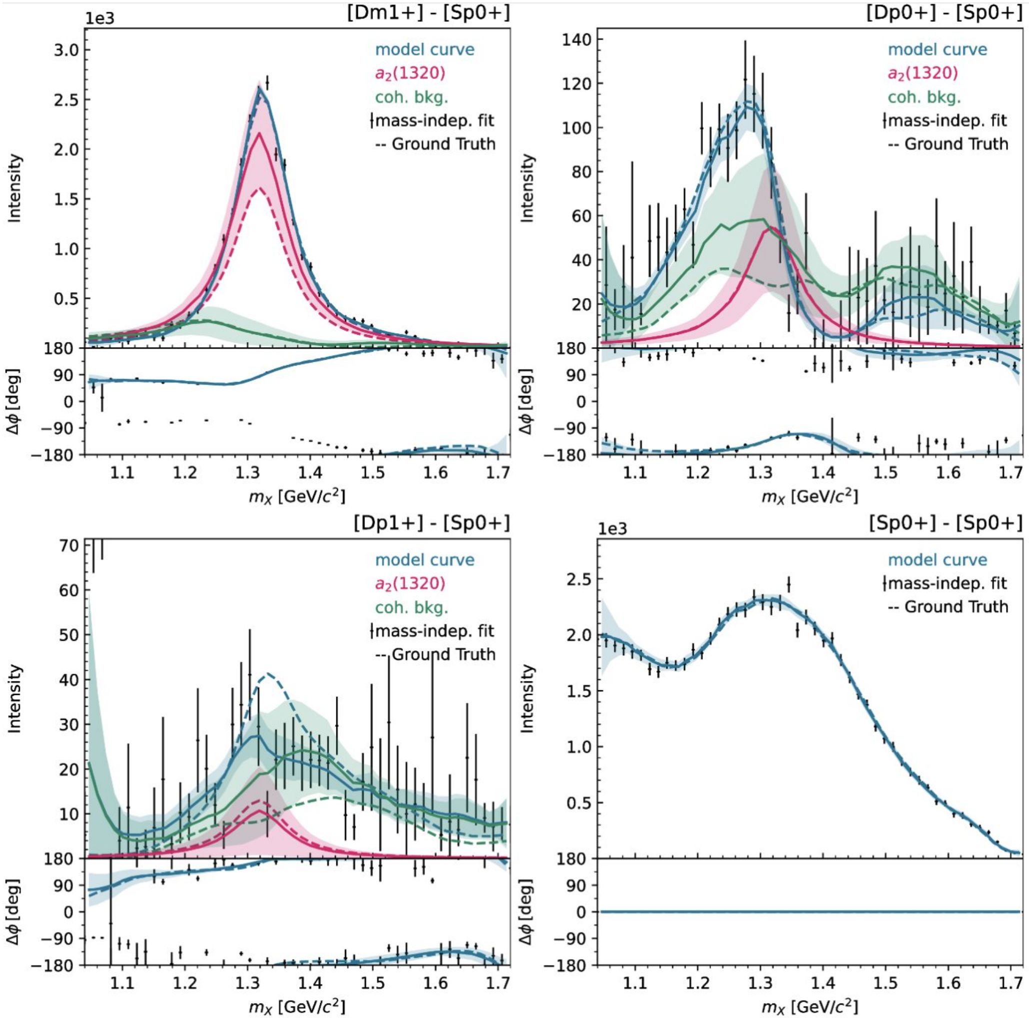


Single Prior Sample

model curve

$a_2(1320)$

coh. bkg.



model curve
$a_2(1320)$
coh. bkg.

Individual components are mostly recovered (within uncertainties)