

Amplitude Analysis Tools at BESIII

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Outline

- Introduction
- Designs of PWA library
- TF-PWA
- Automatic Differentiation and its application in TFPWA.
- Performances of TF-PWA.
- Current development
- Summary

Introduction

- Amplitude analysis / Partial wave analysis (PWA) is a powerful method to study multi-body decay processes, e.g.
 - to search for (exotic) resonances and measure their properties
 - to understand CP violation over phase space
- Most of previous fitters are designed for special processes or are time-consuming.
- A general PWA framework using modern acceleration technology (such as GPU, AD, ...) is eagerly needed.



Main tools in BESIII

- Closed source / hand coded
 - Tensor formulism: most of charm decays. $[D^+ \rightarrow K_S^0 \pi^+ \pi^0 \pi^0: \underline{2305.15879}]$
 - Helicity formulism: $[e^+e^- \rightarrow \omega \pi^+\pi^-: \underline{2303.09718}]$
- <u>GPUPWA</u>:
 - First PWA tools use GPU.
 - Used in most of partial wave analysis.
 - $[J/\psi \to \gamma \eta \eta: \underline{\text{PRD.87.092009(2013)}}, J/\psi \to \gamma \eta \eta': \underline{\text{PRD.106.072012(2022)}}$
- <u>FDC-PWA</u>:
 - Use Feynman Diagram Calculation.
 - Used in some baryon decay.
 - $[\psi' \to p\bar{p}\eta: \underline{\text{PRD.88.032010(2013)}}, e^+e^- \to pK^-\bar{\Lambda}: \underline{2303.01989}]$
- <u>TF-PWA</u>:
 - Main topics in this talk
 - $[\Lambda_c^+ \rightarrow \Lambda \pi^+ \pi^0 : \underline{\text{JHEP12}(2022)033}]$
- Other tools:
 - <u>Amptools</u>: Some charmonium. $[\chi_{c1} \rightarrow \eta \pi^+ \pi^-: \underline{\text{PRD.95.032002(2017)}}]$
 - <u>PAWIAN</u>: $[J/\psi \rightarrow \phi \eta \eta: 10.13154/294-6468]$
 - ComPWA: $[D^0 \to K_S K^+ K^-: 2006.02800]$

Properties and Requirement of PWA

- Complex Formula
 - Avoid hand written code, automatic.
 - Rule based amplitude evaluation.
 - Constraints in special process.
- Multiple Dimension.
 - Study relation between many variables: masses and angles.
 - Proper way to consider resolution. (see backup)
 - Large size of MC for integration to normalize the PDF.
- Large size of data (e.g., 10B J/ψ in BESIII)
 - Fast calculation to reduce time cost.
 - Distribute the calculation into multi devices.

Configurable

High performance calculation.

Configuration

- Why Configurable?
 - Global representation for automation and transferability.
 - General way to support more decays
- Difference level
 - No configuration:
 - Hand coded / code templates
 - Decay Card like:
 - Key-value / command-parameters / structured .
 - Specify all possible decays (interactions).
 - With addition simplification rules.
 - Auto search:
 - Provide a large particles dataset.
 - Use rules to find all possible intermediate states.
 - Filter with requirement.



Symbolic and numeric approaches

- Symbolic approach
 - Requires a Computer Algebra System (CAS) to simplify formulas.
 - Write/generate code from CAS outputs
 - Procedure:
 - configuration -> CAS -> formula -> generated code -> function -> amplitude
 - Simplify the formula is difficult and time-consuming.
- Numeric approach
 - Combine Function directly,
 - Rule based evaluation
 - Procedure:
 - configuration -> function call -> amplitude
 - Without simplified formula, more computation might required
 - Allow caching rule to reduce computation

<u>FDC-PWA</u> series (REDUCE) <u>ComPWA</u> series (SymPy)

AmpGen
GPUPWASelf hold
tensor library

<u>TF-PWA</u> <u>PAWIAN</u> <u>TensorFlowAnalysis</u>

TFPWA

TF-PWA: Partial Wave Analysis with TensorFlow

• Fast

• General

• Easy to use

- GPU based
- Vectorized calculation
- Automatic differentiation Quasi-Newton Method: scipy.optimize
- Custom model available
- Simple configuration file (example provided)
- Most of the processing is automatic
- All necessary functions implemented
- Developing more functions
- Open access and well supported

https://github.com/jiangyi15/tf-pwa



Configuration as global representation



Configuration

- What is needed?
 - Particles (Resonances, line) and their properties
 - Decays (interaction, vetex) and their properties
- Possible process in this Λ_c decay $\Lambda_c^+ \to \Lambda \pi^+ \pi^0$







Automatically calculated from decay structure

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Factor system: automatic factorization of amplitude

• Amplitude can be written as the combination of summation and production.

$$A = (\sum g_i A_i) (\sum g'_j A'_j) \dots \Rightarrow A = \sum_{ij} (g_i g'_j) (A_i A'_j)$$
$$G_{(i,j)} = g_i g'_j = \begin{cases} 1 & i, j = (a, b) \\ 0 & i, j \neq (a, b) \end{cases} \Rightarrow A = B_{(i,j)} = A_i A'_j$$

- No need known for the exact formula A_i , just use the parameters g_i .
- Some special treatment is implemented as option for better performances. (comparing in Page 21)
 - Amplitude caching method Allow fit parameters related
 - mass dependent:

$$A(p_i^{\mu}) = \sum g_i R(m) A_i(p_i^{\mu}) \Rightarrow A(m) = \sum g_i R(m) B_i$$

- factor only: (only for MC integration)
 - $\sum |A|^2 \to G_i G_j^* (\sum C_{ij})$ calculate only once

Add control options, the processes are automatics.

- Required all shape parameters fixed
- Special in simultaneous fit
 - Mixed likelihood, avoid small size data

$$-\ln L_1 - \ln L_1 = -\sum_{data1+data2} \ln |A|^2 + N_1 \ln \sum_{mc1} |A|^2 + N_2 \ln \sum_{mc2} |A|^2$$



 \vec{p}_{B}^{A} means momentum of B in the rest frame of A ϕ means the rotation is anticlockwise, while $-\phi$ for clockwise The sign Is dependent on data



TF-PWA also provide reverse process: Mass + helicity angle \rightarrow 4-monmenta

Amplitude as a function

- Reverse process of angle calculation
 - Mass + Helicity angle -> 4- momenta

•
$$(m_0, \phi_0, \theta_0, m_{12}, \phi_{12}, \theta_{12}) \xrightarrow{\text{transform}} p_1^{\mu}, p_2^{\mu}, p_3^{\mu}$$

- Factor system:
 - Eval amplitude of special partial wave though control of parameters
 - $A(p_1^{\mu}, p_2^{\mu}, p_3^{\mu}) \xrightarrow{g_{i\neq j}=0} g_i A_i(p_1^{\mu}, p_2^{\mu}, p_3^{\mu})$
- Combine Together: Lineshape function of special wave
 - Set angle to 0, $D_{m,m'}(0,0,0) = \delta_{m,m'}$ is constant.
 - Vary mass, then get the shape of masses
 - $f(m_{12}) = g_i A_i (m_0, \phi_0 = 0, \theta_0 = 0, m_{12}, m_{12}, \phi_{12} = 0, \theta_{12} = 0)$
 - No worries for the complex formula
- 2D function of amplitude
 - 2D plot Dalitz variables
 - 2D plot of Mass and $\cos \theta$

f1 = config.get_particle_function("R1")
f2 = config.get_particle_function("R2")
m = f1.mass_linspace(1000)
plot the first wave
amp = tf.abs(f1(m)[:,0] + f2(m)[:,0])**2
plt.plot(m, amp)

Uncertainties from error propagation



Automatic Differentiation(AD)

- Widely used in Optimize problem
 - Calculate gradient automatically
 - No need for exact formula.
 - Recorded the compute graphs.
 - Operator: used function (sin, g)
 - Intermediate value: (z= 1¹)
 - Mostly matrix form (Jacobian).
 - Just combine the operator (Chain Rules)

Chain Rules

• X:
$$\frac{\partial f(g(x))}{\partial x_i} = \frac{df}{dg} \times \frac{\partial g}{\partial x_i}$$

• +: $\frac{\partial f(h(x), g(x))}{\partial x_i} = \frac{\partial f}{\partial h} \frac{\partial h}{\partial x_i} + \frac{\partial f}{\partial g} \frac{\partial g}{\partial x_i}$

The same rule based way for our amplitude calculation.





AD in amplitude fit

- Minimize of $-\ln L(\vartheta)$
 - $-\frac{\partial \ln L}{\partial \vartheta}$ is the steepest descent direction, used by most of optimizer
 - Error matrix $V_{ij} = \left[-\frac{\partial^2 \ln L}{\partial \vartheta_i \partial \vartheta_j} \right]^{-1}$ can also be estimated though AD
 - AD advantage:
 - Automatic.
 - Fast estimation: Time cost for eval $-\ln L(\vartheta)$ and $-\frac{\partial \ln L}{\partial \vartheta}$ are on the same level.
 - Accurate gradient: more stable results.
 - AD disadvantage:
 - Require well defined gradients (continuous).
 - Avoid step function, delta function.
 - Only support function with predefined gradients.
 - Use TensorFlow only, but also have an interface to define functions.
 - Large (GPU) memory cost for recording intermediate values.
 - Split data into small batches (discuss later).

AD for error propagation

- Error propagation
 - $\sigma_y^2 = \frac{\partial y}{\partial x} \sigma_x^2 \frac{\partial y}{\partial x}$, $\frac{\partial y}{\partial x}$ can be calculated by AD
 - Simple interface (see right)
 - Example: uncertainties of fit fractions in TF-PWA
- Advance usage
 - Define function with gradient
 - AD + some part of numerical function
 - $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial g} \frac{\partial g}{\partial h} \frac{\partial h}{\partial x}$, numerical: $\frac{\partial g}{\partial x} = \frac{g(x + \Delta x) g(x \Delta x)}{2\Delta x}$
 - Example: Solve pole mass in TF-PWA (a iteration process)
 - Systematic of fixed parameters (fixed mass and width)
 - $-\ln L = -\ln L(\vartheta, z)$, ϑ : fit parameters, *z*: fixed parameters
 - Minimum condition as implicit function

•
$$-\frac{\partial \ln L}{\partial \vartheta} = 0 \Rightarrow \frac{\partial \vartheta_i}{\partial z} = -\left[\frac{\partial^2 \ln L}{\partial \vartheta_i \partial \vartheta_j}\right]^{-1} \frac{\partial^2 \ln L}{\partial \vartheta_j \partial z}$$

with config.params_trans() as pt: # g1 is fixed to 1 g2_r = pt["Lmdc->piz.Sigma(1385)p_g_ls_1r"] g2_phi = pt["Lmdc->piz.Sigma(1385)p_g_ls_1i"] alpha = 2*g2_r*tf.cos(g2_phi) / (1+g2_r*g2_r) print(alpha, pt.get_error(alpha))



AD in Large size of data

- Basic Log-Likelihood function
 - $\ln L(\vartheta) = \sum \ln \left[(1 f_2) \frac{P_1(x;\vartheta)}{\int P_1(x;\vartheta) dx} + f_2 \frac{P_2(x;\vartheta)}{\int P_2(x;\vartheta) dx} \right]$
 - $I_i = \int P_i(x) dx \approx \sum \omega_j P_i(x_j)$
 - Required recording all $P_i(x_j)$ and intermediate values before gradients evaluations.
- Split large data into small batches (only record value of a small batch)

•
$$\ln L(\vartheta) \Rightarrow \ln L(\vartheta; I_i)$$

• $\frac{\partial \ln L(\vartheta)}{\partial \vartheta} \Rightarrow \frac{\partial \ln L(\vartheta; I_i)}{\partial \vartheta} + \sum_i \frac{\partial \ln L(\vartheta; I_i)}{\partial I_i} \frac{\partial I_i}{\partial \vartheta}$
• $\frac{\partial I_i}{\partial \vartheta} = \frac{\partial [\sum \omega_j P_i(x_j)]}{\partial \vartheta} + \frac{\partial [\sum \omega_j P_i(x_j)]}{\partial \vartheta} + \cdots$
Batch 1 Batch 2

• Expand the power of AD to multi GPU, even multi cluster

Base fit results

- $\Lambda_c^+ \to \Lambda(\to p\pi^-)\pi^+\pi^0$
 - Simultaneous fit
 - 7 energy points
 - Total around 10k events, 854k MC
 - 38 free parameters
 - Dominated by $\Lambda_c^+ \rightarrow \Lambda \rho$: 57.2 ± 4.2%
 - Clear peak for $\Lambda_c^+ \to \pi \Sigma(1385)$

Plot thought TF-PWA with simple config.yml All decay chain will add automatic





Real analysis performance

Environment: NVIDIA RTX 3080 TensorFlow 2.2 CUDA 10.1

- Optimized method in Factor System page
 - Caching method (in <u>Page 14</u>)
 - Large time for caching
 - required more memory
 - limited to special cases
 - All the process is automatic (from config.yml to all basic results)



Implement of Covariant tensor formula

- Covariant tensor formula
 - Covariant orbital-spin scheme for any spin based on irreducible tensor
 - Traditional covariant tensor formula Eur. Phys. J. A 16 537-547(2003) Zou, Hugg
- Include some symbolic method for automation.
- Angular distribution consist in simple cases.
 - $0^- \to R_1(1^+)0^-, R_1(1^+) \to R_2(1^-)0^-, R_2(1^-) \to 0^-0^-$
- Preliminary implement, working in process.

Fluctuations due to MC sample size



arxiv:2301.01575

Summary

- BESIII have already used many tools.
- TF-PWA
 - Convenient configuration, general proposed
 - Automatic for all procedure though numeric approach.
 - Use powerful AD in fitting and error propagation.
 - Achieve high performance
 - Developing more functions

Thank you for your attentions!

Backup

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Formula of Resolution

- Detector: Combine effect of resolution and efficiency
- An event x was detected as y with probability
 - $p(x \to y) = \epsilon_x(x) R_x(x \to y)$
- The real probability of y: $p(y) = \int |A|^2(x)p(x \to y)dx$

$$\epsilon_{y}(y) = \int \epsilon_{x}(x)R_{x}(x \to y)dx, R_{y}(x \to y) = \frac{p(x \to y)}{\epsilon_{y}(y)}$$
$$p(y) = \int |A|^{2}(x)p(x \to y)dx = \epsilon_{y}(y)\int |A|^{2}(x)R_{y}(x \to y)dx$$

- $\epsilon_y(y)$ can be obtained by Phase Space MC. The distribution of reconstructed variables
- $R_y(x \rightarrow y)$ in normalize probability function that y from all possible x.
- Use $R_y(x \to y)$ to do the convolution,
 - Use phase space MC for flat x, then $R_y(x \to y)$ is the projection of p(x, y) with fixed y
 - Normalized $\int R_y(x \to y) dx = 1$.
- Use MC truth to do the integration
 - $\int |A|^2(x) \int \epsilon_y(y) R_y(x \to y) dy dx = \int |A|^2(x) \epsilon_x(x) dx.$

Alignment angle

Boost: $B_z(\omega)$, Rotation: $R_z(\phi)$, $R_y(\theta)$

For final state $|out\rangle = |p_1\rangle \otimes |p_2\rangle \otimes |p_3\rangle$, choose a single particle state $|p_1\rangle$. The final state define in $0 \rightarrow R, 2; R \rightarrow 1, 3$:

$$|p_1\rangle_R = B_z(\omega_1)R_z(0)R_y(\theta_1)R_z(\phi_1)|p_1\rangle = L_1|p_1\rangle$$

$$|p_1\rangle_1 = B_z(\omega_2)R_z(0)R_y(\theta_2)R_z(\phi_2)|p_1\rangle = L_2|p_1\rangle_R$$

On the other decay chain $0 \rightarrow R'$, 3; $R' \rightarrow 1$, 2:

$$|p_1\rangle_{R'} = B_z(\omega_1')R_z(0)R_y(\theta_1')R_z(\phi_1')|p_1\rangle = L_1'|p_1\rangle$$

$$|p_1\rangle_2 = B_z(\omega_2')R_z(0)R_y(\theta_2')R_z(\phi_2')|p_1\rangle = L_2'|p_1\rangle_{R'}$$

The alignment angle is the rotation

$$|p_1\rangle_2 = L_r |p_1\rangle_1 = B_z(\omega)R_z(\gamma)R_y(\beta)R_z(\alpha)|p_1\rangle_1$$

So

$$L_{r} = B_{z}(\omega)R_{z}(\gamma)R_{y}(\beta)R_{z}(\alpha) = L_{2}'L_{1}'L_{1}^{-1}L_{2}^{-1}$$

In general

$$L_r = L_a L_b^{-1} = \left(\prod_i L_{n-i}'\right) \left(\prod_j L_j^{-1}\right)$$



choose SU(2) representation as

$$\omega = \operatorname{arccosh} \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad B_z(\omega) = \begin{pmatrix} e^{-\frac{\omega}{2}} & 0\\ 0 & e^{\frac{\omega}{2}} \end{pmatrix}, R_z(\phi) = \begin{pmatrix} e^{-\frac{i\phi}{2}} & 0\\ 0 & e^{\frac{i\phi}{2}} \end{pmatrix}, R_y(\theta) = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2}\\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}$$

$$L_{ab} = B_z(\omega)R_z(\gamma)R_y(\beta)R_z(\alpha) = \begin{pmatrix} e^{-\frac{\omega}{2}}\cos\frac{\beta}{2}e^{-\frac{i(\alpha+\gamma)}{2}} & -e^{-\frac{\omega}{2}}\sin\frac{\beta}{2}e^{\frac{i(\alpha-\gamma)}{2}} \\ e^{\frac{\omega}{2}}\sin\frac{\beta}{2}e^{-\frac{i(\alpha-\gamma)}{2}} & e^{\frac{\omega}{2}}\cos\frac{\beta}{2}e^{\frac{i(\alpha+\gamma)}{2}} \end{pmatrix}$$

$$\cos \beta = \cos^2 \frac{\beta}{2} - \sin^2 \frac{\beta}{2} = L_{11}L_{22} + L_{12}L_{21}, \beta \in [0, \pi]$$

$$\omega = \ln \left| \frac{L_{22}}{L_{11}} \right|$$

$$\alpha + \gamma = -2 \arg L_{11} = 2 \arg L_{22}, \alpha - \gamma = -2 \arg L_{12} = -2 \arg L_{21}$$

$$|L_{ab}| = 1$$
 $L_{ab}^{-1} = \begin{pmatrix} L_{22} & -L_{12} \\ -L_{21} & L_{11} \end{pmatrix}$

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Custom Model

Line: R(M; a) = M + a

from tf_pwa.amp import register_particle
from tf_pwa.amp import Particle

```
@register_particle("Line")
class LineModel(Particle):
```

```
def init_params(self): # define parameters
    self.a = self.add_var("a")
```

```
def get_amp(self, *args, **kwargs):
    """ model as m + a """
    m = args[0]["m"]
    zeros = tf.zeros_like(m)
    return tf.complex(m + self.a(), zeros)
```

Use register_particle to register it, then it can be used in config.yml

$$\begin{split} H_{[\lambda_R\lambda_B]}(x;\vartheta) D^{j_A\star}_{[\lambda_A,\lambda_R-\lambda_B]}(x) R(x;\vartheta) H_{[\lambda_C,\lambda_D]}(x;\vartheta) D^{j_R\star}_{[\lambda_R,\lambda_C-\lambda_D]}(x) \\ D^{j_B\star}_{[\lambda_B,\lambda'_B]}(x) D^{j_C\star}_{[\lambda_C,\lambda'_C]}(x) D^{j_D\star}_{[\lambda_D,\lambda'_D]}(x) \to A_{[\lambda_A,\lambda'_B,\lambda'_C,\lambda'_D]}(x;\vartheta) \end{split}$$

 $\lambda_{[RB][ARB][][CD][RCD][BB'][CC'][DD'] \rightarrow [AB'C'D']$ The shape is (number of events,), type is complex128

 $R(x; \vartheta) = \begin{cases} x: all data, (*args, **kwargs) \\ \vartheta: all parameters (self.a, ...) \end{cases}$

here the data, (*args, **kwargs) is passed from DecayChain.

For convenience, different data will be divided into different parts to pass to get_amp(self, *args, **kwargs)

The parameters are directly defined in the class, and the values are obtained from VarsManager.

Batch for Hessian

•
$$\frac{\partial \ln L(\vartheta)}{\partial \vartheta} = \frac{\partial \ln L(\vartheta,I)}{\partial \vartheta} + \frac{\partial \ln L(\vartheta,I)}{\partial I} \frac{\partial I}{\partial \vartheta}$$

•
$$\frac{\partial^2 \ln L(\vartheta)}{\partial \vartheta \partial \vartheta} = \left[\frac{\partial^2 \ln L(\vartheta,I)}{\partial \vartheta \partial \vartheta} + \frac{\partial^2 \ln L(\vartheta,I)}{\partial \vartheta \partial \vartheta} \frac{\partial I}{\partial \vartheta}\right] + \left(\frac{\partial^2 \ln L(\vartheta,I)}{\partial I \partial \vartheta} \frac{\partial I}{\partial \vartheta} + \frac{\partial^2 \ln L(\vartheta,I)}{\partial I \partial \vartheta} \frac{\partial I}{\partial \vartheta}\right) + \frac{\partial \ln L(\vartheta,I)}{\partial I} \frac{\partial^2 I}{\partial \vartheta \partial \vartheta}$$

• Step1: eval $(I, \frac{\partial I}{\partial \vartheta}, \frac{\partial^2 I}{\partial \vartheta \partial \vartheta})$ in small batch
• Step2: eval $(\ln L(\vartheta'), \frac{\partial \ln L(\vartheta')}{\partial \vartheta'}, \frac{\partial \ln L(\vartheta')}{\partial \vartheta'})$ in small batch
• Here: $\vartheta'_i = (\vartheta_i, I), \frac{\partial \vartheta'_i}{\partial \vartheta_j} = (\delta_{ij}, \frac{\partial I}{\partial \vartheta_j})$
• Step3:
$$\frac{\partial^2 \ln L(\vartheta)}{\partial \vartheta_i \partial \vartheta_j} = \frac{\partial^2 \ln L(\vartheta')}{\partial \vartheta'_k \partial \vartheta'_l} \frac{\partial \vartheta'_k}{\partial \vartheta_i \partial \vartheta'_j} + \frac{\partial^2 \ln L(\vartheta')}{\partial I} \frac{\partial^2 I}{\partial \vartheta_i \partial \vartheta_j}$$

FDC-PWA

- FDC: Feynman Diagram Calculation
 - Construct the Lagrangian and deduce Feynman rules automatically
 - Generation of all Feynman diagrams and amplitudes for a given process.
- FDC-PWA:
 - Construct effective strong interaction model
 - Generate Fortran code to calculate Partial waves amplitudes
 - Fit for coupling parameters with TensorFlow on GPU (include AD)

Many steps, but automatic

