

# AI for Partial Wave Analysis

## 分波分析与深度学习

董翔，潘楚铨，蔡浩  
武汉大学



# AI for Science

思路方法

解决问题

# 分波分析

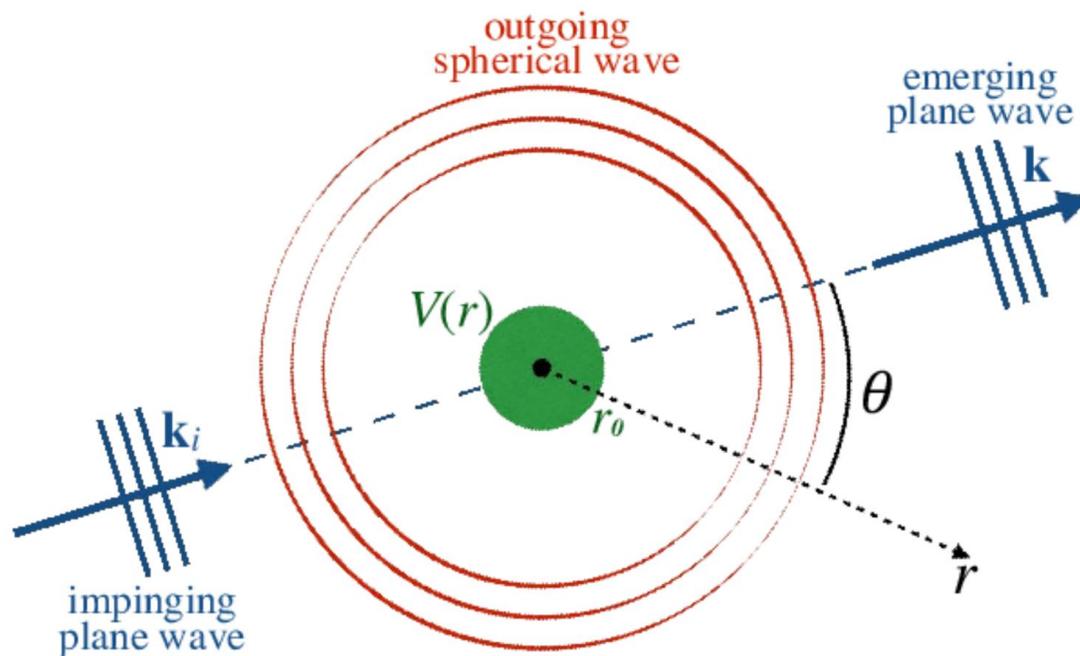
The stationary Schrödinger equation

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \Psi(\mathbf{r}) = E \Psi(\mathbf{r})$$

$$\Psi(\mathbf{r}) \rightarrow \Psi^{(+)}(\mathbf{r}) = \exp(ikz) + f(\theta, k) \frac{\exp(ikr)}{r}$$

**Differential cross section**

$$\frac{d\sigma}{d\Omega} = |f(\theta, k)|^2$$



# 分波分析与最大似然拟合

The probability to observe the event characterized by the measurement  $\zeta$

$$P(\zeta : \alpha) = \frac{\omega(\zeta, \alpha)\epsilon(\zeta)}{\int d\zeta \omega(\zeta, \alpha)\epsilon(\zeta)}$$

$\omega(\zeta, \alpha) = d\sigma/d\Omega$  is the differential cross section, and the standard likelihood is

$$P(\zeta_1, \zeta_2, \dots, \zeta_n : \alpha) = \prod_{i=1}^N P(\zeta : \alpha) = \prod_{i=1}^N \frac{\omega(\zeta_i, \alpha)\epsilon(\zeta_i)}{\int d\zeta \omega(\zeta, \alpha)\epsilon(\zeta)} = L$$

The second item of the log likelihood could be dropped

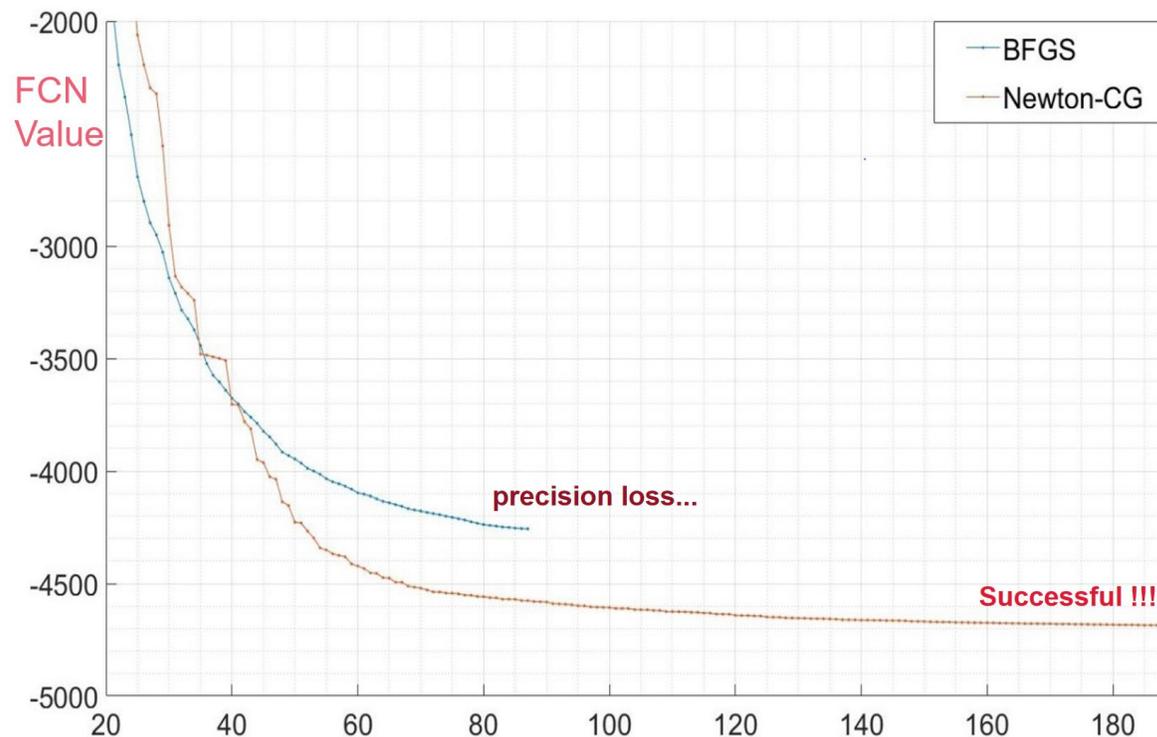
$$\ln L = \sum_{i=1}^N \ln \left( \frac{\omega(\zeta_i, \alpha)}{\int d\zeta \omega(\zeta, \alpha)\epsilon(\zeta)} \right) + \sum_{i=1}^N \epsilon(\zeta_i)$$

And the **normalized integral** could be approximated as

$$\sigma' = \int d\zeta \omega(\zeta, \alpha)\epsilon(\zeta) \simeq \frac{1}{N_{gen}} \sum_{i=1}^{N_{acc}} \omega(\zeta_i, \alpha)$$

## scipy.optimize.minimize

- 'Nelder-Mead' (see here)
- 'Powell' (see here)
- 'CG' (see here)
- 'BFGS' (see here)
- 'Newton-CG' (see here)
- 'L-BFGS-B' (see here)
- 'TNC' (see here)
- 'COBYLA' (see here)
- 'SLSQP' (see here)
- 'trust-constr' (see here)
- 'dogleg' (see here)
- 'trust-ncg' (see here)
- 'trust-exact' (see here)
- 'trust-krylov' (see here)



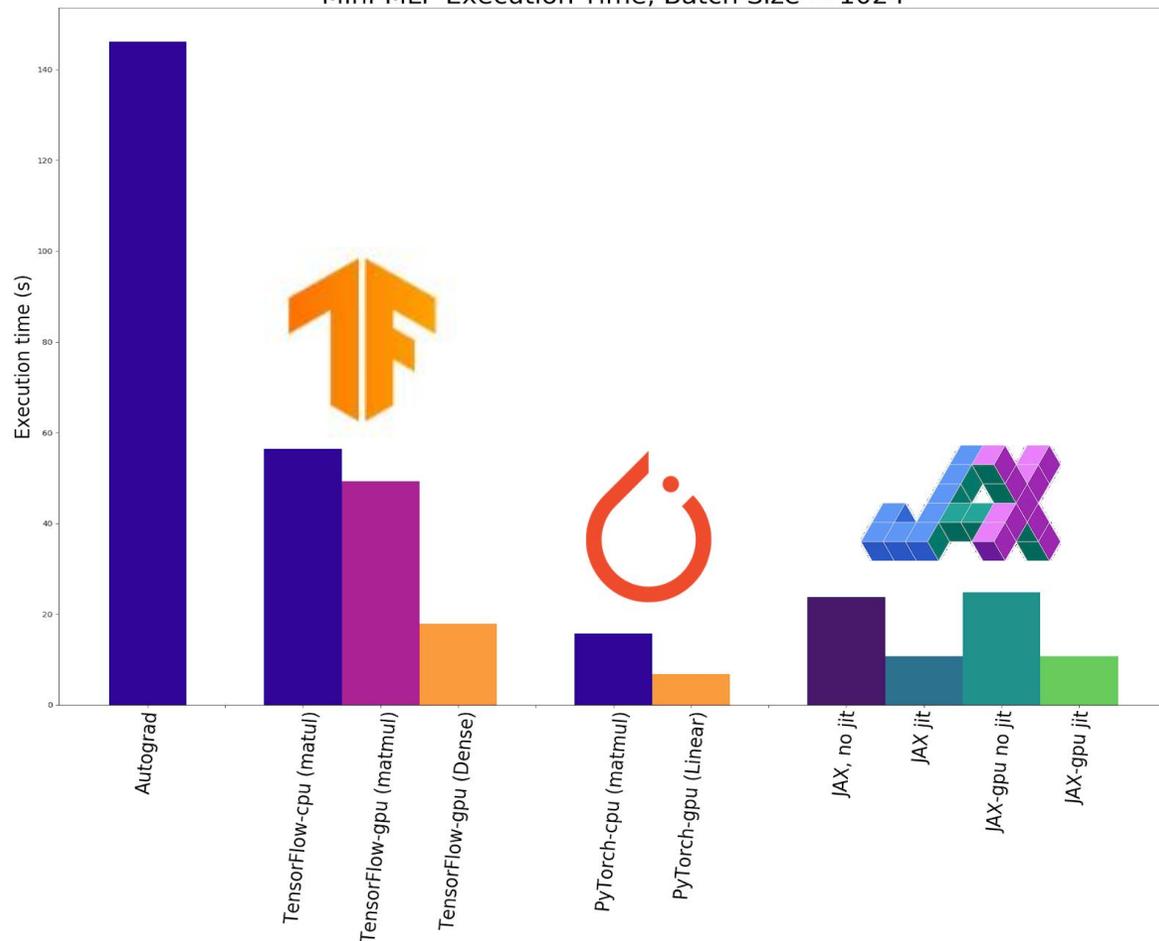
精确的二阶导数矩阵（Hessian matrix）保证了极点的性质，同时提供了可靠的统计误差！

# 自动微分

- 分波分析使用最大似然法拟合数据，而在拟合过程中通常使用梯度下降类型的方法进行优化；
- 梯度的计算精度对拟合性能有决定性影响；
- 基于GPU的自动微分算法在精度和性能两方面相对于数值微分和解析微分都有明显优势：
  - TensorFlow
  - PyTorch
  - JAX

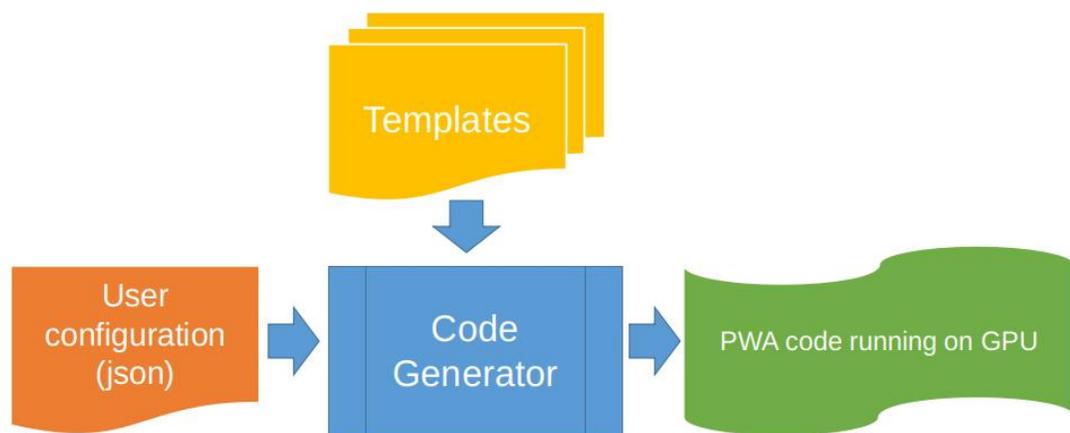
## Results: JAX Dominates with matmul, PyTorch Leads with Linear Layers

Mini-MLP Execution Time, Batch Size = 1024



# 代码生成

- JAX作为底层的自动微分工具，受框架限制更少；
- 代码生成技术的优点：
  - 性能优势；
  - 节约显存；
  - 多GPU支持；
  - 适应各种分波分析需要脚本。



```
Every 0.1s: nvidia-smi

Mon Jun 28 10:10:13 2021

+-----+
| NVIDIA-SMI 455.45.01      Driver Version: 455.45.01      CUDA Version: 11.1      |
+-----+-----+
| GPU  Name                Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf    Pwr:Usage/Cap|      Memory-Usage | GPU-Util  Compute M. |
|                                           | MIG M.         |
+-----+-----+-----+
|   0   GeForce RTX 3090      Off   | 00000000:1A:00.0 Off |             N/A   |
| 67%   68C    P2     304W / 350W | 23171MiB / 24268MiB |   98%      Default  |
|                                           |                 |
+-----+-----+-----+
|   1   GeForce RTX 3090      Off   | 00000000:68:00.0 Off |             N/A   |
| 68%   69C    P2     298W / 350W | 23169MiB / 24265MiB |   98%      Default  |
|                                           |                 |
+-----+-----+-----+

+-----+
| Processes:                                     |
| GPU  GI    CI          PID    Type   Process name          GPU Memory |
|                                           | Usage   |
+-----+-----+-----+
|   0   N/A  N/A     2744169    C     python3              23169MiB |
|   1   N/A  N/A     2744169    C     python3              23167MiB |
+-----+-----+-----+
```

多GPU下可以让显卡达到满载的水平。

# 分波分析示例

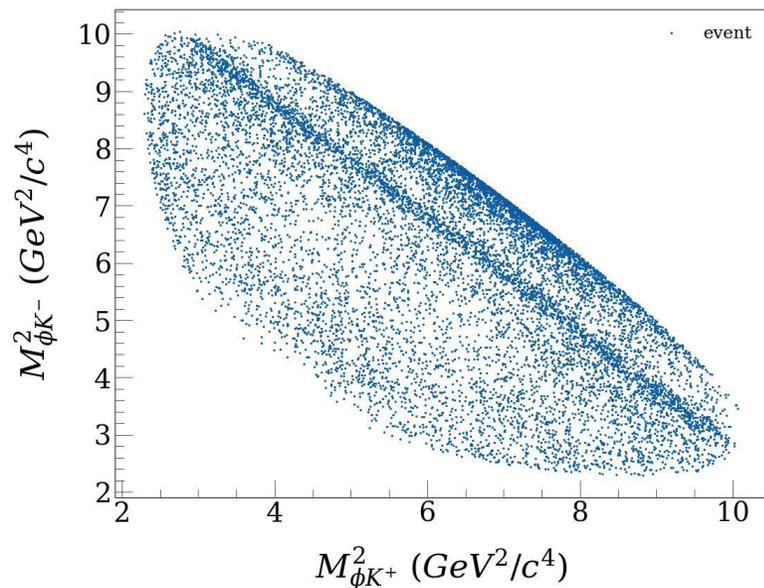
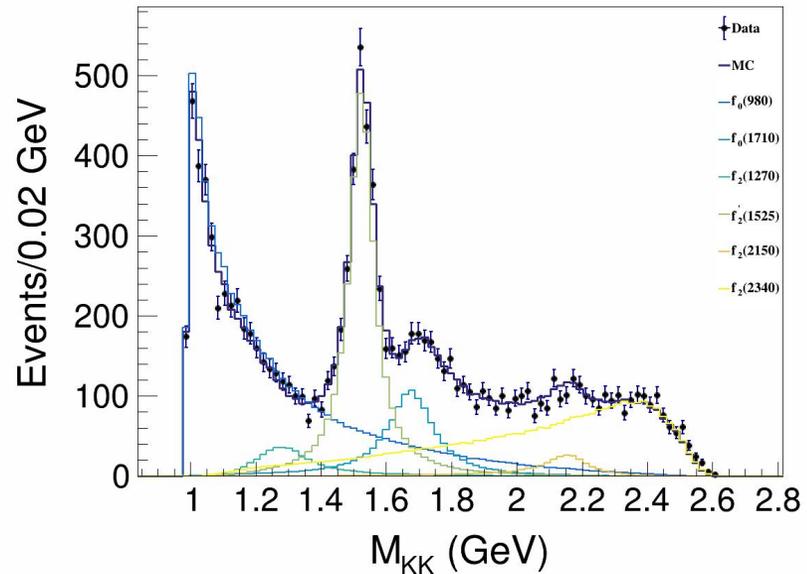


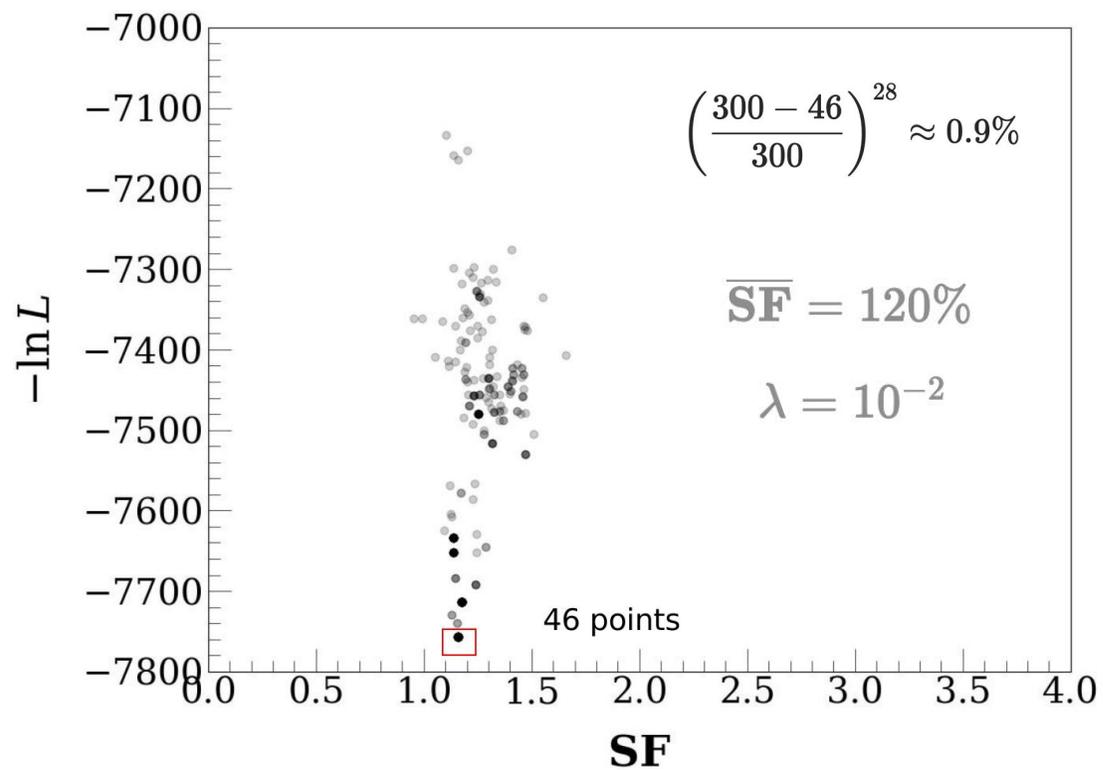
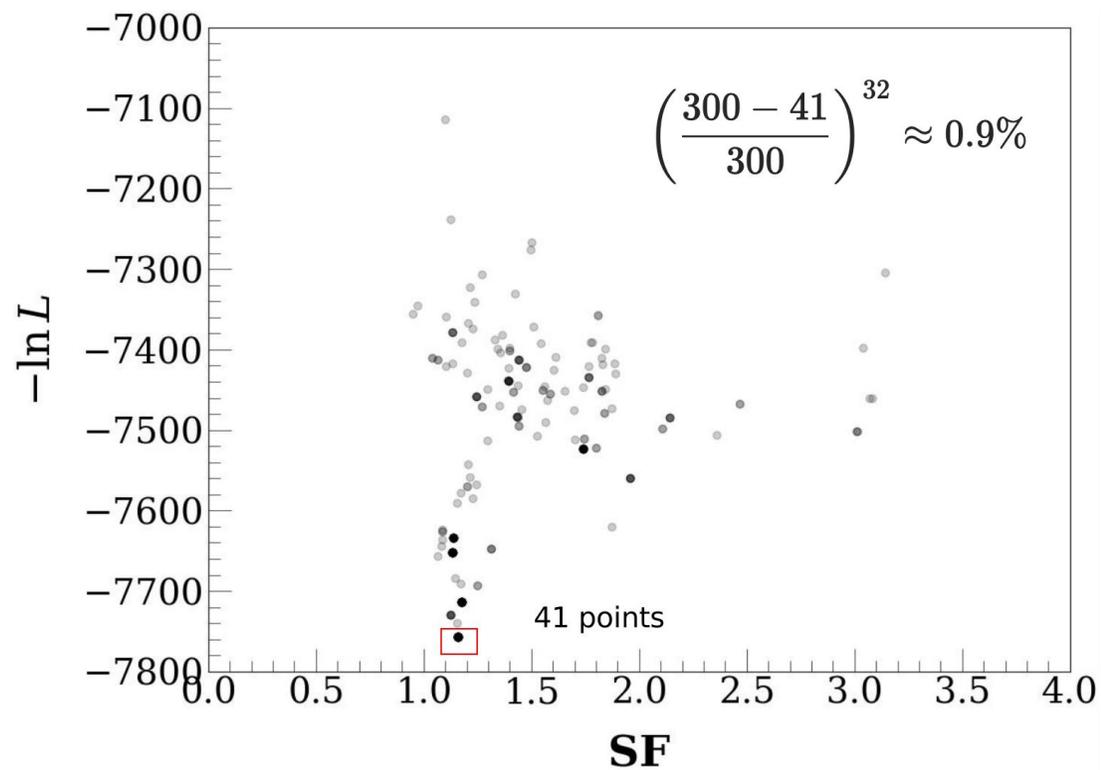
Table 1: The partial wave analysis model  $R_0$  used to generate the data.

$R_0$	Name	$F_i$ (%)	Mass(GeV)	width
1	$f_0(980)$	39.5	0.979	0.107
2	$f_2(2340)$	37.1	2.548	0.324
3	$f_2'(1525)$	24.7	1.5223	0.0858
4	$f_0(1710)$	8.30	1.6762	0.1627
5	$f_2(1270)$	3.16	1.290	0.196
6	$f_2(2150)$	2.22	2.162	0.159
	<b>SF</b>	115.0		

$$\mathbf{F}_k = \sum_{i=1}^N \frac{|c_k M_k(\zeta_i)|^2}{|\sum_k c_k e^{i\phi_k} M_k(\zeta_i)|^2}$$

$$\mathbf{SF} = \sum_k \mathbf{F}_k$$

# 组分约束



$$-\ln L \quad \longrightarrow \quad \tilde{L} = -\ln L + \lambda N (\mathbf{SF} - \overline{\mathbf{SF}})^2$$

# 组分约束对误差的影响

Table 2: Fitting results of the partial wave analysis model  $R_0$  using  $-\ln L$ .

$R_0$	Name	$F_i$ (%)	Mass(GeV)	Width(GeV)
1	$f_0(980)$	$39.2 \pm 1.5$	$1.015 \pm 0.043$	$0.102 \pm 0.030$
2	$f_2(2340)$	$37.5 \pm 1.6$	$2.571 \pm 0.015$	$0.281 \pm 0.017$
3	$f_2'(1525)$	$23.5 \pm 1.0$	$1.5233 \pm 0.0015$	$0.0841 \pm 0.0031$
4	$f_0(1710)$	$8.66 \pm 0.93$	$1.6714 \pm 0.0047$	$0.159 \pm 0.010$
5	$f_2(1270)$	$2.68 \pm 0.57$	$1.288 \pm 0.013$	$0.181 \pm 0.027$
6	$f_2(2150)$	$2.52 \pm 0.63$	$2.152 \pm 0.012$	$0.170 \pm 0.026$
	<b>SF</b>	114.0		

Table 3: Fitting results of the partial wave analysis model  $R_0$  using  $\tilde{L}$ .

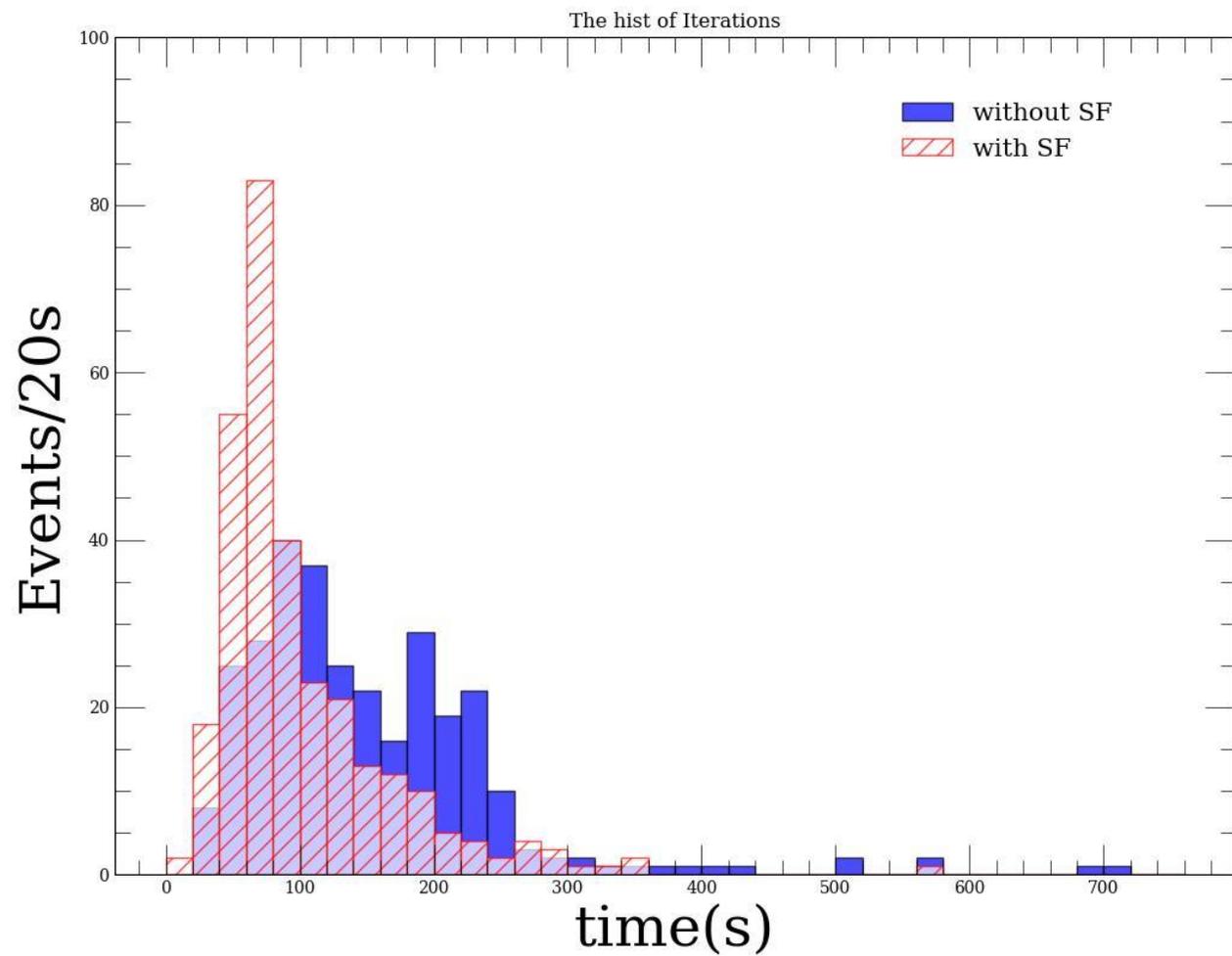
$R_0$	Name	$F_i$ (%)	Mass(GeV)	Width(GeV)
1	$f_0(980)$	$39.3 \pm 1.6$	$1.017 \pm 0.039$	$0.101 \pm 0.035$
2	$f_2(2340)$	$37.5 \pm 1.8$	$2.571 \pm 0.016$	$0.282 \pm 0.018$
3	$f_2'(1525)$	$23.6 \pm 1.0$	$1.5233 \pm 0.0015$	$0.0842 \pm 0.0031$
4	$f_0(1710)$	$8.72 \pm 0.96$	$1.6712 \pm 0.0047$	$0.159 \pm 0.010$
5	$f_2(1270)$	$2.72 \pm 0.58$	$1.288 \pm 0.014$	$0.182 \pm 0.026$
6	$f_2(2150)$	$2.52 \pm 0.62$	$2.152 \pm 0.012$	$0.170 \pm 0.027$
	<b>SF</b>	114.3		

$$\overline{\text{SF}} = 120\%$$

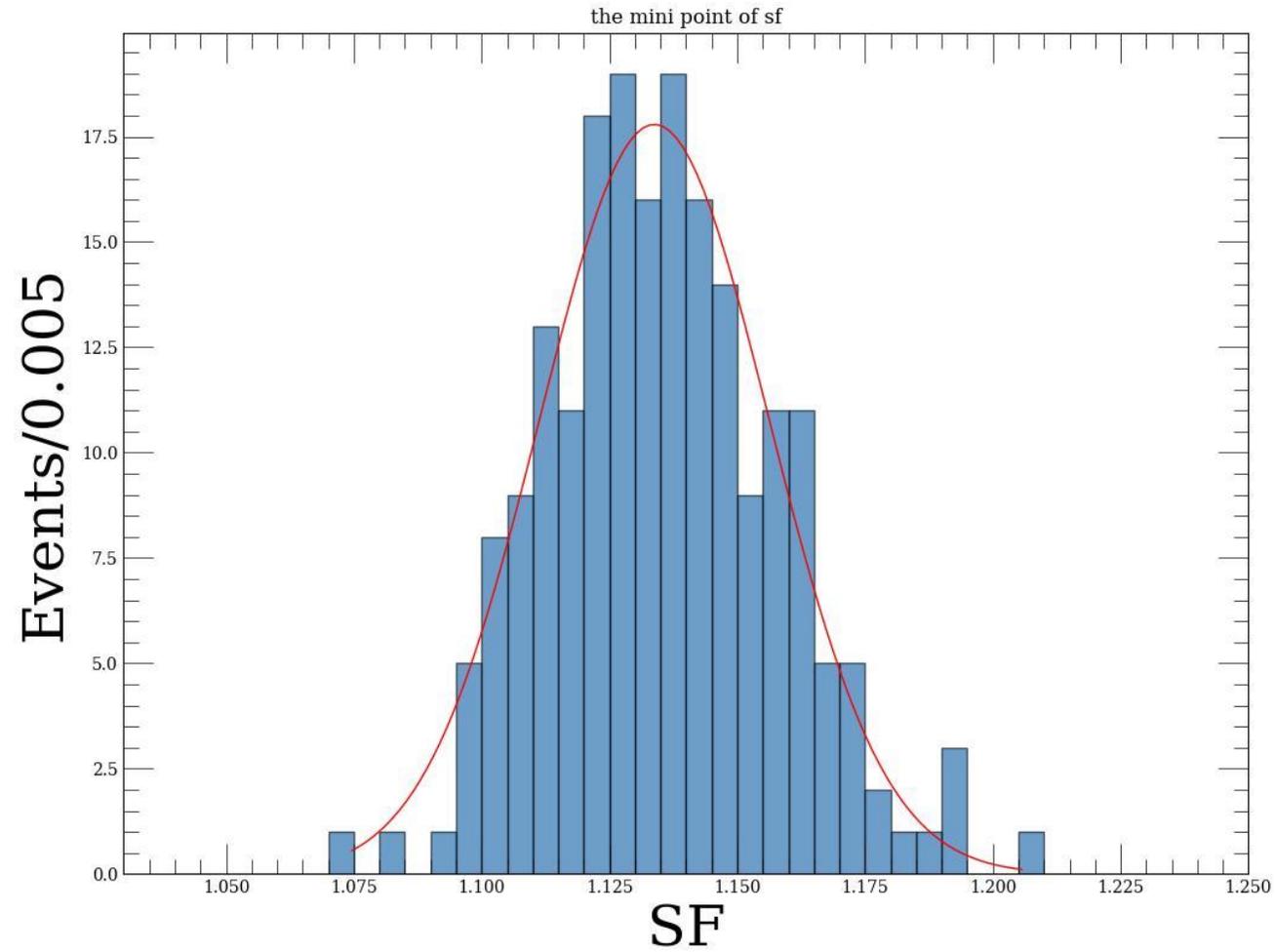
$$\lambda = 10^{-2}$$

组分约束对误差基本没有影响！

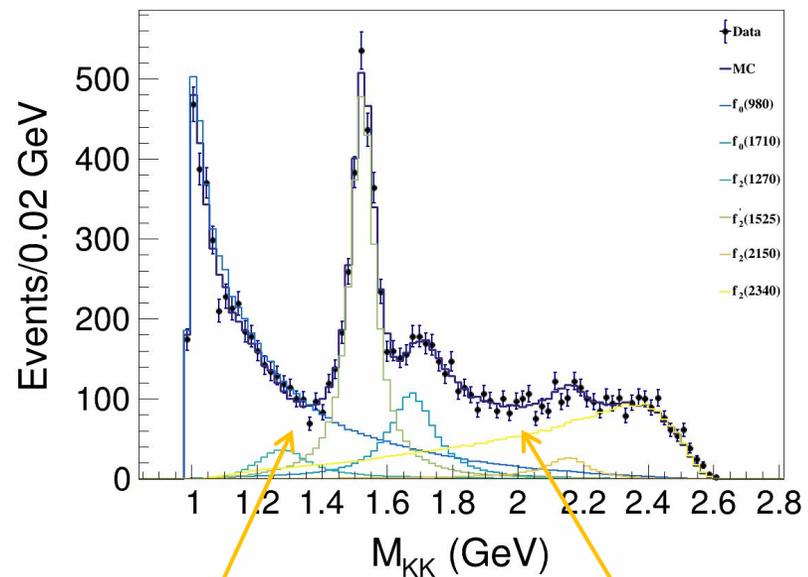
# 组分约束的性能



# 组分的涨落

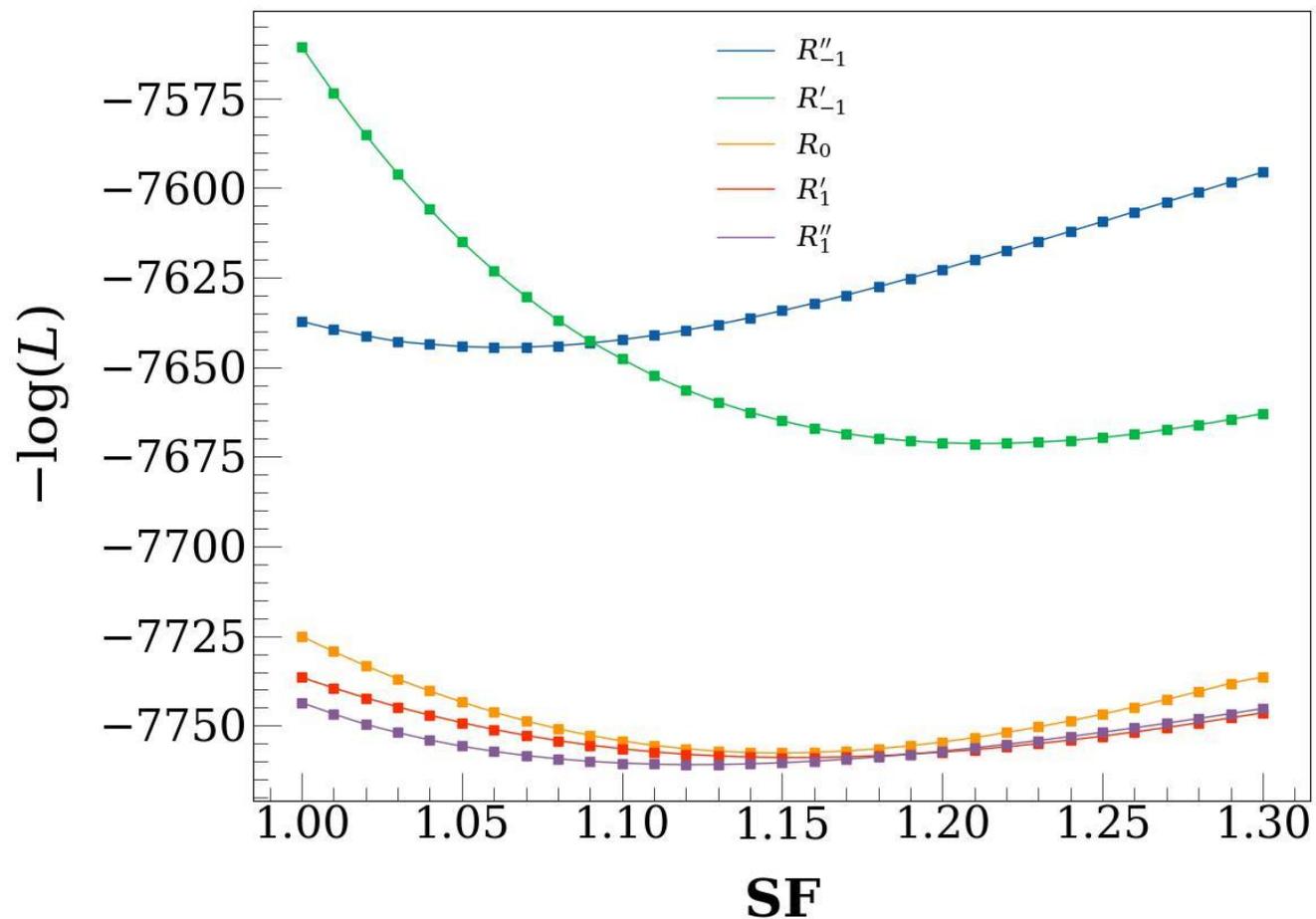


# 组分扫描



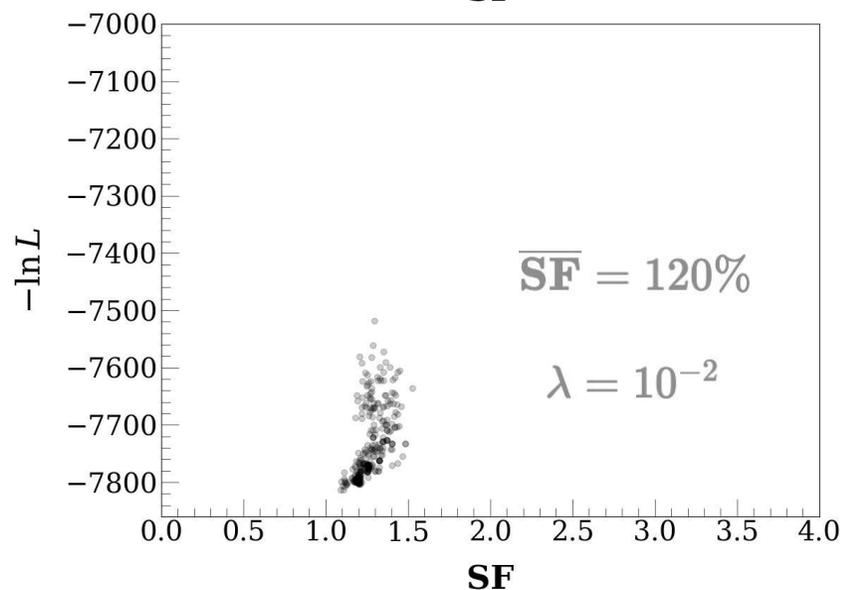
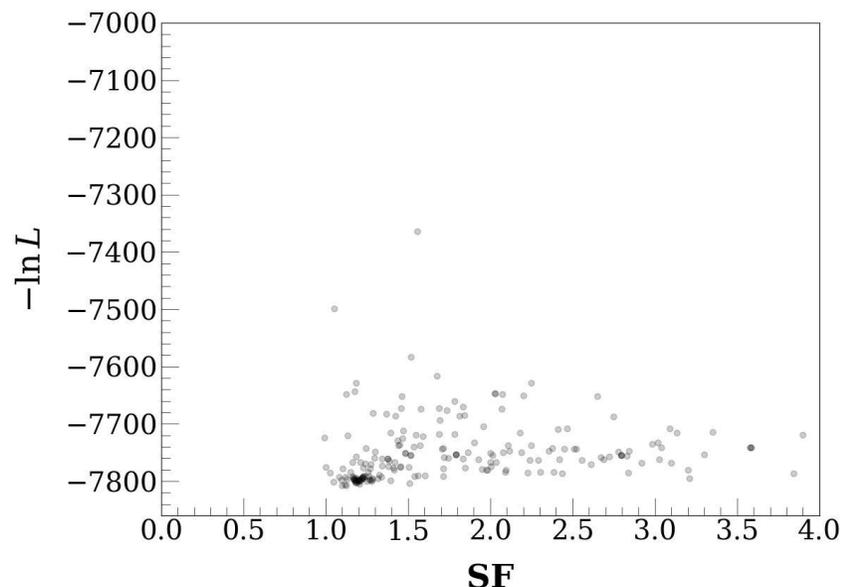
$f_0(1370)$

$f_2(2010)$



组分扫描的结果可以作为共振态选择的参考指标。

# 组分约束对多余共振态的抑制

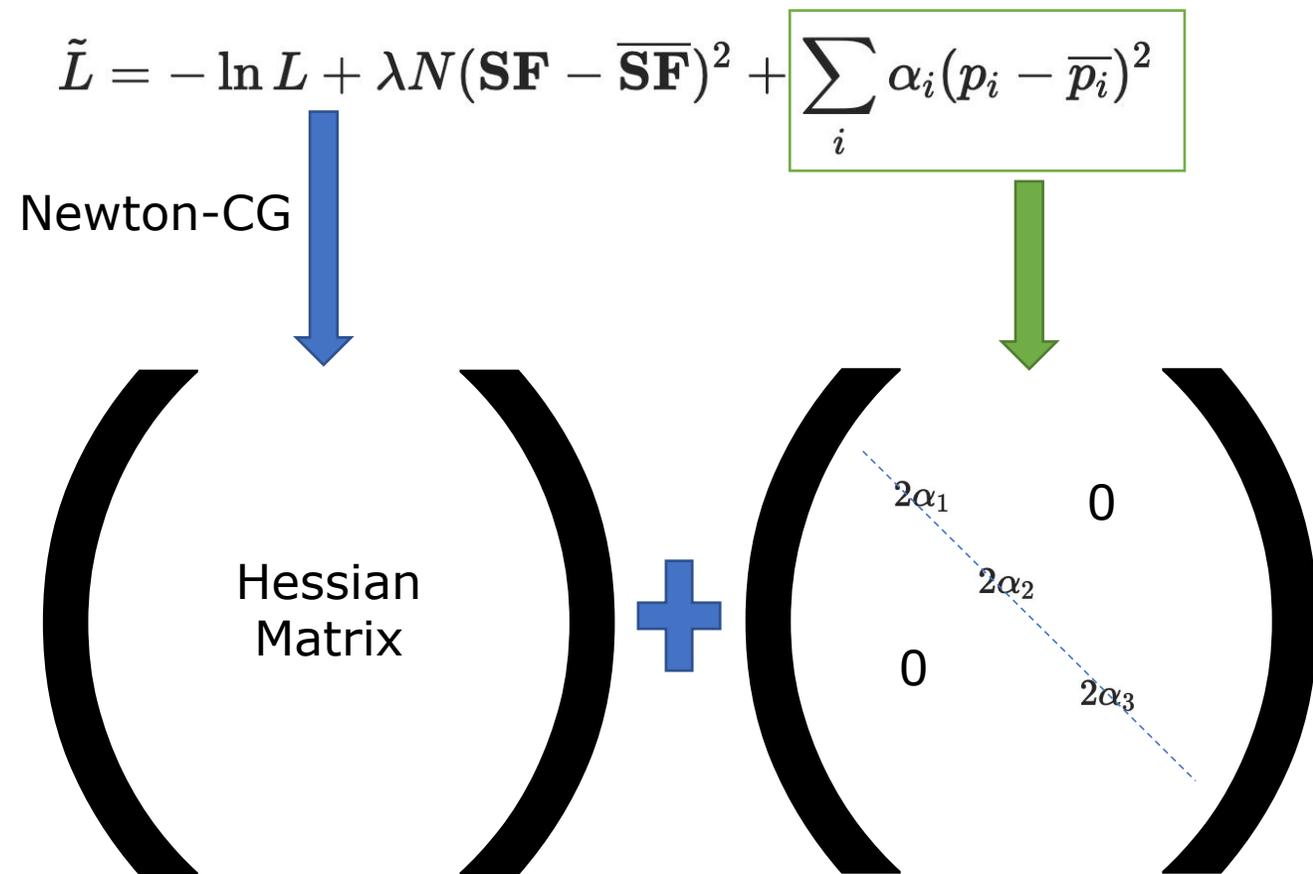
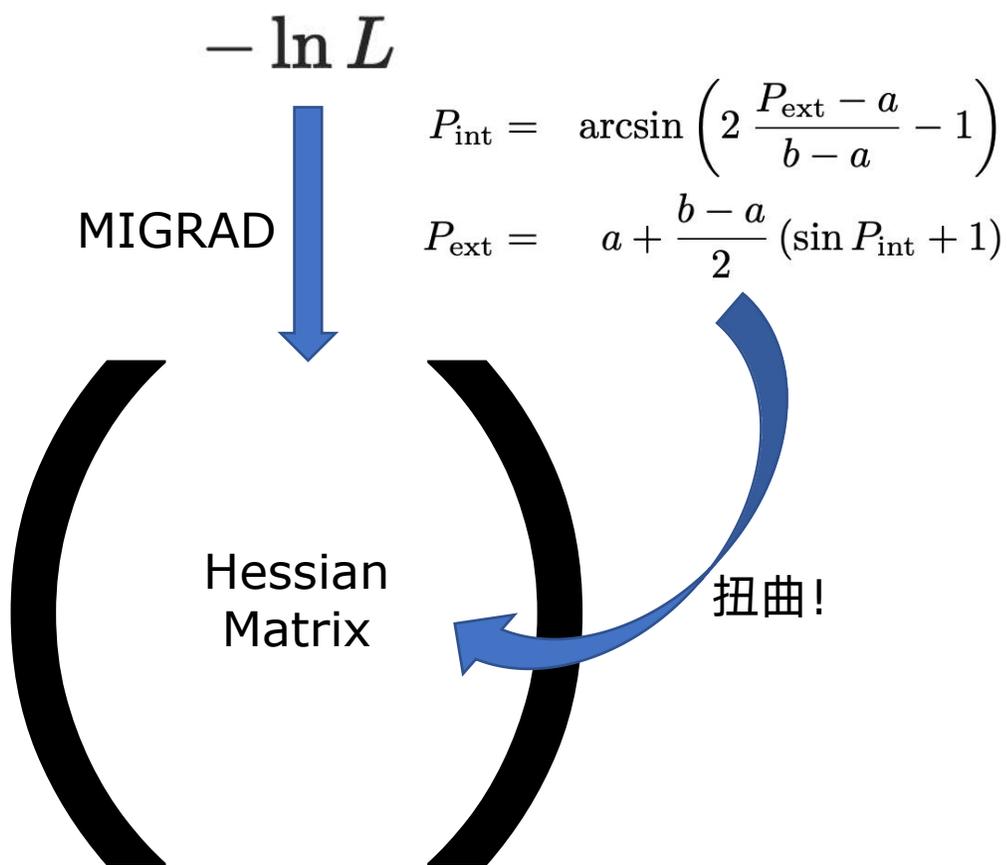


$$\lambda = 10^2, \overline{SF} = 115.0\%$$

Table 4: Results of fitting using the model  $R_{+4}$ .

	Name	$F_i$ (%)	Mass(GeV)	Width(GeV)
0	$f_2(2340)$	40.0	2.577	0.296
1	$f_0(980)$	34.3	1.007	0.094
2	$f_2'(1525)$	24.8	1.524	0.088
3	$f_0(1710)$	9.88	1.666	0.162
4	$f_2(1270)$	2.92	1.279	0.184
5	$f_2(2150)$	2.23	2.140	0.134
6	$f_2(2010)$	0.37	2.011	0.202
7	$f_0(1500)$	0.20	1.507	0.112
8	$f_0(1370)$	0.15	1.347	0.200
9	$f_2(1640)$	0.08	1.639	0.099
	<b>SF</b>	115.0		

# 参数约束与误差



$\alpha_i \rightarrow 0$  能够确保平滑过渡到标准误差矩阵!

# AI高精度蒙卡模拟研究现状

- 传统蒙卡模拟已被广范应用在高能物理事例产生当中，但在特定的物理过程及物理分析之中，蒙卡模拟由于其速度及计算资源限制，制约了相应的物理研究。部分高能物理学家考虑使用深度学习等技术来进行数据驱动式的快模拟
- 深度学习已在图像生成（如人脸，AI作画）以及文本生成（如AI自动对话，文章生成）领域已达到可实用的级别，计算机领域学者将图像，文本视为一种特定的高维分布问题，常规深度学习产生使用VAE和GAN进行数据驱动式的模型训练，在训练完成后则可高效完成所需目标。同时深度学习前沿考虑使用最优传输理论进行更为稳定的训练
- 高能物理学家已使用VAE，GAN在事例产生中作出一定成果，基本实现和目标高维分布大体趋势相同，但实际产生高维分布并不能达到同分布的实用要求，因此在做相关物理分析当中无法有效的代替蒙卡模拟

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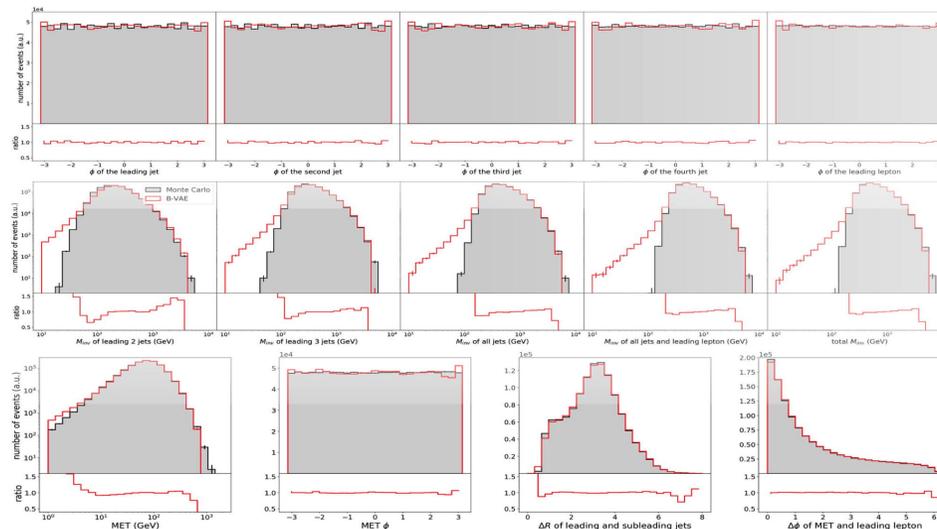
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## Event generation and statistical sampling for physics with deep generative models and a density information buffer

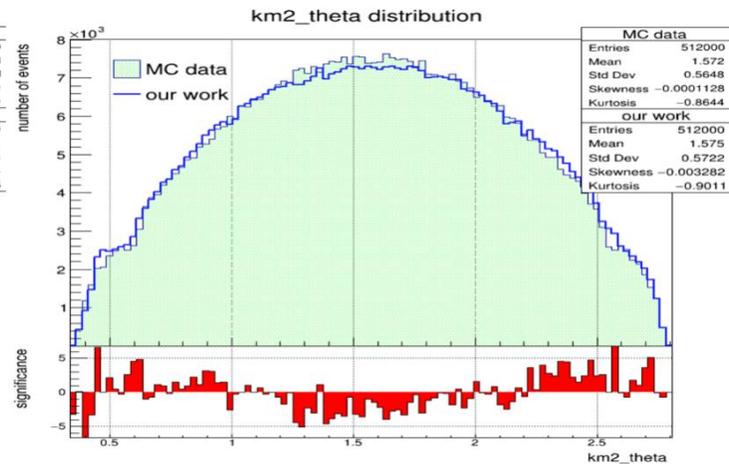
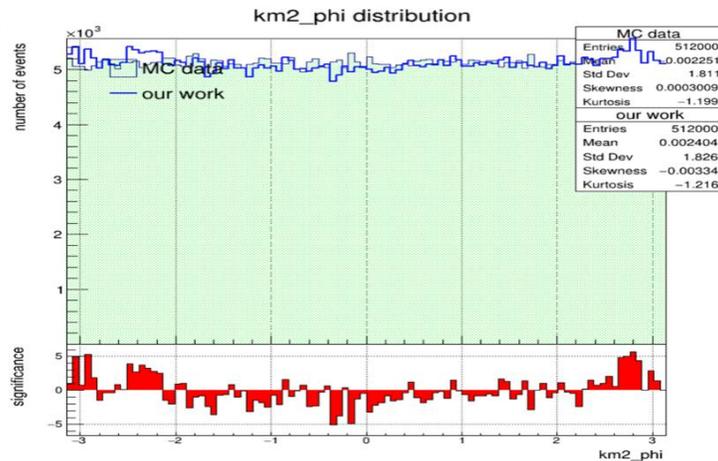
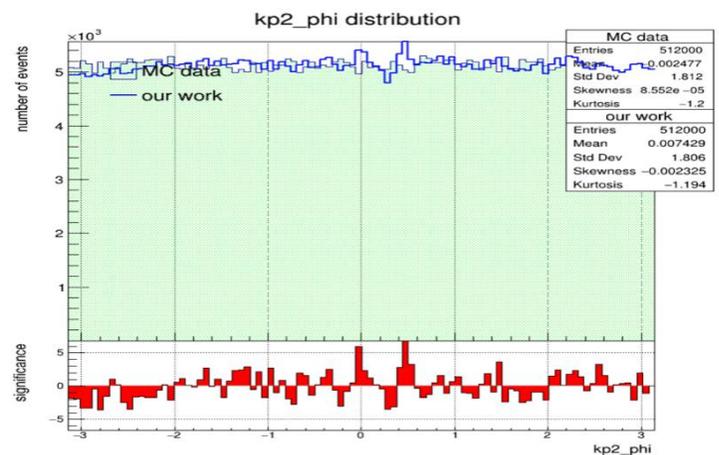
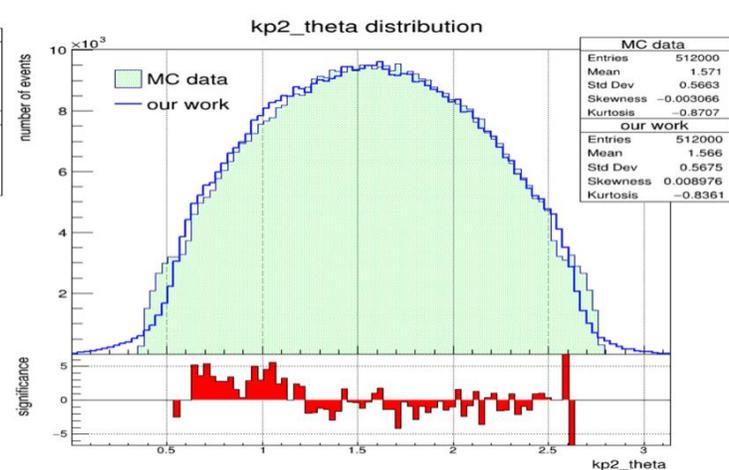
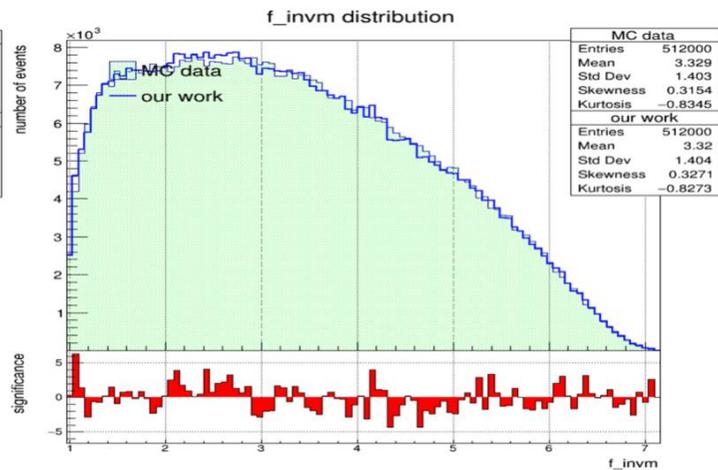
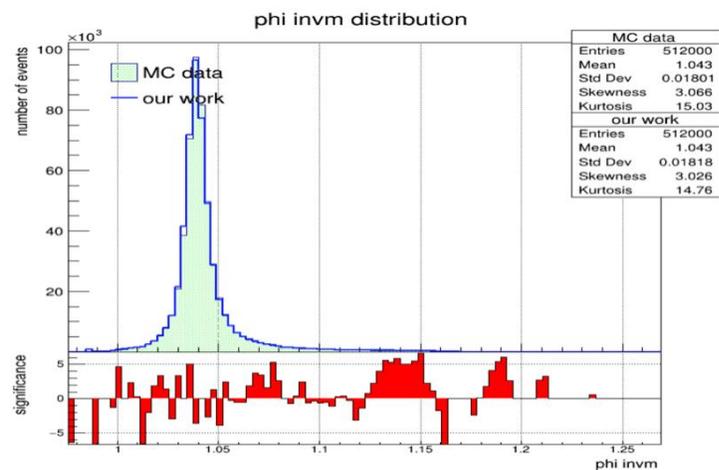
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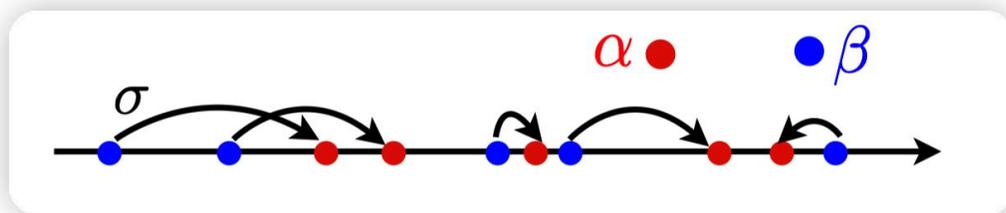
# 课题组早期工作



# 利用最优传输理论构造损失函数

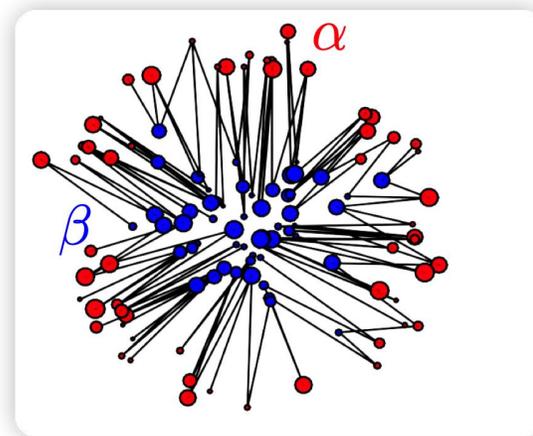
## □ 最优传输运输功

对两个高维分布样本A和B，我们可以计较从A如何最优的搬运到B的运输功，该功的物理意义则为两个高维分布的距离，从深度学习训练角度，其也可以理解为一个连续可微的损失函数，并已被验证为有极优的收敛性质



## □ 训练步骤

1. 从目标分布中进行随机抽样作为单次迭代的训练目标
2. 输入随机种子进入注意力模型，产生结果
3. 计算二者的最优传输运输损失
4. 更新模型参数，循环以上步骤直至收敛



# 注意力机制与分布变换

## □ 注意力机制

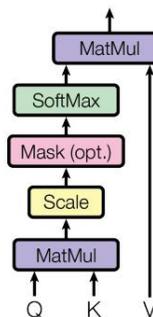
使用注意力机制，我们可以使模型更加关注不同物理量之间的相互关系，相对于全连接神经网络以及卷积神经网络在事例产生当中有着很大的优势

## □ 分布变换

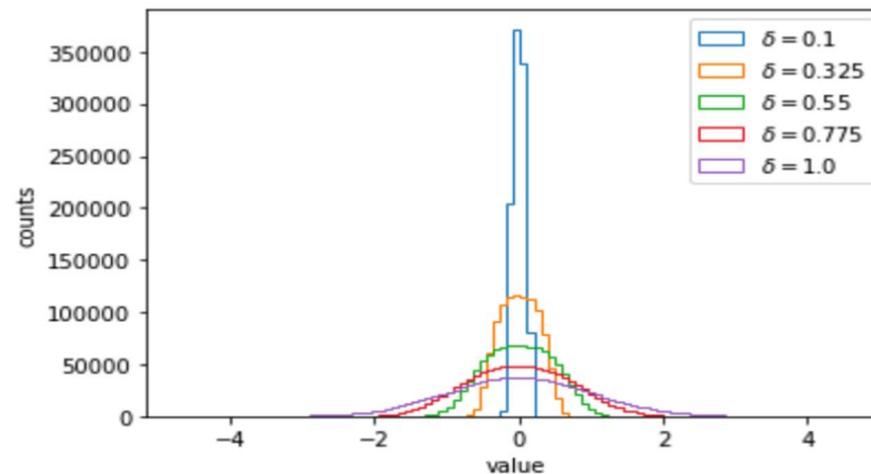
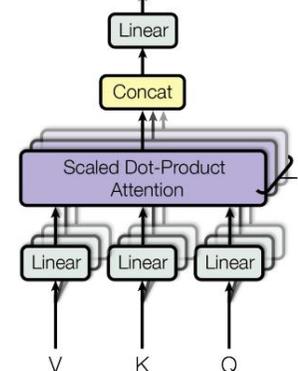
我们针对神经网络对高峰度的物理量（如个别粒子的质量）进行有效的产生的问题，从数学上进行变换，使产生器实际产生低峰度物理量，再人为转换即可有效解决

$$Z = \sinh \left\{ \epsilon + \delta \sinh^{-1} (X) \right\}$$

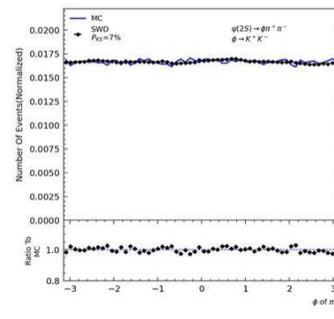
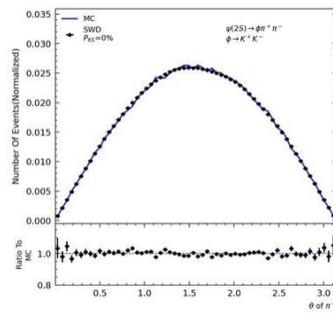
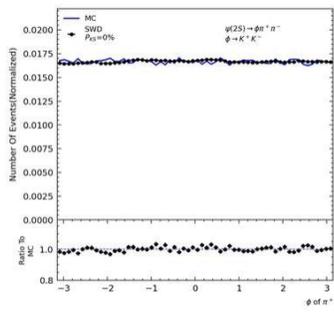
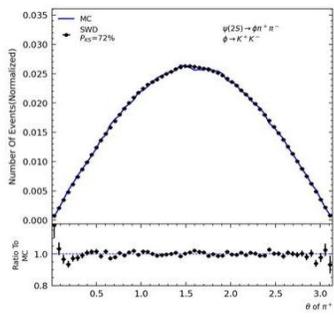
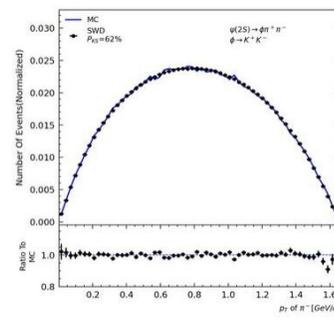
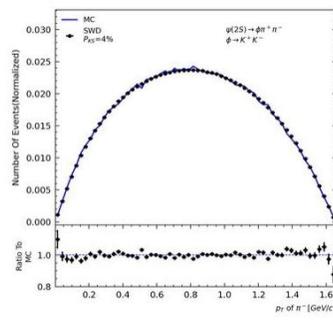
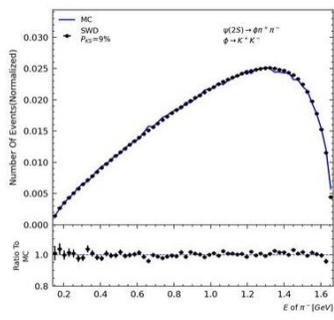
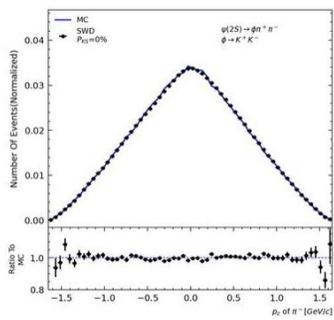
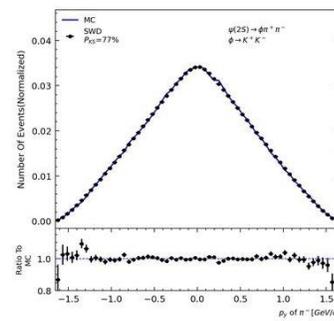
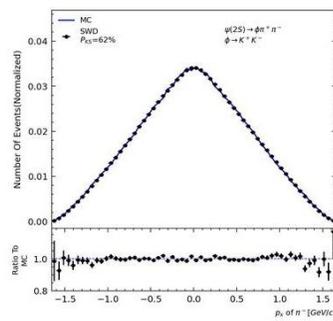
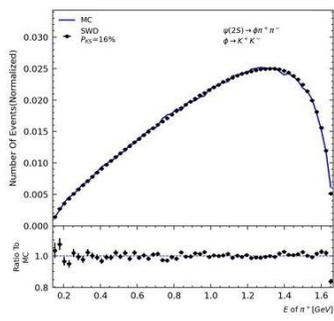
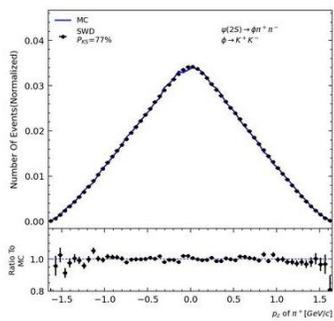
Scaled Dot-Product Attention



Multi-Head Attention

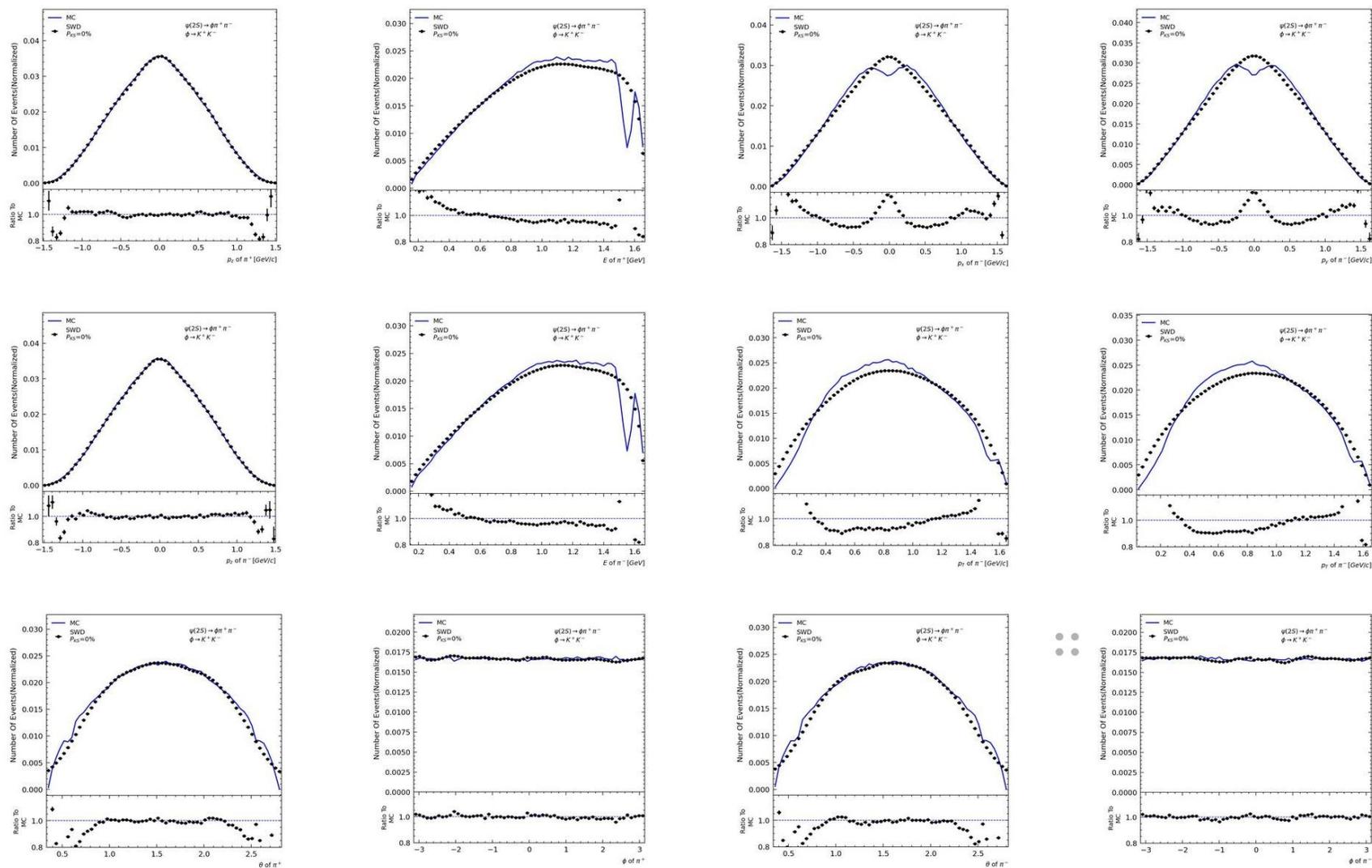


# 针对相空间产生子的模拟



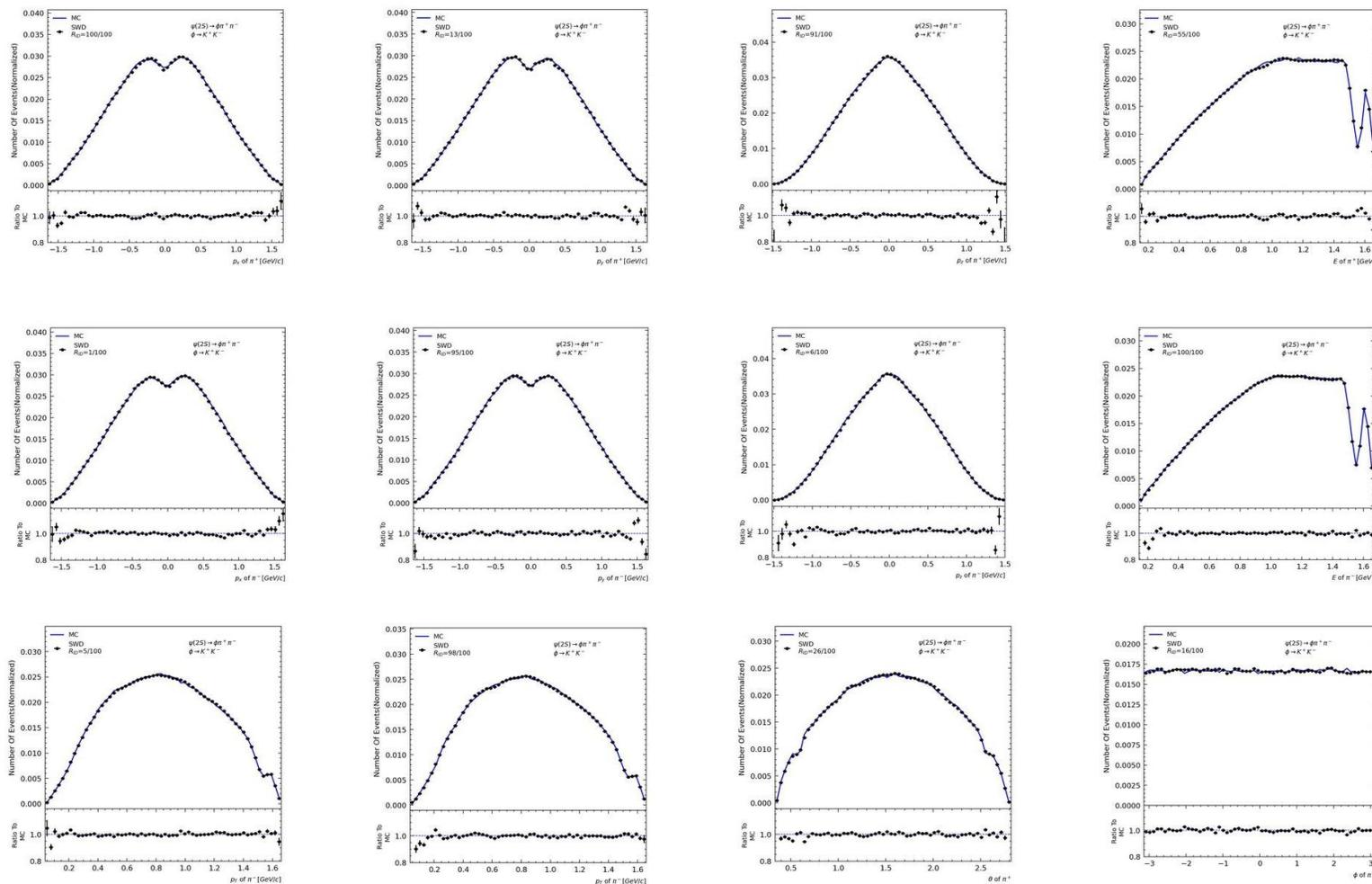
深度学习可以学习到数据分布特征，同时满足必要的物理约束。

# 探测效率对模拟的影响



探测器效率是高精度模拟的重要挑战!

# 高精度蒙卡模拟



修正的最优传输理论缔造了目前最高精度的AI数据模拟方法!

AI时代我们应该如何“计算/评估”高维数据的差异？



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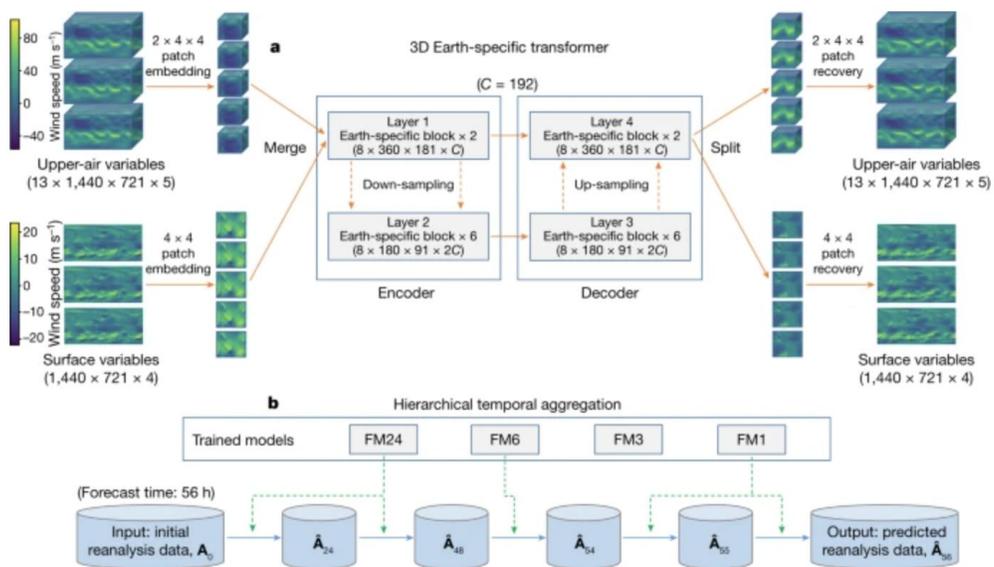
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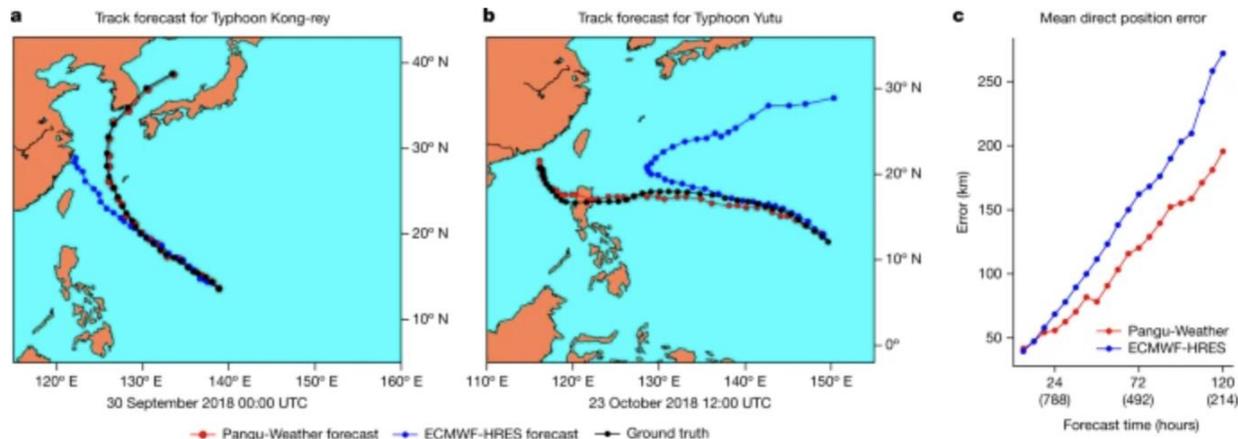
### Accurate medium-range global weather forecasting with 3D neural networks

[Kaifeng Bi](#), [Lingxi Xie](#), [Hengheng Zhang](#), [Xin Chen](#), [Xiaotao Gu](#) & [Qi Tian](#) ✉

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### 盘古气象大模型



## 高能物理实验大模型?

# 总结

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- 通过借鉴AI领域的思路方法，修正的最大似然函数能够帮助我们高效的解决分波分析中的极值搜索问题；

$$\tilde{L} = -\ln L + \lambda N(\mathbf{SF} - \overline{\mathbf{SF}})^2 + \sum_i \alpha_i (p_i - \bar{p}_i)^2$$

- AI能够我们解决大统计量分波分析中的一些关键技术问题；
- 高维数据处理方法的进步将从多方面推动高能物理的发展。

谢谢大家！