Machine learning-based line shape analysis of exotic hadron candidates

Denny Lane Sombillo

National Institute of Physics, University of the Philippines Diliman

LM Santos, VAA Chavez, DLBS, JPG (2025) 52 015104

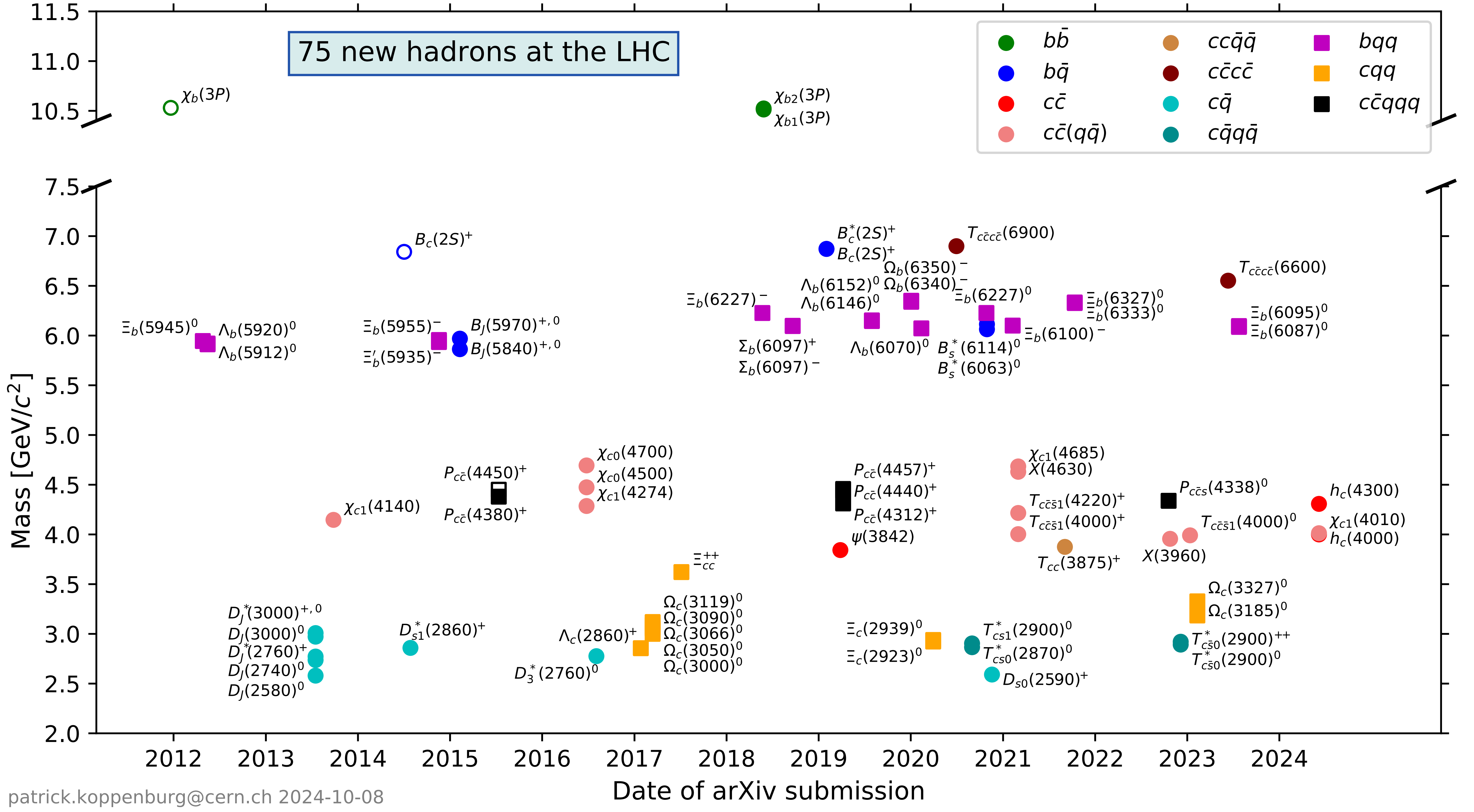
DAO Co, VAA Chavez, DLBS, arXiv:2403.18265 Accepted in PRD

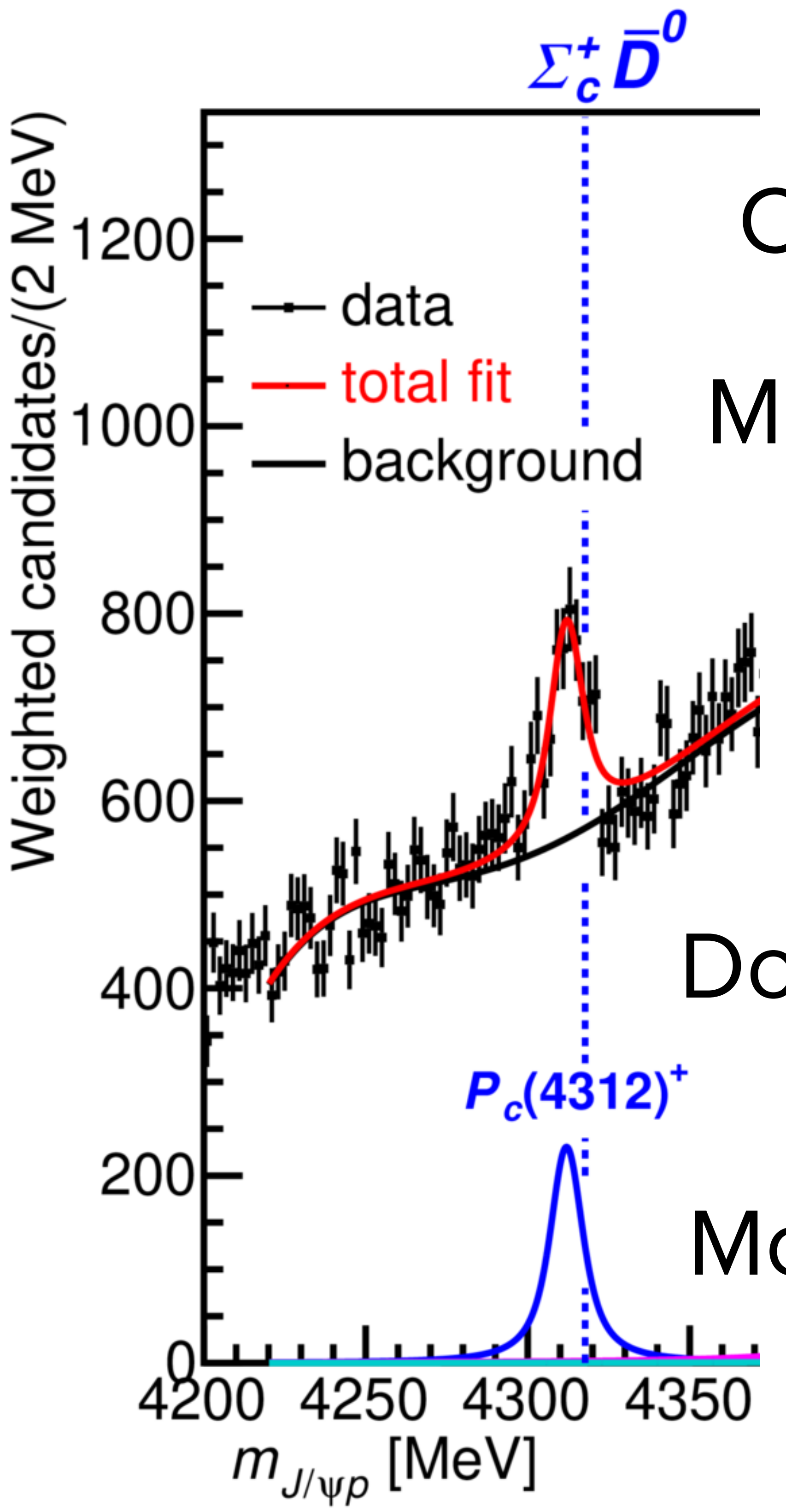
DLBS, Y Ikeda, T Sato, A Hosaka PRD 102 016024 (2020)
DLBS, Y Ikeda, T Sato, A Hosaka Few-Body Syst. 62, 52 (2021)

Hadron spectroscopy - line shape interpretation

- Many observations of possible new states.
- Some are near hadron-hadron thresholds.

- Experiments give us the line shape.
- How do we interpret/ classify them?





[LHCb, PRL 122 222001 (2019)]

Compact: [A Ali, AY Parkhomenko PLB 793 (2019)]

Molecular: [ML Du, V Baru, FK Guo, C Hanhart, UG Meißner, J A Oller, Q Wang PRL 124 072001 (2020)]

Virtual: [JPAC, PRL 123 092001 (2019)]

Double TS: [SX Nakamura, PRD 103 L111503 (2021)]

Molecule coupled to compact:

[Y Yamaguchi, H García-Tecocoatzi, A Giachino, A Hosaka, E Santopinto, S Takeuchi, M Takizawa, PRD 101 091502(R) (2020)]

Hadron spectroscopy - line shape interpretation

Why use machine learning in line shape analysis?

Line shape interpretation - classification problem

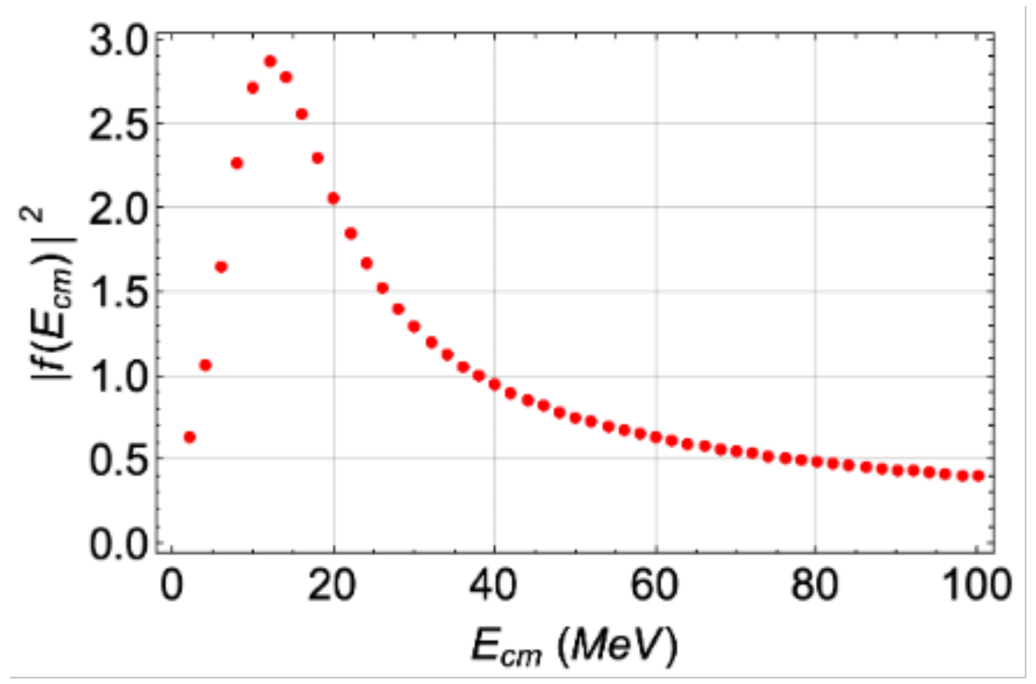
Deep neural network (DNN) as a universal approximator (universal map).

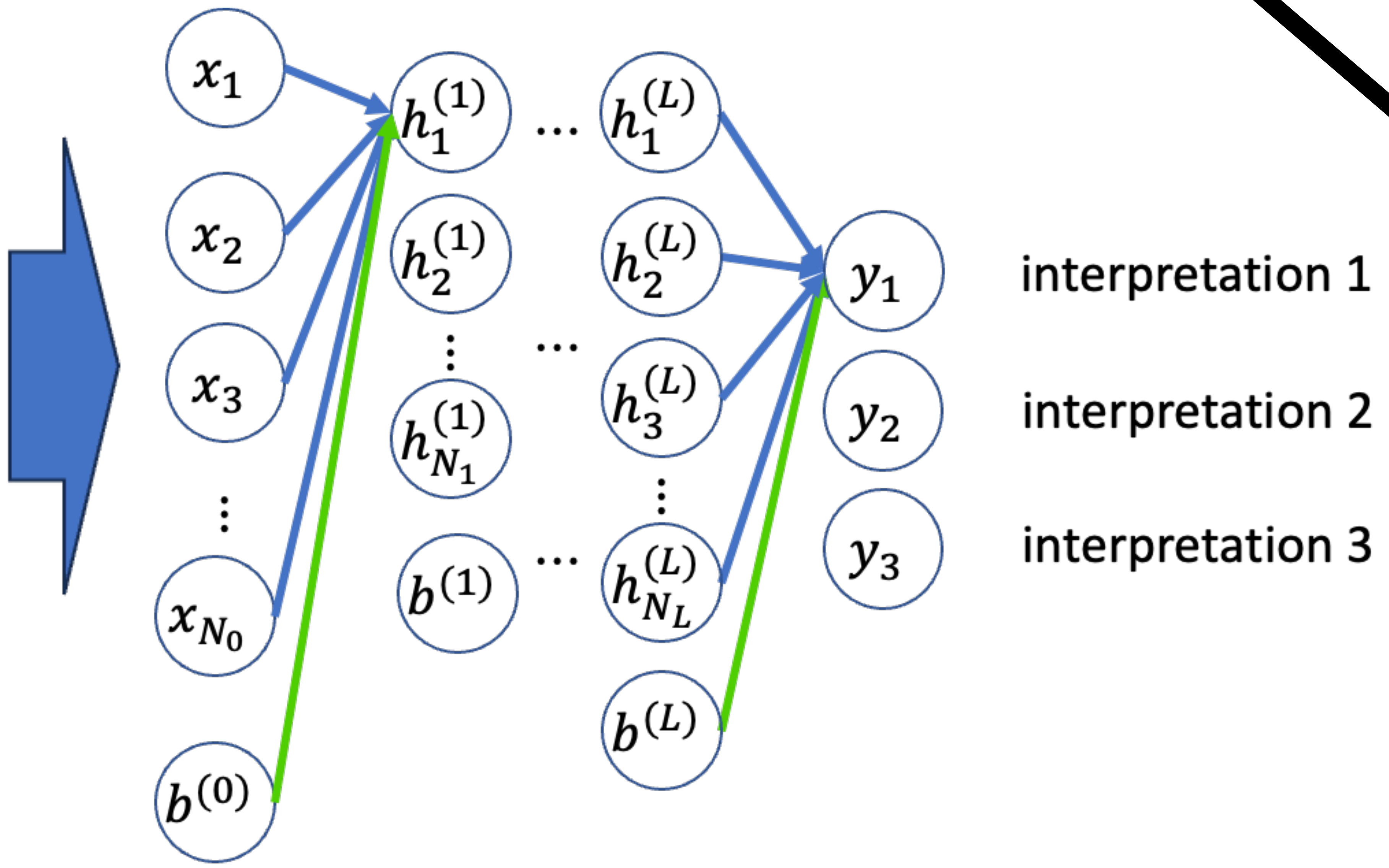
K Hornik, M Stinchcomber, H White, Neural Net., 2 5 (1989)

Linear transformation + non-linear activations and squashing

$$z_j^{(0)} = W_{ij}^{(0)} x_i + b_j^{(0)}$$
$$h_j^{(1)} = \mathrm{ReLU}(z_j^{(1)})$$
$$\vdots$$
$$z_j^{(n)} = W_{ij}^{(n)} h_i^{(n)} + b_j^{(n)}$$
$$h_j^{(n+1)} = \mathrm{ReLU}(z_j^{(n)})$$
$$\vdots$$
$$z_j^{(L)} = W_{ij}^{(L)} h_i^{(L)} + b_j^{(L)}$$
$$y_j = \frac{\exp(z_j^{(L)})}{\sum_i \exp(z_i^{(L)})}$$

DNN can be trained to map input line shape space into output interpretation space.





Backpropagation to minimize the cost:

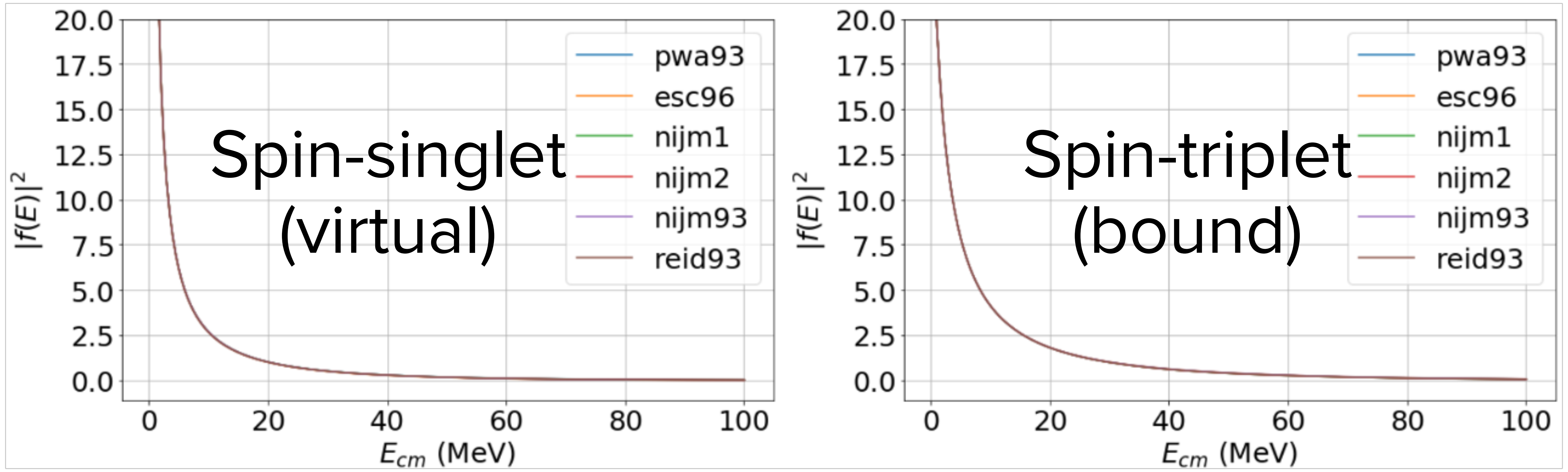
$$C\left(\hat{W}, \vec{b}\right) = \frac{1}{X} \sum_{\vec{x}}^{X} \vec{a}\left(\vec{x}\right) \cdot \log\left[\vec{y}_{W,b}\left(\vec{x}\right)\right]$$

DE Rumelhart, GE Hinton, RJ Williams, Nature 323, 533-536 (1986)

Deep learning: proof of principle

Benchmarked on the known nucleon-nucleon bound state

Given only the s-wave cross section, the origin of enhancement can be unambiguously identified.



For near-threshold pole:

$k \cot \delta \sim -1/a$ (constant)

$$|f(k)|^{-2} = |k \cot \delta - ik|^2 \sim \frac{1}{a^2} + k^2$$

Not possible to distinguish bound vs virtual pole enhancements.

S-matrix can have distant singularities on the unphysical sheet.

Use different (unitary, analytic) backgrounds to help DNN distinguish bound and virtual enhancements.

$$S(k) = \exp\left[2i\delta_{bg}(k)\right] \frac{k + i\gamma}{k - i\gamma}; \quad \delta_{bg} = \alpha \tan^{-1}\left(\frac{k}{\beta}\right)$$

Deep learning: proof of principle

DLBS, YI, TS, AH PRD 102 016024 (2020)
DLBS, YI, TS, AH Few-Body Syst. 62, 52 (2021)

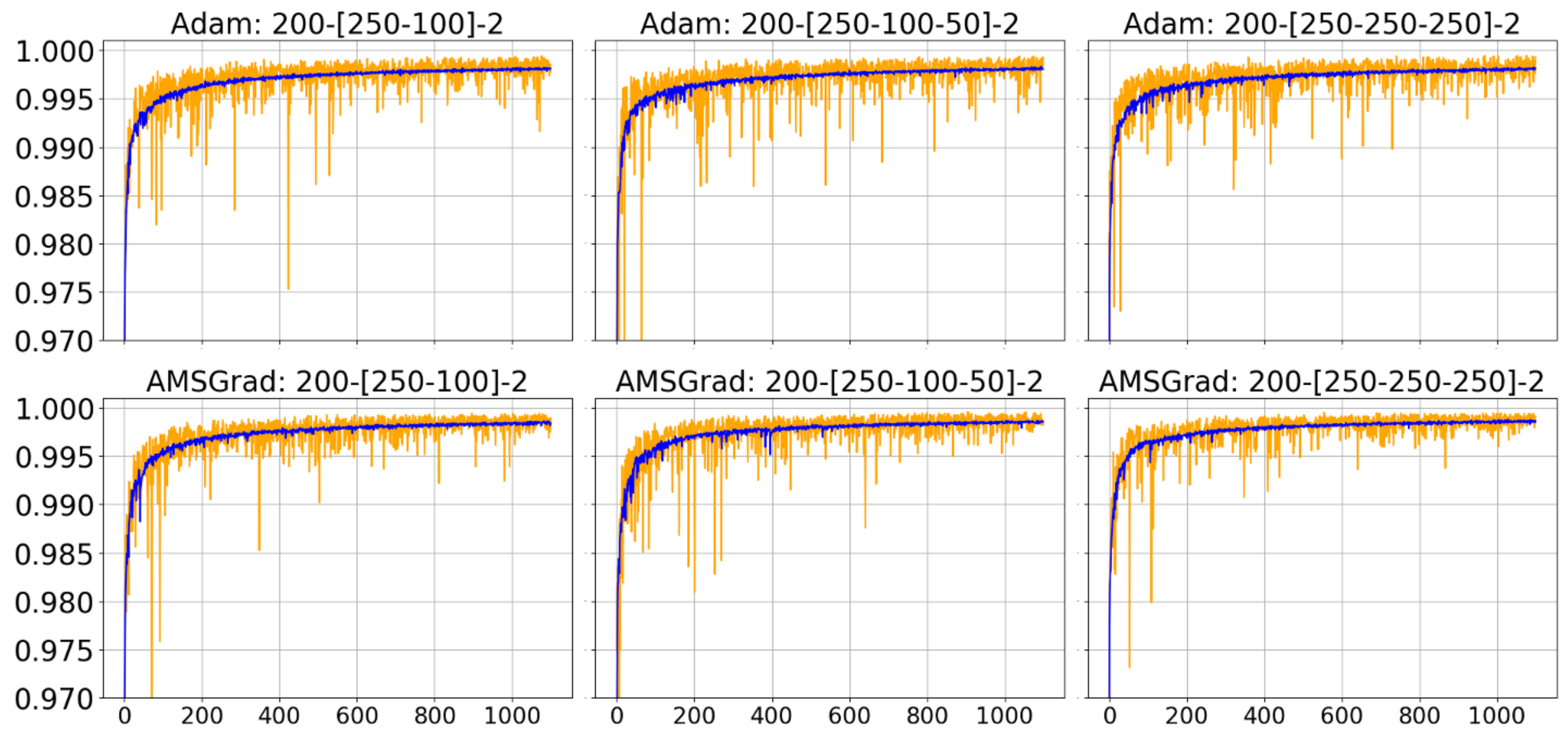
Optimize parameters of DNN using mock amplitudes:

$$S(k) = \exp\left[2i\delta_{bg}(k)\right]\frac{k+i\gamma}{k-i\gamma}$$

3,200,000 training data

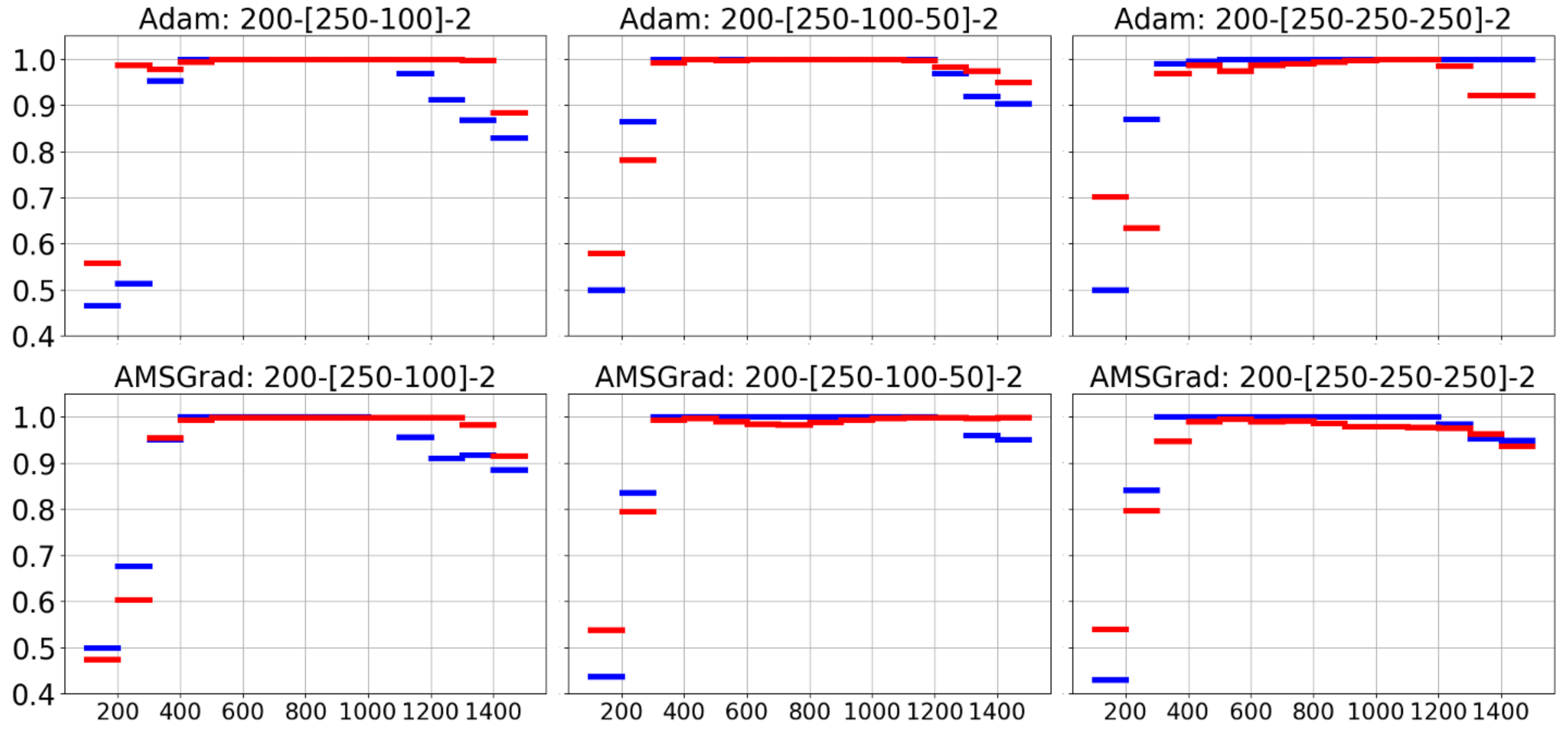
800,000 testing data

Accuracy vs training epoch

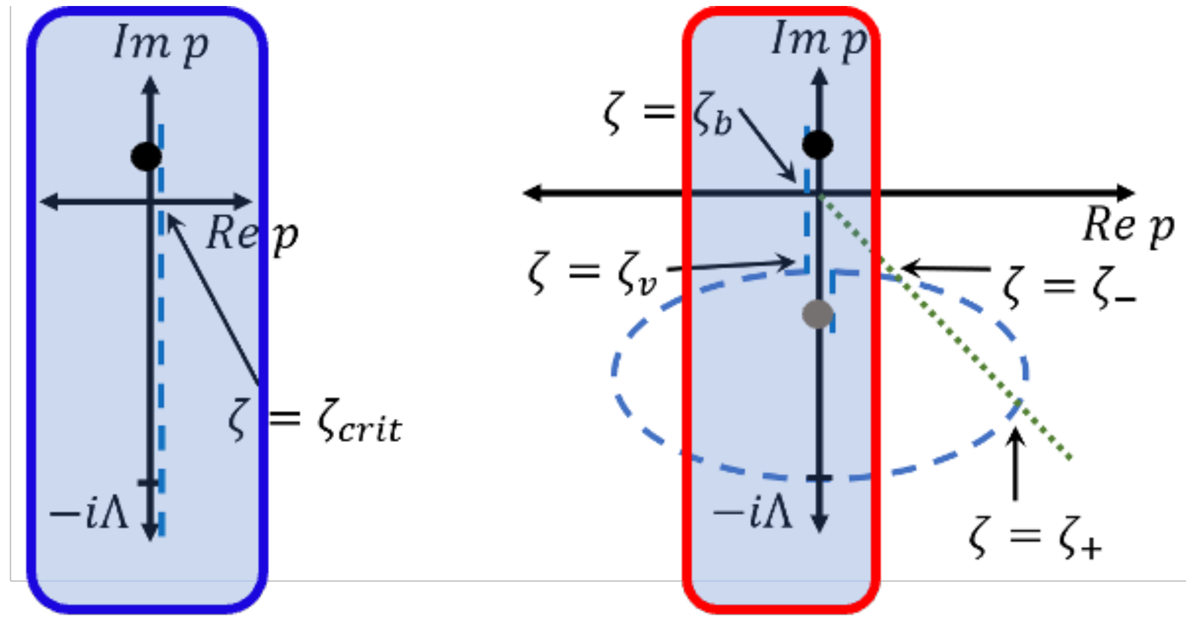


Validation using separable potential model

$$v(p,p') = \zeta\left(\frac{\Lambda^2}{p^2+\Lambda^2}\right)\left(\frac{\Lambda^2}{p'^2+\Lambda^2}\right)$$



Cut-off parameter Λ



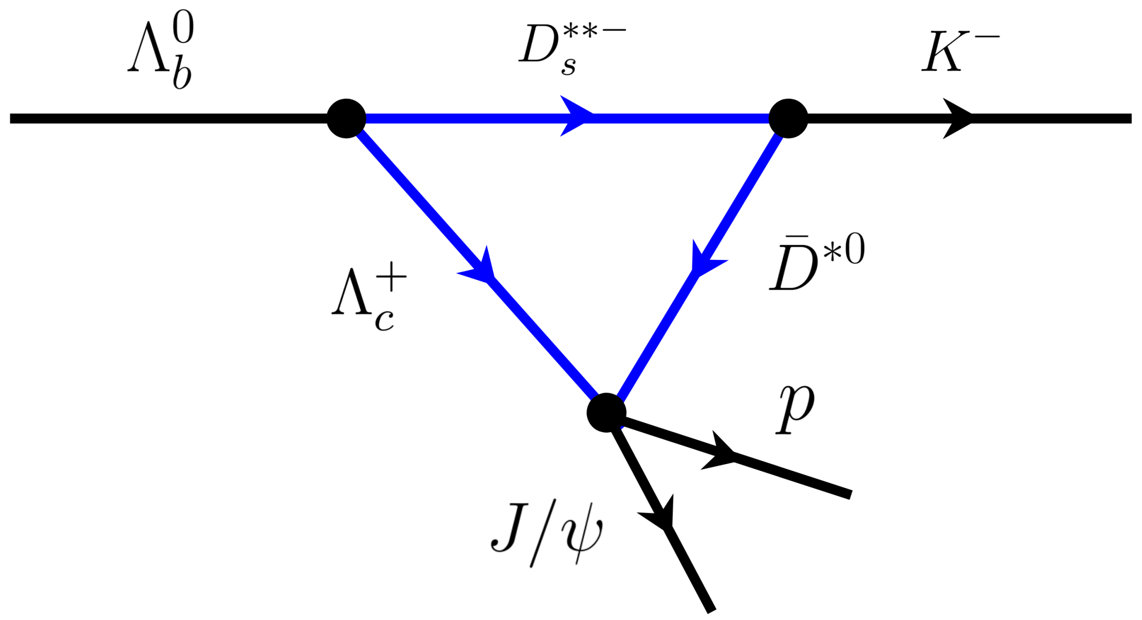
Energy independent coupling
$\zeta \to$ constant

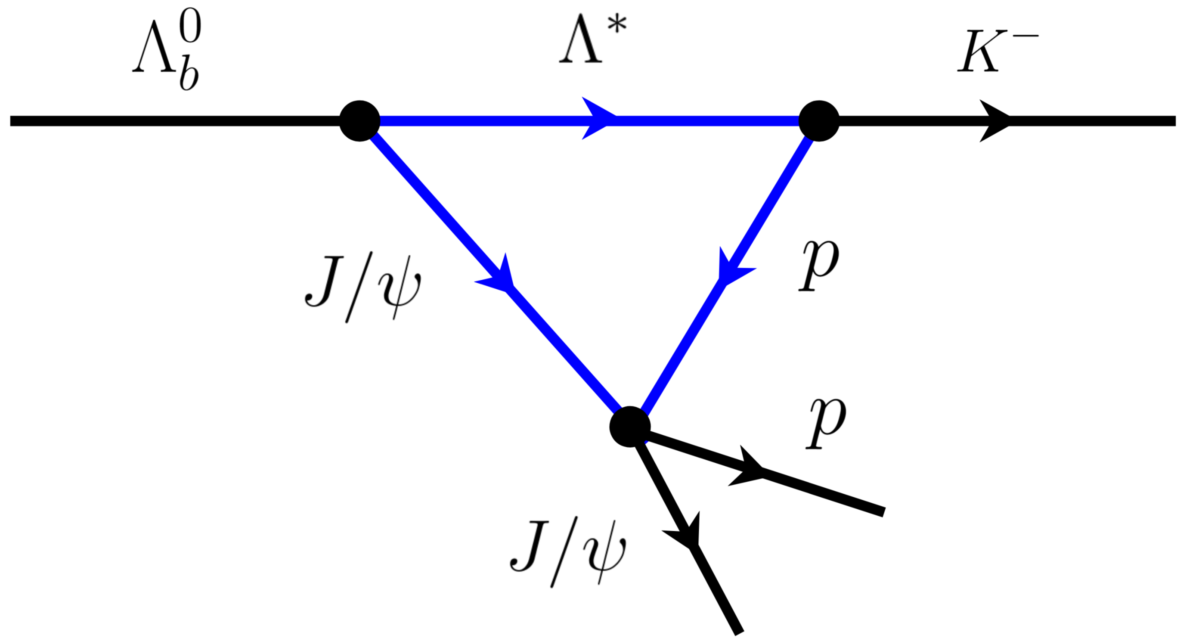
Energy independent coupling
$\zeta \to (E - M_{sep})\zeta$

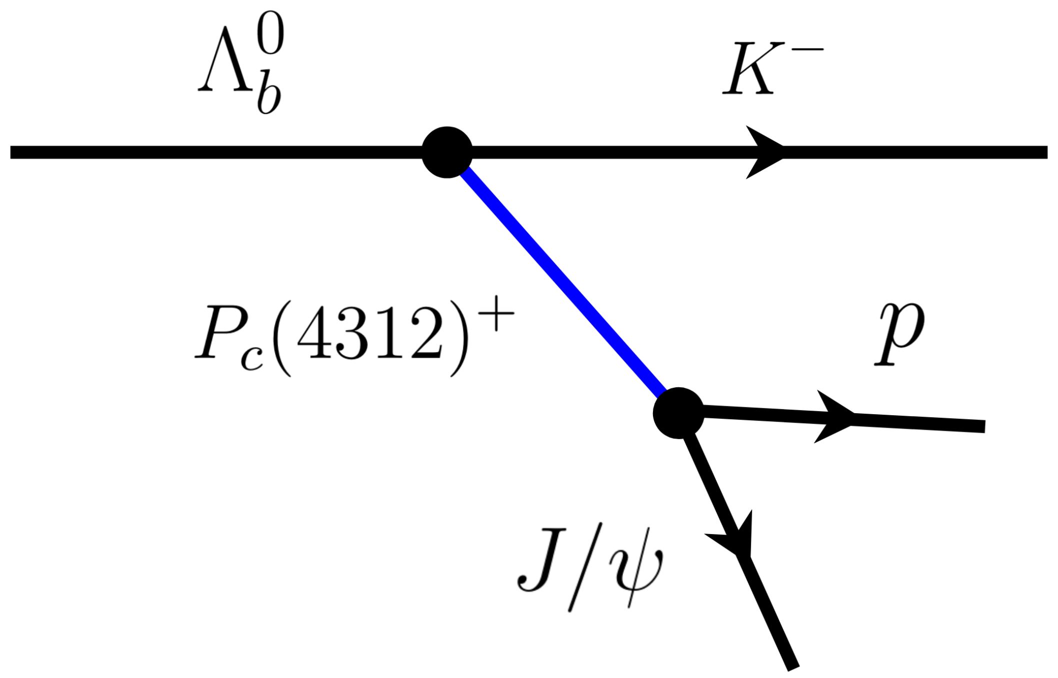
Trained and validated DNN deployed to probe the nucleon-nucleon

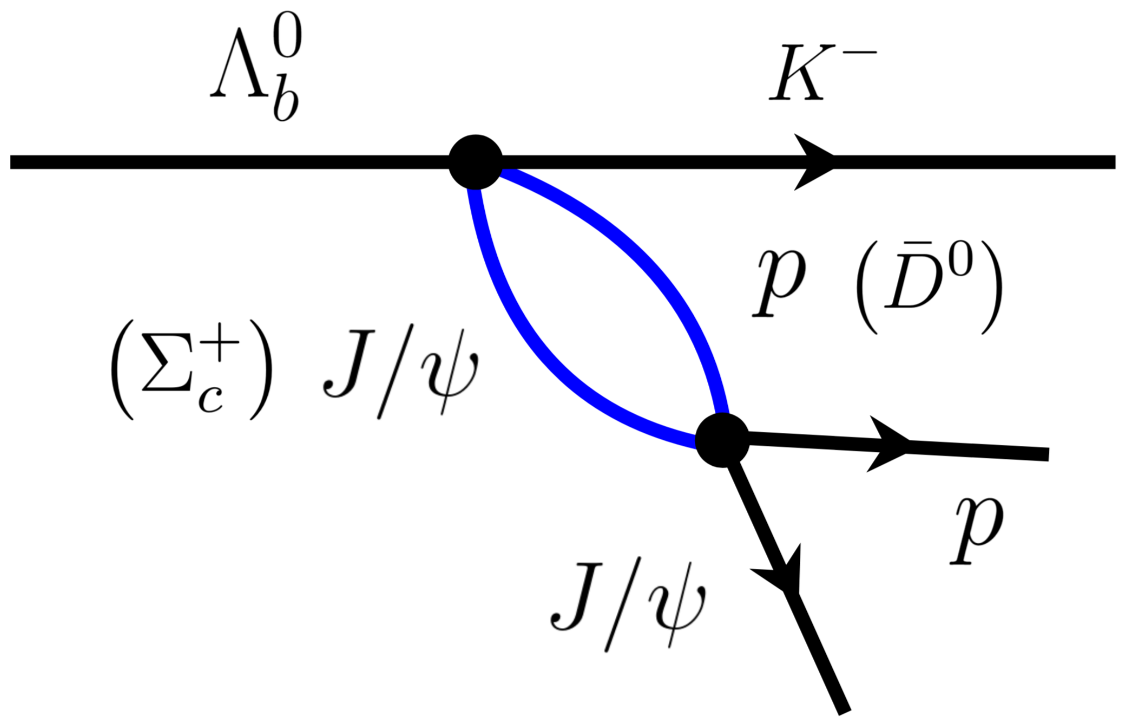
	PWA93	ECS96	NijmI	NijmII	Nijm93	Reid93
$^1S_0$	virtual	virtual	virtual	virtual	virtual	virtual
$^3S_1$	bound	bound	bound	bound	bound	bound

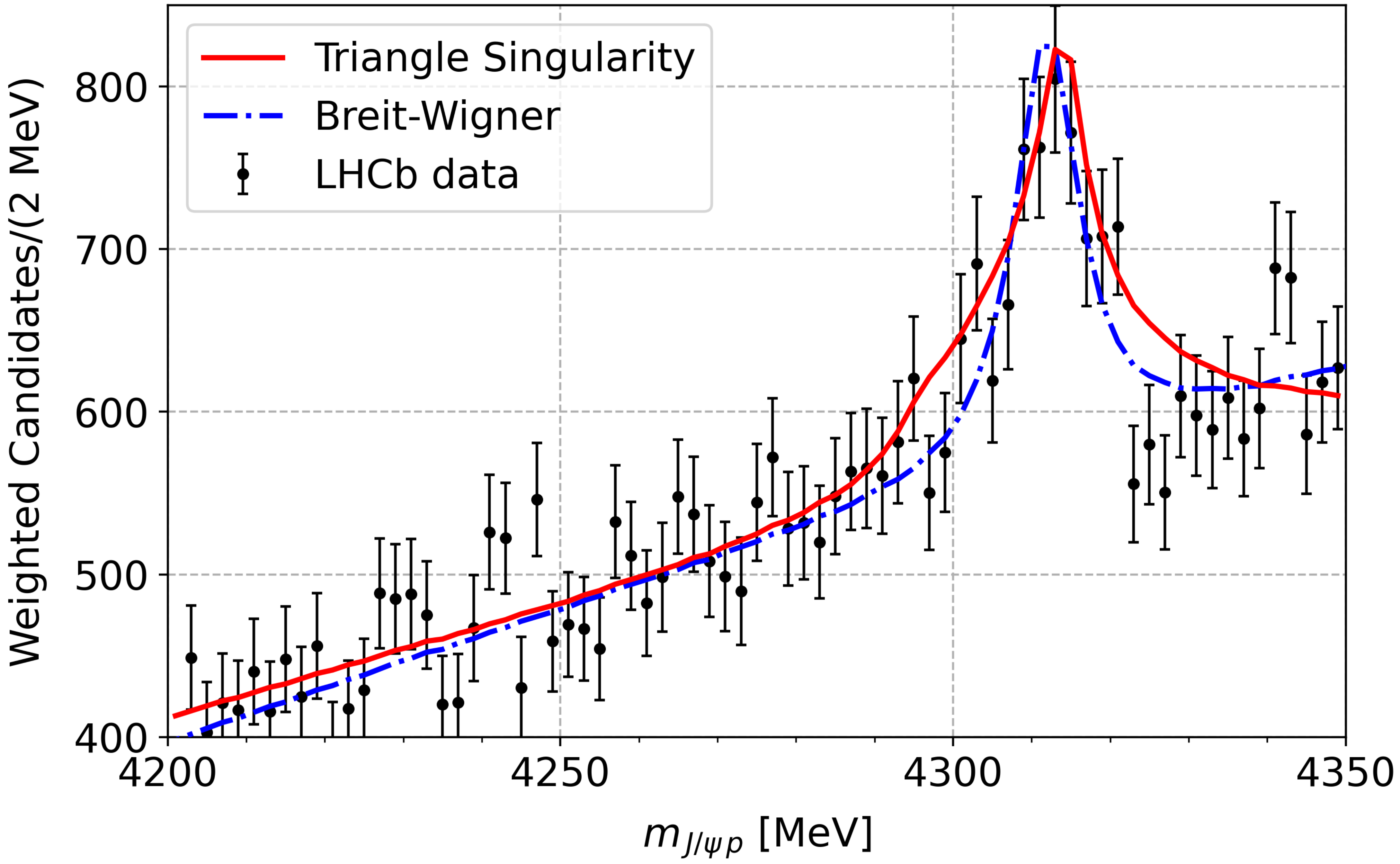
Kinematical vs Dynamical enhancements











Can we train a DNN to discriminate different origin of enhancements?

- Triangle mechanism
- Coupled-channel effects
- True resonance

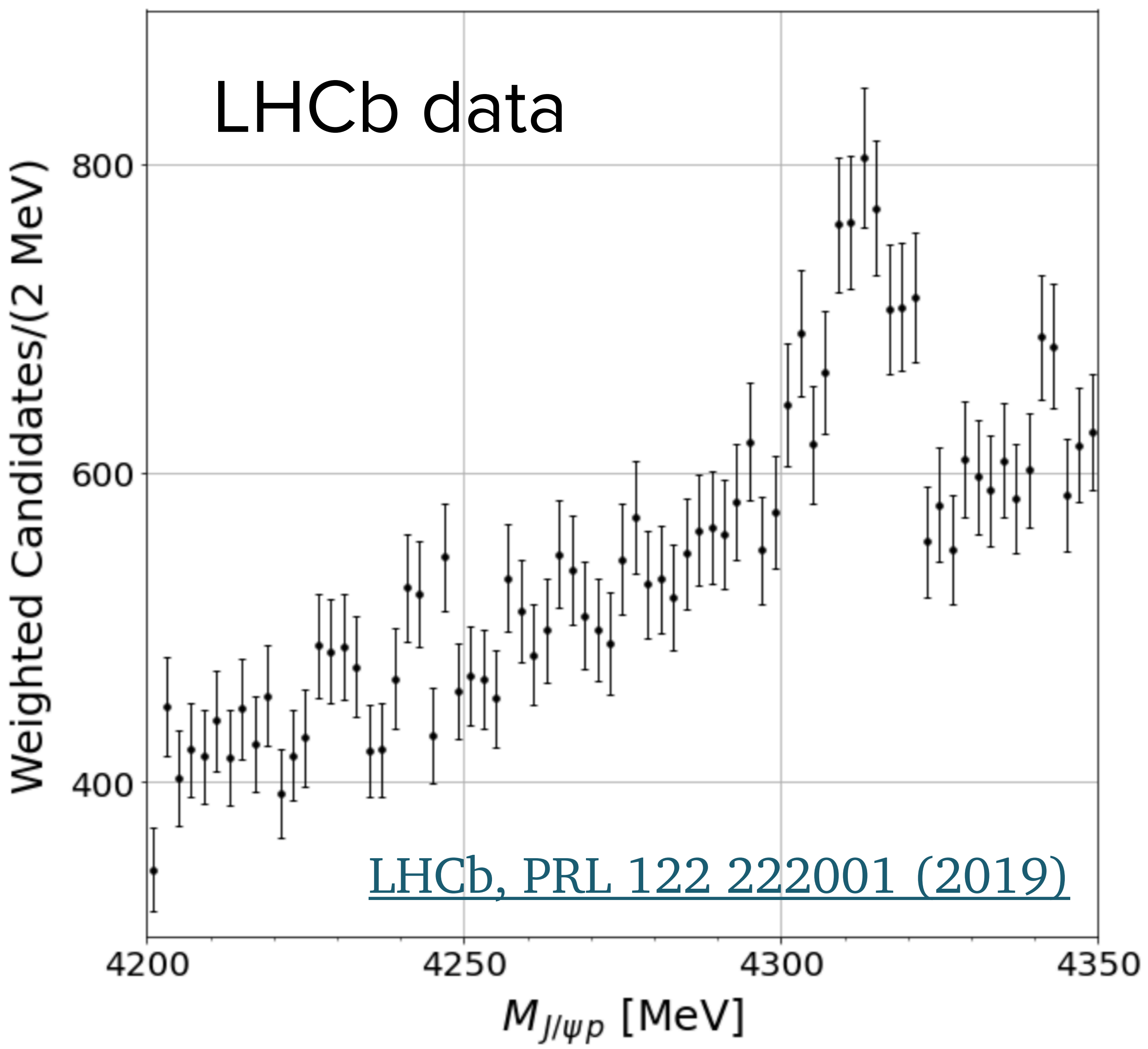
DAO Co, VAA Chavez, DLBS, arXiv:2403.18265
Accepted in PRD

If yes, then ML can supplement our analysis.

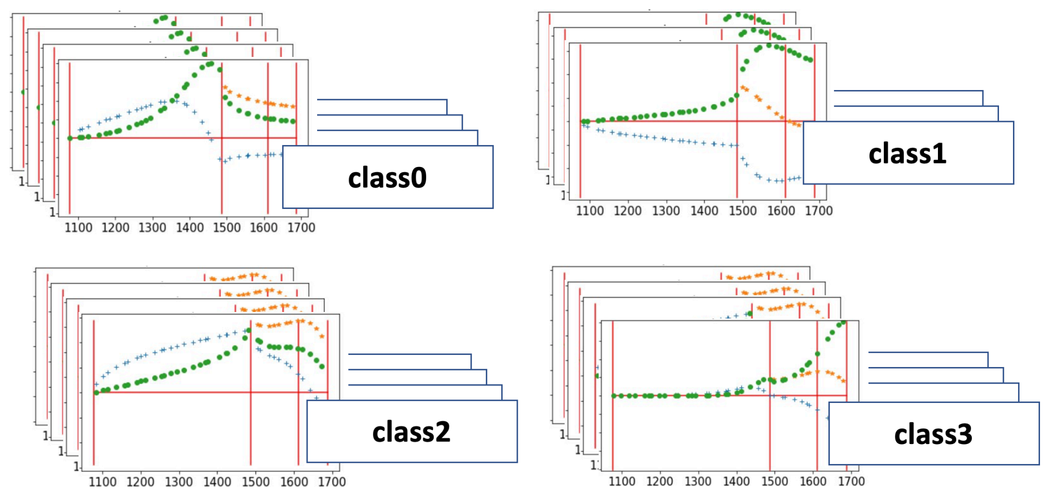
If no, then TS and pole enhancements are inherently ambiguous.

ML framework

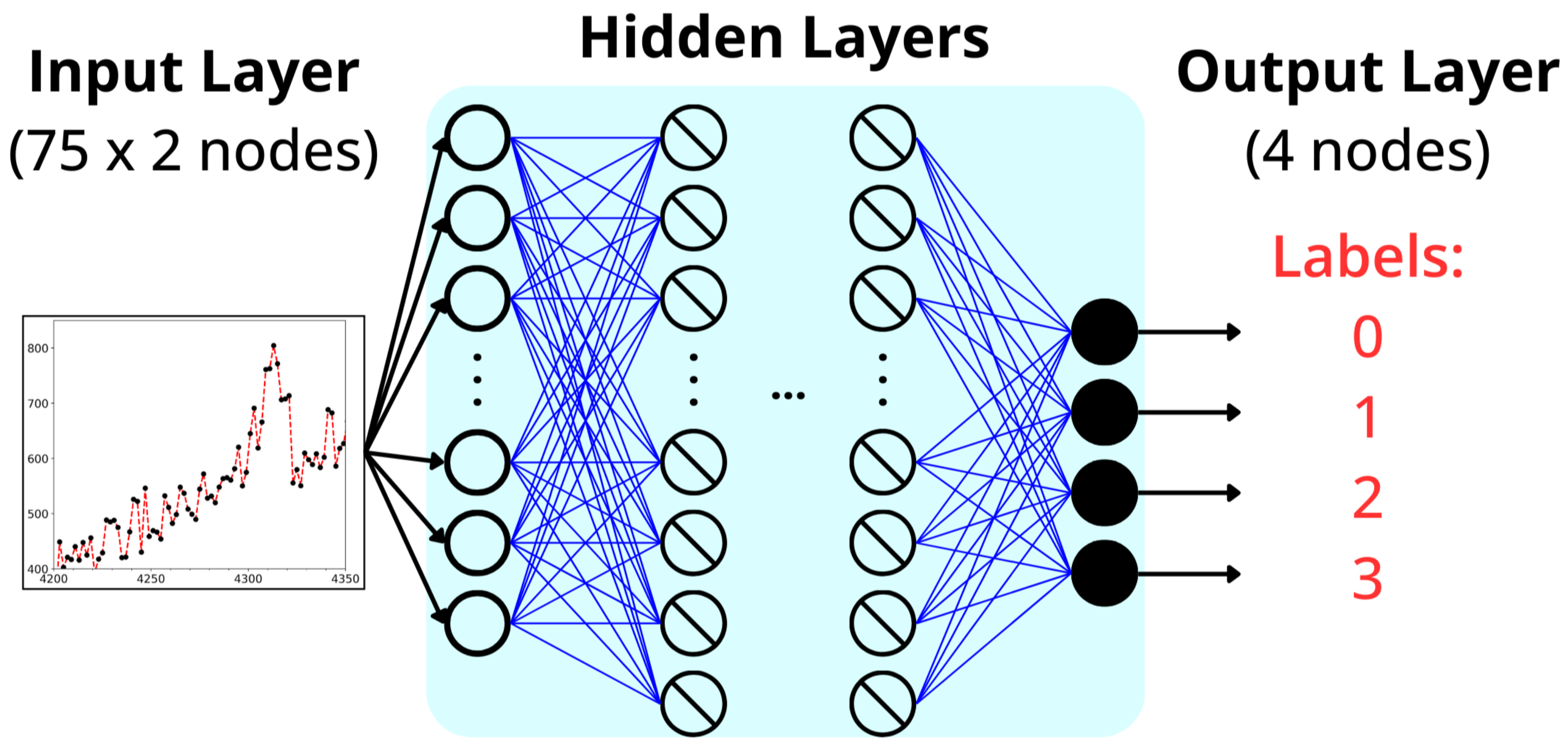
1. Choose the region of interest: [4200 MeV - 4350 MeV]



2. Generate the training dataset
- Triangle singularity
- Pole of S-matrix
  - 1 pole in 2nd RS
  - 1 pole in 4th RS
  - 1 pole each in 2nd and 3rd RS

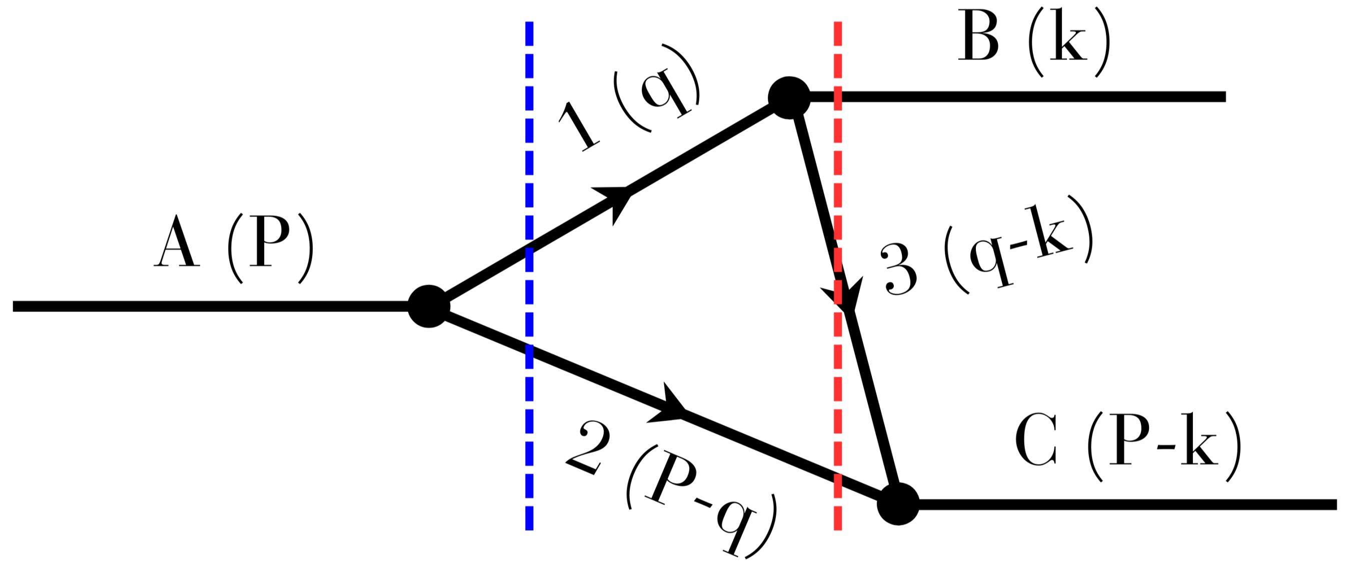


3. Design a set of DNN to solve the classification problem



4. Train, test, and validate the DNN
5. Use the trained DNN to interpret the experimental data

(Single) Triangle mechanism



$$I(k) \propto \int_0^\infty \frac{q^2 f(q)\, dq}{P^0 - \sqrt{m_1^2+q^2} - \sqrt{m_2^2+q^2} + i\epsilon}$$

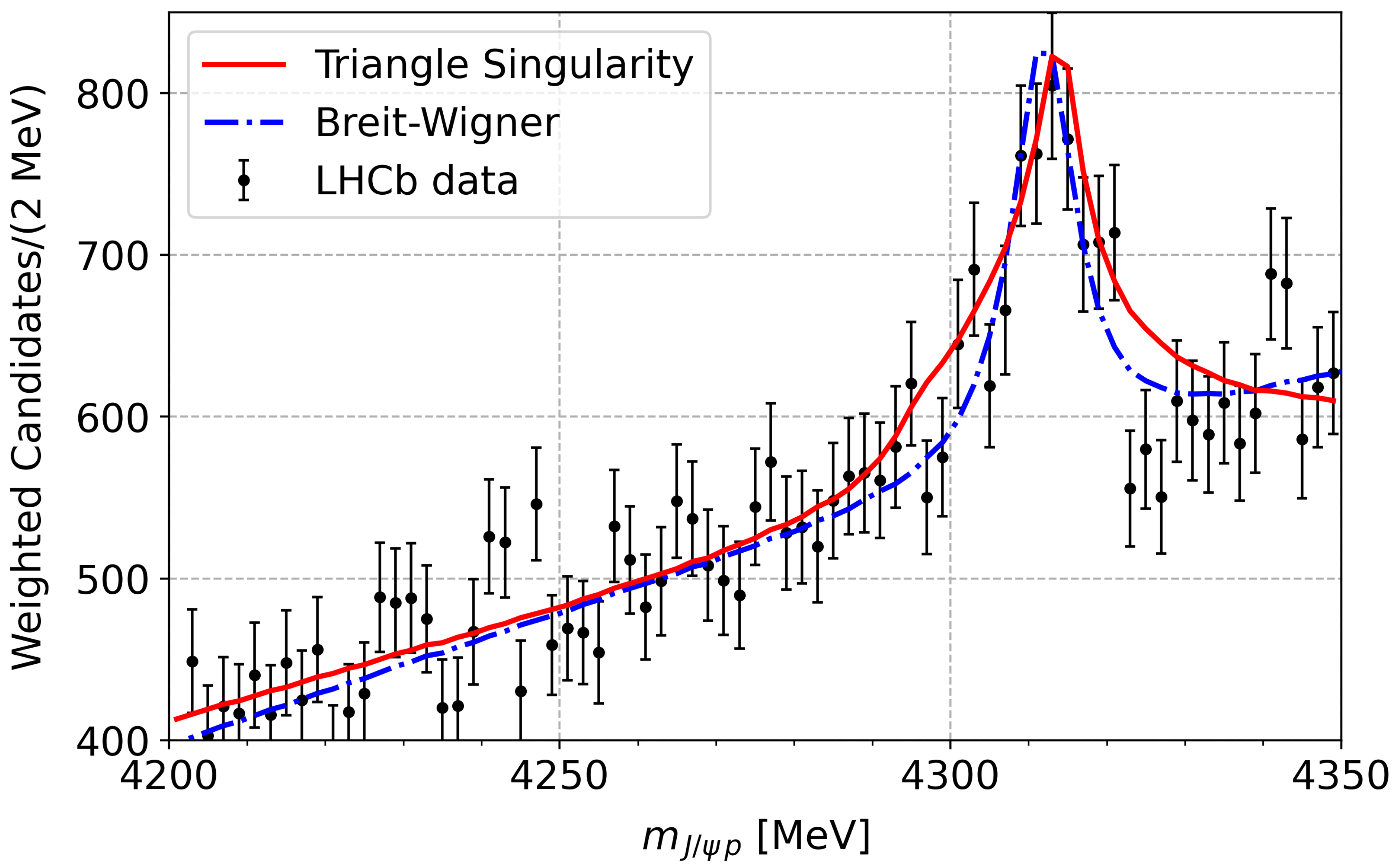
$$f(q) = \int_{-1}^{1} \frac{dz}{E_C - \omega(q) - \sqrt{m_3^2+q^2+k^2-2qkz} + i\epsilon}$$

M Bayar, F Aceti, FK Guo, E Oset, PRD 126 074039 (2016)

FK Guo, XH Liu, S Sakai, PPNP 122 103757 (2020)

The amplitude has no singularity (no pole)

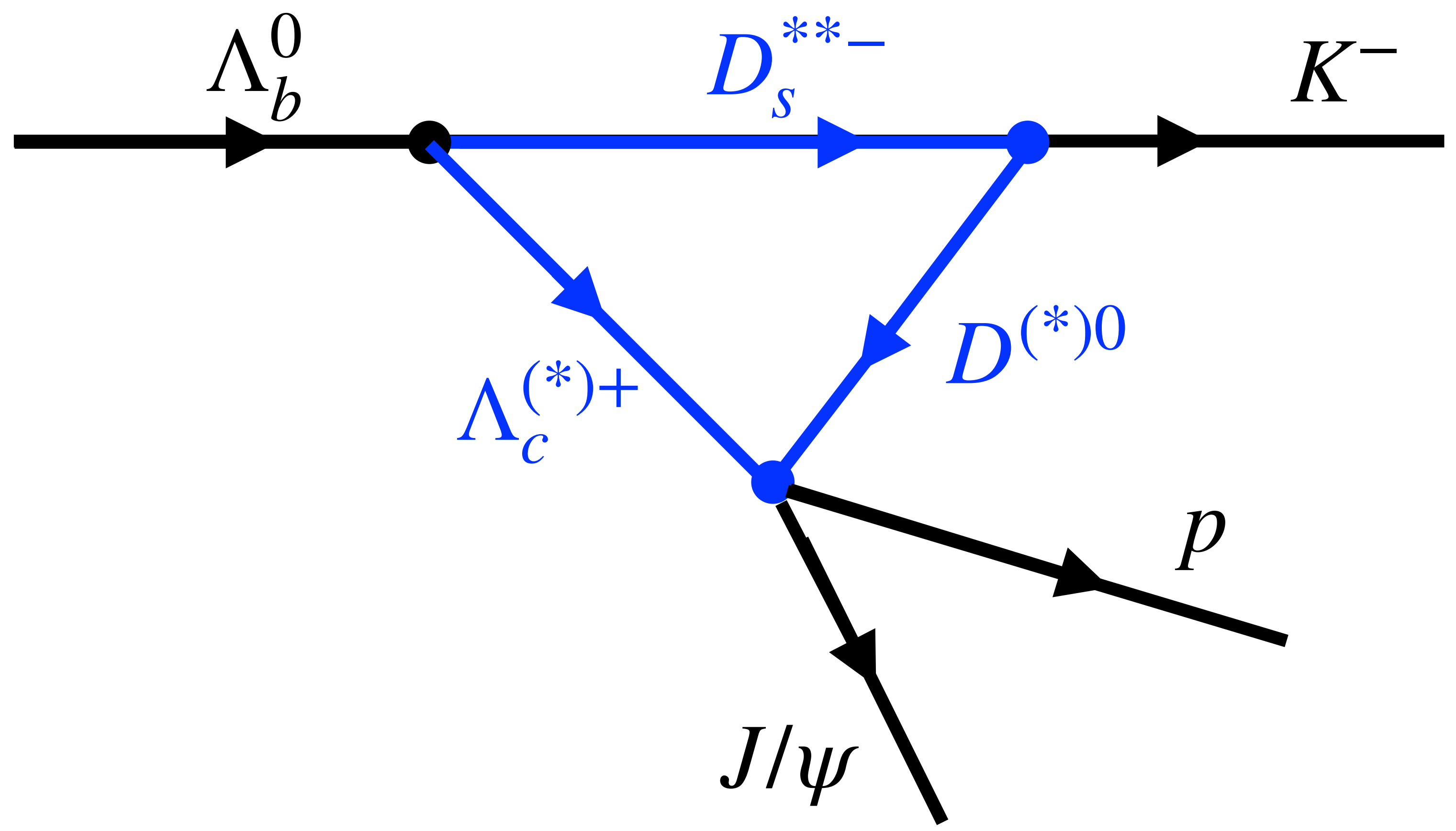
$$m_1^2 \in \left[\frac{M_A^2 m_3 + M_B^2 m_2}{m_2+m_3} - m_2 m_3,\ (M_A - m_2)^2\right] \qquad m_C^2 \in \left[(m_2+m_3)^2,\ \frac{M_A m_3^2 - M_B^2 m_2}{M_A - m_2} + M_A m_2\right]$$



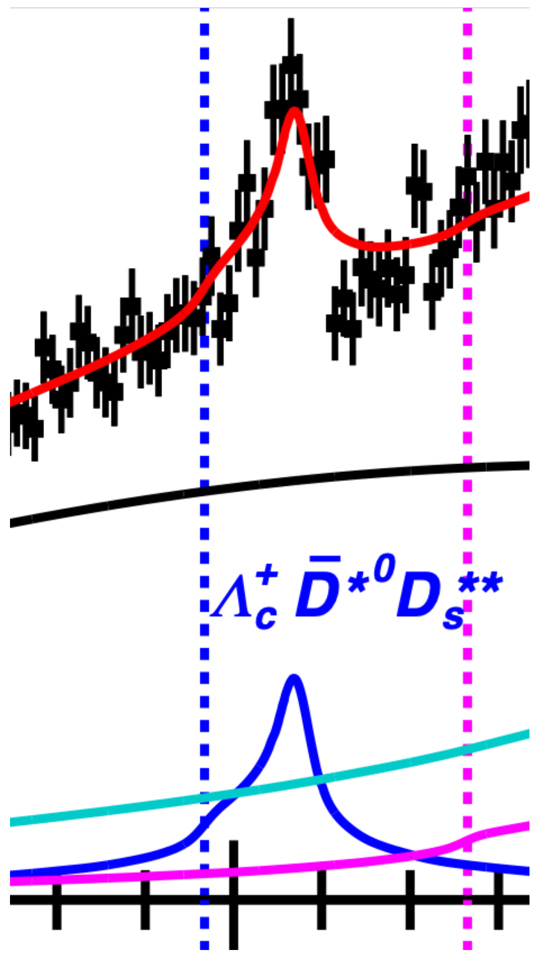
No need to introduce new hadron to explain the enhancement.

Mass condition - crucial in generating mock dataset

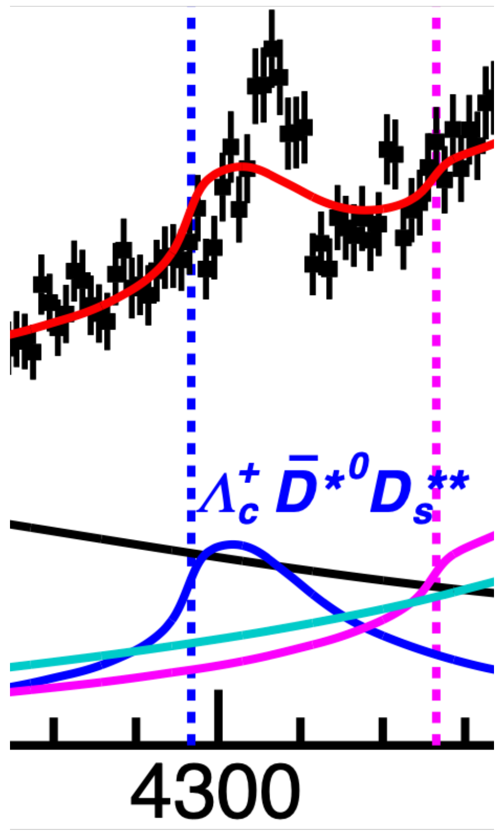
(Single) Triangle mechanism



Good fit but with unrealistic $\Gamma \sim 1\text{MeV}$ for D_s^{**}



Bad fit with realistic $\Gamma \sim 50\text{MeV}$ for D_s^{**}



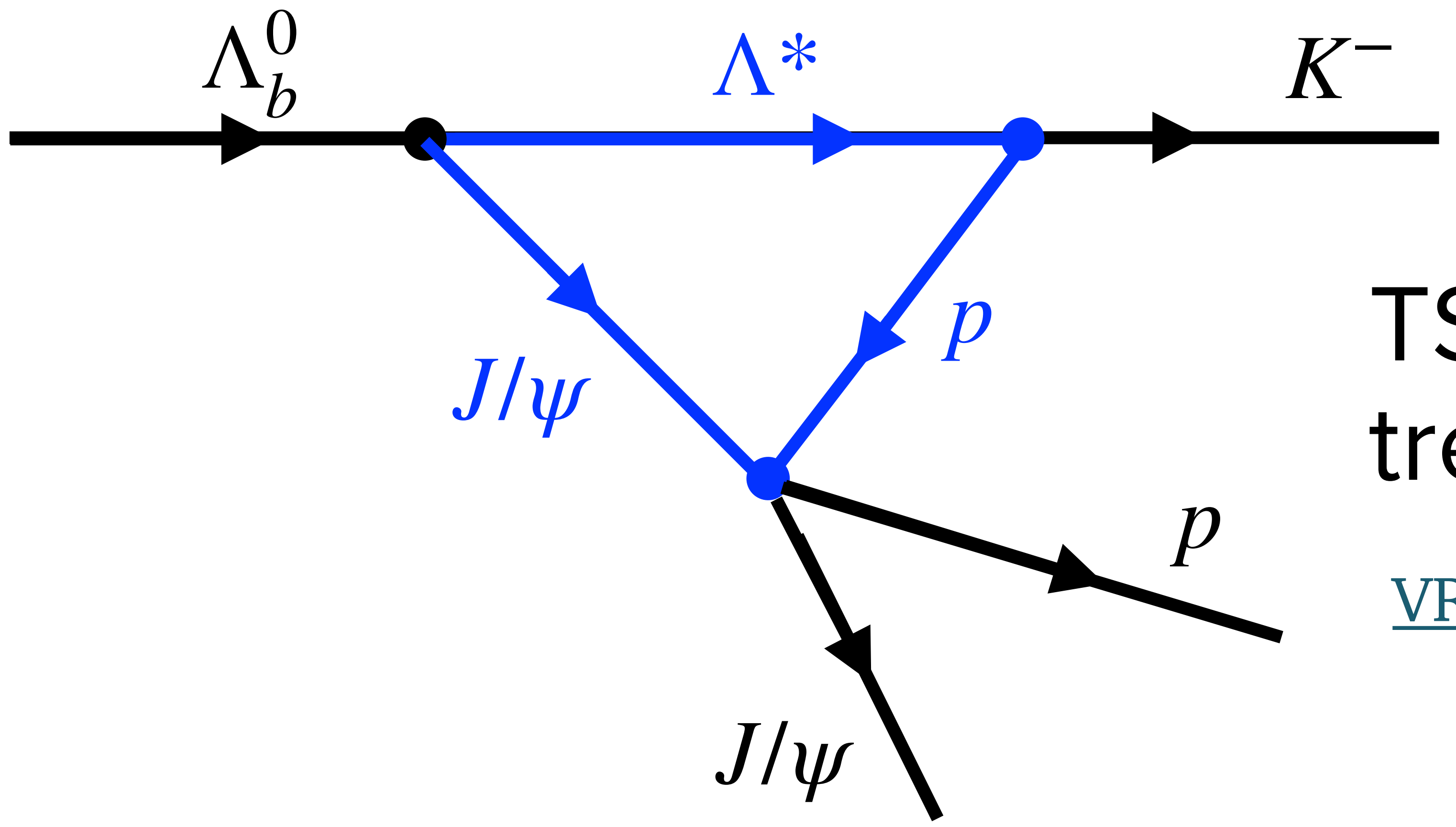
$D_s^{**-}(3288)$

Not in PDG

TS interpretation for the $P_{c\bar{c}}(4312)^+$ - ruled out

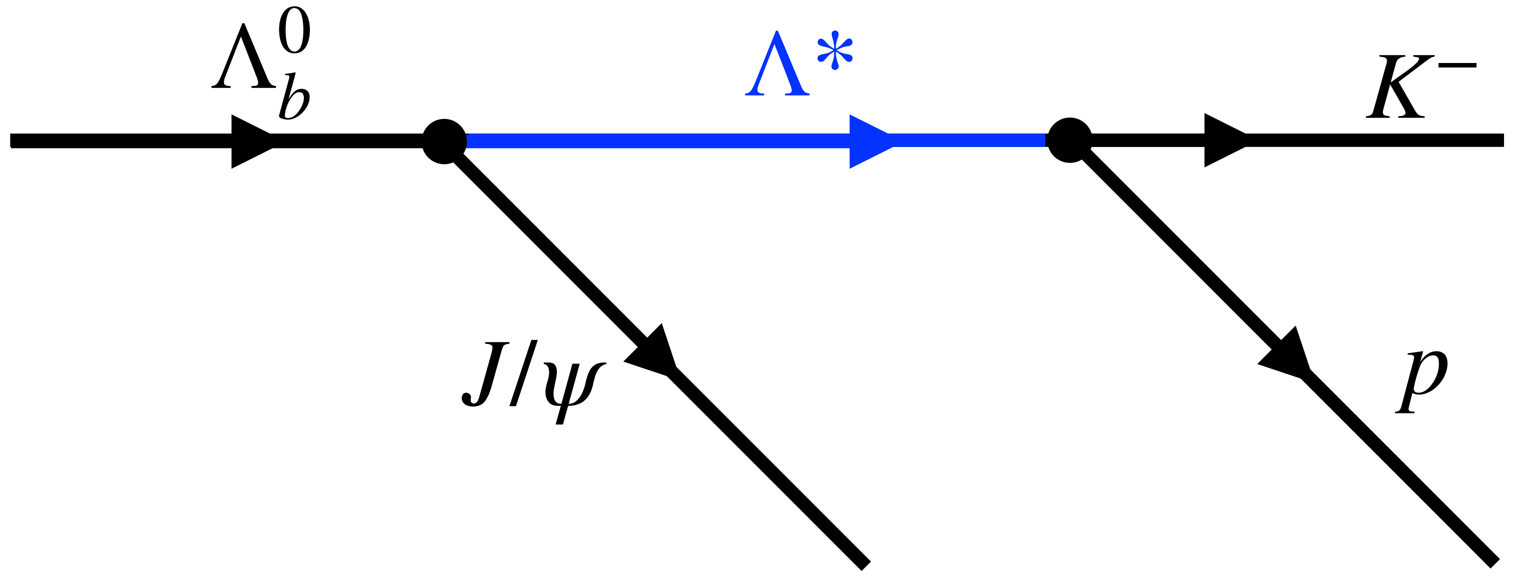
LHCb, PRL 122 222001 (2019)

Other possible Triangle Mechanism



TS enhancement is drowned by the tree-level decay. (Schmid theorem)

VR Debastiani, S Sakai, E Oset, EPJC, 79, 69 (2019)

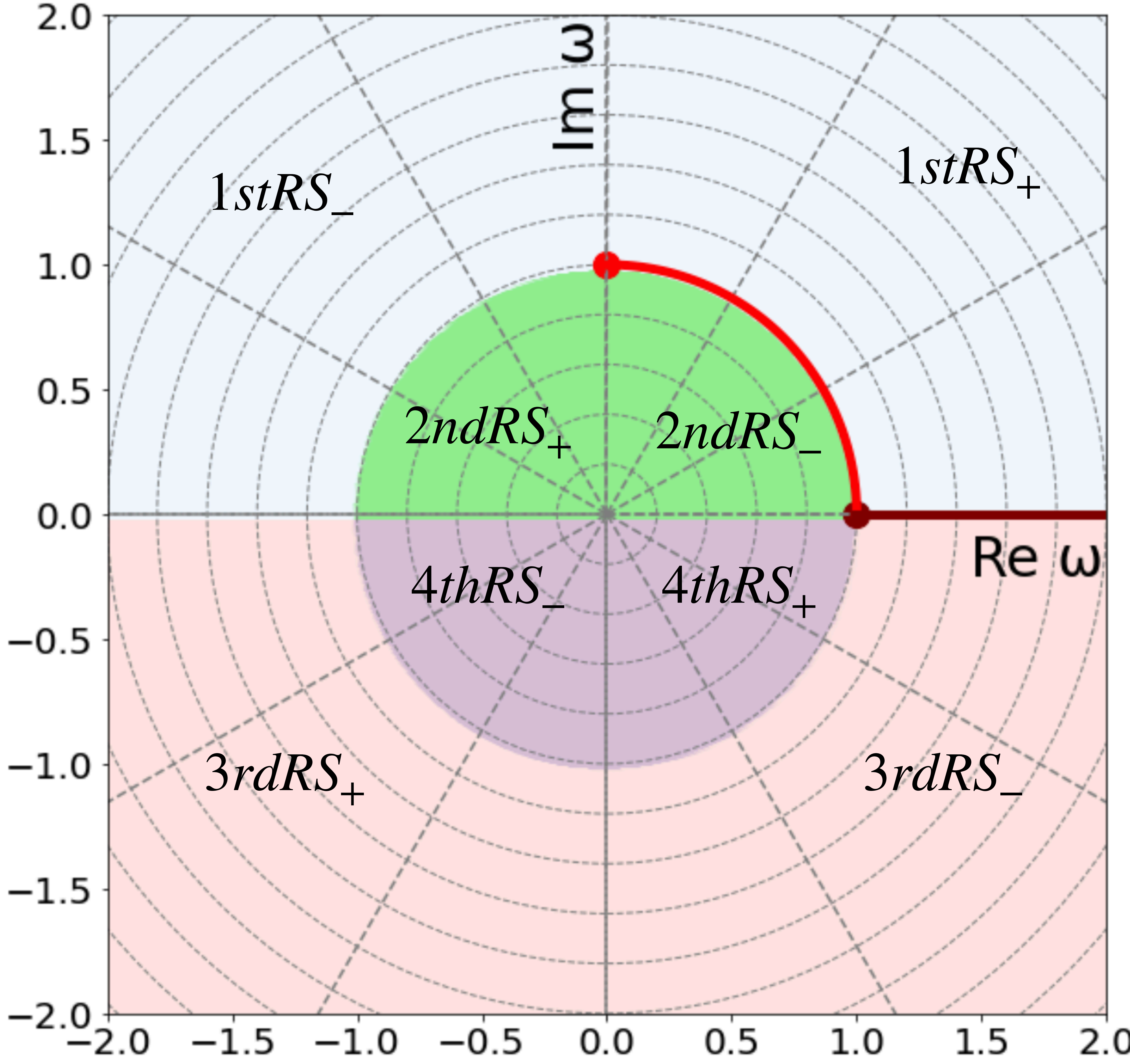


General S-matrix parametrization

$$S_{11}(p_1,p_2)=\prod_m \frac{D_m(-p_1,p_2)}{D_m(p_1,p_2)}$$

KJ Le Couteur, Proc. Roy. Soc (London) A256 (1960)
RG Newton J. Math. Phys. 2, 188 (1961)

$$p_k \to q_k; \quad s=q_k^2+\epsilon_k^2; \quad \omega=\frac{q_1+q_2}{\sqrt{\epsilon_2^2-\epsilon_1^2}} \quad \frac{1}{\omega}=\frac{q_1-q_2}{\sqrt{\epsilon_2^2-\epsilon_1^2}}$$



One pole per $D_m(q_1,q_2)$: ω_m

$$D_m(q_1,q_2)=D_m(\omega)$$

M Kato, Ann. Phys., 31 1 (1965)

$$=\frac{1}{\omega^2}\left(\omega-\omega_m\right)\left(\omega+\omega_m^*\right)\left(\omega-\omega_{\bar{m}}\right)\left(\omega+\omega_{\bar{m}}^*\right)$$

$\omega_{\bar{m}}$ needed only to ensure $\lim\limits_{\omega\to\infty} S_{11}\to 1;$

$$|\omega_m\omega_{\bar{m}}|=1$$

- Poles are introduced independently.
- Cusp at the threshold can be controlled via pole placement.

LMS, DLBS PRC 108 045204 (2023)

General S-matrix parametrization

$$S_{11}(p_1,p_2) = \prod_m \frac{D_m(-p_1,p_2)}{D_m(p_1,p_2)}$$

KJ Le Couteur, Proc. Roy. Soc (Lo
RG Newton J. Math. Phys. 2, 188

$$p_k \to q_k; \quad s = q_k^2 + \epsilon_k^2; \quad \omega = \frac{q_1+q_2}{\sqrt{\epsilon_2^2-\epsilon_1^2}}$$

One pole per $D_m(q_1,q_2)$: ω_m

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M Kato, Ann. Phys., 31 1 (1965)

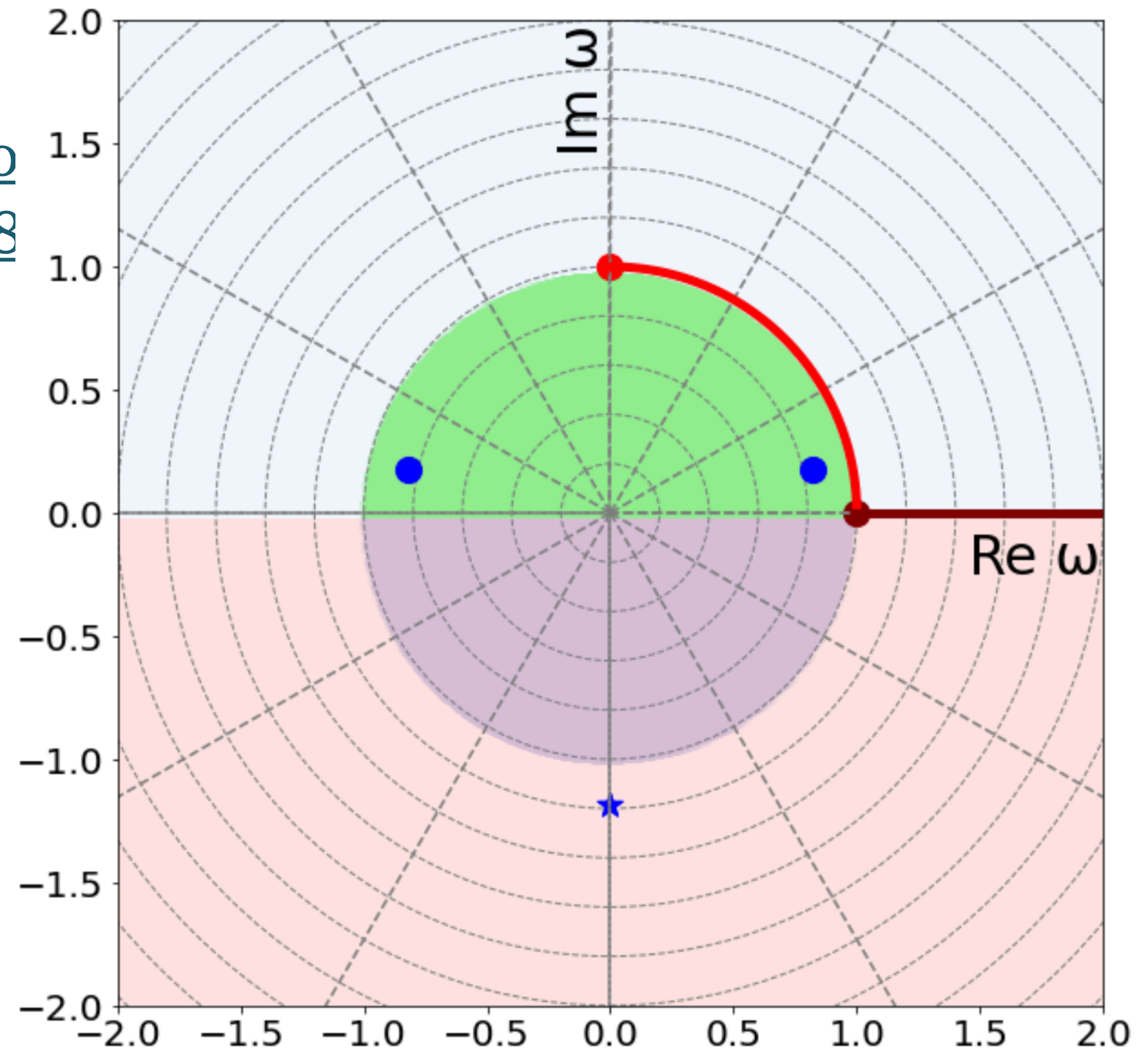
$$= \frac{1}{\omega^2}\left(\omega-\omega_m\right)\left(\omega+\omega_m^*\right)\left(\omega-\omega_{\bar{m}}\right)\left(\omega+\omega_{\bar{m}}^*\right)$$

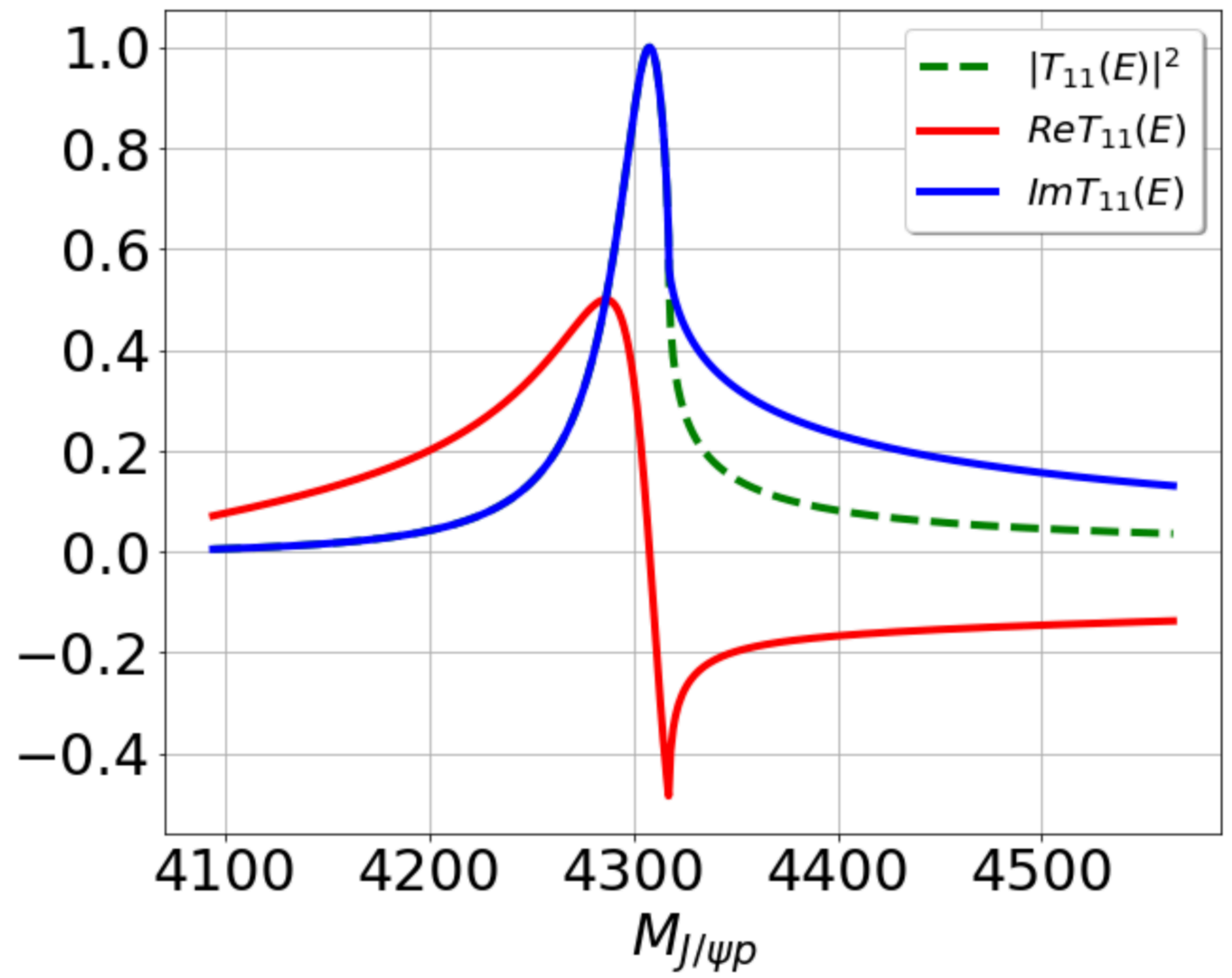
$\omega_{\bar{m}}$ needed only to ensure $\lim_{\omega\to\infty} S_{11} \to 1;$

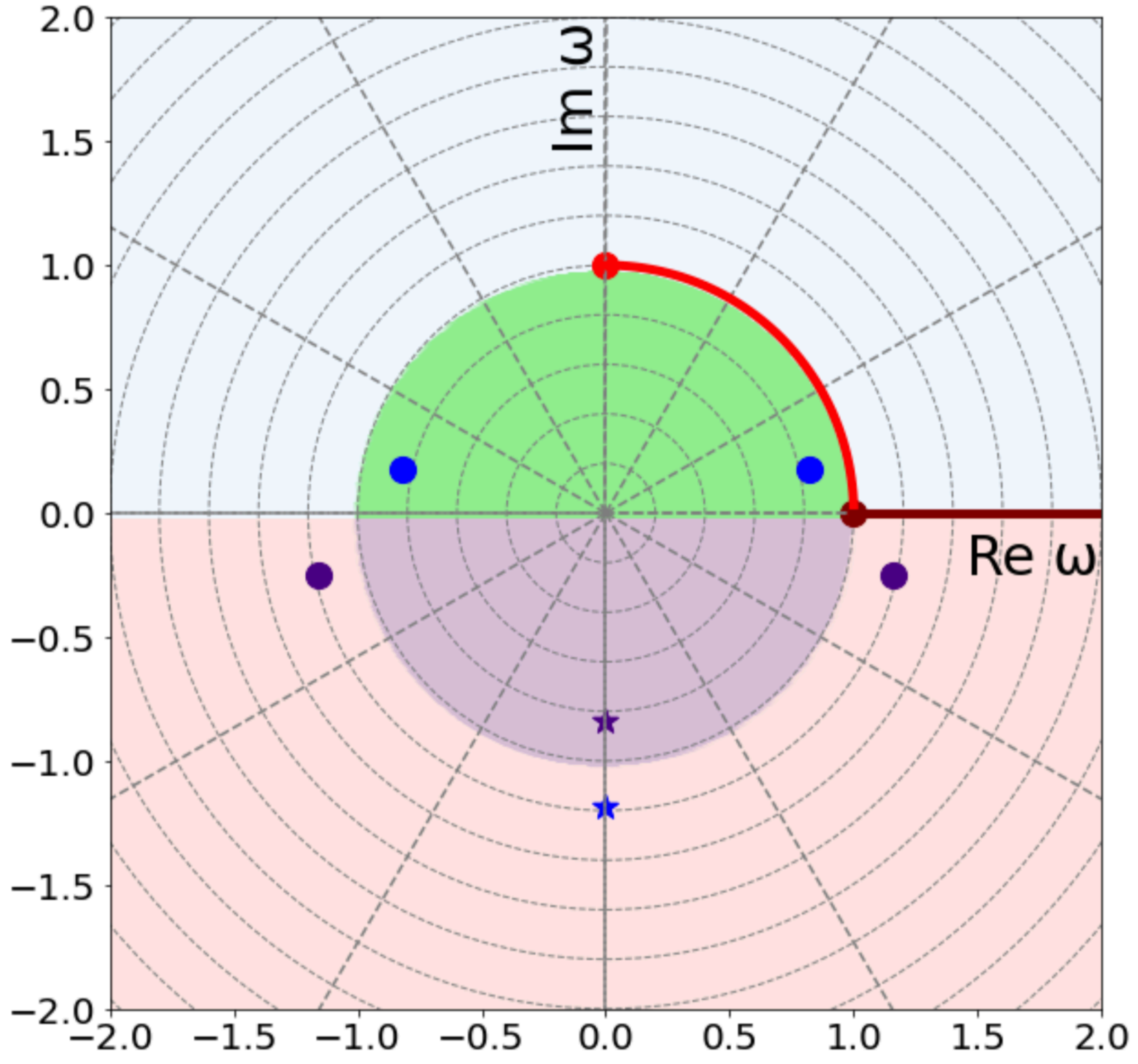
$$|\omega_m\omega_{\bar{m}}| = 1$$

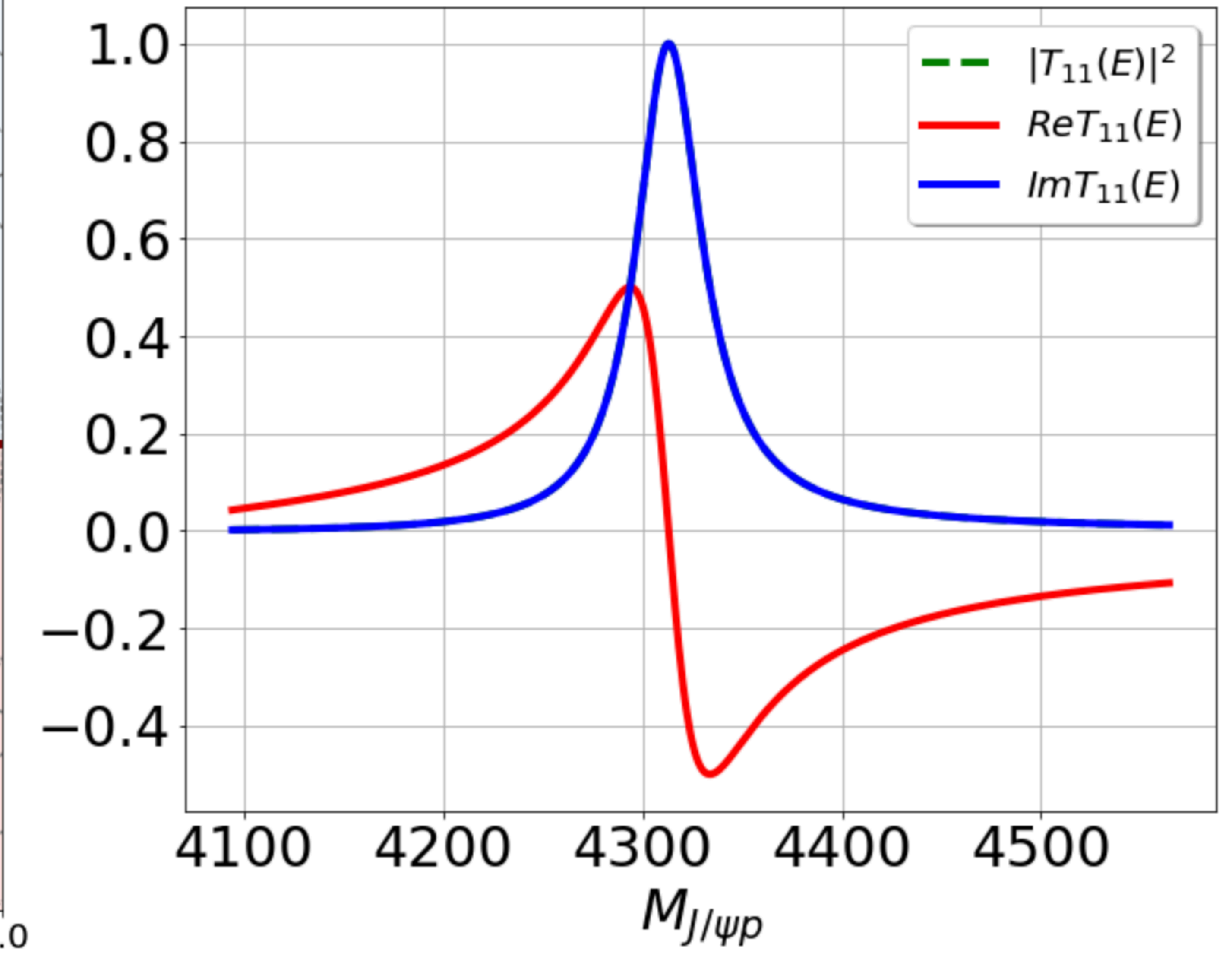
- Poles are introduced independently.
- Cusp at the threshold can be controlled via pole placement.

LMS, DLBS PRC 108 045204 (2023)





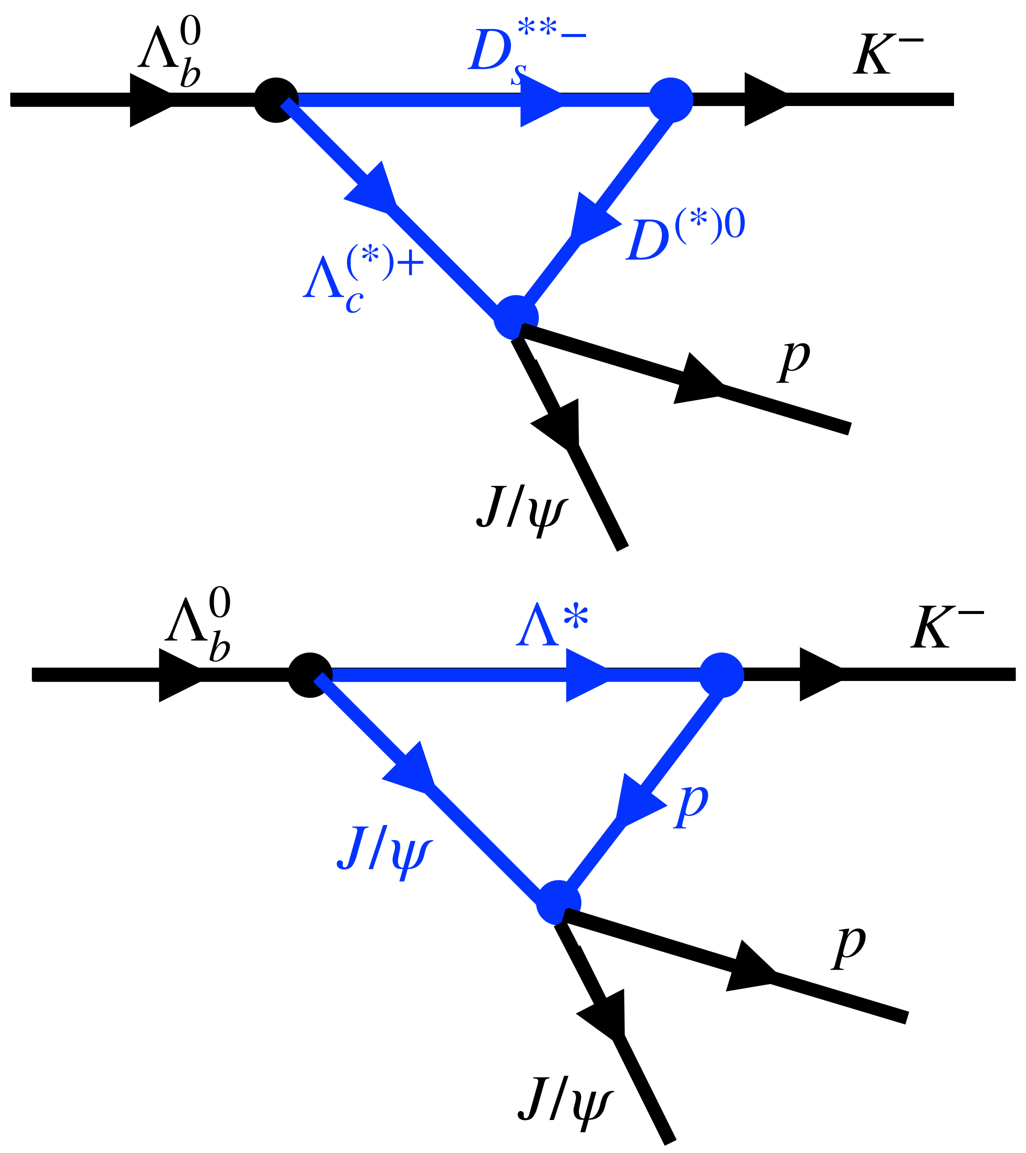




Sample training datasets

Triangle singularity

Parameter	Range of values [MeV]
$m_{\Lambda_b^0}$	5619.60 ± 0.17
m_{K^-}	493.677 ± 0.016
$m_{\Lambda_c^+}$	2286.46 ± 0.14
$m_{\bar{D}^{*0}}$	2006.85 ± 0.05
$m_{J/\psi}$	3096.9 ± 0.006
$m_{D_s^{**}}$	[3209.80, 3315.00]
m_{Λ^*}	[2490.00, 2522.70]
Λ	[2000.0, 2500.0]
ϵ	[1.0, 10.0]

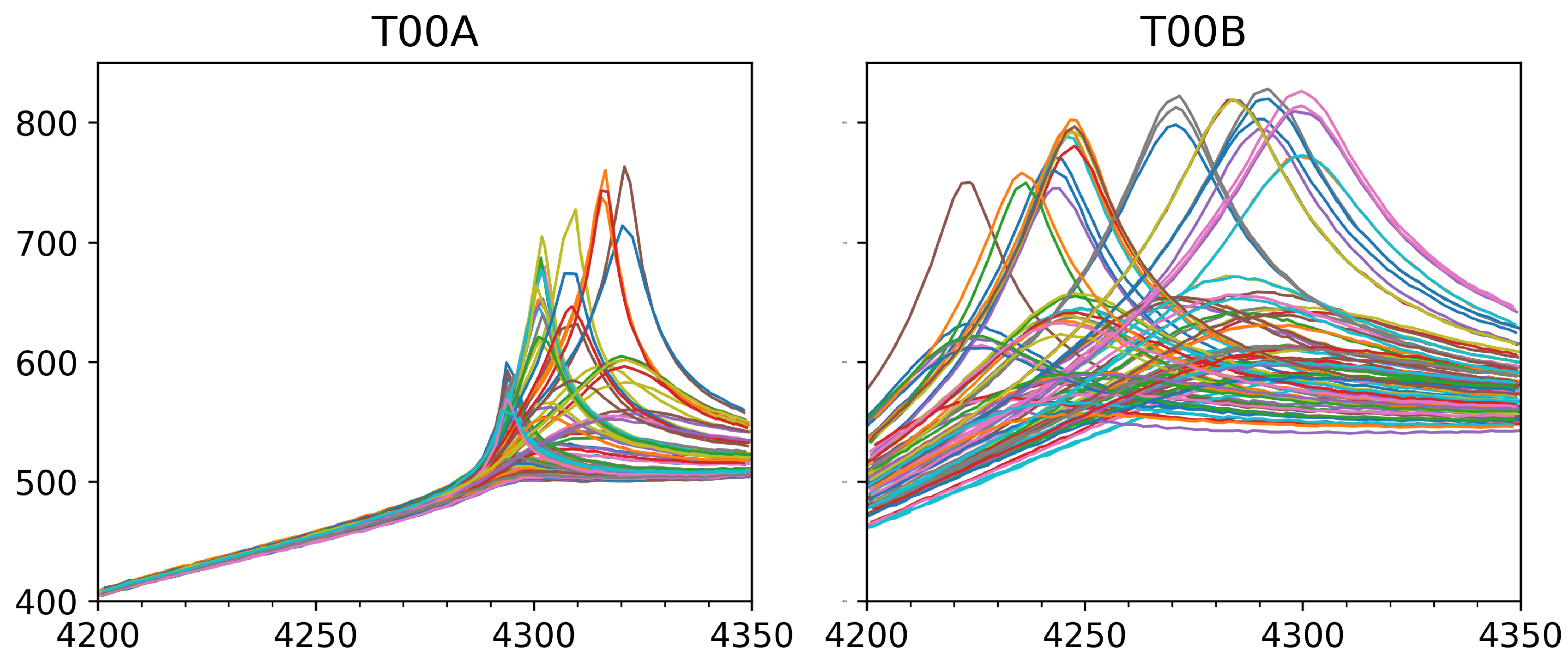


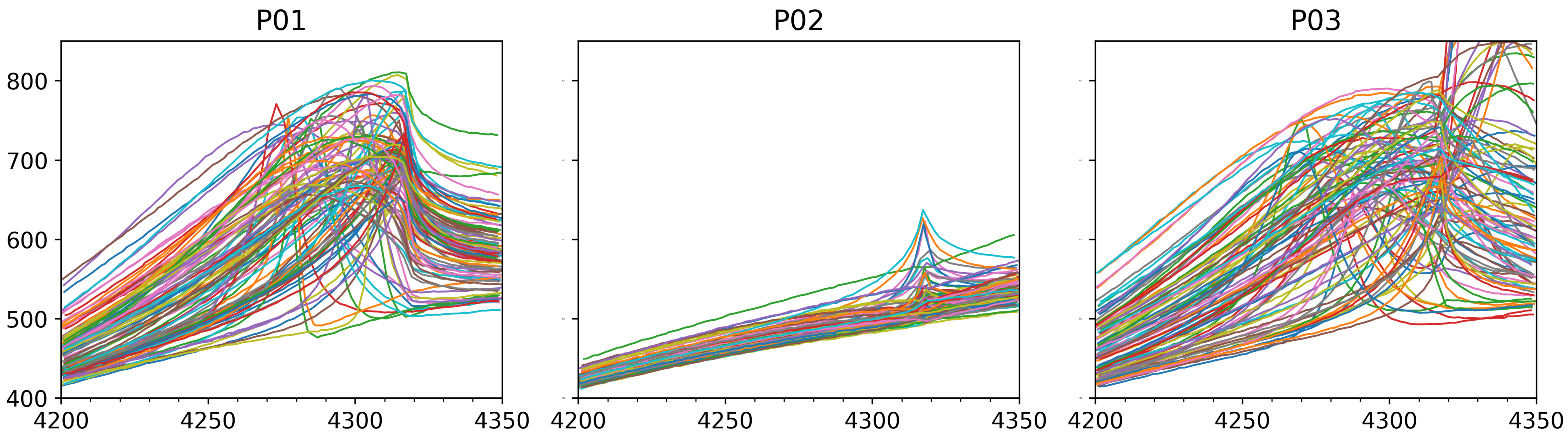
Pole-based enhancements

$$\begin{cases} T_2 - 50 \le \mathrm{Re}\,E_{\text{pole}} \le 4350 & \text{all RS} \\ -100 \le \mathrm{Im}\,E_{\text{pole}} < 0 & [bt]\ \&\ [bb] \\ 0 < \mathrm{Im}\,E_{\text{pole}} \le 100 & [tb] \end{cases}$$

$4 \times 10{,}000$
Training dataset generated

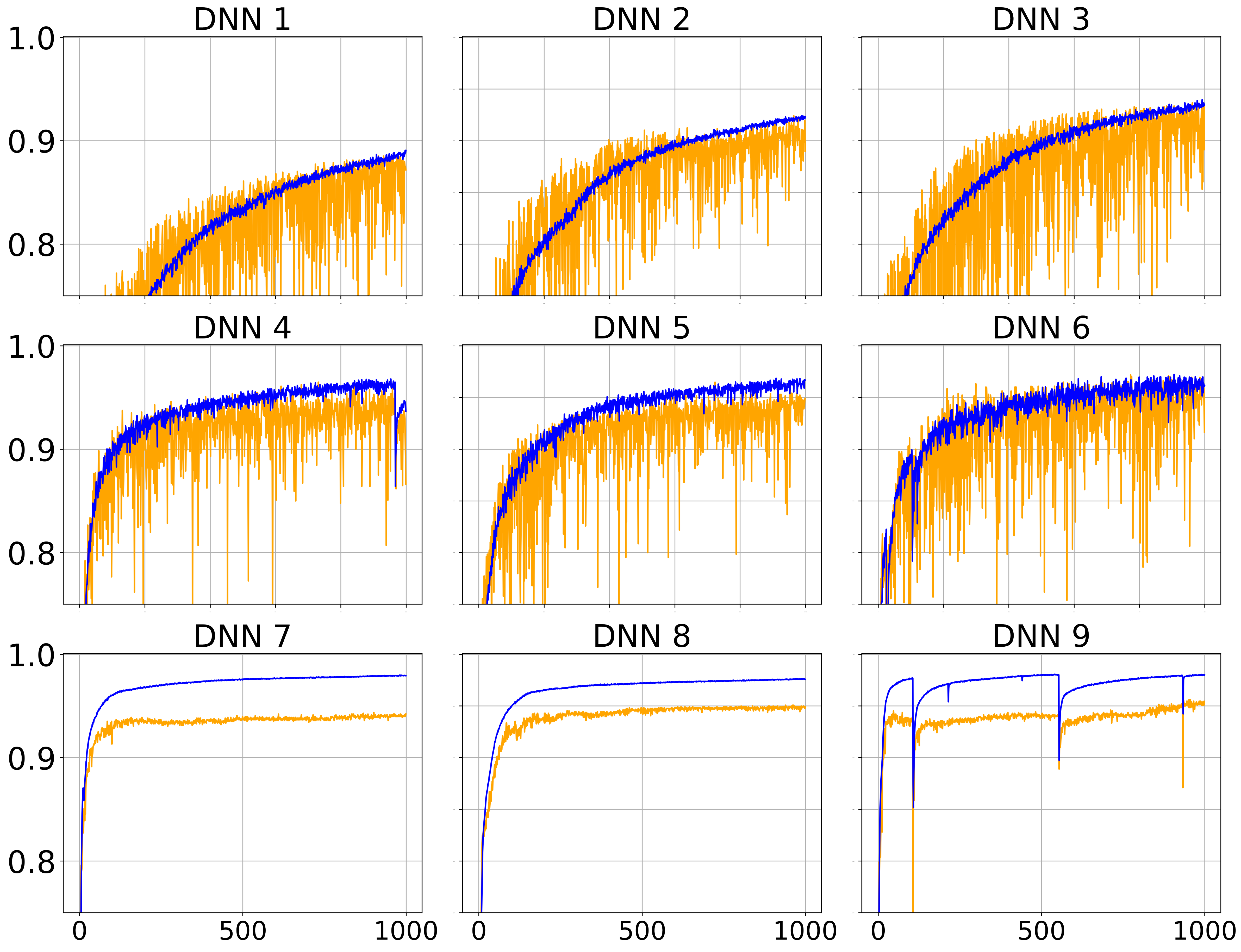
4×320
Testing dataset generated





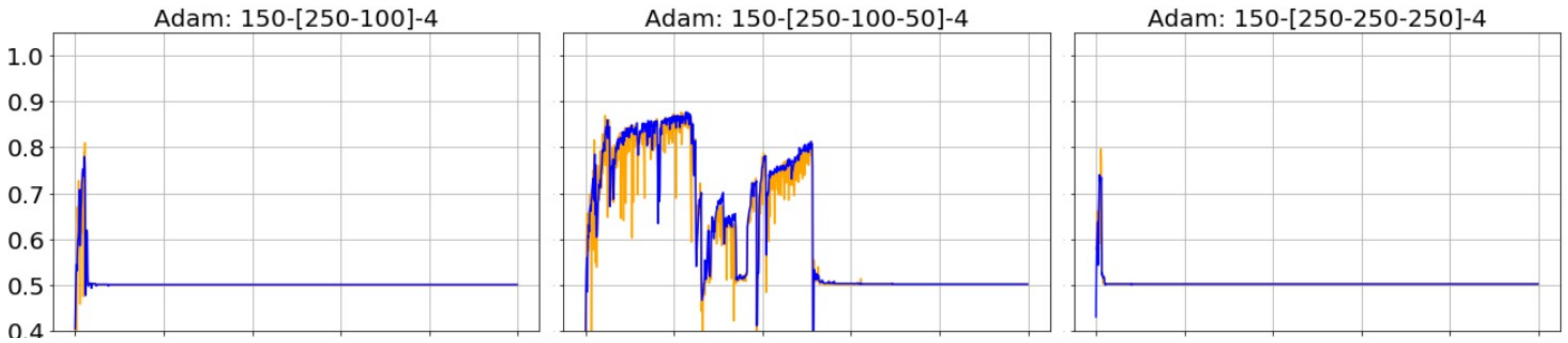
Training performance

Model	Optimizer and Architecture
DNN 1	AdaGrad: 150-[250-100]-4
DNN 2	AdaGrad: 150-[250-100-50]-4
DNN 3	AdaGrad: 150-[250-250-250]-4
DNN 4	AMSGrad: 150-[250-100]-4
DNN 5	AMSGrad: 150-[250-100-50]-4
DNN 6	AMSGrad: 150-[250-250-250]-4
DNN 7	SMORMS3: 150-[250-100]-4
DNN 8	SMORMS3: 150-[250-100-50]-4
DNN 9	SMORMS3: 150-[250-250-250]-4



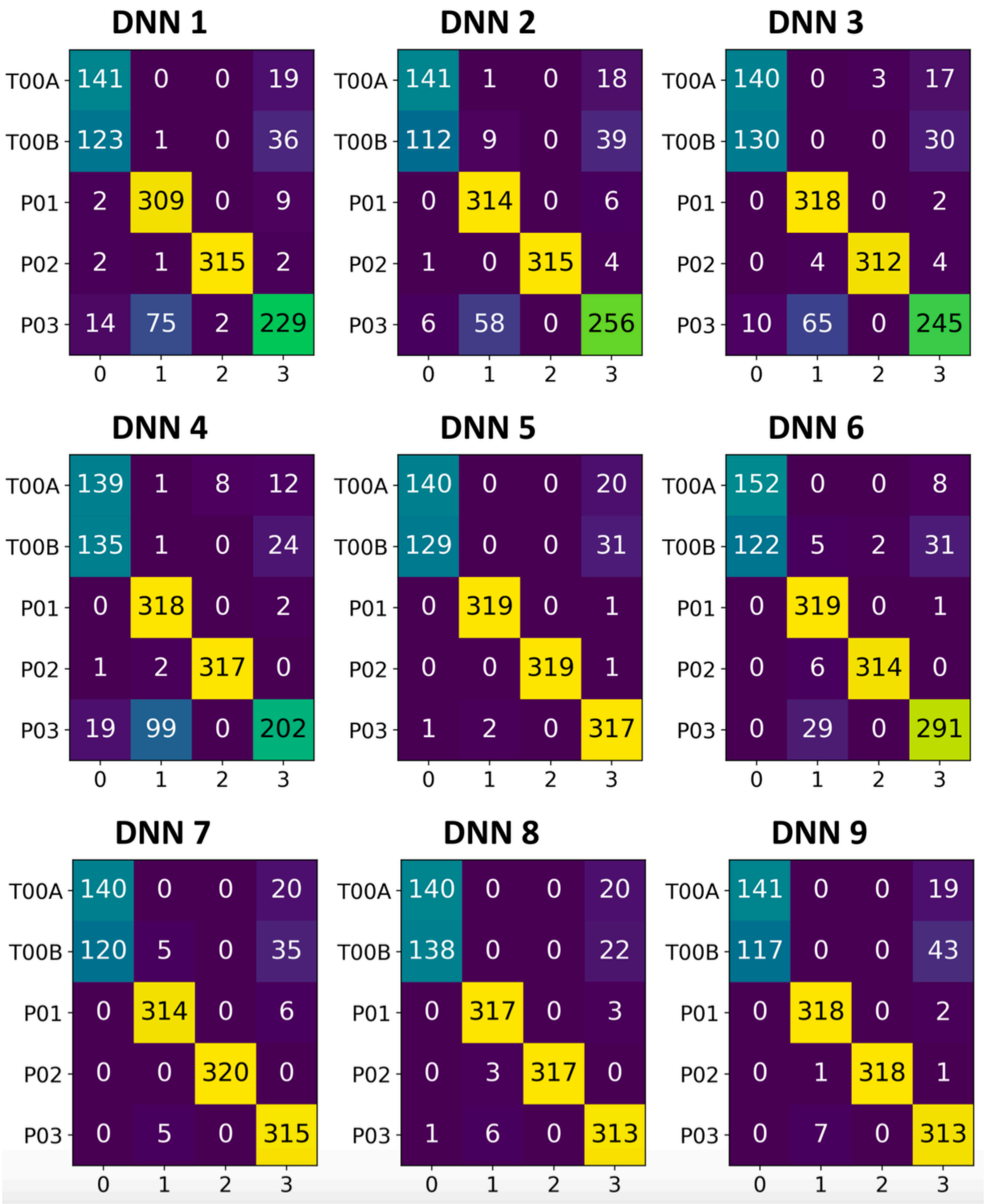
Training epoch vs accuracy

Other optimizers cannot even learn the classification task.

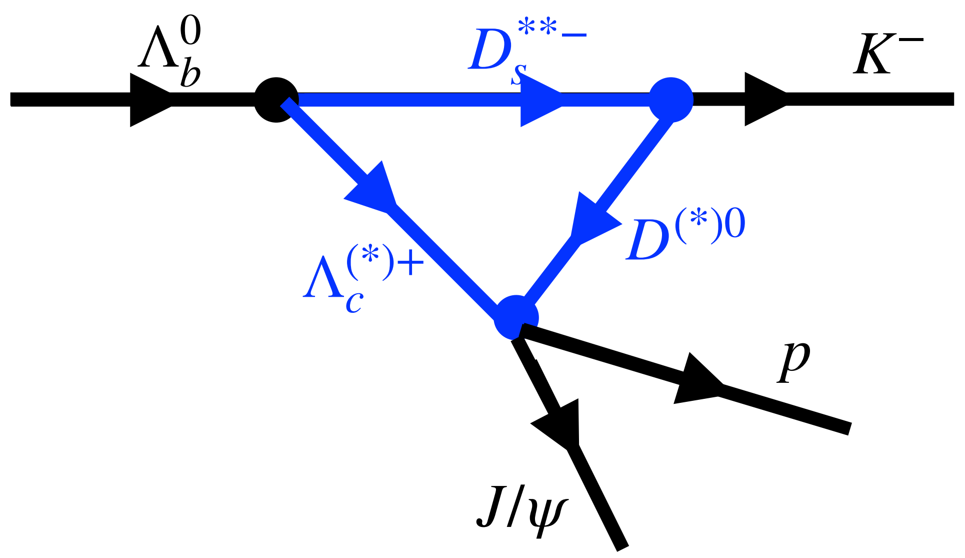


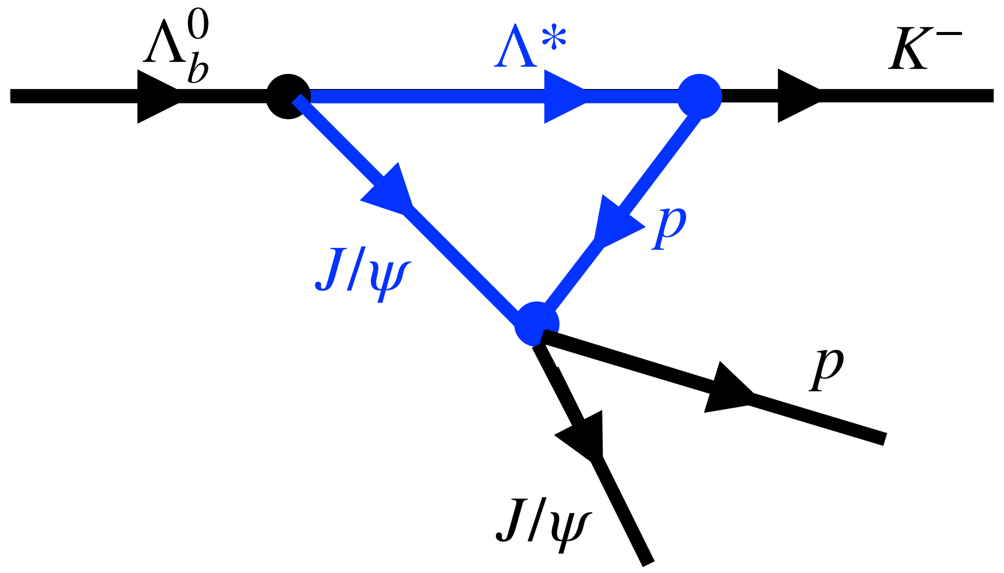
The classification task is non-trivial.

Confusion Matrix



Generate a different set of 320 validation dataset per classification.



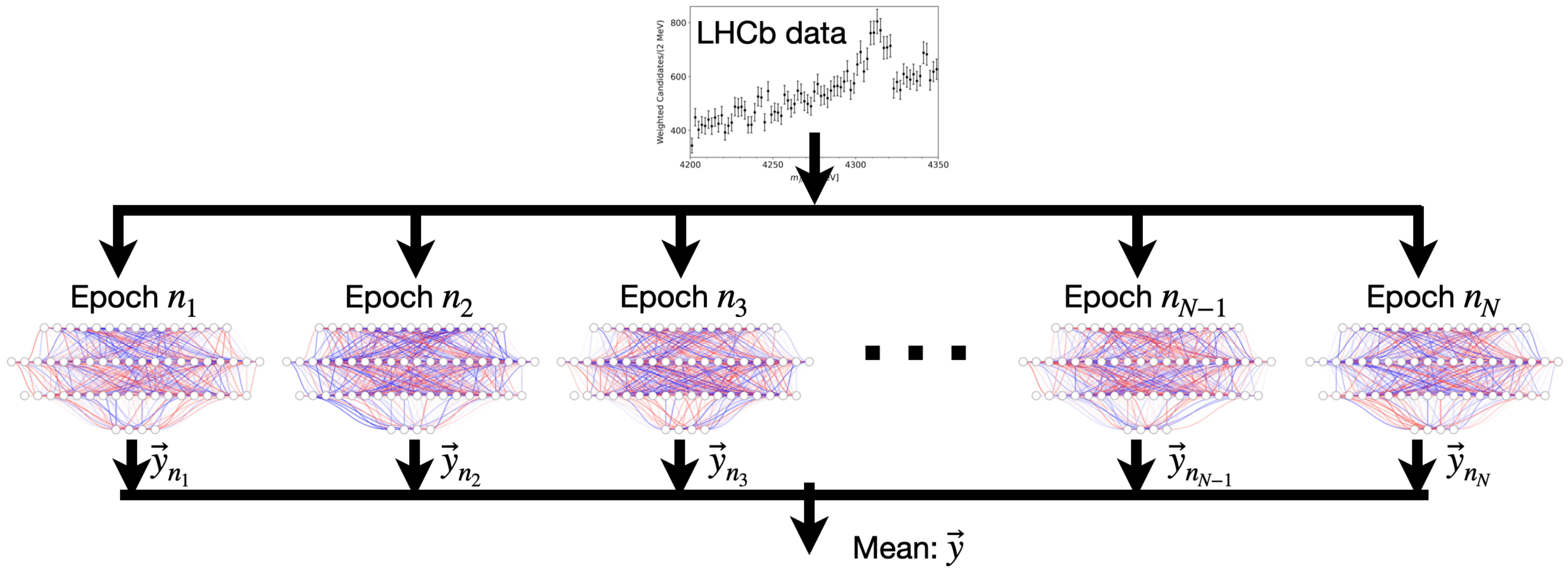


Label	Description
0	Triangle mechanism
1	1 pole in 2nd RS
2	1 pole in 4th RS
3	1 pole in 2nd and 1 pole in 3rd RSs

Slight confusion between TS and BW-like line shapes.

If the experimental data will favor either the TS or class 3, further analysis must be done.

Inference stage (snapshot ensemble)



- Bootstrapped 3000 line shapes from the experimental data. (Uniform distribution)
- Feed to the DNN state at epoch n
- Get the mean count

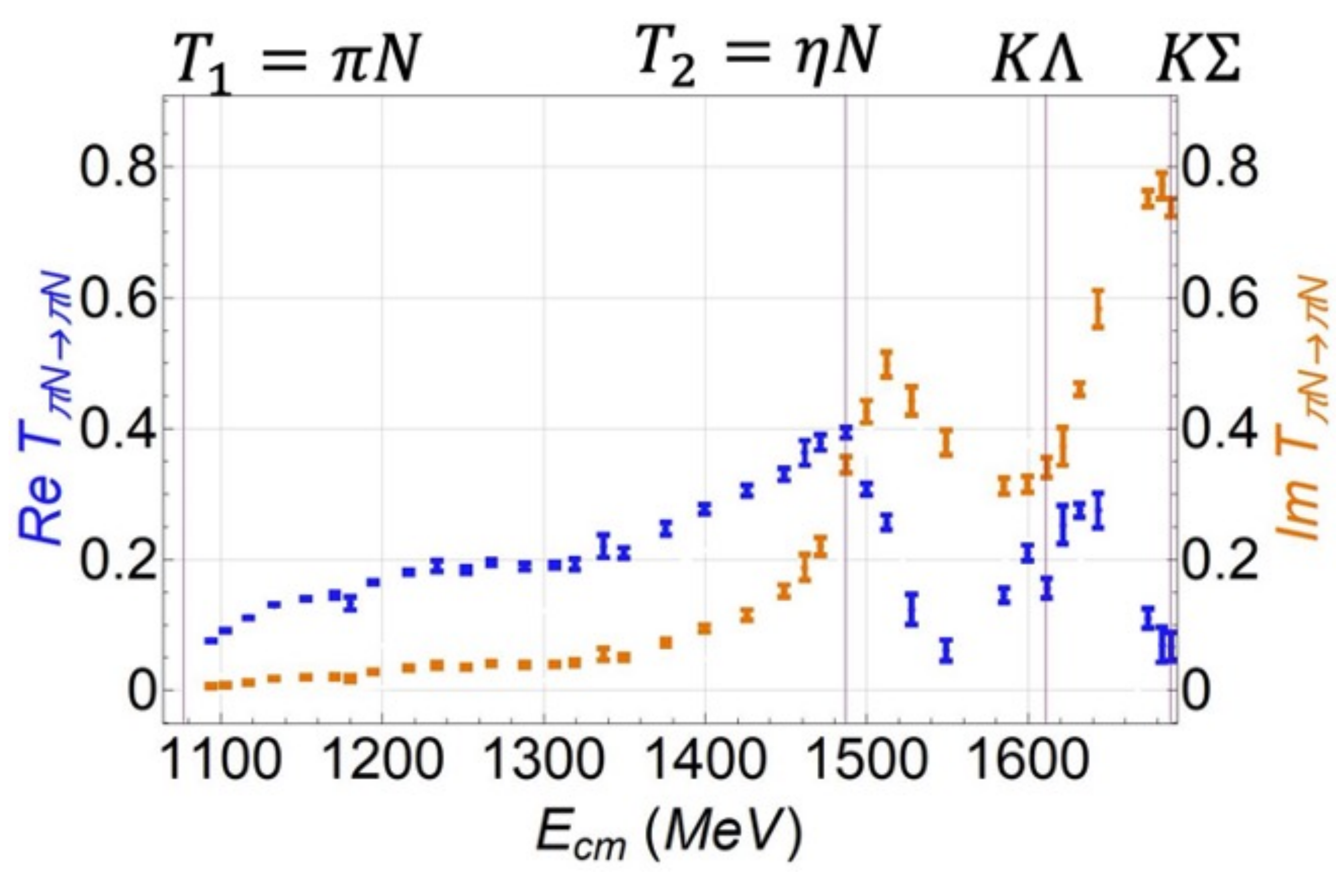
Model	TS	1 pole in RS2	1 pole in RS4	1 pole each in RS2 & RS4
DNN 1	261	1930	0.248	804
DNN 2	18.4	1998	969	14.5
DNN 3	0.653	2960	0	36
DNN 4	0	2990	0	14.2
DNN 5	0	2660	0	337
DNN 6	0.436	2999	0	0.891
DNN 7	1	2590	0	414
DNN 8	0	2999	0	1.06
DNN 9	0	2970	0	127

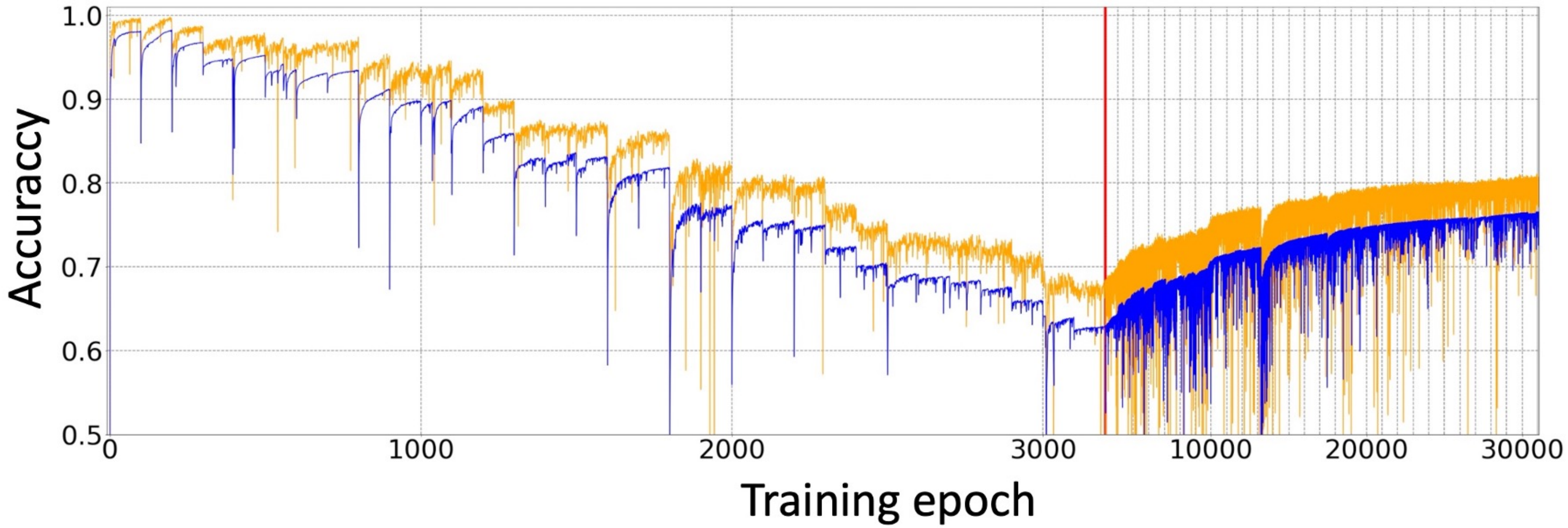
- TS is ruled out by pure line shape analysis!
- It is possible to distinguish kinematical cusp vs pole despite the presence of experimental uncertainty.
- The data favored the pole-based interpretation:
  1 pole in 2nd RS

DAO Co, VAA Chavez, DLBS, arXiv:2403.18265

Probe deeper: Pole structure of $P_{c\bar{c}}(4312)^+$

DNN designed to probe the pole structure is difficult to train.





Label	S-matrix pole configuration
0	no nearby pole
1	1 pole in [bt]
2	2 poles in [bt]
⋮	⋮ ⋮ ⋮ ⋮
32	1 pole in [bt], 2 poles in [bb] and 1 pole in [tb]
33	1 pole in [bt], 1 pole in [bb] and 2 poles in [tb]
34	1 pole in [bt], 1 pole in [bb] and 1 pole in [tb]

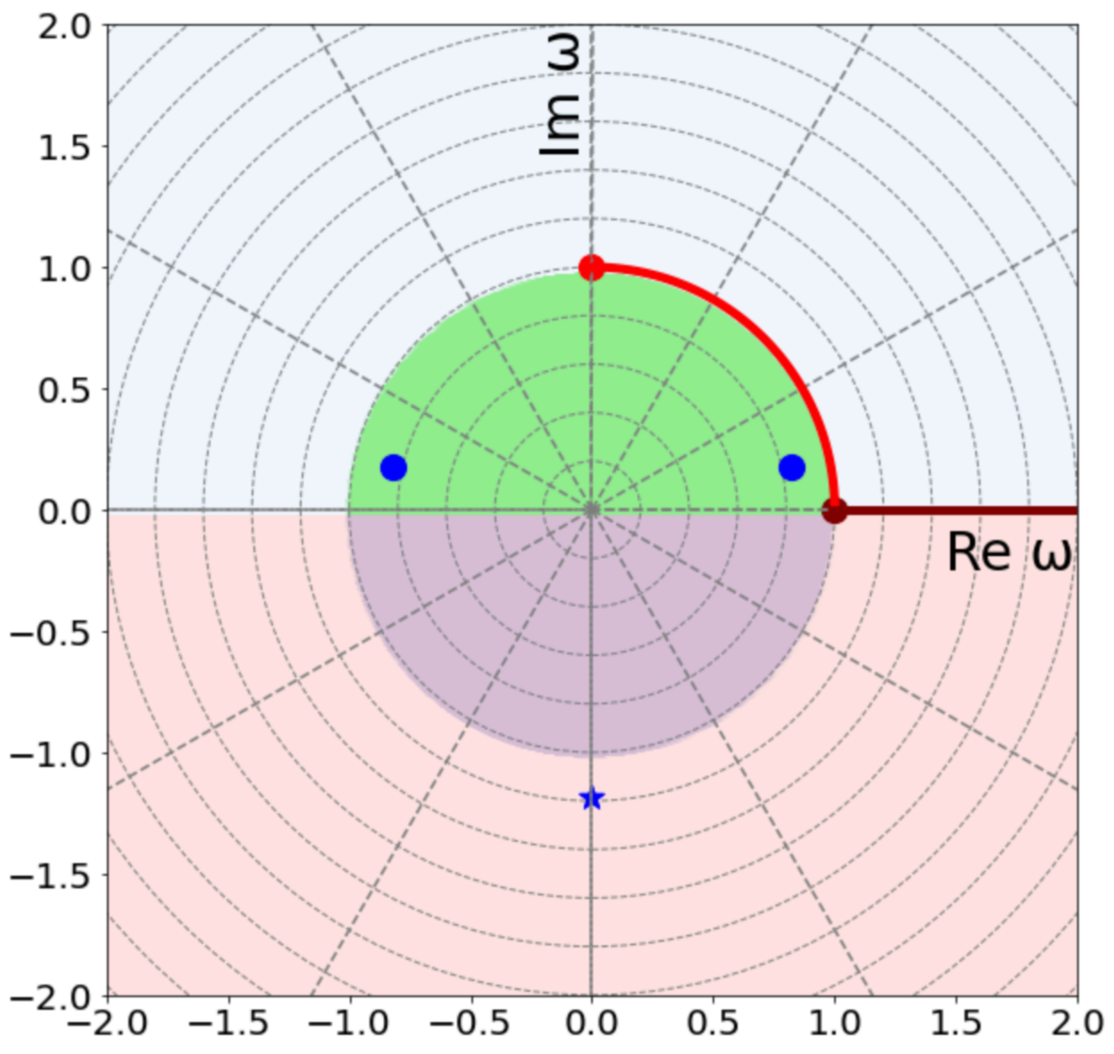
DLBS, YI, TS, AH PRD 104 3 036001 (2021)

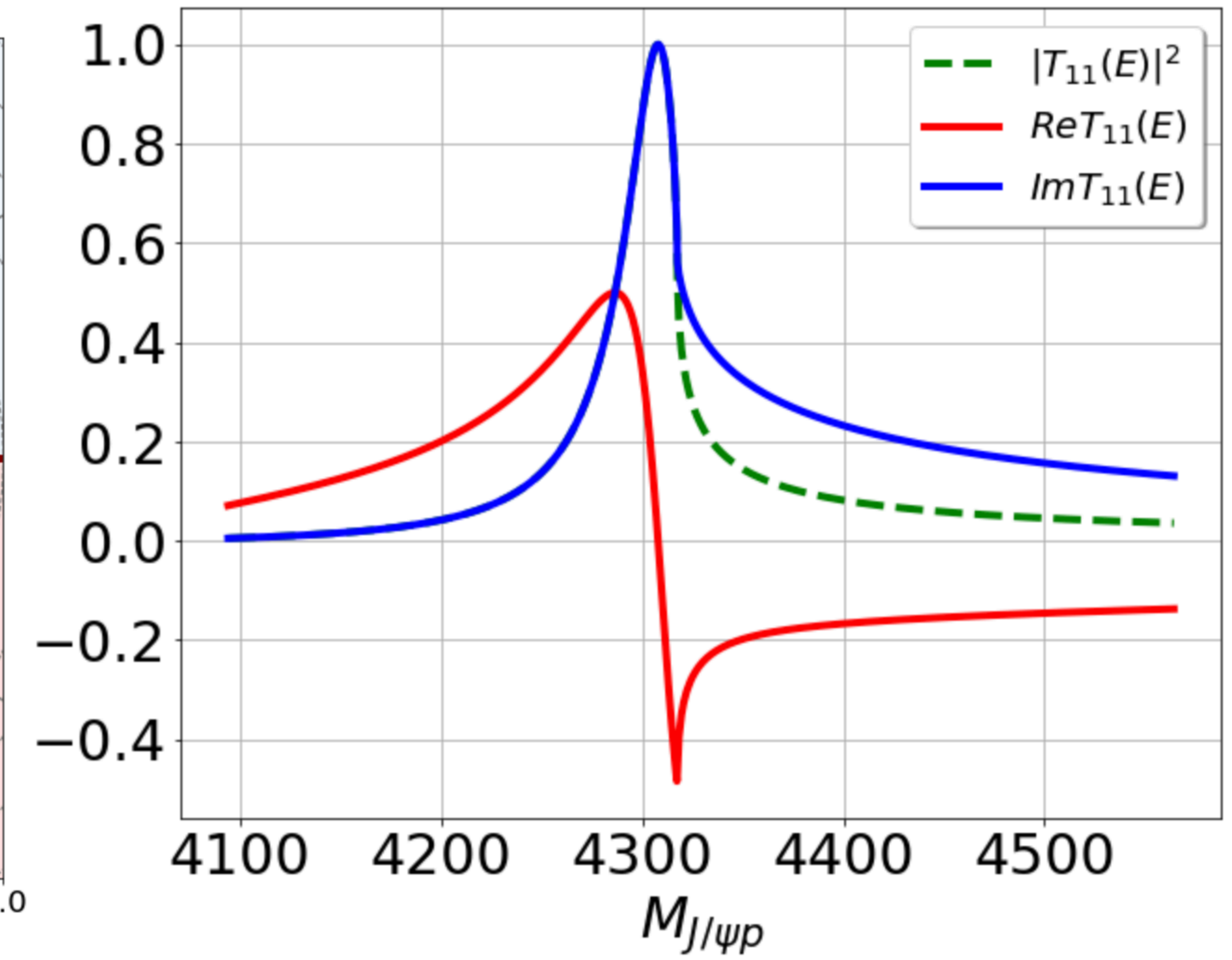
There is an ambiguity in the line shape of T_{11}.

Different pole structures can give rise to the same line shape.

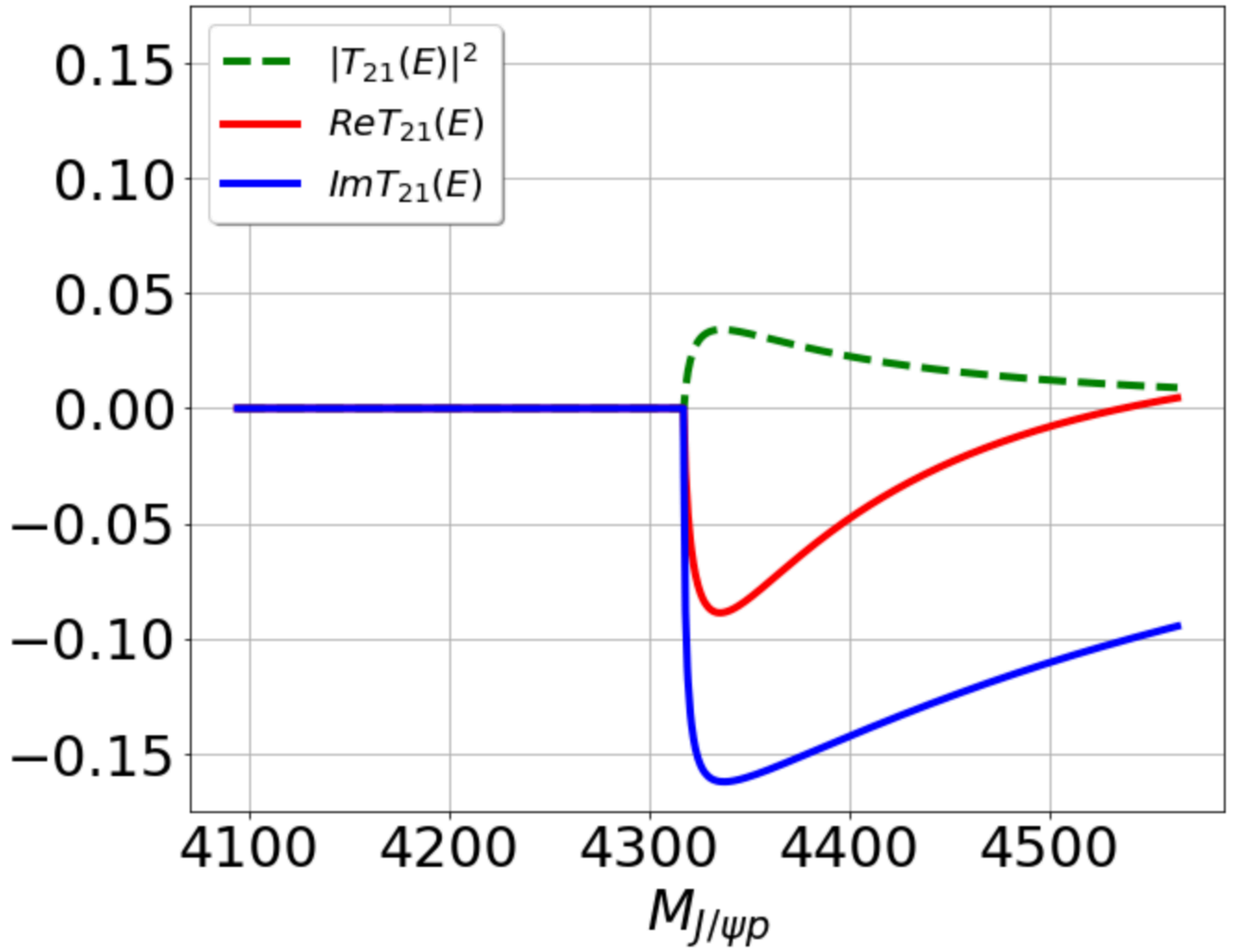
Probe deeper: Pole structure of $P_{c\bar{c}}(4312)^+$

1 pole in the 2nd RS

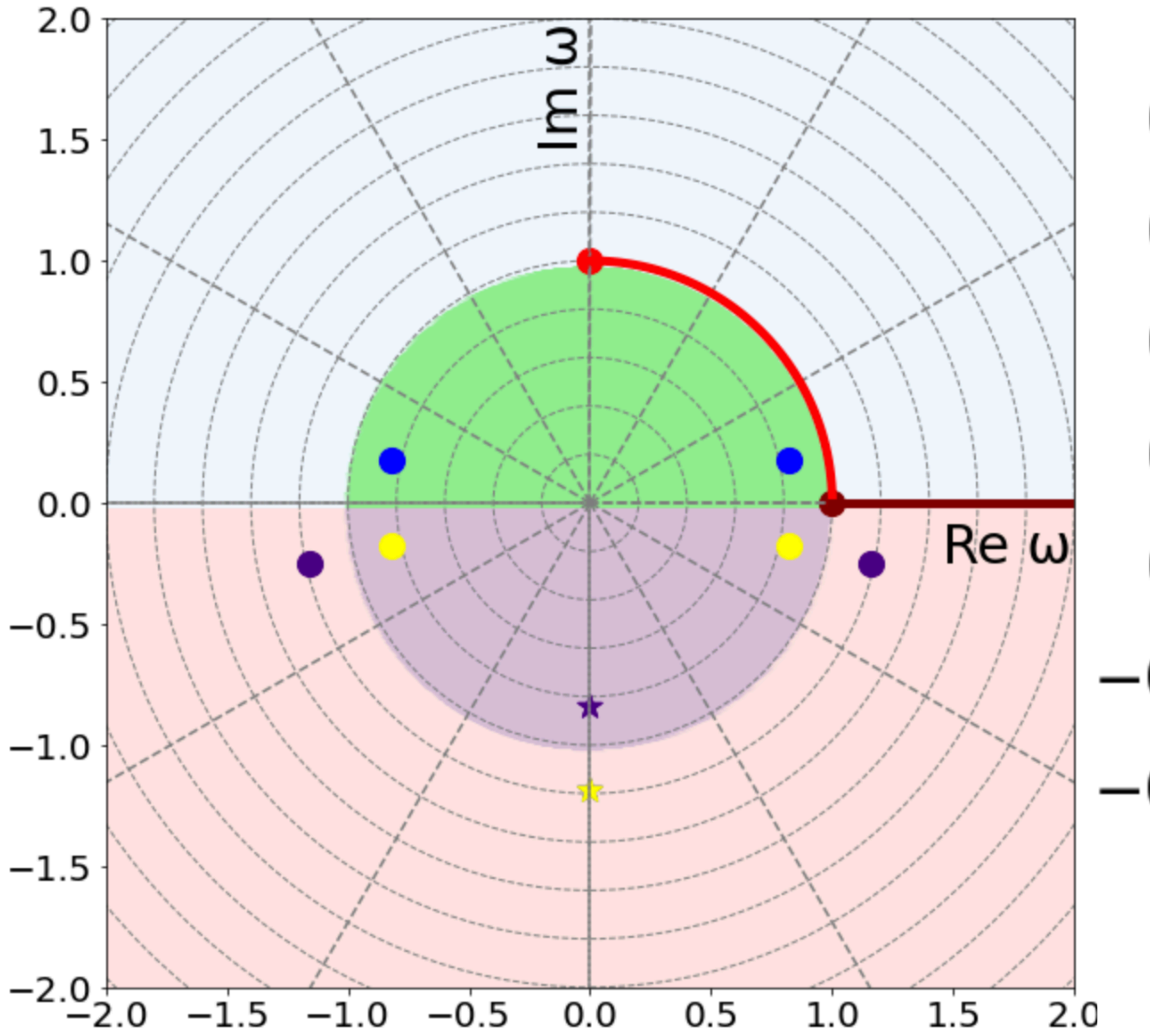


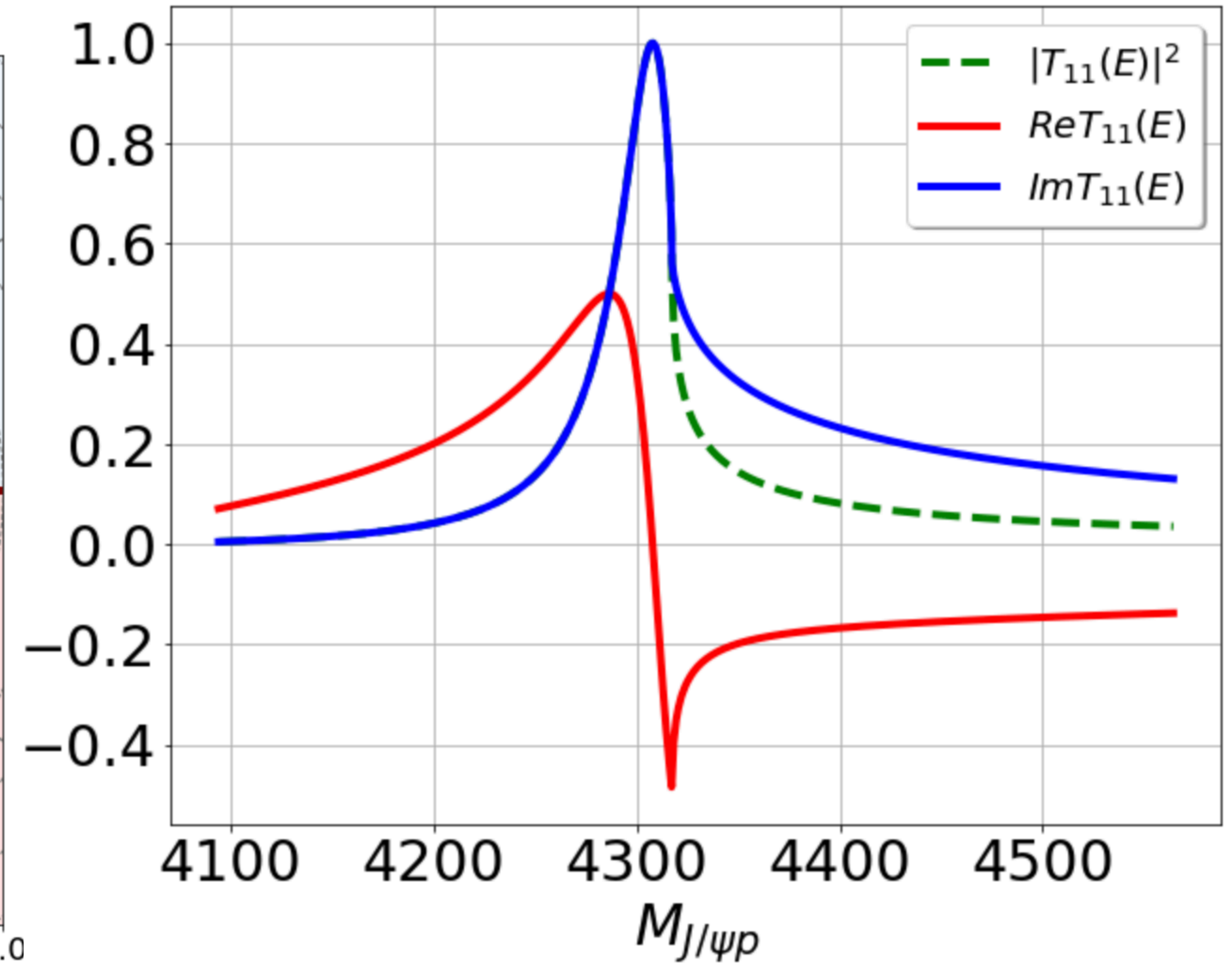


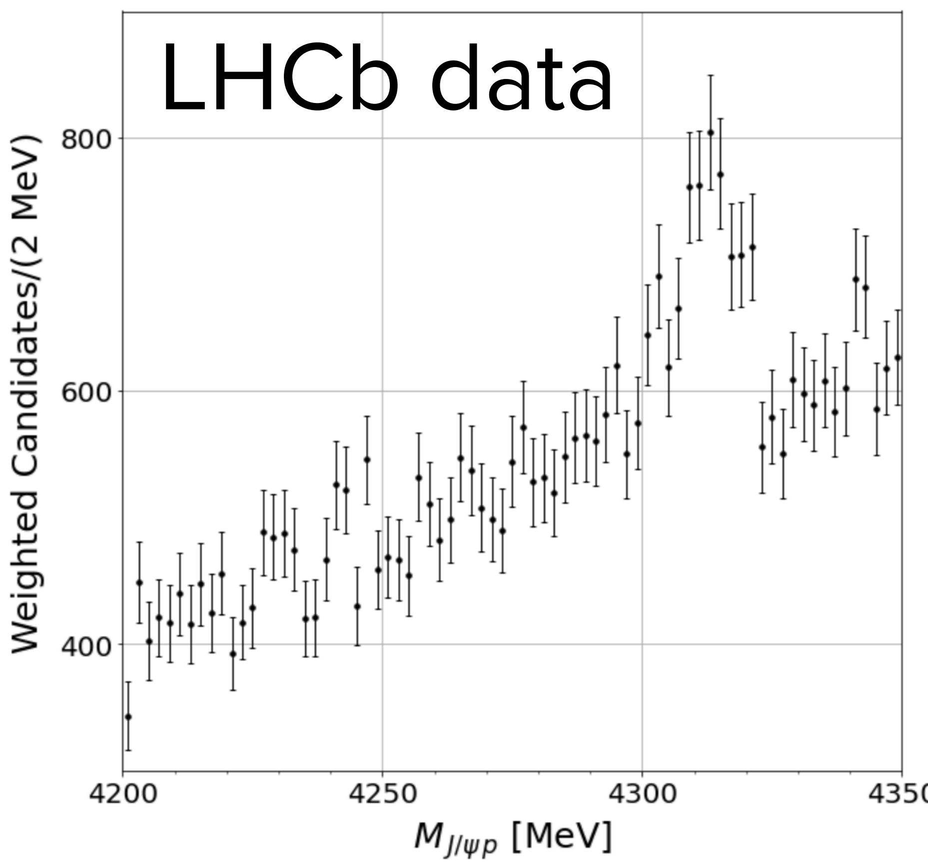
It is not enough to use one element of the T-matrix.
We need to include the off-diagonal element.



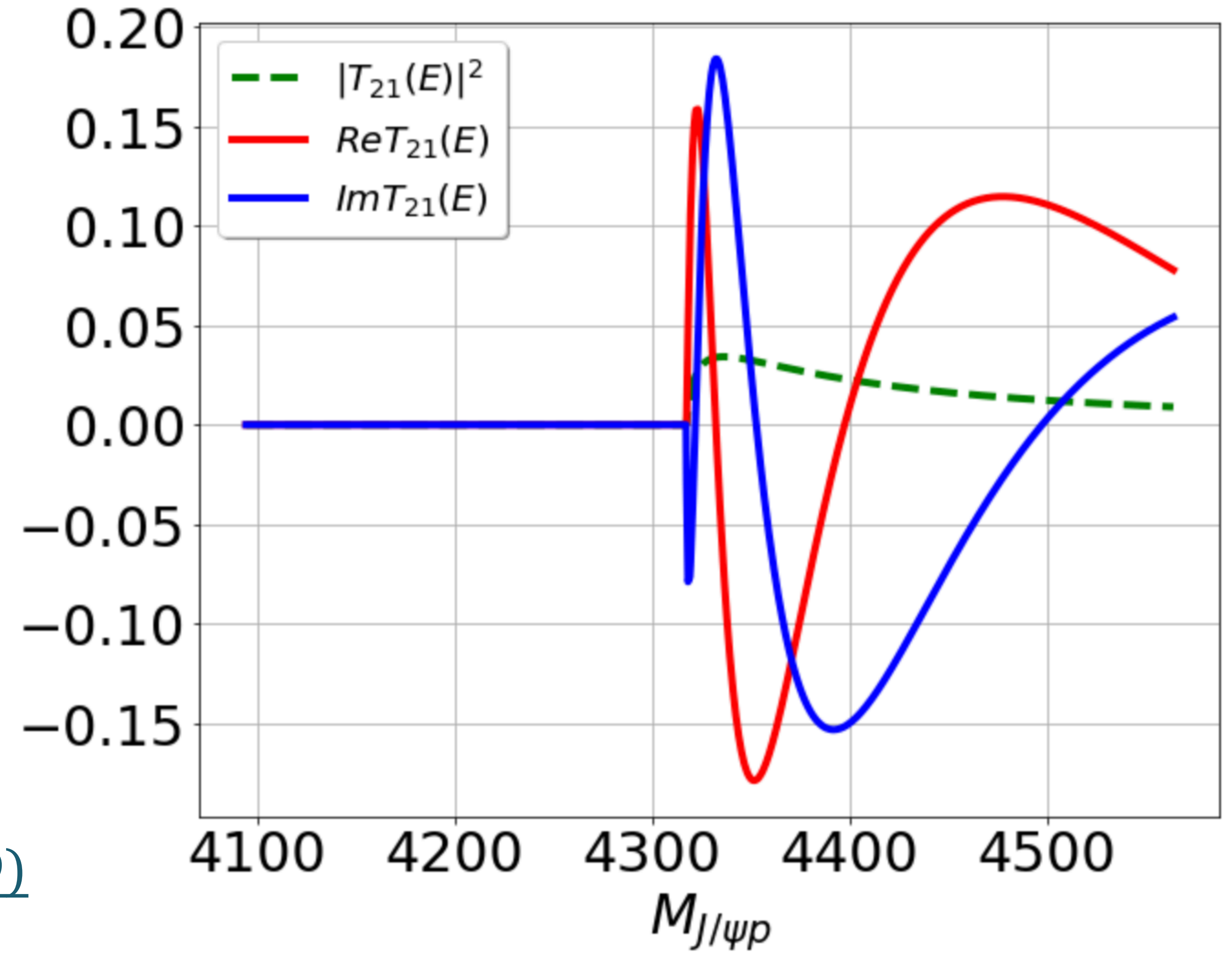
1 pole in each RS







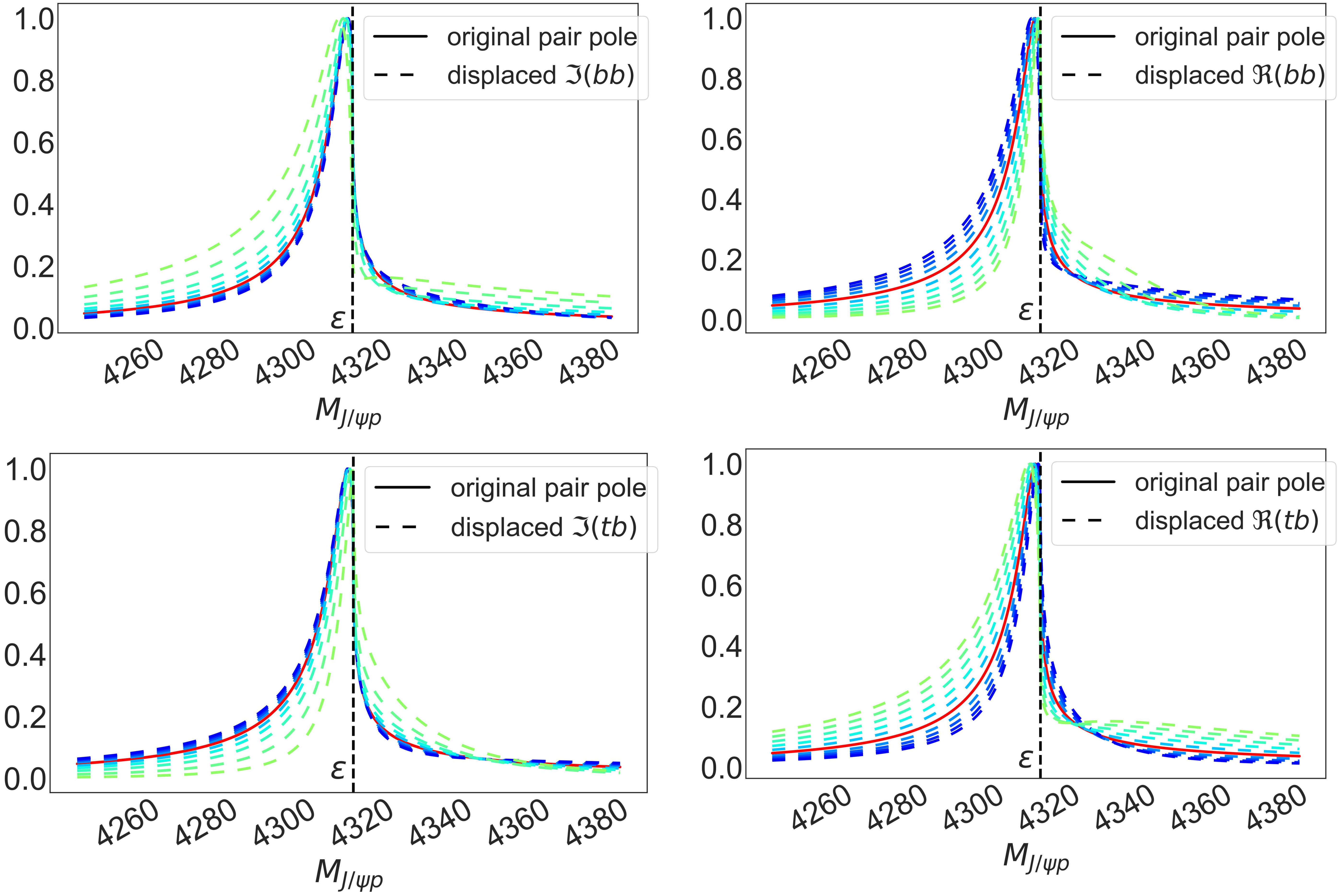
LHCb, PRL 122 222001 (2019)

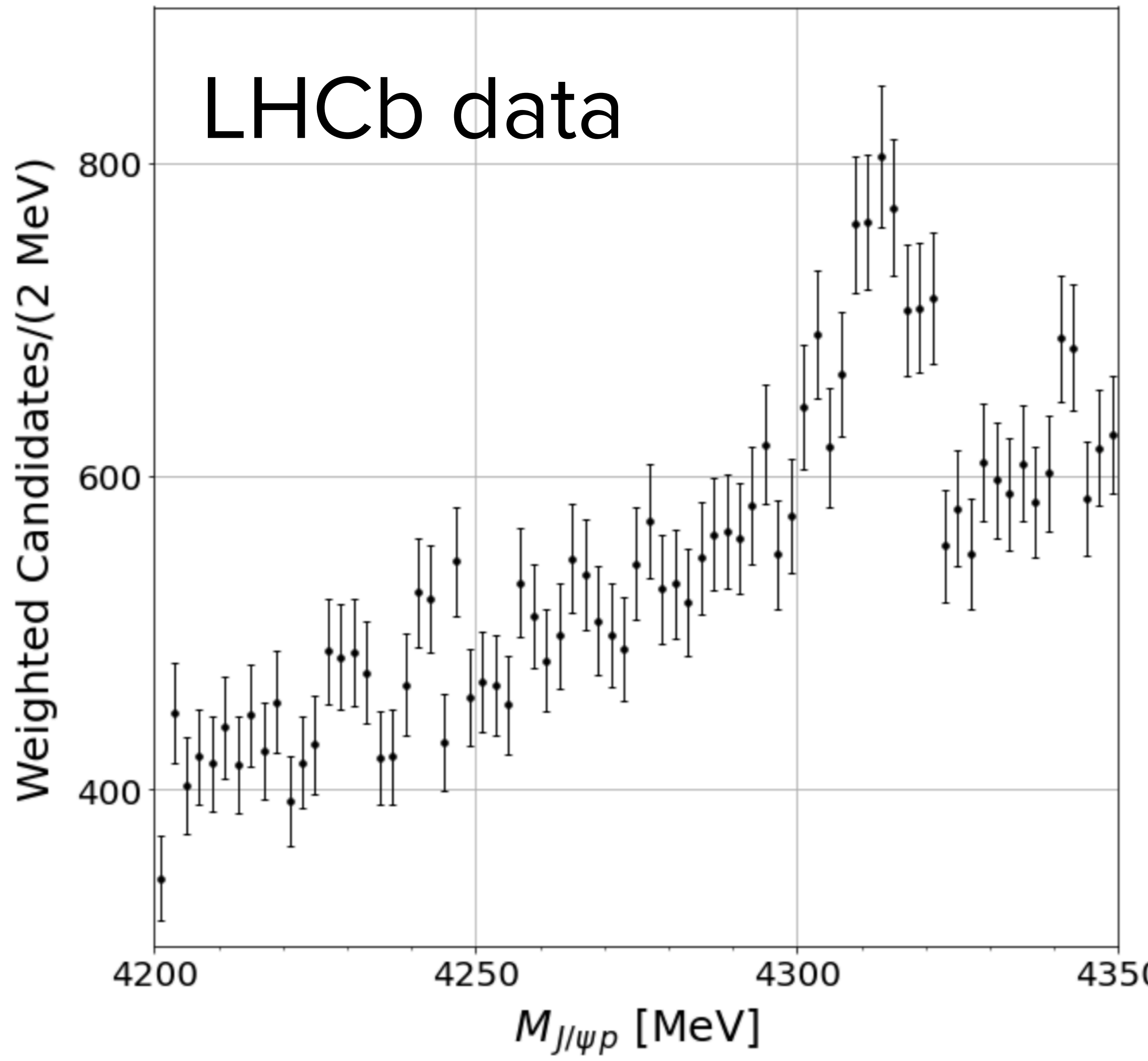


LMS, DLBS PRC 108 045204 (2023)

Probe deeper: Pole structure of $P_{c\bar{c}}(4312)^+$

Maybe unlikely to happen -
to produce ambiguous pole structure, the poles must have the same position.





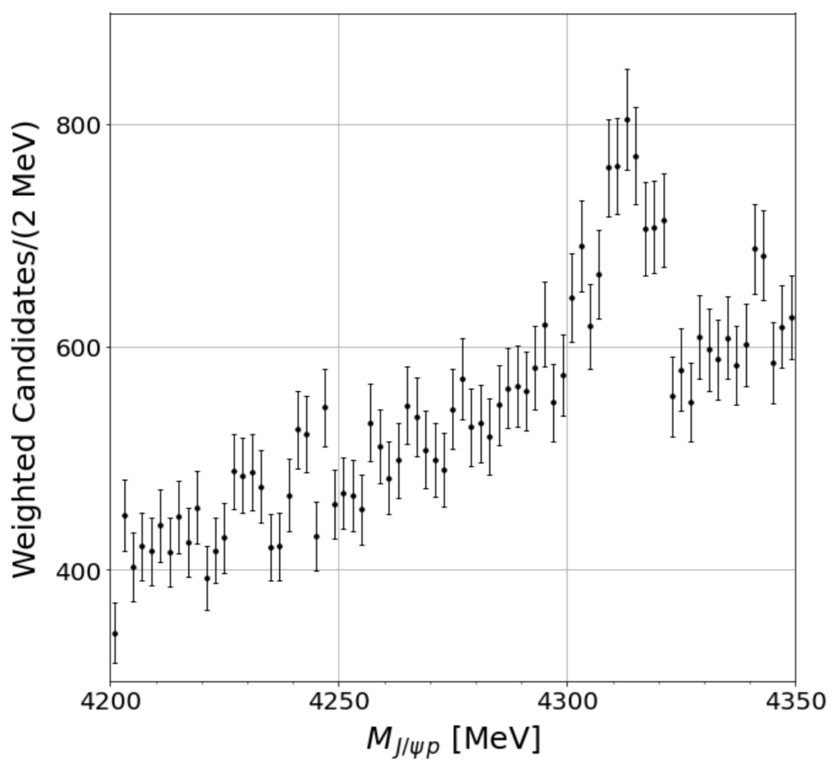
LHCb, PRL 122 222001 (2019)

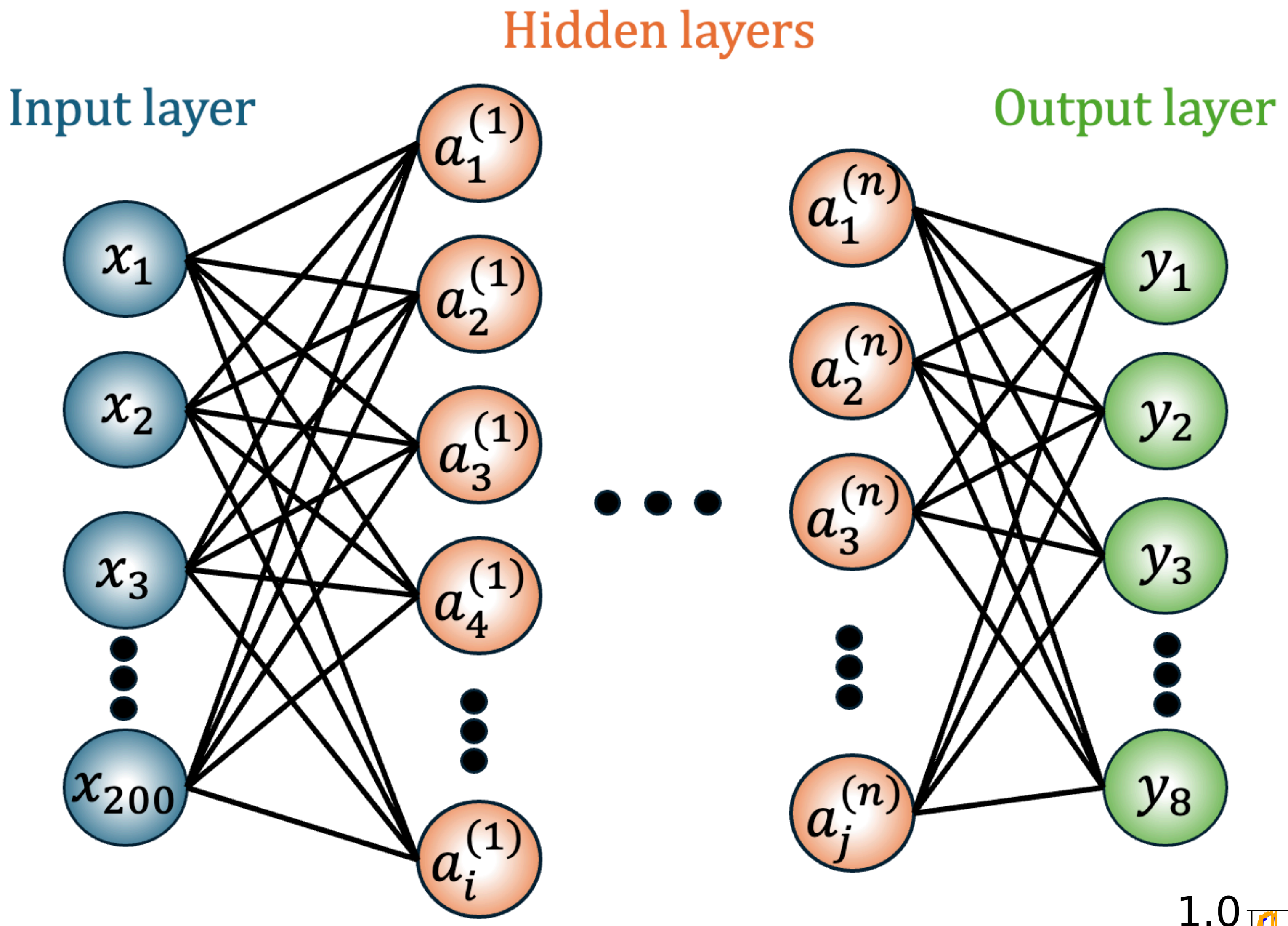
Slight variation in the line shape

Experimental uncertainty might hide them.

LMS, DLBS PRC 108 045204 (2023)

Probe deeper: Pole structure of $P_{c\bar{c}}(4312)^+$





Class label	S-matrix pole configuration
0	1 pole on $[bt]$
1	1 pole on $[bb]$
2	1 pole on $[tb]$
3	1 pole on $[bt]$ and 1 pole on $[bb]$
4	1 pole on $[bb]$ and 1 pole on $[tb]$
5	1 pole on $[bb]$, 1 pole on $[tb]$, 1 pole on $[bt]$
6	2 poles on $[bb]$, 1 pole on $[tb]$
7	1 pole on $[bb]$, 2 poles on $[tb]$

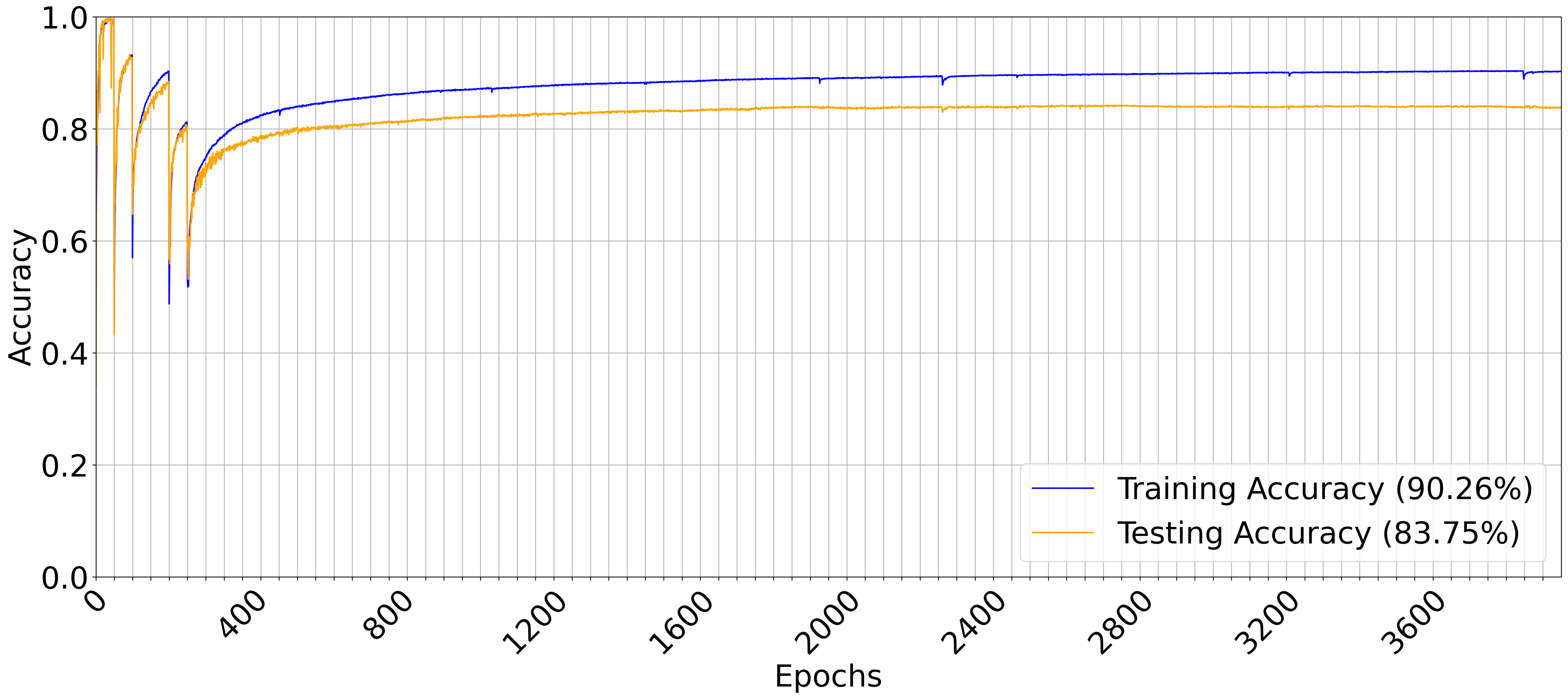
$$\frac{dN}{d\sqrt{s}} = \rho(s)\Big[\,|F(s)|^2 + B(s)\Big];$$

$$F(s) = \alpha_1 T_{11}(s) + \alpha_2 T_{21}(s)$$

$$S_{11}(\omega) = \prod_m \frac{D_m(-1/\omega)}{D_m(\omega)} \qquad S_{11}S_{22} - S_{12}S_{21} = \prod_m \frac{D_m(-\omega)}{D_m(\omega)}$$

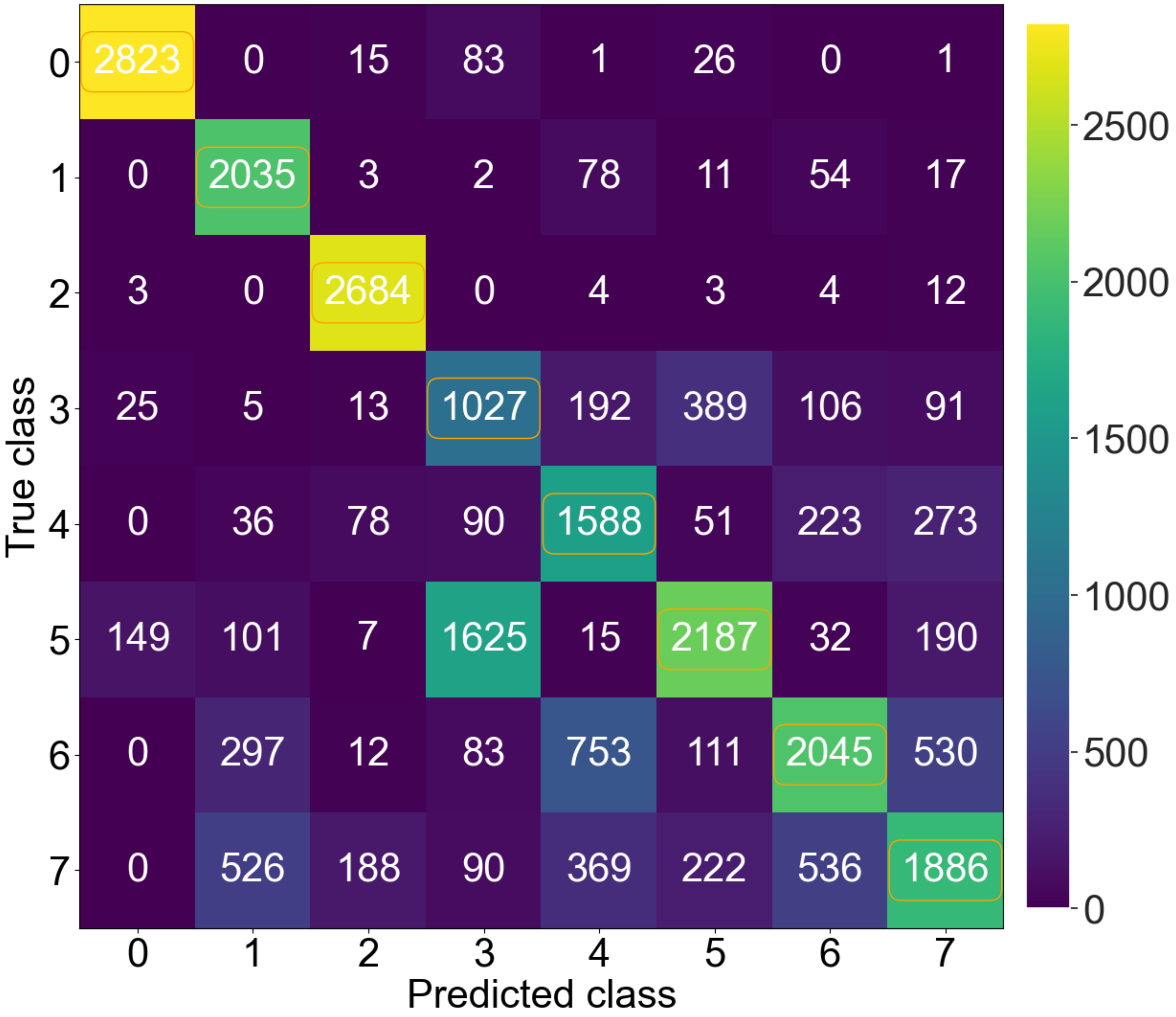
$$S_{22}(\omega) = \prod_m \frac{D_m(1/\omega)}{D_m(\omega)}$$

$$\hat{S} = \hat{1} + 2i\hat{T}$$

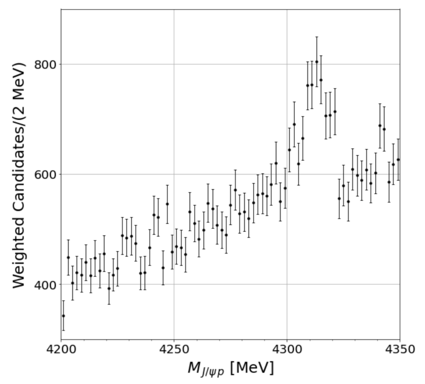


LM Santos, VAA Chavez, DLBS, JPG (2025) 52 015104

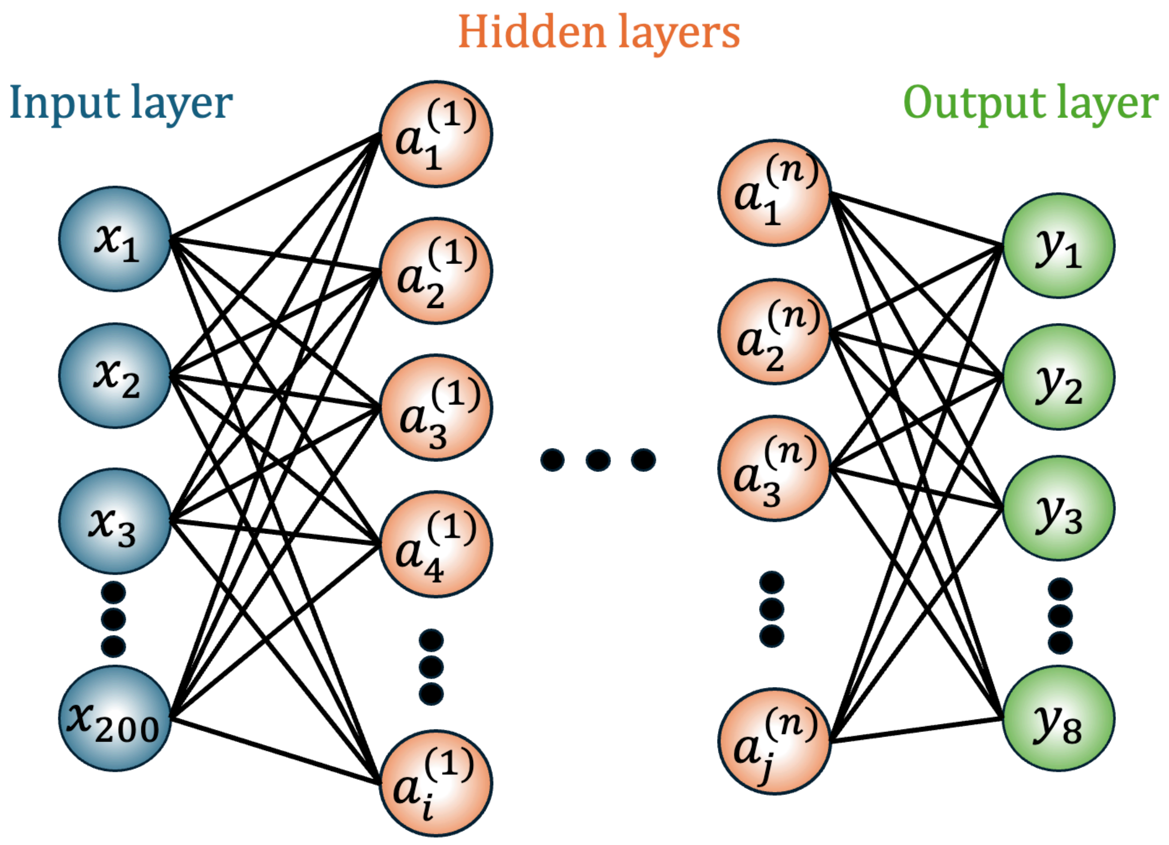
Probe deeper: Pole structure of $P_{c\bar{c}}(4312)^+$



Class label	S-matrix pole configuration
0	1 pole on $[bt]$
1	1 pole on $[bb]$
2	1 pole on $[tb]$
3	1 pole on $[bt]$ and 1 pole on $[bb]$
4	1 pole on $[bb]$ and 1 pole on $[tb]$
5	1 pole on $[bb]$, 1 pole on $[tb]$, 1 pole on $[bt]$
6	2 poles on $[bb]$, 1 pole on $[tb]$
7	1 pole on $[bb]$, 2 poles on $[tb]$



Bootstrapped 3000



All output: Class 5

1 pole in each unphysical RS.

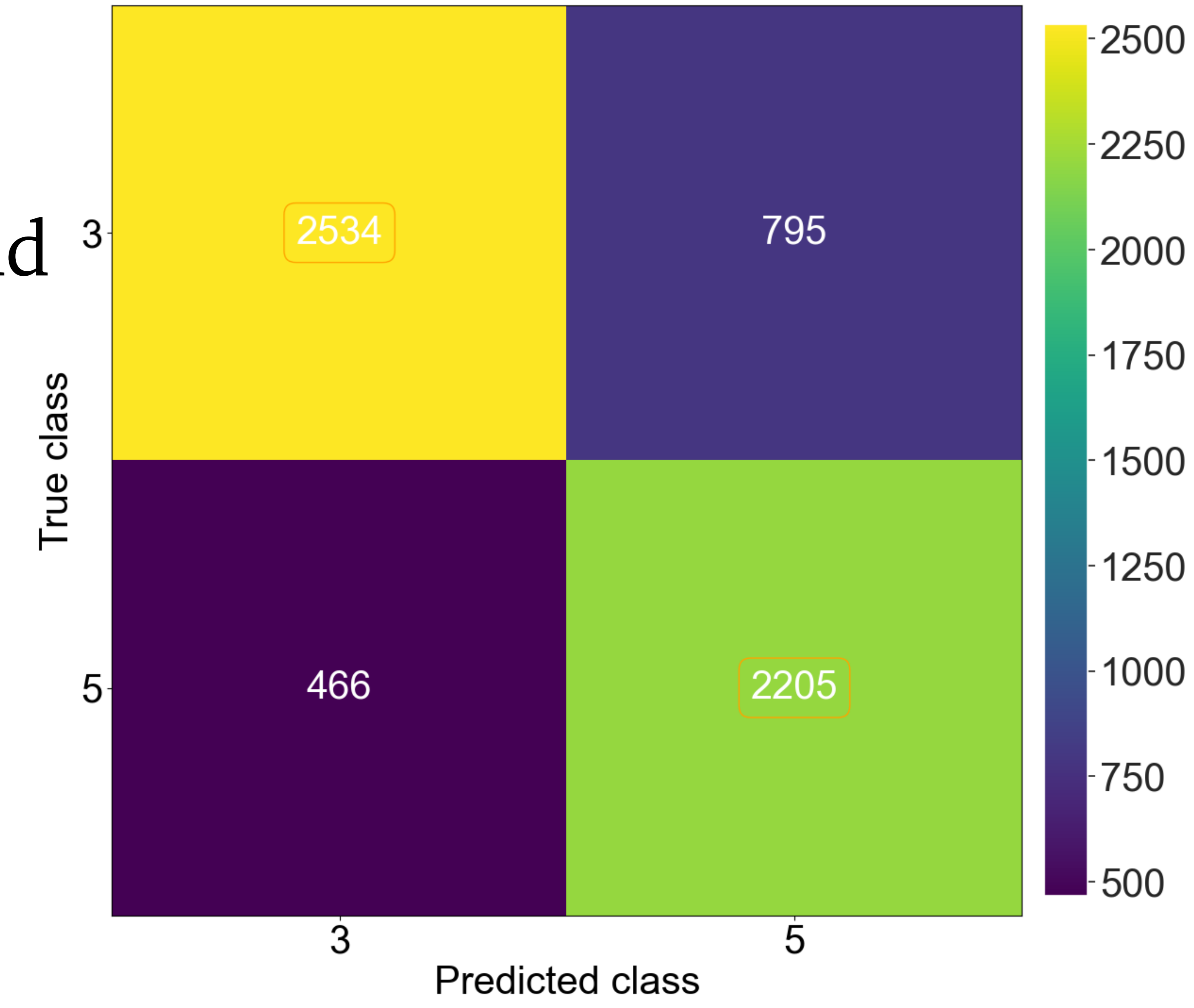
LM Santos, VAA Chavez, DLBS, JPG (2025) 52 015104

Probe deeper: Pole structure of $P_{c\bar{c}}(4312)^+$

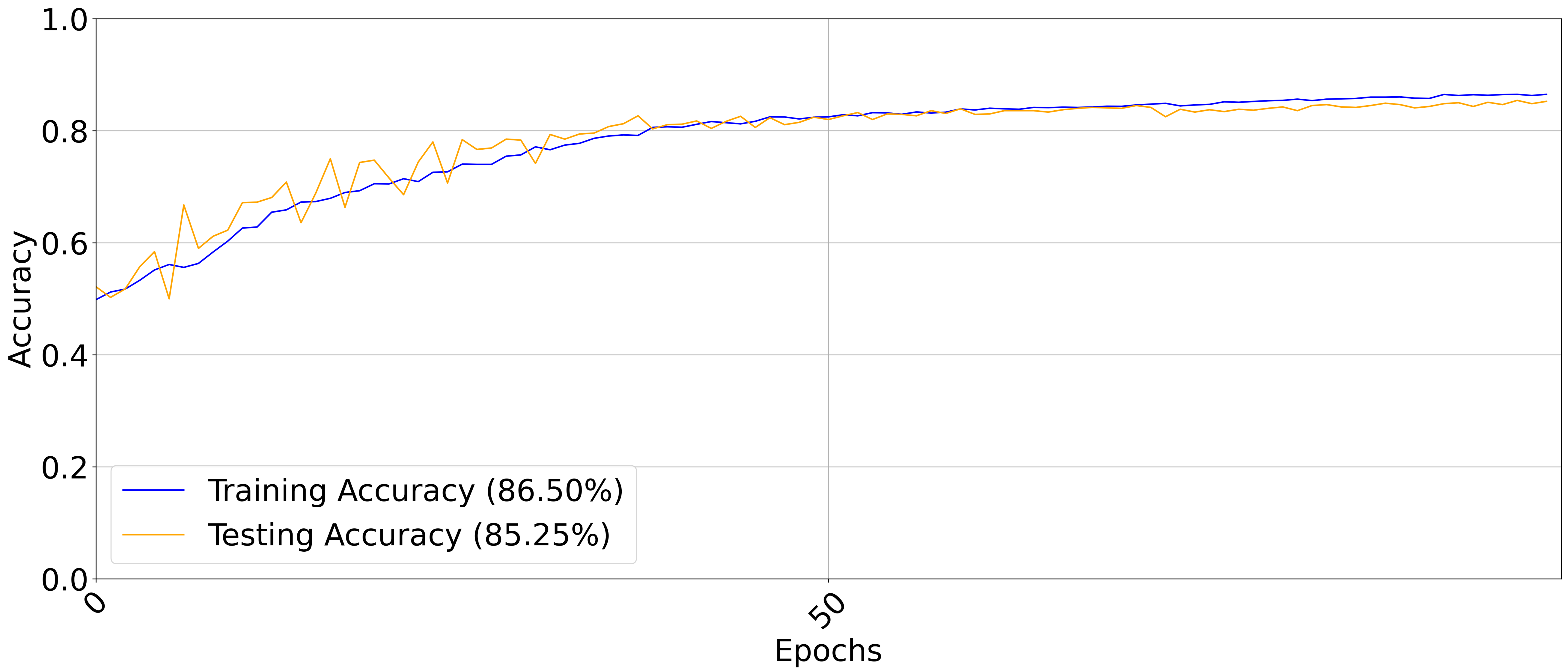
Focus only on two confusing classes: class 3 vs class 5
- Retrain new DNN model but with only two outputs.
- Apply again to the experimental data.

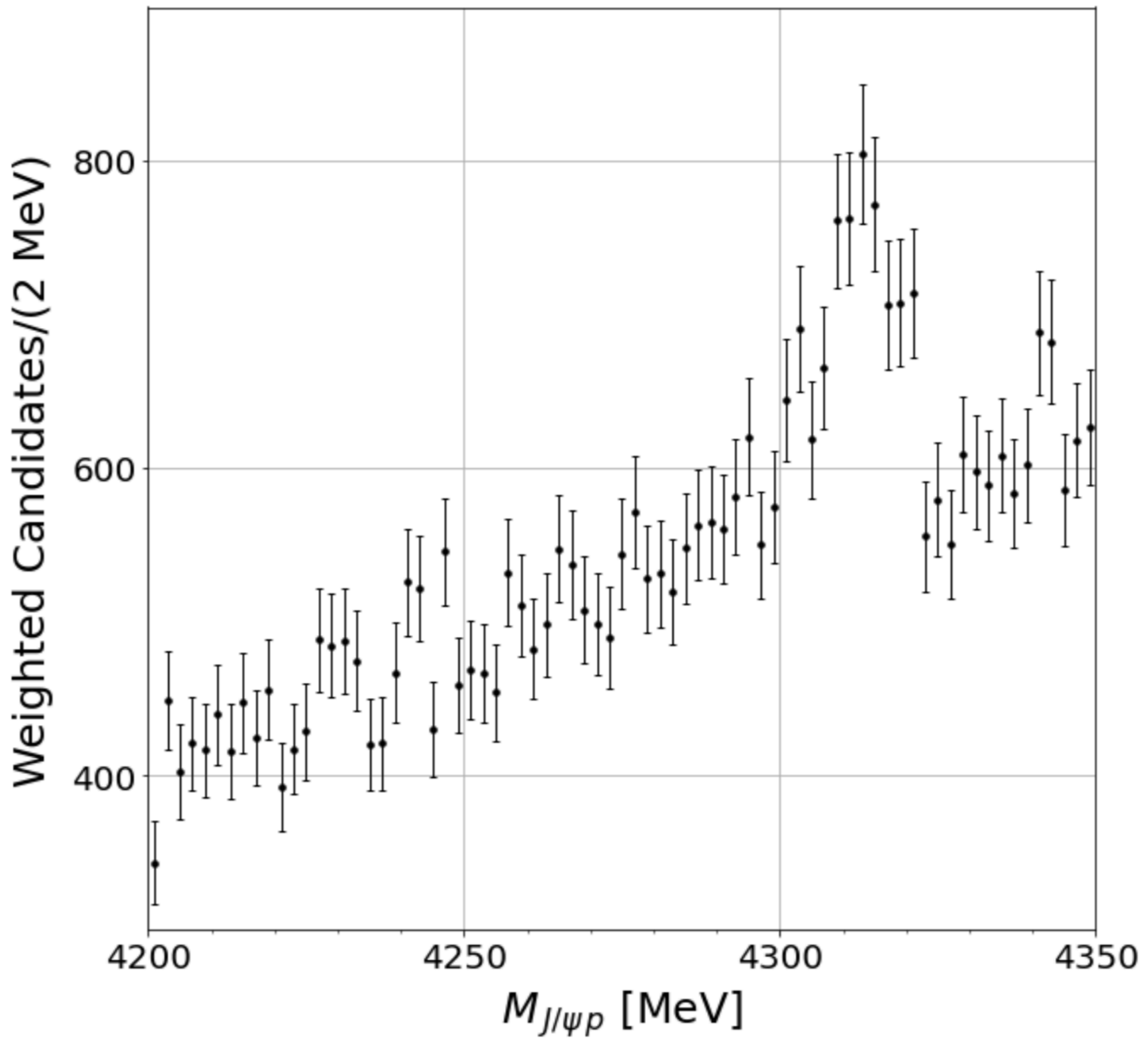
Class 3:
1 pole in 2nd RS and
1 pole in the 3rd

Class 5:
1 pole in each
unphysical RS



When the binary DNN model is applied to the experimental data, class 5 is still favored.





Pole in 2nd and 3rd RS
-resemble pole-shadow pair
-possible true resonance decaying into $J/\psi p$

Pole in 4th RS
-Virtual state of $\Sigma_c\bar{D}$ coupled to $J/\psi p$

LM Santos, VAA Chavez, DLBS, JPG (2025) 52 015104

Conclusion and Outlook

- It is possible to distinguish kinematical enhancements with dynamical pole-based enhancements despite the presence of experimental uncertainty.

- To fully utilized the power of ML, use it a as a model-selection framework.
  - Multi-parameter of a DNN can be used to cover a wider model space.

- Using the ML approach, we have shown that
  - $P_{c\bar{c}}(4312)^+$ is NOT due to (single) triangle singularity
  - $P_{c\bar{c}}(4312)^+$ is a possible true resonance that is contaminated by the coupled-channel interaction of $\Sigma_c\bar{D}$ (having a virtual state) with $J/\psi p$.

Outlook

- Include the Double Triangle Singularity interpretation in the ML model-selection framework.
- Apply the method to other near-threshold phenomena.
- Apply the method to correlation function.

Thank you for your attention.

Back Up: General parametrization

$$S_{11}(p_1, p_2) = \prod_m \frac{D_m(-p_1, p_2)}{D_m(p_1, p_2)}$$

KJ Le Couteur, Proc. Roy. Soc (London) A256 (1960)
RG Newton J. Math. Phys. 2, 188 (1961)

ERE - Scattering length approx.

$$D(p_1, p_2) = \left(M_{11} - ip_1\right)\left(M_{22} - ip_2\right) - M_{12}^2$$

$D(p_1, p_2)$ can only vanish when the $\bar{p}_1$ and $\bar{p}_2$ have opposite imaginary parts. W Frazer and A Hendry, Phys. Rev., 134, B1307 (1964)

Flatté-like parametrization

$$D(p_1, p_2) = E - M + ip_1 + i\gamma_2 p_2$$

Shadow poles may appear on the physical sheet.

RJ Eden, JR Taylor, Phys. Rev. 133, B1575 (1974)

$$\left[\left(p_1 - i\beta_1\right)^2 - \alpha_1^2\right] + \lambda\left[\left(p_2 - i\beta_2\right)^2 - \alpha_2^2\right] = 0$$

$$\left[\left(p_1 - i\beta_1\right)^2 - \alpha_1^2\right]\left[\left(p_1 - i\beta_1\frac{1-\lambda}{1+\lambda}\right)^2 - \left(\alpha_1^2 + \frac{4\lambda\beta_2^2}{(1+\lambda)^2}\right)\right] = 0$$

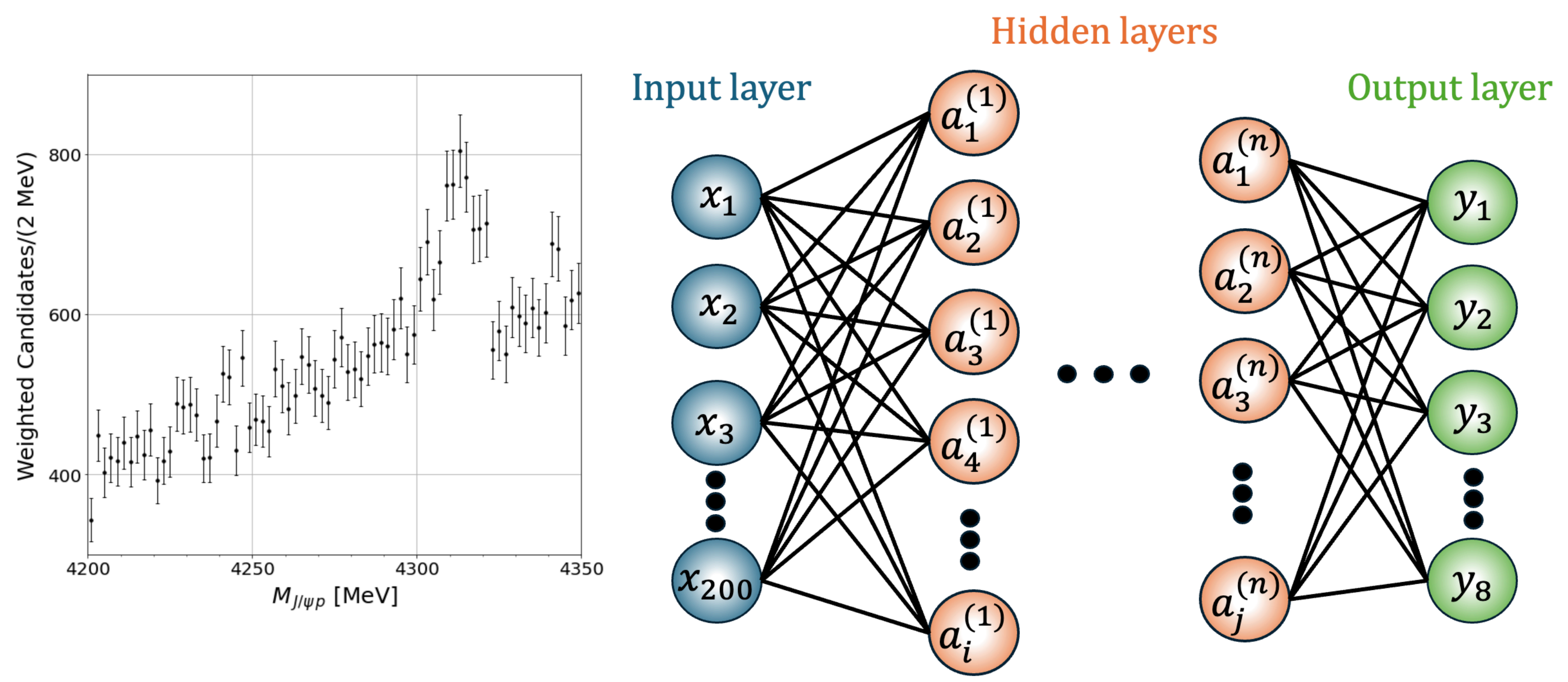
$$\left[\left(p_2 - i\beta_2\right)^2 - \alpha_2^2\right]\left[\left(p_2 + i\beta_2\frac{1-\lambda}{1+\lambda}\right)^2 - \left(\alpha_2^2 + \frac{4\lambda\beta_1^2}{(1+\lambda)^2}\right)\right] = 0$$

Main pole — Shadow poles

We need a general parametrization:

- Pole position can be controlled and RS can be assigned.
- Poles are independent of each other.

Back Up: $P_{c\bar{c}}(4312)^+$



Pole in 2nd and 3rd RS
-resemble pole-shadow pair
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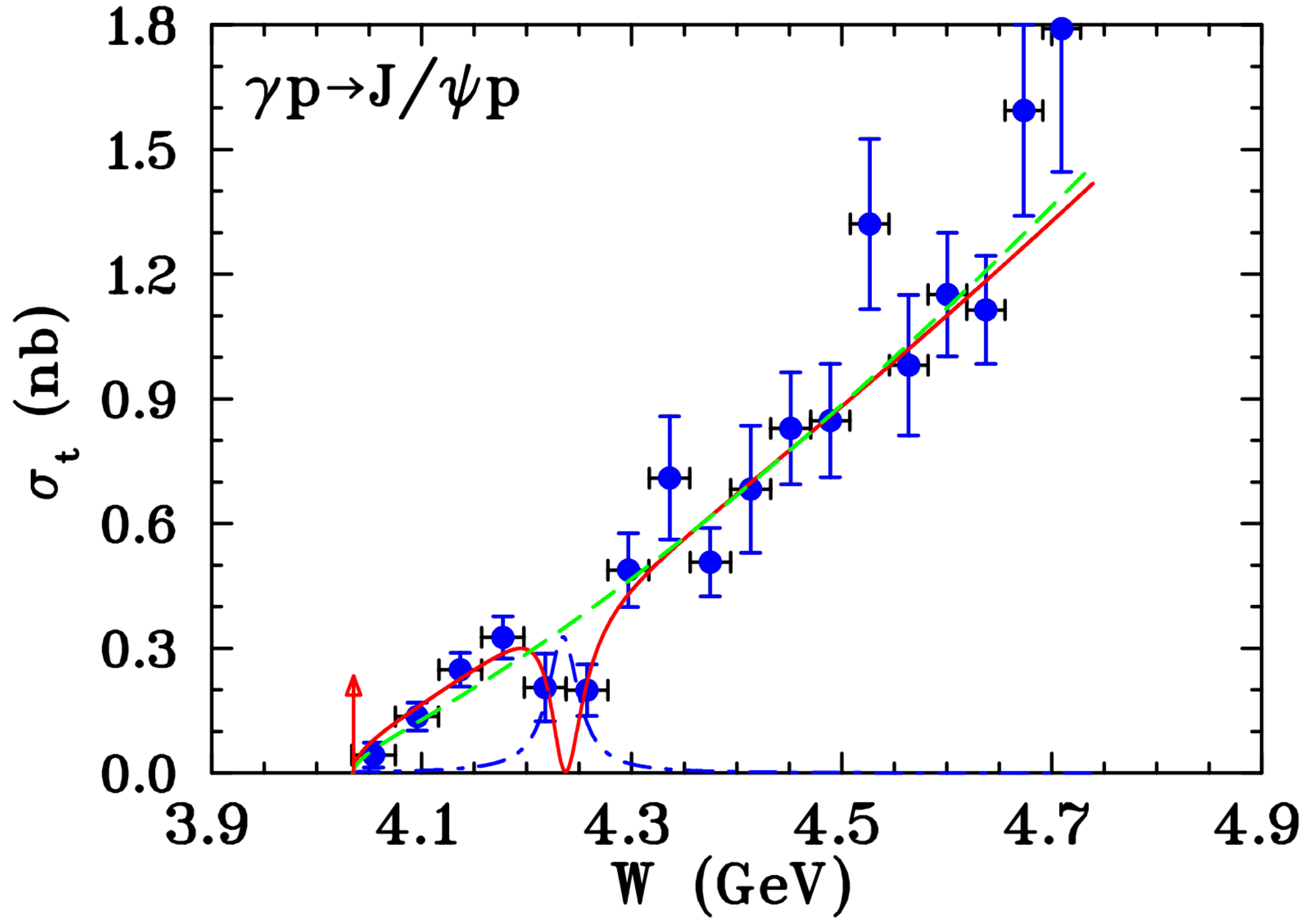
Pole in 4th RS
-Virtual state of $\Sigma_c\bar{D}$ coupled to $J/\psi p$



In contrast with the analysis of JPAC in 2019

JPAC, PRL 123 092001 (2019)

GlueX: J/ψ photo-production 2023 result - structure found in the J/ψ-p cross-section

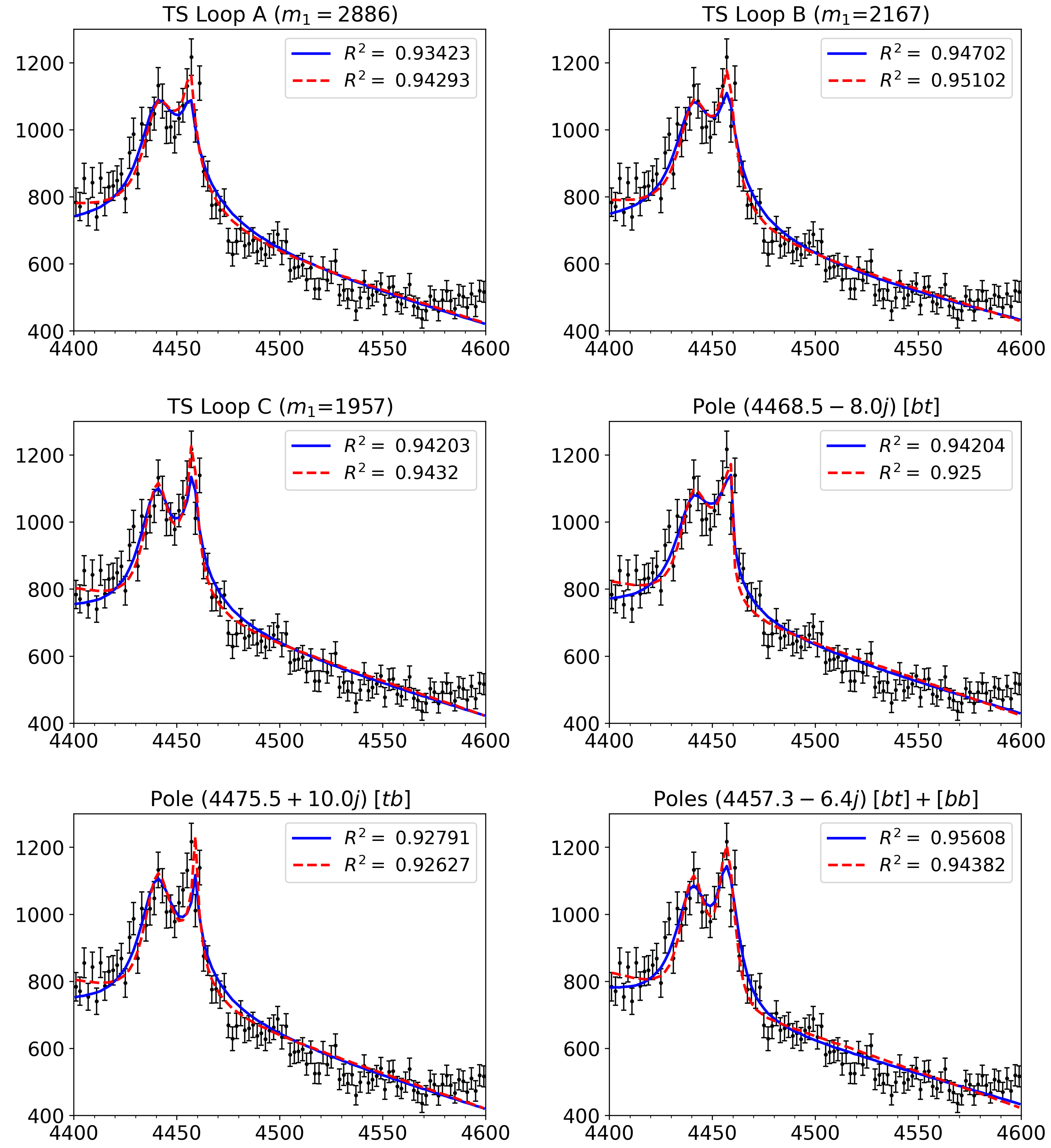
GlueX, PRC 108 025201 (2023)

The dip structure can be interpreted as a resonance that interfere with the non-resonant background.

I Strakovsky, et al, PRC 108 015202 (2023)

No contribution from the $\Sigma_c\bar{D}$ - cannot be interpreted as molecular.

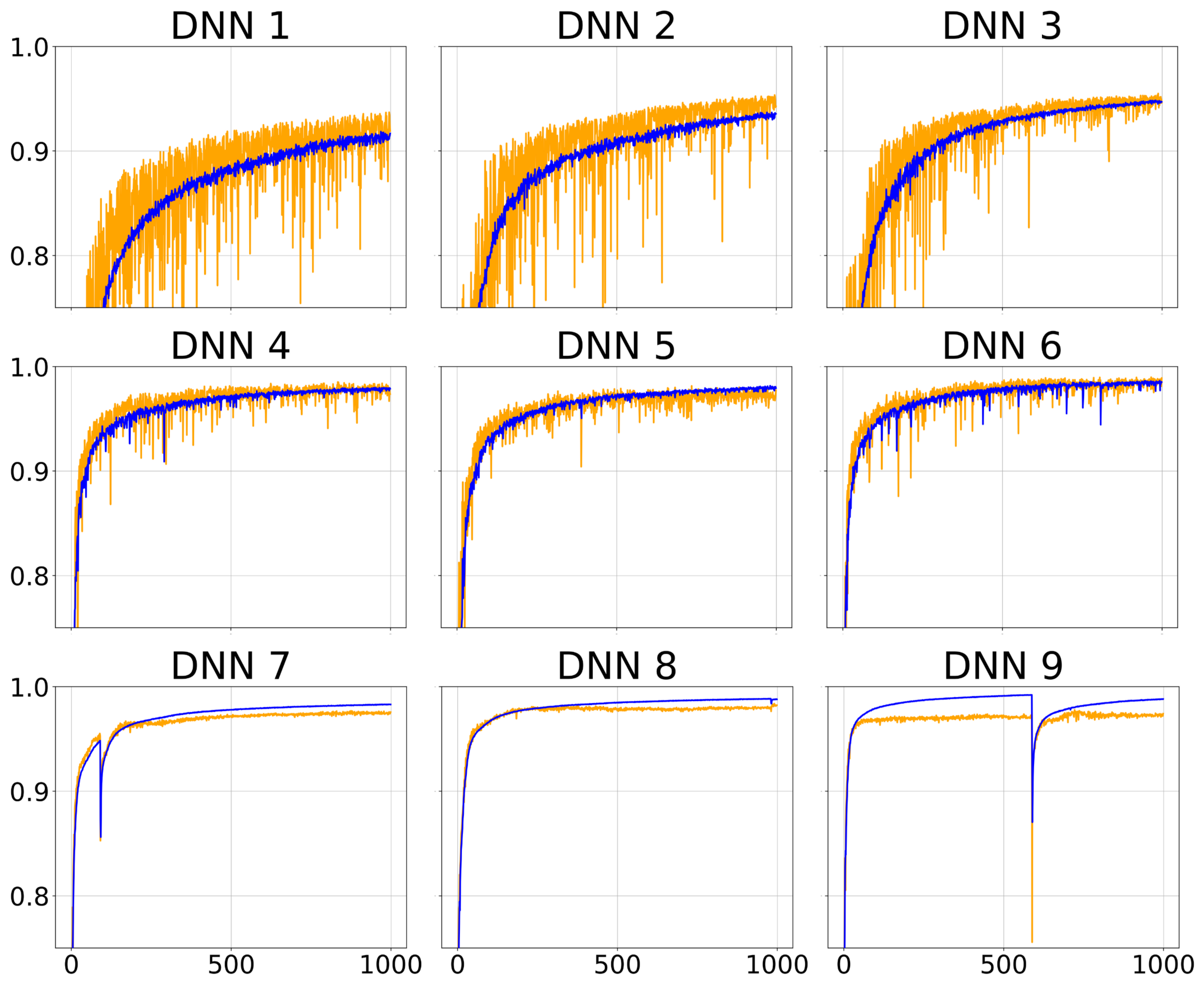
Back Up: $P_{c\bar{c}}(4457)^+$

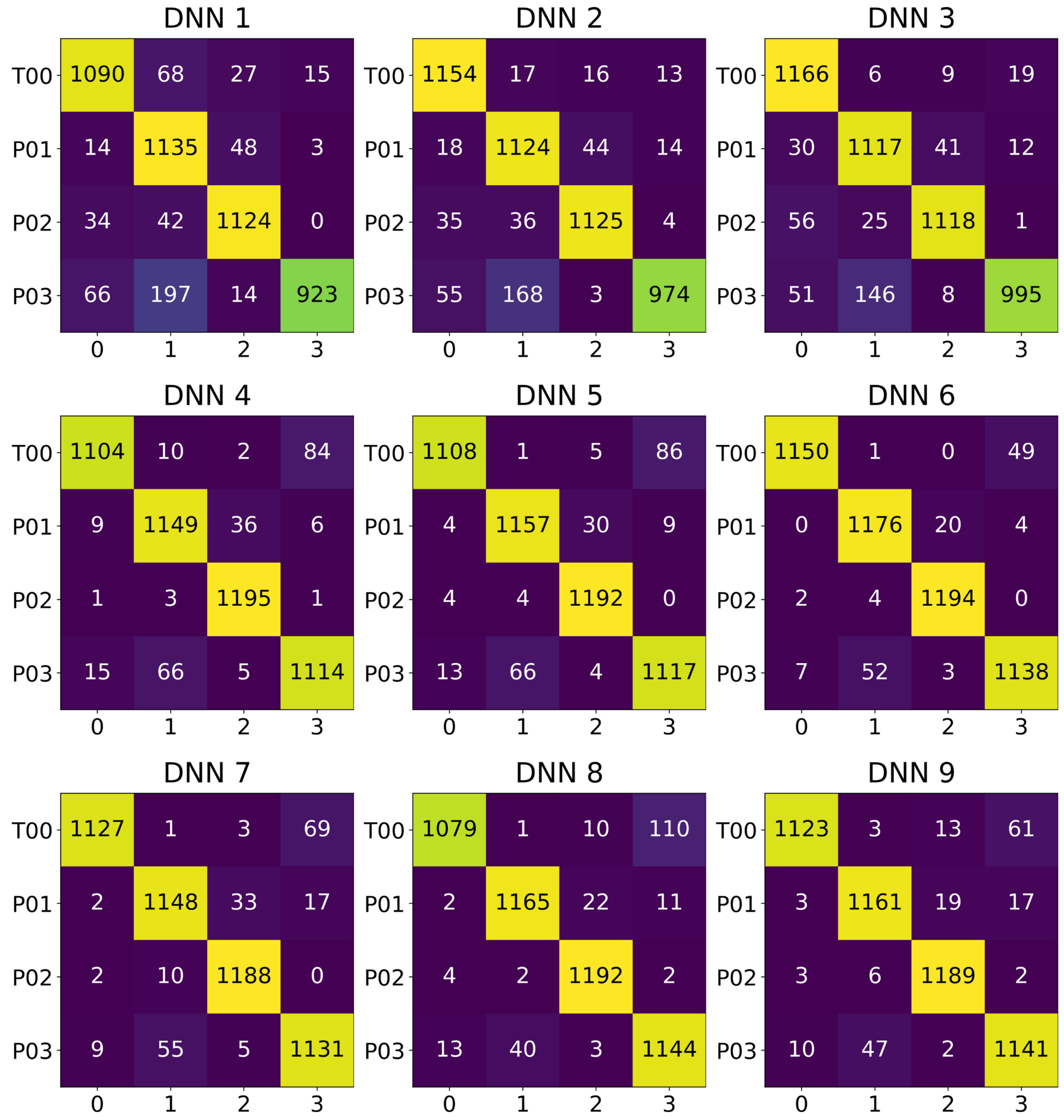


DNN model	Optimizer and architecture
DNN 1	AdaGrad: 200-[350-250]-4
DNN 2	AdaGrad: 200-[350-300-250]-4
DNN 3	AdaGrad: 200-[350-400-350]-4
DNN 4	AMSGrad: 200-[350-250]-4
DNN 5	AMSGrad: 200-[350-300-250]-4
DNN 6	AMSGrad: 200-[350-400-350]-4
DNN 7	SMORMS3: 200-[350-250]-4
DNN 8	SMORMS3: 200-[350-300-250]-4
DNN 9	SMORMS3: 200-[350-400-350]-4

DAO Co and DLBS, arXiv:2411.14044

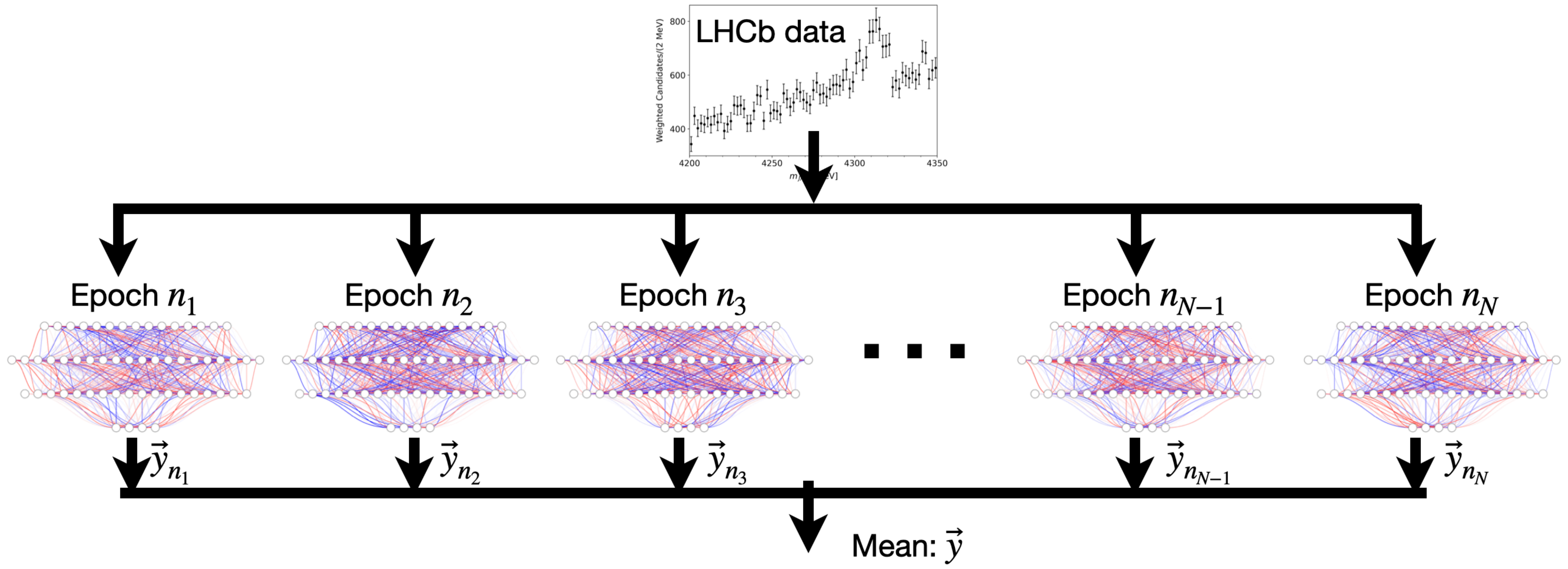
Back Up: $P_{c\bar{c}}(4457)^+$





[DAO Co and DLBS, arXiv:2411.14044]

Back Up: $P_{c\bar{c}}(4457)^+$



DAO Co and DLBS, arXiv:2411.14044

	Triangle	1 pole in $[bt]$	1 pole in $[tb]$	1 pole each in $[bt]$ and $[bb]$
DNN 1	376	320	1	2303
DNN 2	36	0	0	2964
DNN 3	14	287	1008	1691
DNN 4	181	317	0	2502
DNN 5	0	0	0	3000
DNN 6	0	0	0	3000
DNN 7	0	0	0	3000
DNN 8	12	2	0	2986
DNN 9	0	5	0	2995