ML based classification of scattering amplitude poles. A case of $P_c(4312)$

INT Program 22-1 Machine Learning for Nuclear Theory, Seattle, Mar 31, 2022

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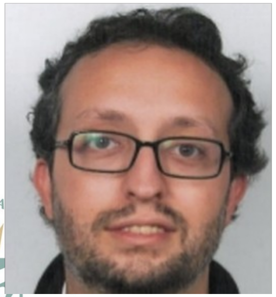

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Outline

- Motivation
- Physical model
- ML model
- Feature refinement
- Model predictions and explanation
- Outlook and open questions

Motivation

Plethora of potentially multiquark states observed in last decade

PHYSICAL REVIEW LETTERS **122**, 222001 (2019)

Editors' Suggestion **Featured in Physics**

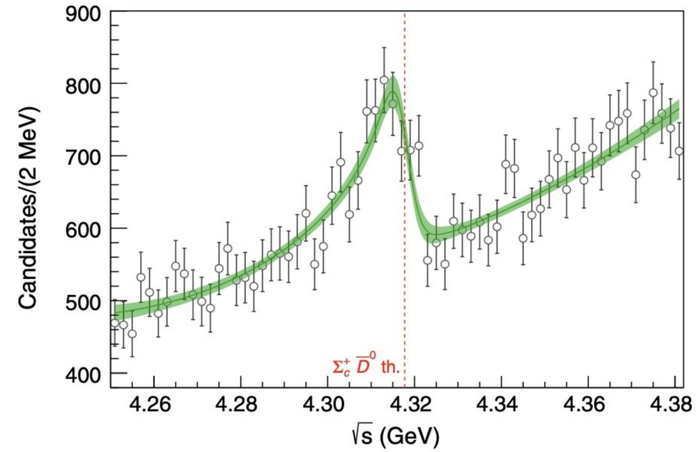
Observation of a Narrow Pentaquark State, $P_c(4312)^+$, and of the Two-Peak Structure of the $P_c(4450)^+$

R. Aaij *et al.*[*]
(LHCb Collaboration)

(Received 6 April 2019; published 5 June 2019)

A narrow pentaquark state, $P_c(4312)^+$, decaying to $J/\psi p$, is discovered with a statistical significance of 7.3σ in a data sample of $\Lambda_b^0 \to J/\psi p K^-$ decays, which is an order of magnitude larger than that previously analyzed by the LHCb Collaboration. The $P_c(4450)^+$ pentaquark structure formerly reported by LHCb is

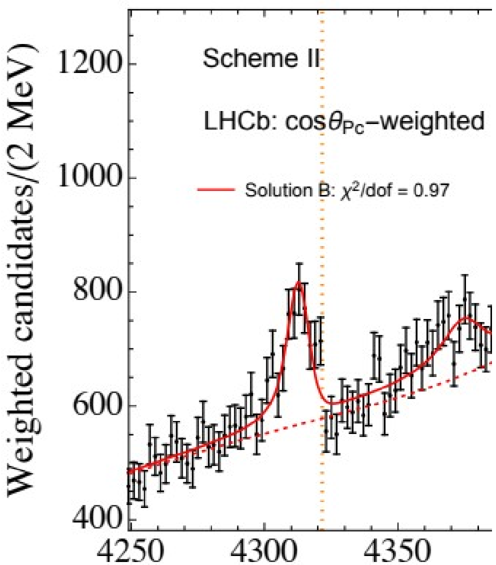
Possible interpretation as $duuc\bar{c}$ pentaquark



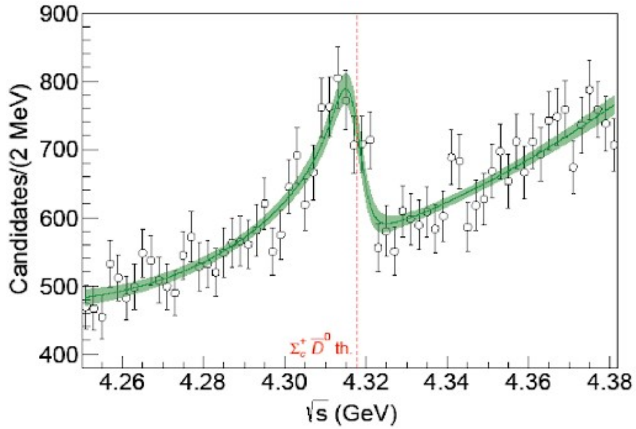
Intensity in the $P_c(4312)$ neighbourhood and the JPAC fit *C. Fernandez-Ramirez Phys.Rev.Lett. 123 (2019) 9, 092001*

- There is a close relation between QCD spectrum and the analytic structure of amplitudes (production thresholds → branch points, resonaces/bound states → poles)
- Currently this relationship is impossible to derive from first principles of QCD (top down approach)
- One can utilize the general properties of amplitudes, like unitarity, analyticity or crossing symmetry, but then some interaction parameters must be derived from data – bottom up approach

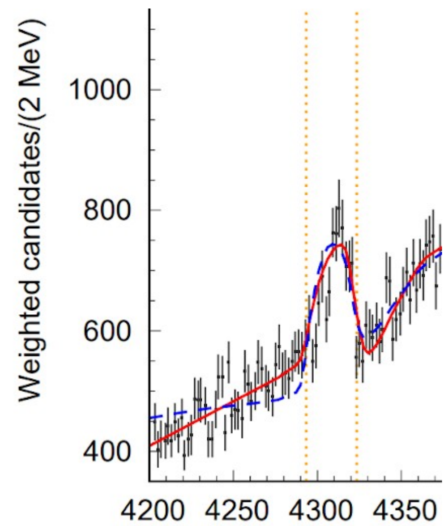
Discrepant interpretations of the $P_c(4312)$ nature



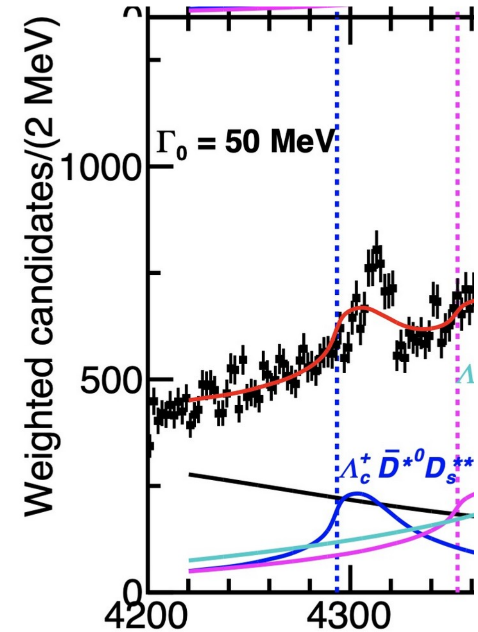
Molecule
Du et al., 2102.07159



Virtual
C. F-R et al. (JPAC), Phys. Rev. Lett. 123, 092001 (2019)



Double-triangle (w. complex coupl. in the Lagrangian)
Nakamura, Phys. Rev. D 103, 111503 (2021)



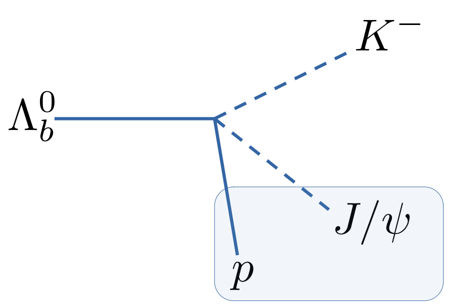
Single triangle (ruled out)
LHCb, Phys. Rev. Lett. 122, 222001 (2019)

We want to use ANN to:

- Go beyond the standard χ^2 fitting
- Specific questions:
  - Can we train a neural network to analyze a lineshape and get as a result what is the probability of each posible dynamical explanation ?
  - If posible, what other information can we gain by using machine learning techniques?
- First attempts to use Deep neural networks as model classifiers for hadron spectroscopy:

  Sombillo et al., 2003.10770, 2104.141782, 2105.04898

Physics model



- $P_c(4312)$ seen as a maximum in the pJ/ψ energy spectrum
- $P_c(4312)$ has a well defined spin and appears in single partial wave
- Background contributes to all other waves
- $\Sigma^+_c \bar{D}^0$ channel opens at 4.318 GeV -coupled channel problem

- Intensity

$$\frac{dN}{d\sqrt{s}} = \rho(s) \left[|P_1(s) T_{11}(s)|^2 + B(s) \right]$$

where

$$\rho(s) = pqm_{\Lambda_b}$$ phase space

$$p = \lambda^{\frac{1}{2}}(s, m^2_{\Lambda_b}, m^2_K)/2m_{\Lambda_b}, \;\; q = \lambda^{\frac{1}{2}}(s, m^2_p, m^2_\psi)/2\sqrt{s}$$

$$P_1(s) = p_0 + p_1 s$$ production term

$$B(s) = b_0 + b_1 s$$ background term

Physics model

- Coupled channel amplitudes

$$T^{-1}_{ij} = M_{ij} - ik_i\delta_{ij} \quad \text{where} \quad k_i = \sqrt{s - s_i}$$

$$s_1 = (m_p + m_{J/\psi})^2 \quad \text{and} \quad s_2 = (m_{\Sigma_c^+} + m_{\bar{D}^0})^2$$

- Unitarity implies that M_{ij} is free from singularities near thresholds s_1 and s_2 so that can be Taylor expanded *Frazer, Hendry Phys. Rev. 134 (1964)*

$$M_{ij}(s) = m_{ij} - c_{ij}s$$

- In principle the off-diagonal term of the amplitude $P_2(s)T_{21}$ could be included but we are interested in the analytical structure ("denominator") – so it's effect can be absorbed to the background and production terms.

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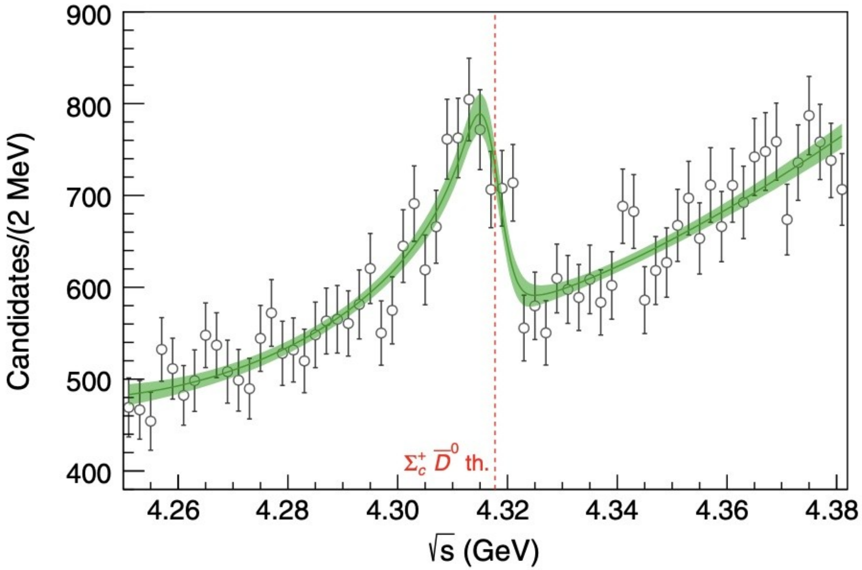
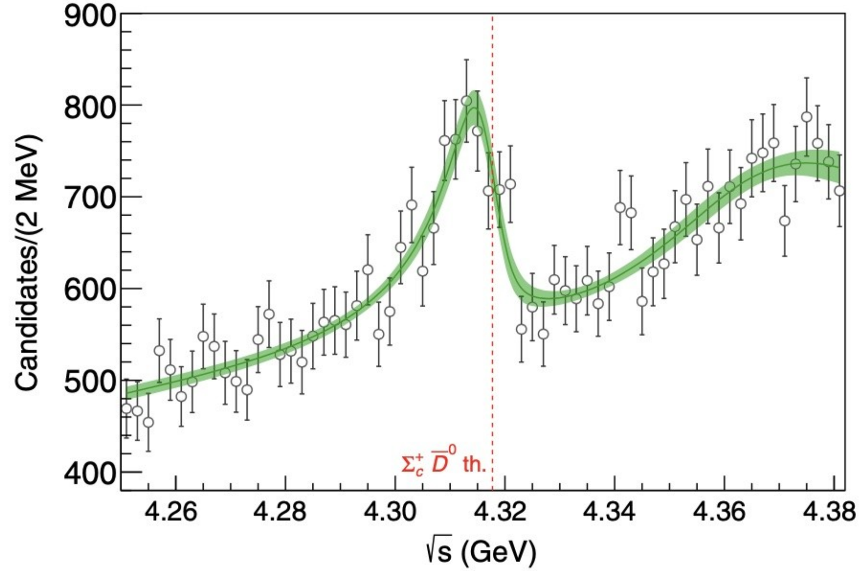
JPAC

Physics model – final version



Scattering length approximation



Effective range approximation

See *C. Fernandez-Ramirez Phys.Rev.Lett. 123 (2019) 9, 092001*

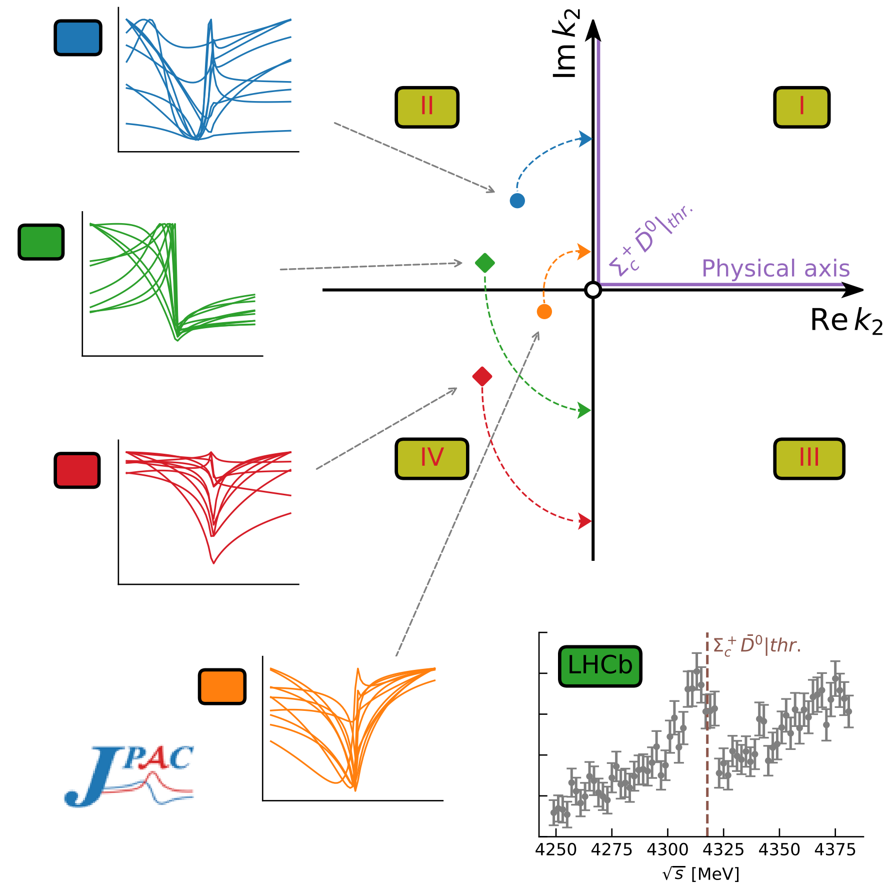
Finally we use the scattering length approximated amplitude as the basis for ML model

$$T_{11} = \frac{m_{22} - ik_2}{(m_{11} - ik_1)(m_{22} - ik_2) - m_{12}^2}$$

7 model parameters in total: m_{11}, m_{22}, m_{12}, p_0, p_1, b_0, b_1.

ML model – general idea

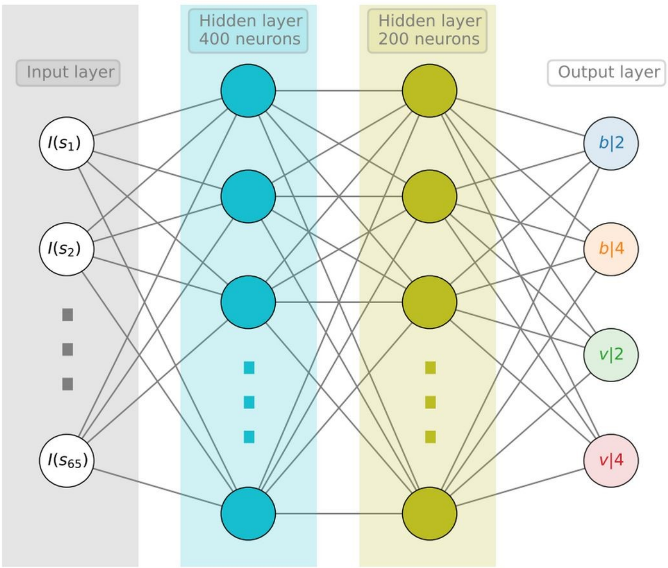
- From the physical model we produce:
  - Sample intensities (computed in 65 energy bins) – produced with randomly chosen parameter samples – **examples**
  - For each parameter sample we are able to compute the **target class** – one of the four: b|2, b|4, v|2, v|4
  - Symbolically:



$$K : \{[I_1, ..., I_{65}](m_{11}, m_{22}, m_{12}, p_0, p_1, b_0, b_1)\} \to \{b|2, b|4, v|2, v|4\}$$

ML model

Layer	Shape in	Shape out
Input		(B, 65)
Dense	(B, 65)	(B, 400)
Dropout(p=0.2)	(B, 400)	(B, 400)
ReLU	(B, 400)	(B, 400)
Dense	(B, 400)	(B, 200)
Dropout(p=0.5)	(B, 200)	(B, 200)
ReLU	(B, 200)	(B, 200)
Dense	(B, 200)	(B, 4)
Softmax	(B, 4)	(B, 4)



Training dataset preparation:

1. Parameters were uniformly sampled from the following ranges: b_0 = [0 ; 700], b_1 = [-40 ; 40], p_0 = [0 ; 600], p_1 = [-35 ; 35], M_{22} = [-0.4 ; 0.4], M_{11} = [-4 ; 4], M_{12}^2 = [0 ; 1.4]
2. The signal was smeared by convolving with experimental LHCb resolution:

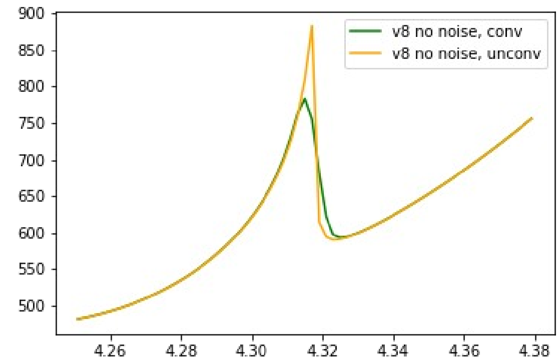
$$I(s) = \int_{m_\psi + m_p}^{m_{\Lambda_b} - m_K} I(s')_{\text{theo}} \exp\left[-\frac{(\sqrt{s}-\sqrt{s'})^2}{2R^2(s)}\right] d\sqrt{s'} \Bigg/ \int_{m_\psi + m_p}^{m_{\Lambda_b} - m_K} \exp\left[-\frac{(\sqrt{s}-\sqrt{s'})^2}{2R^2(s)}\right] d\sqrt{s'}\,,$$

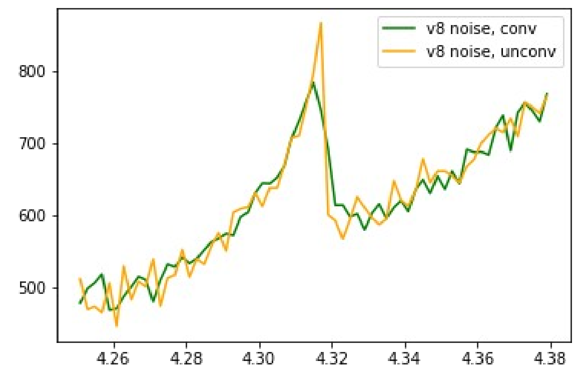
$$R(s) = 2.71 - 6.56 \times 10^{-6-1} \times \left(\sqrt{s} - 4567\right)^2$$

3. To account for experimental encertainty the 5% gaussian noise was added

ML model - training

- Input examples (efect of energy smearing and noise):





- Computing target classes:
  - $m_{22}>0$ – bound state, $m_{22}<0$ – virtual state
  - To localize the poles on Riemann sheets we need to find zeros of the amplitude denominator in the momentum space:

$$p_0 + p_1\, q + p_2\, q^2 + p_3\, q^3 + q^4 = 0$$

with

$$p_0 = (s_1 - s_2)\, m_{22}^2 - \left(m_{12}^2 - m_{11} m_{22}\right)^2$$

$$p_1 = 2\,(s_1 - s_2)\, m_{22} + 2 m_{11} \left(m_{12}^2 - m_{11} m_{22}\right)$$

$$p_2 = -m_{11}^2 + m_{22}^2 + s_1 - s_2$$

$$p_3 = 2 m_{22}$$

Then poles appear on sheets defined with (η_1,η_2) pairs:

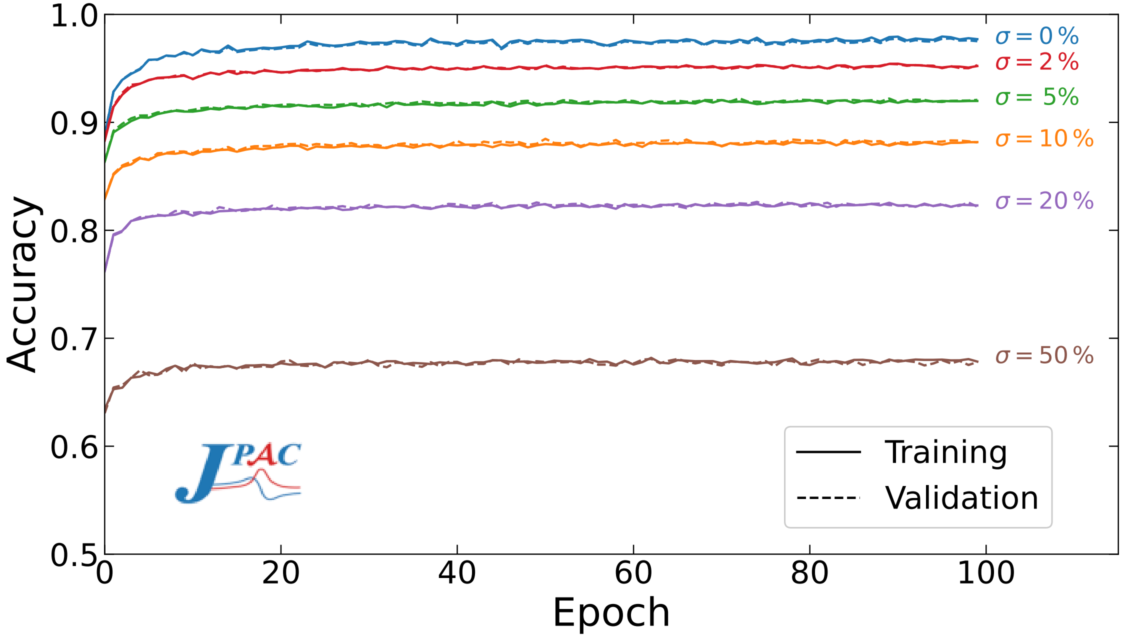
(-,+) - II sheet

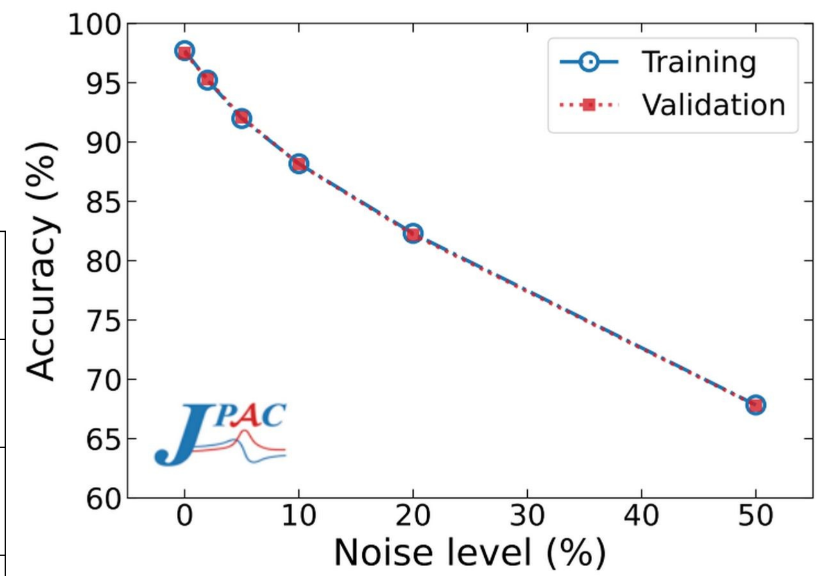
(+,-) - IV sheet

$$\eta_1 = \text{Sign Re}\left(\frac{m_{12}^2}{m_{22}+q} - m_{11}\right) \quad \eta_2 = \text{Sign Re}\, q$$

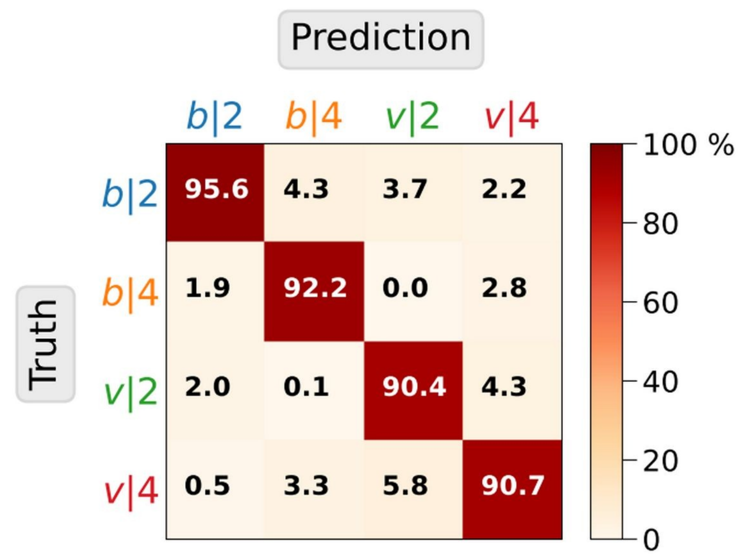
ML model – training results

Accuracy for various noise levels



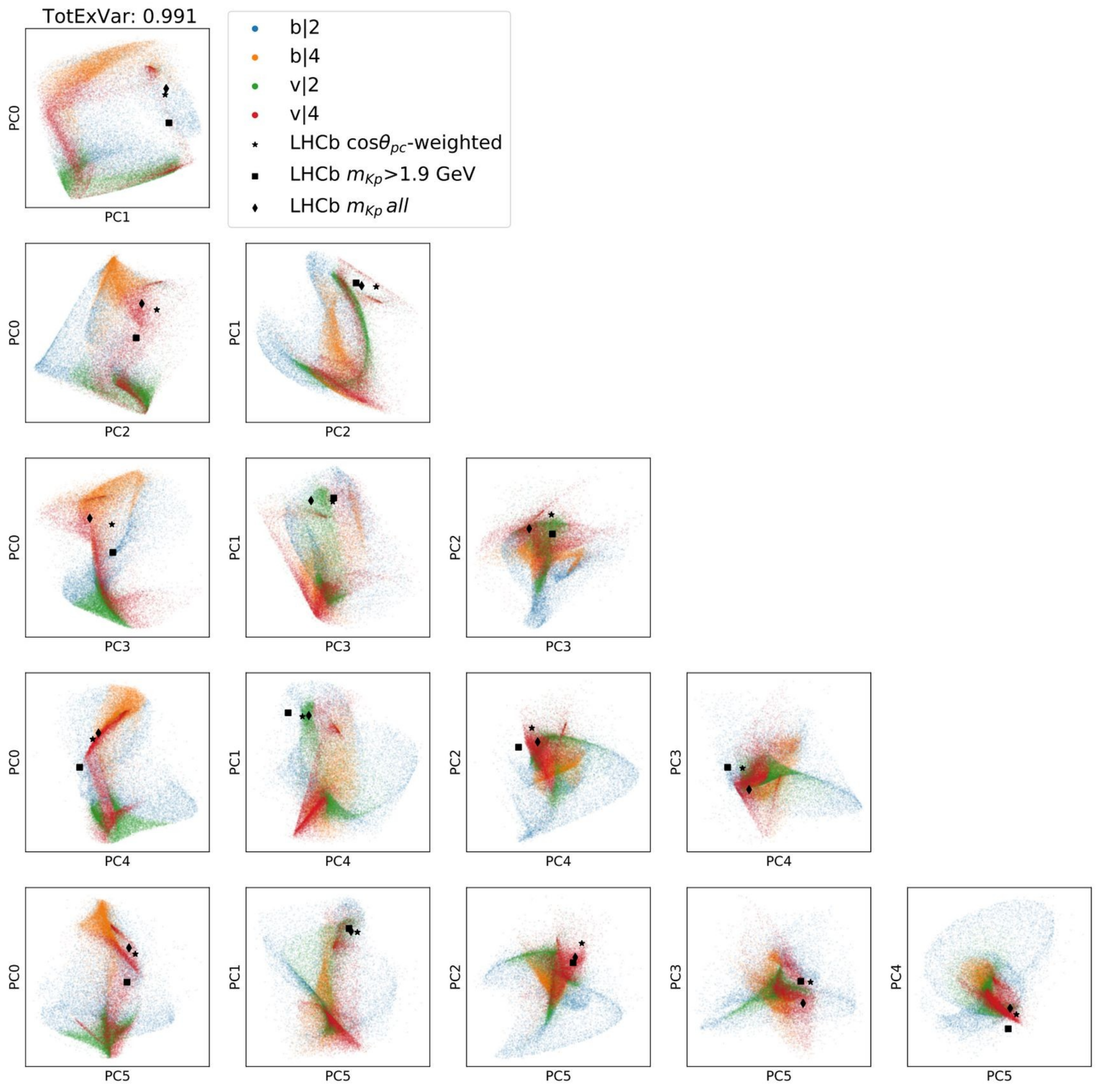


Confusion matrix for the 5% noise



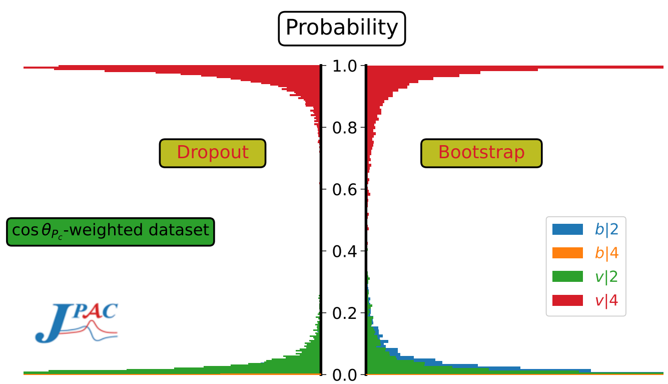
Feature refinement

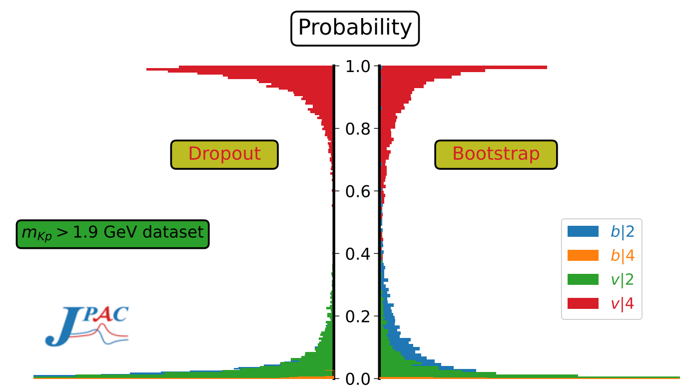
- Dimensionality reduction - Principal Component analysis
- Over 99% of the variance can be explained with just 6 features
- Experimental data projected onto principal components are well encompassed within the training dataset

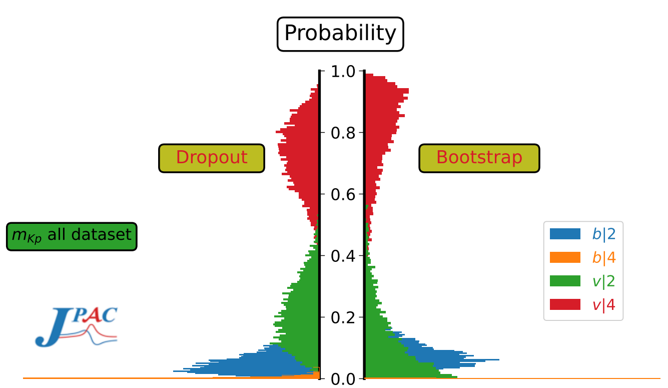


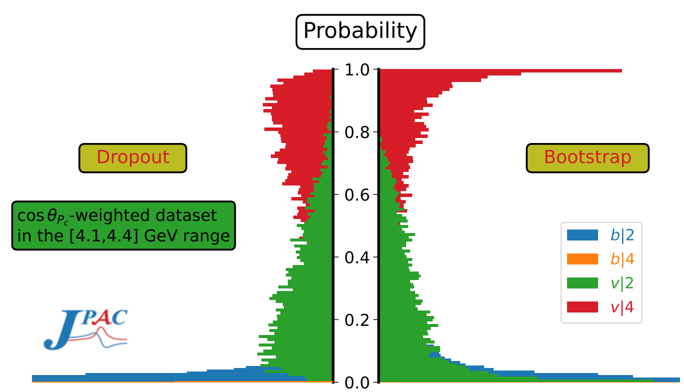
Model predictions – statistical analysis

- The distribution of the target classes was evaluated with
  - the bootstrap (10 000 pseododata based on experimental mean values and uncertainties) and
  - dropout (10 000 predictions from the ML model with a fraction of weights randomly dropped out)





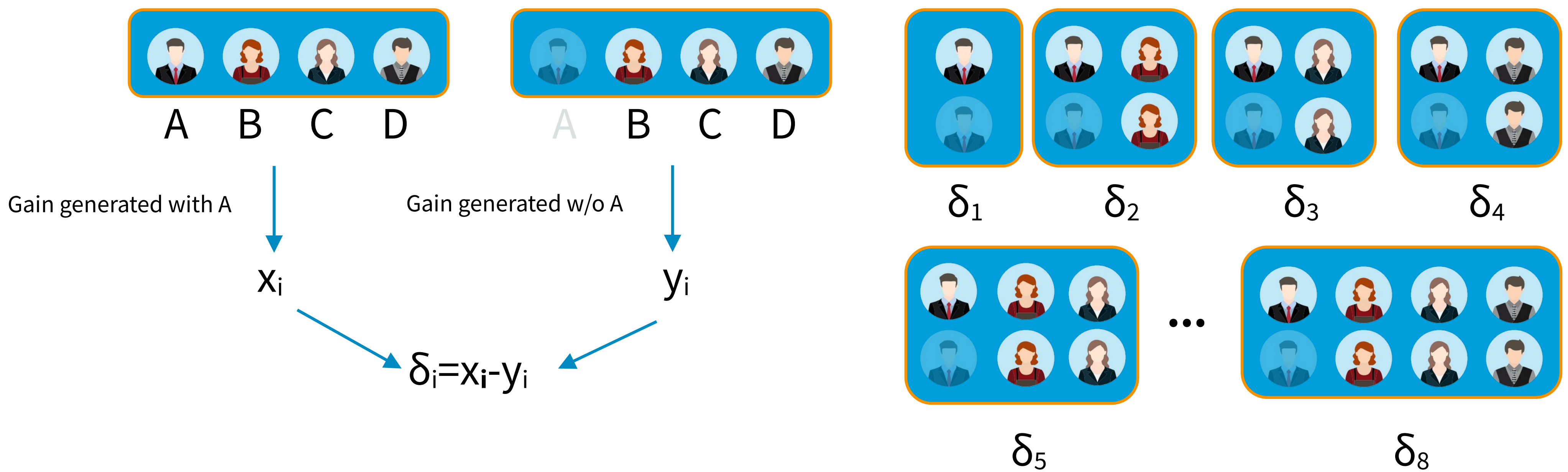




Model explanation with SHAP

- Shapley values and Shapley Additive Explanations

Shapley, Lloyd S. "Notes on the n-Person Game -- II: The Value of an n-Person Game" (1951)



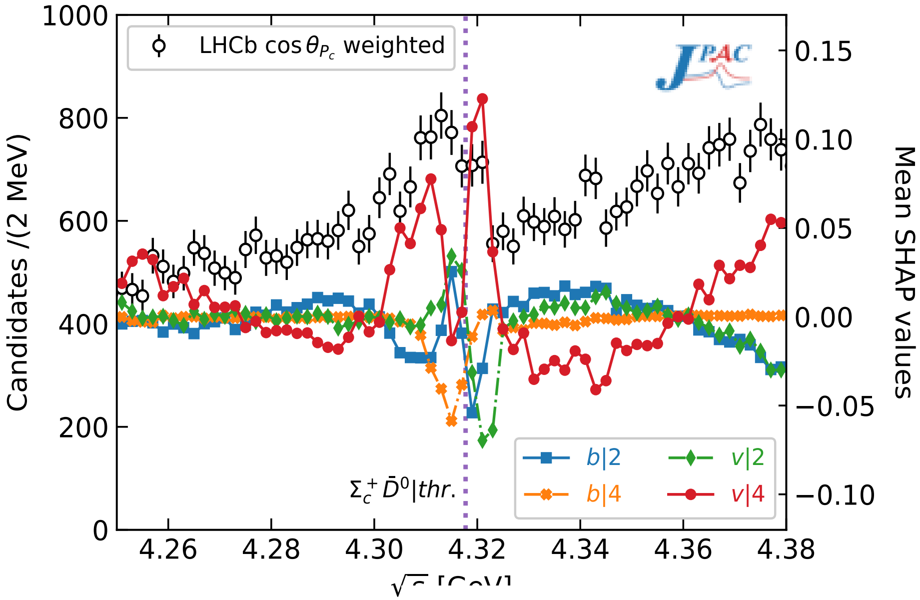
Shapley value for member A: $$\phi_A = \frac{\delta_1 + \delta_2 + \delta_3 + \delta_4 + \delta_5 + \delta_6 + \delta_7 + \delta_8}{8}$$

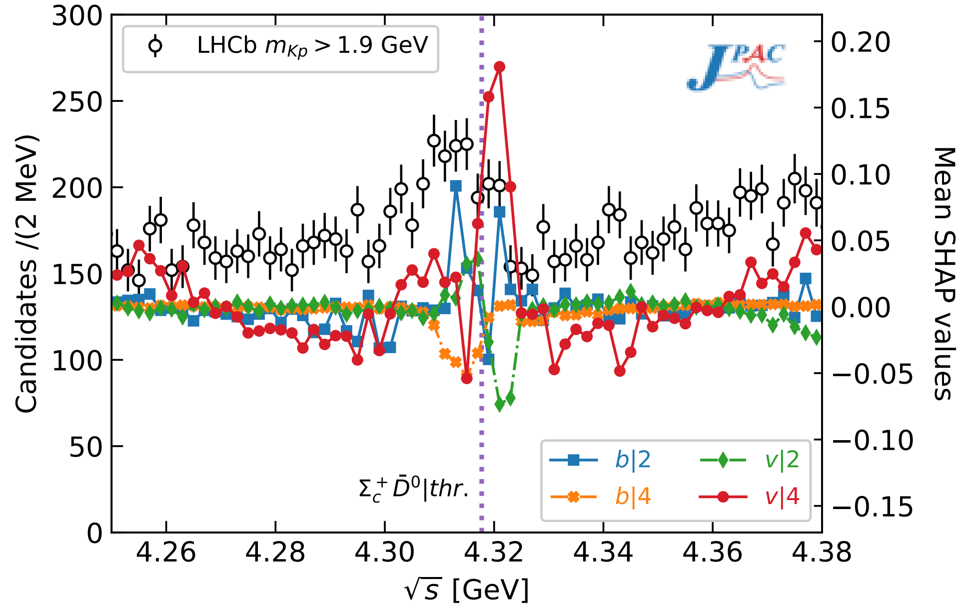
Model explanation with SHAP

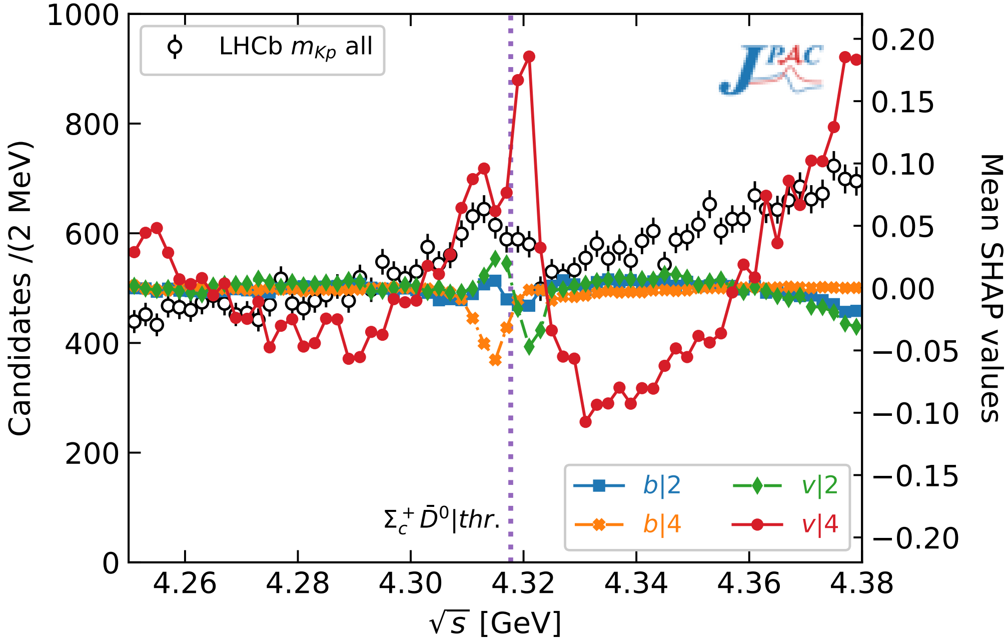
- By making an assotiation:
  - Member of a coalition → Feature
  - Game → Function that generates classification/regression result
  - Gain → Prediction
  - We define the Shapley values for features
- Caveats:
  - A number of possible coalitions grows like 2^N
  - Prohibitively expensive computationally (NP-hard)

Solution: Shapley additive explanations (Lundberg, Lee, arXiv:1705.07874v2, 2017)

Model explanation with SHAP





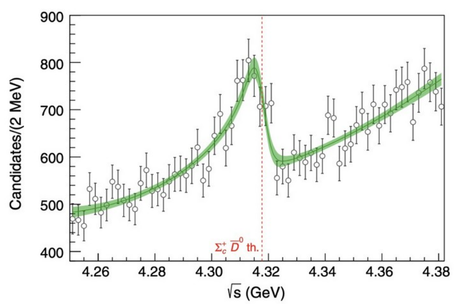


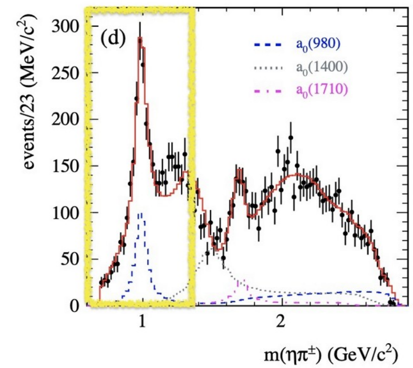
Summary

- Takeaways:
  - Standard χ^2 fit may be unstable, since small change in the input may result in large parameter fluctuations (change physics interpretation)
  - Rather than testing the single model hypothesis with χ^2, we obtained the probabilities of four competitive pole assignments for the $P_c(4312)$ state
  - The approach was model independent – meta model
  - By the analysis of the SHAP values we obtained an *ex post* justification of our scattering length approximation

Questions to be addressed

- Going beyond the limited generalization power - applying the method for larger class of resonances, described by the same physics, eg. $a_0/f_0(980)$ or other resonances located near thresholds





- Eg. we believe that these two resonances can be described by the same physics
  - MLPs and CNNs require inputs of the same size – rebinning required (but also kinematics and resonance parameters change: masses, widths, thresholds, phase spaces,...)
  - Alternatively we can use the length of the signal as part of the input information for RNNs
  - Difference between the models is not always as clear as above (different Riemann sheets) – need for model selection criteria (discussed already on Wednesday)