TF-PWA

Research on the partial wave analysis tools with auto differentiation

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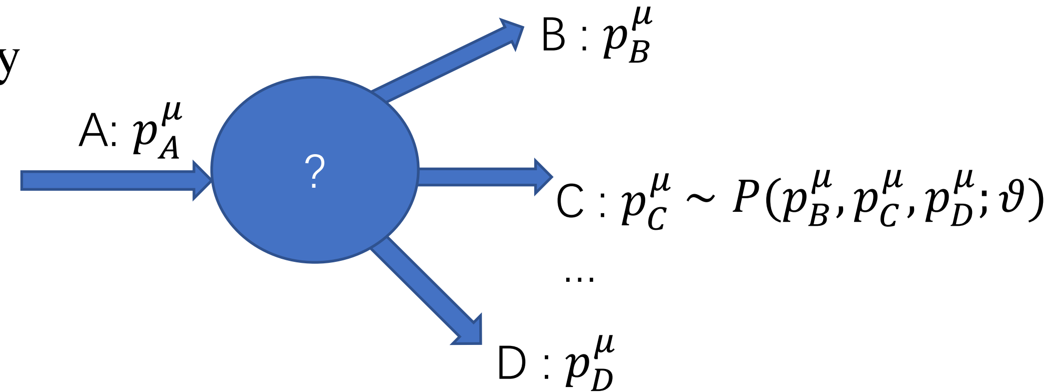
Monday, 6 September 2021

Outline

- Introduction
  - Partial Wave analysis (PWA) and Auto Differentiation (AD)
- TF-PWA
  - Framework (aim for general propose amplitude analysis)
    - Decay process
    - Helicity amplitude
  - Special technology (to make it fast and easy to use)
    - Automatic differentiation
    - Factor system
  - Benchmarks
- Summary

Introduction

- 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



- A powerful fitter is the key factor affecting the performance of PWA tools.

- A general PWA framework using modern acceleration technology (such as GPU, AD, …) is eagerly needed.

- We have developed a new framework using TensorFlow.

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

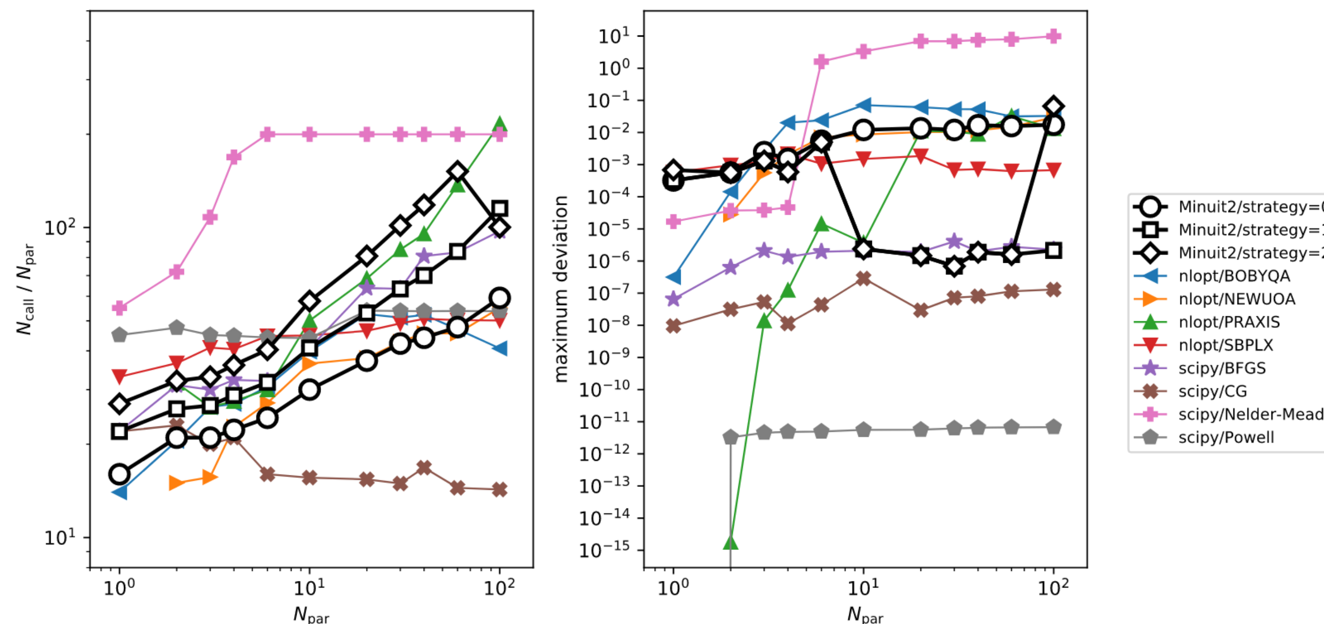
Optimization methods

supported fit method

Fit method	type
Nelder-Mead	no-gradient
BFGS CG	gradient
Newton-CG trust-krylov trust-ncg …	hessian, hessian vector product
iminuit	gradient

scipy

https://iminuit.readthedocs.io/en/stable/benchmark.html



"6.1.1 MIGRAD

… Its main weakness is that it depends heavily on knowledge of the first derivatives, and fails miserably if they are very inaccurate. If first derivatives are a problem…"

From Minuit2 manual(Page 31), F. James and M. Winkler

Gradient and hessian can be calculated by AD precisely!

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial w_1}\frac{\partial w_1}{\partial x} = \left(\frac{\partial y}{\partial w_2}\frac{\partial w_2}{\partial w_1}\right)\frac{\partial w_1}{\partial x} = \left(\left(\frac{\partial y}{\partial w_3}\frac{\partial w_3}{\partial w_2}\right)\frac{\partial w_2}{\partial w_1}\right)\frac{\partial w_1}{\partial x} = \cdots$$

Automatic Differentiation (AD)

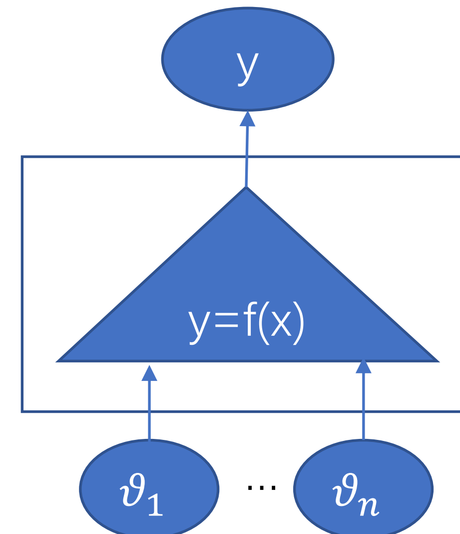
- AD provides a powerful way to calculate gradient automatically
  - Time for calculating gradient

    N is the number of parameters

    t is the time of function evaluation

AD	$[f(x+\delta)-f(x)]/\delta$
$\sim t$	$\sim N\, t$

- Fast Fit
  - can reduce time for many gradient based method
  - $f(x) \approx f(x_0) + \frac{\partial f}{\partial x}(x - x_0) + \frac{\partial^2 f}{\partial x_i \partial x_j}(x-x_0)_i (x-x_0)_j \cdots$
  - $x_{out} = \text{argmin } f(x) \Rightarrow x_{out} \approx \left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)^{-1} \frac{\partial f}{\partial x}$



Reverse accumulation is more efficient than forward accumulation for PWA!

https://en.wikipedia.org/wiki/Automatic_differentiation

- Error propagation
  - $\sigma_y = \sqrt{\frac{\partial y}{\partial x_i} V_{ij} \frac{\partial y}{\partial x_j}}$
  - Calculate uncertainties of physical observables , (such as fit fractions)
  - Easy to use in TFPWA

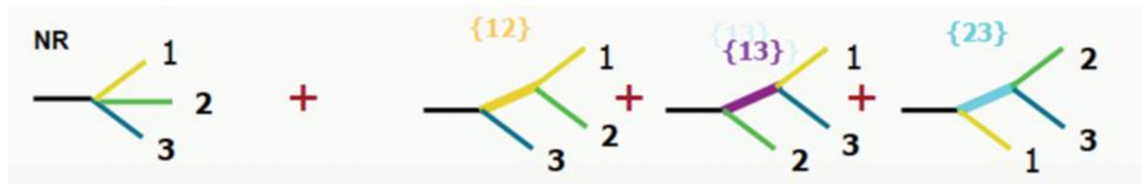
TF-PWA: Partial Wave Analysis with TensorFlow

- Fast
  - GPU based
  - Vectorized calculation
  - Automatic differentiation

    Quasi-Newton Method: scipy.optimize
- General
  - Custom model available
- Easy to use
  - Simple configuration file (example provided)
  - Most of the processing is automatic
  - All necessary functions implemented (details later)
- Open access and well supported

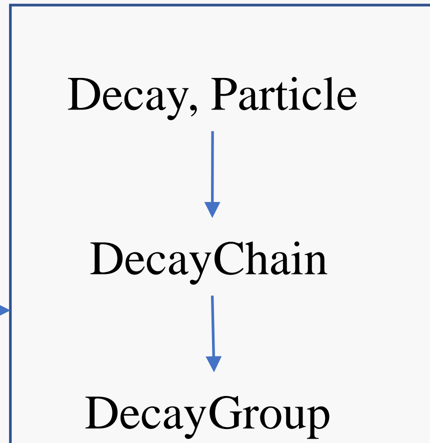
https://github.com/jiangyi15/tf-pwa

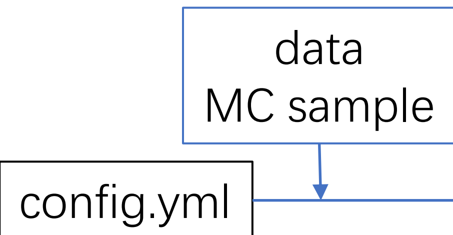
The Framework



Automatic generations of different kinds of fitting outputs

General Decay Description.

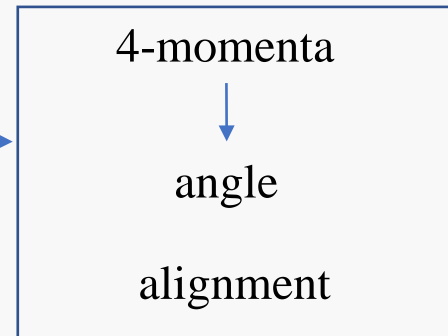




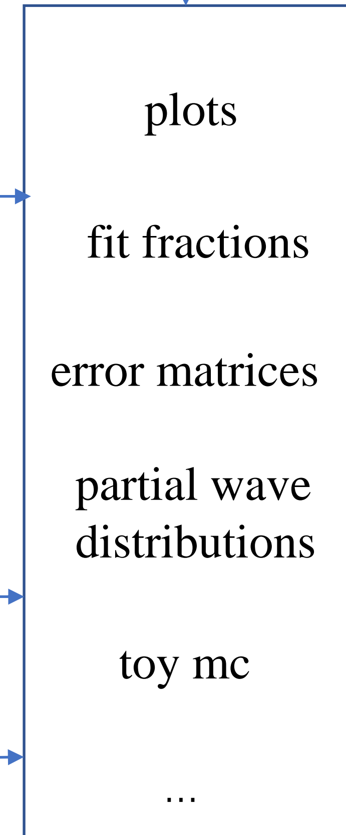
Configuration file

structure

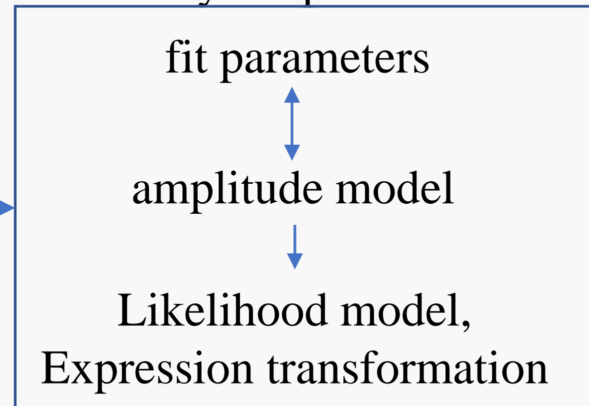
General Helicity Angle Process



Results



Helicity Amplitude Rule



fit

Fast Evaluation

users only need to take care of the input files

Can be a black box for beginners

Configuration File

YAML (YAML Ain't Markup Language) format https://yaml.org

- Widely used in other packages
- Easy to read and write
- Easy to rewrite in scripts

- Basic Parameters

  Decay:

  in state, out states

  model (helicity amplitude as default)

  model parameters.

  Particle:

  spin parity (J^P),

  mass (m_0)

  width (Γ_0),

  model (Breit-Wigner),

  model parameters.

config.yml — Full example

```yaml
decay:
  B0:
  - [DK , Dst, model:
default, p_break: True]
  - [DstK , D, p_break: True]
  - [DstD , K, p_break: True]
  DstD: [Dst, D]
  DstK: [Dst, K]
  DK: [D, K]
  Dst: [D0, pi]
```

Resonances.yml

```yaml
Zc(3900): {J: 1, P: +1, mass:
3.8817, width: 0.0266, model:
default}
Ds1(2700): {J: 1, P: -1,
mass: 2.7083, width: 0.120}
Ds2(2573): {J: 2, P: +1,
mass: 2.5691, width: 0.0169}
```

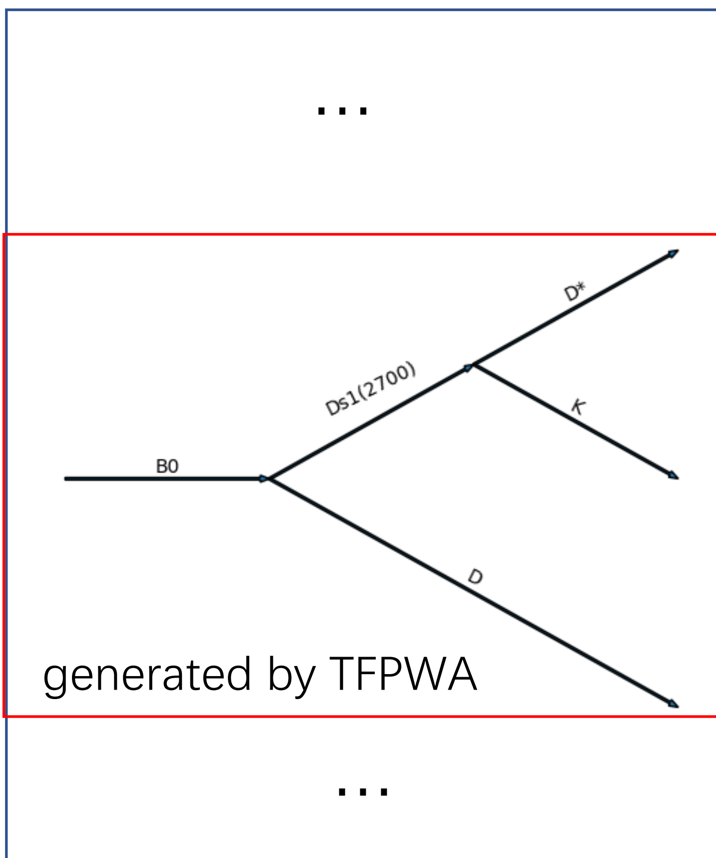
$B^0 \to D^{*-}D^0K^+, D^{*-} \to D^0\pi^-$

config.yml

```yaml
particle:
  $top:
    B0: {J: 0, P: -1, mass: 5.2}
  $finals:
    D: {J: 0, P: -1, mass: 1.86}
    K: {J: 0, P: -1, mass: 0.5 }
    D0: {J: 0, P: -1, mass: 1.86}
    pi: {J: 0, P: -1, mass: 0.14}
  DstD: [Zc(3900)]
  DstK: [Ds1(2700), Ds2(2573)]
  DK: []
  Dst: {J: 1, P: -1, mass: 2.01,
model: one}
  $include: Resonances.yml
```

The only places users need to modify for different decay processes

Topology based algorithm



$B^0 \to D^{*-} D^0 K^+$: decay group

Automatically built from config.yml

One decay chain

$B^0 \to D^*_{s1}(2700)^+ (\to D^0 K^+)\ D^{*-}$

Decays

$B^0 \to D^*_{s1}(2700)^+ D^{*-}$

$D^*_{s1}(2700)^+ \to D^0 K^+$

etc.

Particles

initial state (B^0),
final states (D^{*-}, D^0, K^+)
propagator ($D^*_{s1}(2700)$)

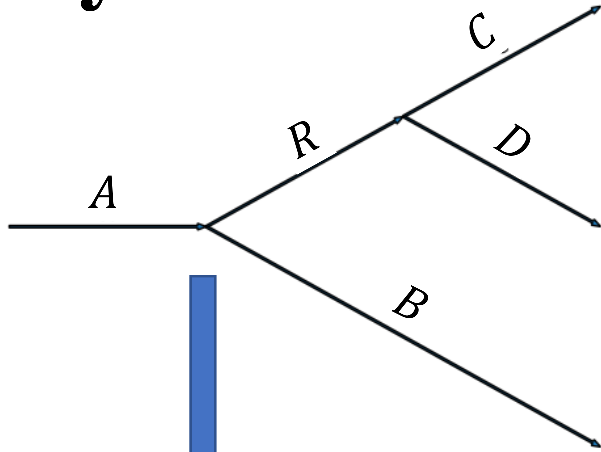
```
Ds1 = Particle("Ds1(2700)",J=1, P=-1)
Dst = Particle("Dst", J=1, P=-1)
B = Particle("B", J=0, P=-1)
...
```

```
d1 = Decay(B, [Ds1, D])
```

```
dec1 = DecayChain([d1, d2, d3])
```

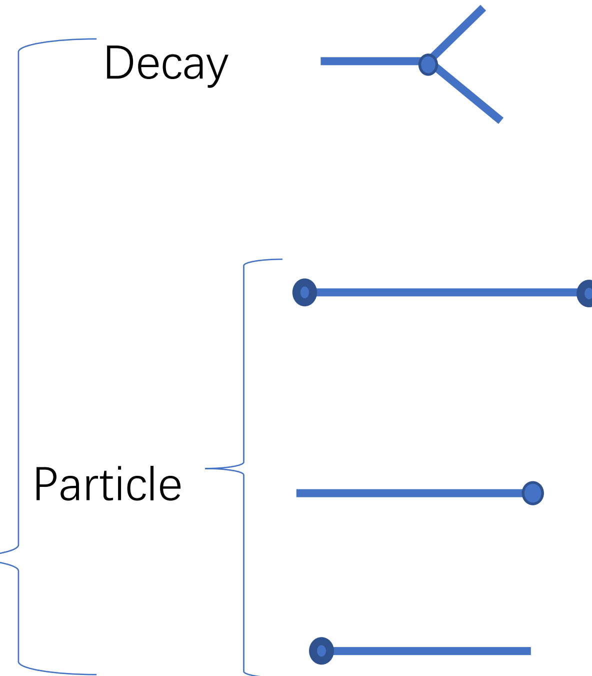
```
dg = DecayGroup([dec1, dec2, dec3])
```

Helicity formalism



Feynman rules

User defined



$F_{\lambda_1,\lambda_2} D^{j_0\star}_{\lambda_0,\lambda_1-\lambda_2}(\varphi,\theta,0)$

Wigner-D matrix

$R(M) = \frac{1}{m_0^2 - M^2 - i m_0 \Gamma}, \cdots$

1

$D^{j_1\star}_{\lambda_1,\lambda_1'}(\alpha,\beta,\gamma)$

alignment

$A^R_{\lambda_A,\lambda_B',\lambda_C',\lambda_D'}$

$=$

$$\sum_{\lambda} F_{\lambda_R\lambda_B} D^{j_A\star}_{\lambda_A,\lambda_R-\lambda_B}(\varphi_1,\theta_1,0) R(M) F_{\lambda_C,\lambda_D} D^{j_R\star}_{\lambda_R,\lambda_C-\lambda_D}(\varphi_2,\theta_2,0)$$

$$D^{j_B\star}_{\lambda_B,\lambda_B'}(\alpha_B,\beta_B,\gamma_B) D^{j_C\star}_{\lambda_C,\lambda_C'}(\alpha_C,\beta_C,\gamma_C) D^{j_D\star}_{\lambda_D,\lambda_D'}(\alpha_D,\beta_D,\gamma_D)$$

$$\frac{d\sigma}{d\Phi} \propto \sum_{\lambda_A} \sum_{\lambda_B,\lambda_C,\lambda_D} \left| \sum_R A^R_{\lambda_A,\lambda_B,\lambda_C,\lambda_D} \right|^2$$

Automatically calculated from decay structure

probability: $|\mathcal{A}|$^2

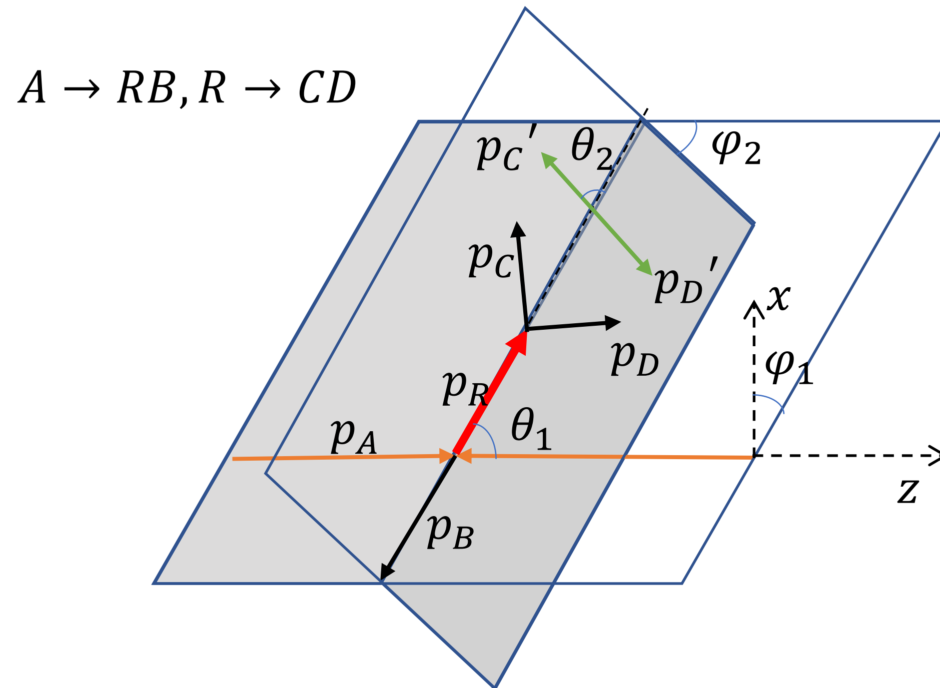
Decay Group: $\mathcal{A} = \tilde{A}_1 + \tilde{A}_2 + \cdots$

Decay Chain: $\tilde{A} = A_1 R A_2 \cdots$

Decay: Wigner D-matrix, $A = F D^{*J}(\phi,\theta,0)$

Particle: Breit-Wigner: $R(m)$, user defined

General Helicity Angle Process



- Data inputs from user

  4-momenta (p^μ), weights

- Converted into amplitude variables

  Invariant masses (m)

  Helicity angles (φ_i, θ_i)

  Alignment angles (α, β, γ)

Automatically calculated based on decay structure,
using Euler rotation system, boost sequence, and SU(2) relationship.

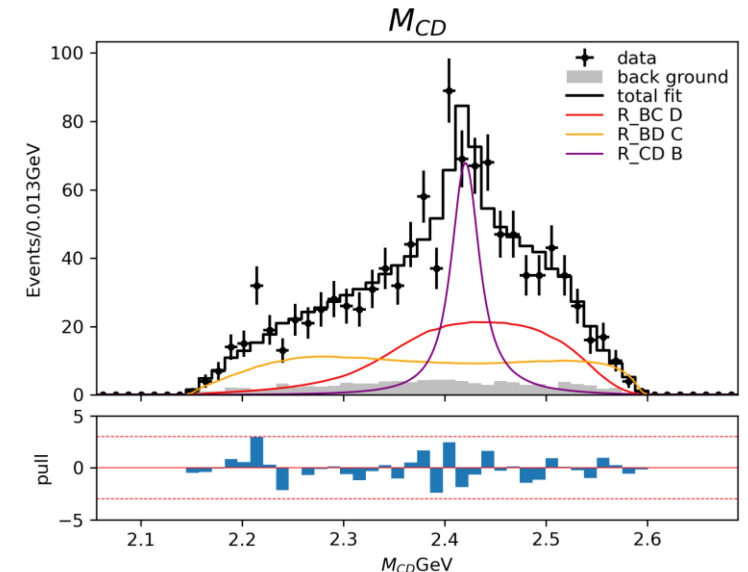
M. Wang, Y. Jiang, Y. Liu el.al., Chinese Physics C Vol. 45, No. 6 (2021) 063103

Factor system: automatic factorization of amplitude

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

$$A = (\sum g_i A_i)(\sum g'_j A'_j)\cdots \Rightarrow A = \sum_{ij} (g_i g'_j)(A_i A'_j)$$

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



- Some special treatment is implemented
  - Plotting of partial waves ($P_i = |A_i|^2$)
  - Amplitude caching
    - mass dependent:

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

      fit parameters related

    - factor only: $\sum |A|^2 \rightarrow G_i G_j^* (\sum C_{ij})$

      calculate only once

method	Time for Calculating –ln L (s)	Time for Single fit (s)	Memory (MB)
original	1.00243	224.1	4371
mass dependent	0.41840	103.2	2323
factor only	0.17831	31.56	2323

Benchmarks

CPU: i7-9750H@2.6 Hz with 12 cores
GPU: Nvidia 1660 Ti, a cheap GPU

Test based on simple MC (200000) sample of a simple amplitude model of $e^+e^- \to R_1(1^+)\pi, R_1 \to D^*D^*$

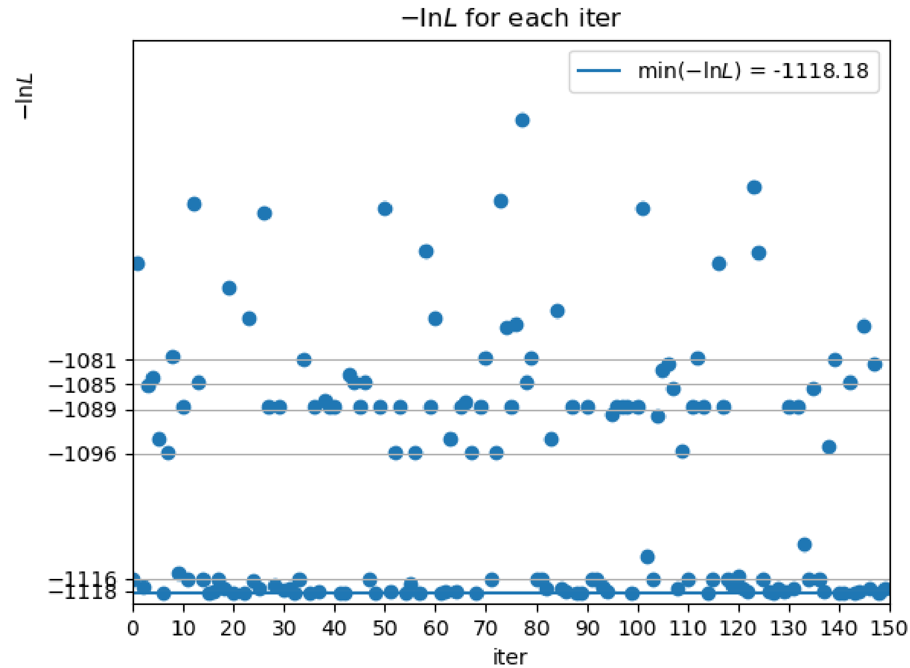
Both based on TF-PWA

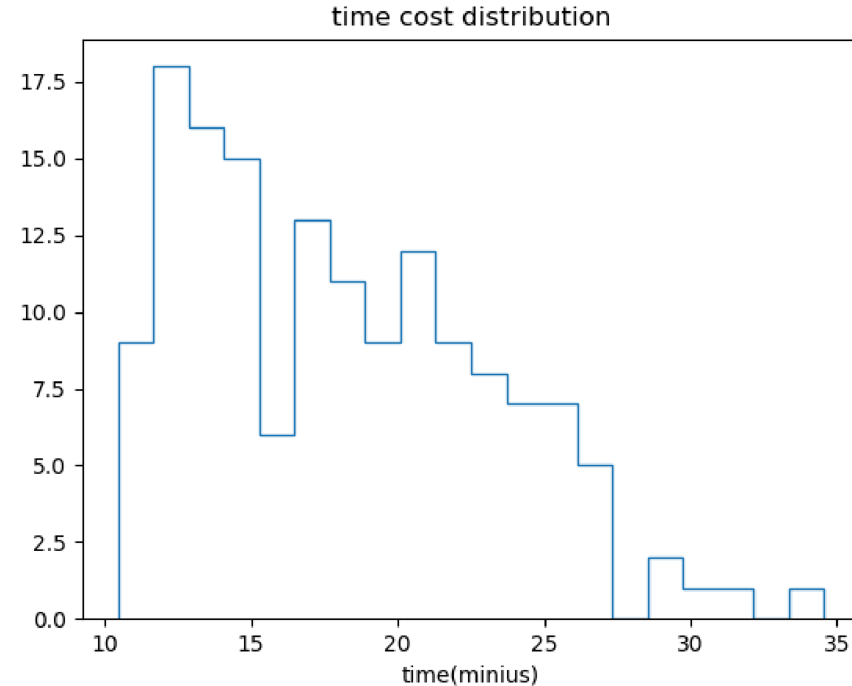
process	CPU (ms)	GPU (ms)	Ratio
Sum of log(PDF)	725 X 12	91	~8 X 12 = 96
Sum + differential	1417 X 12	188	~7.5 X 12 = 90

Almost a factor of 100 times faster for GPU than single CPU

Performance in a real fit

average ~ 10 – 30 minutes





- Randomizing of initial parameters, better searching for global minimum
- Toy studies
- Uncertainty studies etc.

Functions implemented

- Toy studies
- Plotting
- Fit fractions, interference fractions
- Simultaneous fit between different datasets
- Parity conservation, isospin constraints
- Gaussian constraints on parameters
- 2D chi2 test
- CP violation fit
- Final states with identical particles
- Amplitude factorization
- Resolution
- Simple symbolic formula
- Error propagation
- …

TF-PWA

Summary

- A general framework is developed for PWA based on TensorFlow
- Fast, easy to use and still in active development
- TF-PWA cross-checked with other fitters used in BESIII and LHCb collaborations
- Have been used for a large variety of amplitude analyses
- Well supported , welcome to use and provide feedback.

Thank you for your attentions!

Back Up

Fit process: maximum likelihood

$$P(x_i;\vartheta) = \frac{1}{\sigma_{tot}}\frac{d\sigma}{d\Phi}(x_i;\vartheta),\ \sigma_{tot} = \sum_{x_i\in MC}\omega_i\frac{d\sigma}{d\Phi}(x_i;\vartheta),\ \omega_i = \frac{1}{N_{MC}}$$

Negative Log-Likelihood (NLL):

$$-\ln L = -\alpha\sum_{x_i\in \text{data}} w_i \ln P(x_i;\vartheta),\ \alpha = \frac{\sum w_i}{\sum w_i^2}$$

Can either subtract background using weights or directly include background in the fit

$$\hat{\vartheta} = \text{argmin}\,(-\ln L)$$

BFGS:

$$\vartheta_{i+1} = \vartheta_i + kp_i$$
$$p_i = -B_i g_i$$
$$B_{i+1} = B_i + \frac{y_i y_i^T}{y_i^T s_i} - \frac{B_i s_i s_i^T B_i}{s_i^T B_i s_i}$$
$$s_i = \vartheta_{i+1} - \vartheta_i,\ y_k = g_{i+1} - g_i$$

$$g_i = -\frac{\partial \ln L}{\partial\vartheta}$$

Automatic differentiation:

- Reduce the number of calculation of $-\ln L$, speed up the fit.
- More accurate gradient, improve the fit result

error matrix: $V_{ij}^{-1} = -\frac{\partial \ln L}{\partial\vartheta_i\partial\vartheta_j}|_{\vartheta=\hat{\vartheta}}$

also calculated by automatic differentiation

$V \approx B$

Custom Model

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

```python
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

$$F_{[\lambda_R \lambda_B]}(x;\vartheta) D^{j_A\star}_{[\lambda_A,\lambda_R-\lambda_B]}(x) R(x;\vartheta) F_{[\lambda_C,\lambda_D]}(x;\vartheta) D^{j_R\star}_{[\lambda_R,\lambda_C-\lambda_D]}(x)$$

$$D^{j_B\star}_{[\lambda_B,\lambda_B']}(x) D^{j_C\star}_{[\lambda_C,\lambda_C']}(x) D^{j_D\star}_{[\lambda_D,\lambda_D']}(x) \rightarrow A_{[\lambda_A,\lambda_B',\lambda_C',\lambda_D']}(x;\vartheta)$$

$$\lambda_{[RB][ARB][\,][CD][RCD][BB'][CC'][DD'] \rightarrow [AB'C'D']}$$

The shape is (number of events,), type is complex128

$R(x;\vartheta)$
- x: all data, (*args, **kwargs)
- ϑ: all parameters (self.a , ⋯)

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.

Resonant models and LS coupling

Default Model:

- $R(M)$: Breit-Wigner with running width

$$R(M) = \frac{1}{M^2 - m_0^2 + m_0\Gamma(M)},\ \ \Gamma(M) = \Gamma_0 \left(\frac{q}{q_0}\right)^{2l_0+1} \frac{m_0}{m} {B'_{l_0}}^2(q, q_0, d)$$

- LS coupling: from helicity base to LS base
  - F_{λ_1,λ_2}: $J^P(\lambda_0) \to j_1^{\eta_1}(\lambda_1) + j_2^{\eta_2}(\lambda_2)$

Blatt-Weisskopf factor

$$F_{\lambda_1,\lambda_2} = \sum_{ls} g_{ls} \sqrt{\frac{2l+1}{2J+1}} \langle j_1\lambda_1;\ j_2 - \lambda_2 | s\delta\rangle \langle l0; s\delta | J\ \delta\rangle q^l B'_l(q, q_0, d), \delta = \lambda_1 - \lambda_2$$

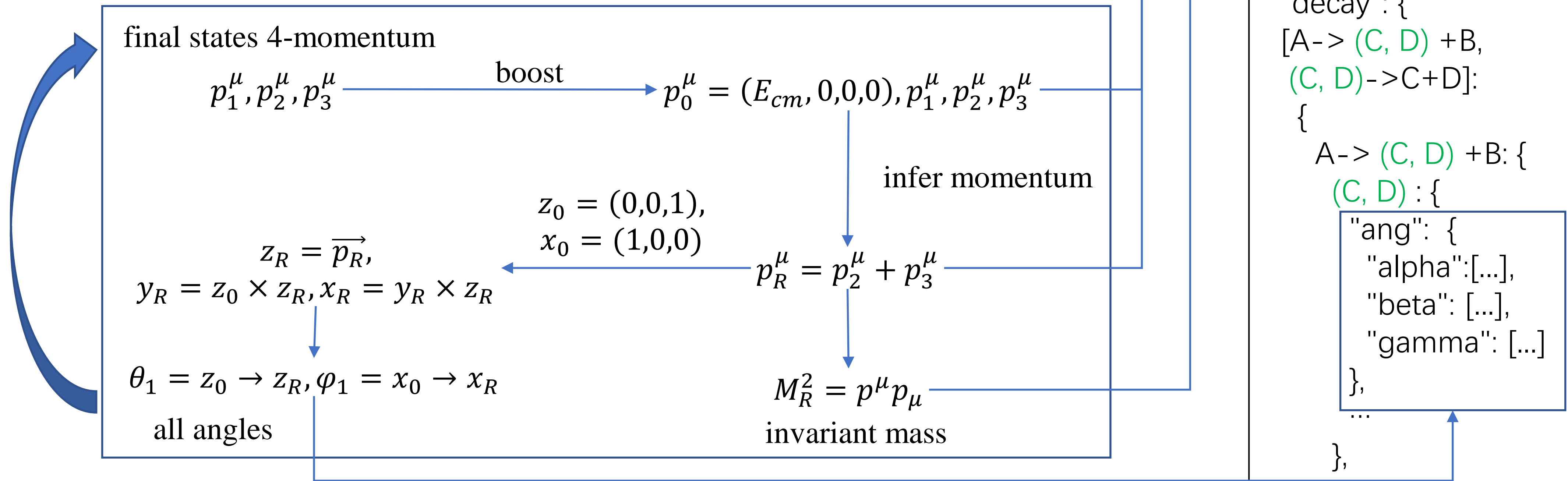
fit parameters　　CG coefficients

LS coupling: $|j_1 - j_2| < s < j_1 + j_2, |l - s| \le J \le l + s$

Parity conversation: $P = \eta_1\eta_2(-1)^l$

Data process: Automatic angle calculation

$p_0 \to p_1 + p_2 + p_3$: $p_0 \to p_1 + p_R, p_R \to p_2 + p_3$



Total data

```
{
 "particle": {
  A:{
   "p":...,
   "m":...
  }
  ...
 },
 "decay": {
 [A-> (C, D) +B,
  (C, D)->C+D]:
  {
   A-> (C, D) +B: {
    (C, D) : {
     "ang": {
      "alpha":[...],
      "beta": [...],
      "gamma": [...]
     },
     ...
    },
    B : {...}
   },
   ...
  }, ...
 }
}
```

loop for decay and decay chain,
so that all angles are calculated automatically

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 $0 \to R, 2; R \to 1, 3$:

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

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

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

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

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

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

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

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

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

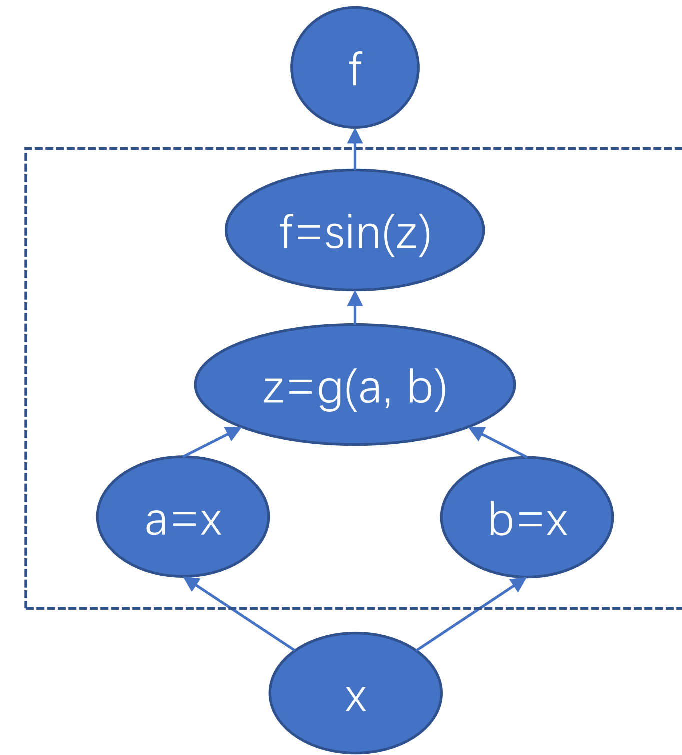
$$\omega = \ln\left|\frac{L_{22}}{L_{11}}\right|$$

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

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

Automatic Differentiation (AD)

- AD provides a powerful way to calculate gradient automatically
- Chain Rules
  - ×: $\frac{\partial f(g(x))}{\partial x_i} = \frac{df}{dg} \times \frac{\partial g}{\partial x_i}$
  - +: $\frac{\partial f(h(x), g(x))}{\partial x_i} = \frac{\partial f}{\partial h}\frac{\partial h}{\partial x_i} + \frac{\partial f}{\partial g}\frac{\partial g}{\partial x_i}$



Only basic operator need for differentiation.
Similar as amplitude rules

Automatic Differentiation (numerically):

$$\frac{df}{dx}(1) = \frac{df}{dz}(1^1)[\frac{\partial g}{\partial a}(1,1) + \frac{\partial g}{\partial b}(1,1)] = 0.5403$$

forward

backward

$$f = \sin(x^x) = \sin(z), z = x^x$$

$$g(a,b) = a^b$$

$$\frac{df}{dz} = \cos z, \frac{\partial g(a,b)}{\partial a} = ba^{b-1}, \frac{\partial g(a,b)}{\partial b} = a^b \ln a$$

Symbolic method:

$$\frac{df}{dx} = \frac{df}{dz}\frac{dg(x,x)}{dx} = \cos z\left[(ba^{b-1})\Big|_{a,b=x} + (a^b \ln a)\Big|_{a,b=x}\right]$$

$$= \cos x^x [x x^{x-1} + x^x \ln x] = x^x \cos x^x (\ln x + 1)$$

AD transform

All parts can be calculated from small batches of data.

- $p(x;\vartheta) = \frac{f(x;\vartheta)}{N_f(y;\vartheta)} + g(x); \mathrm{N_f}(\mathrm{x}) = \sum_{i\in MC} f(x_i;\vartheta)$
- $\frac{\partial p(x;\vartheta)}{\partial\vartheta} = \frac{\partial p(x;\vartheta;N_f)}{\partial\vartheta} + \frac{\partial p(x;\vartheta;N_f)}{\partial N_f}\frac{\partial N_f}{\partial\vartheta}$
- $\frac{\partial N_f}{\partial\vartheta} = \sum_{i\in MC}\frac{\partial f(x_i;\vartheta)}{\partial\vartheta} = \sum_i \sum_{j\in MC_i}\frac{\partial f(x_i;\vartheta)}{\partial\vartheta}$
- $-\frac{\partial \ln L}{\partial\vartheta} = -\alpha\frac{\partial\sum w_i \ln p(x;\vartheta;N_f)}{\partial\vartheta} - \alpha\frac{\partial\sum w_i \ln p(x;\vartheta;N_f)}{\partial N_f}\frac{\partial N_f}{\partial\vartheta}$

```
with config.params_trans() as f:
  real = f["A->R_BD.C_g_ls_1r"]
  imag = f["A->R_BD.C_g_ls_1i"]
  alpha = real / (1 + real * real + imag * imag)
print(alpha, f.get_error(alpha))
```

identical particles

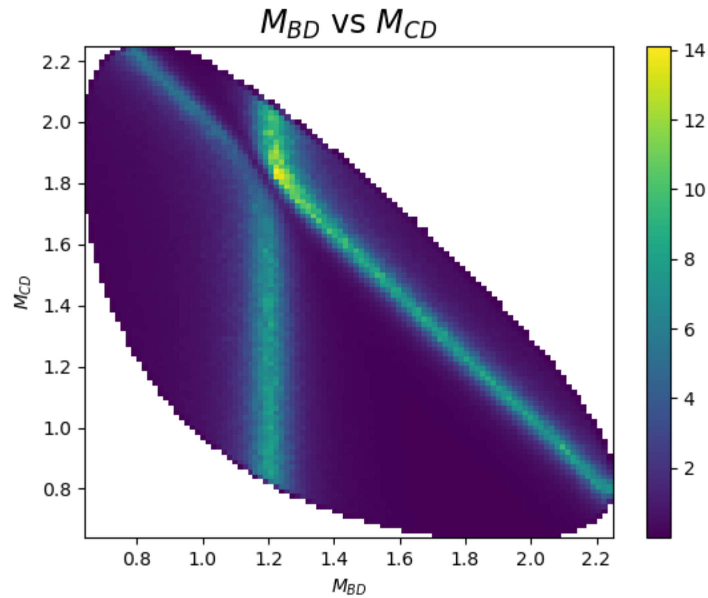
$$A \to BCD$$

$$A \to (BC)D, A \to (BD)C$$

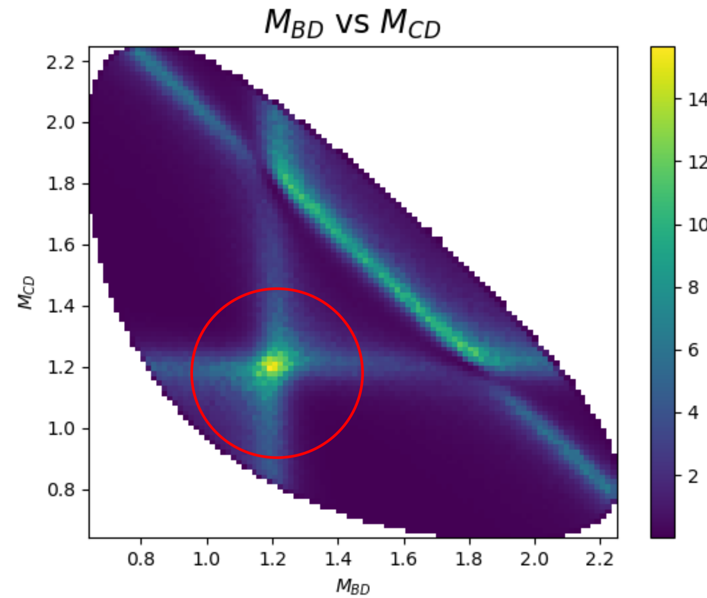
B, C are identical particles

$$Amp(p_B, p_C, p_D) \Rightarrow Amp(p_B, p_C, p_D) \pm Amp(p_C, p_B, p_D)$$

No identical particles



boson :
Interference is enhanced



fermion:
Interference is eliminated