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Complementing the study of exotic hadrons using machine learning

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One of the main challenges in hadron spectroscopy is determining which of the recently observed unstable states qualify as genuine members of the hadronic spectrum. These new states typically appear as enhancements in invariant mass distributions or as structures in scattering cross sections near two-hadron thresholds. They are often associated with hadronic molecules or virtual states on the nearest Riemann sheet, arising from strong channel coupling. However, some of these signals may also be interpreted as genuine compact resonances. Additionally, purely kinematic effects, such as triangle singularities, can produce similar enhancements. Distinguishing among these possibilities based solely on line shapes is challenging, especially given the limited resolution of experimental data. In this contribution, I present a machine learning-based framework for identifying the underlying mechanism responsible for near-threshold enhancements, even in the presence of experimental uncertainties. As a concrete example, we focus on the $P_{c\bar{c}}(4312)^+$ structure observed by LHCb in 2019. I show that the triangle singularity interpretation of the $P_{c\bar{c}}(4312)^+$ can be ruled out using neural network-based line shape analysis. Furthermore, I demonstrate that the pole structure of the observed signal can be probed by training a deep neural network on a generalized S-matrix parametrization. Within this deep learning-assisted framework, we find that the $P_{c\bar{c}}(4312)^+$ exhibits a three-pole structure, one pole in each of the relevant unphysical sheets, suggesting a true resonance associated with a pole-shadow pair, potentially contaminated by a virtual state in the higher-mass channel when coupled to the lower one.

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1. Introduction

The impact of machine learning on science is undeniable, as reflected in the 2024 Nobel Prizes in both Physics and Chemistry. In experimental particle physics, machine learning has already proven to be a powerful and practical tool, with applications ranging from real-time event selection in collider experiments [1] to particle identification [2, 3] and detector calibration [4, 5]. These methods, often originating in computer science and statistics, have been adapted to address the scale and complexity of modern particle physics data. The growing volume of both experimental and simulated datasets has made machine learning indispensable for efficient and accurate data processing. While its early impact was most evident on the experimental side, machine learning is now playing an increasingly important role in theoretical analyses, including studies of hadron spectroscopy [6–8], lattice QCD [9, 10], and amplitude analysis [11–15]. Recent reviews on the intersection of machine learning and hadron physics can be found in Refs. [16–18].

Among these theoretical applications, amplitude analysis presents a particularly compelling case for the use of machine learning. This paper focuses on its application, with an emphasis on deep learning methods, to the interpretation of near-threshold enhancements observed in experimental data. These structures are often attributed to hadronic molecular states, which are theoretically expected to appear near the opening of two-hadron thresholds. However, alternative scenarios must be taken into account. Strong coupled-channel effects can distort resonance signals, and purely kinematic phenomena, such as threshold cusps or triangle singularities, can produce enhancement-like features without requiring the presence of a genuine state. The coexistence of these competing mechanisms complicates the direct identification of observed enhancements with states in the hadron spectrum. To address this challenge, we developed a S-matrix-based learning approach, in which deep neural networks are trained on synthetic amplitudes constructed solely from general properties of the S-matrix, such as unitarity and analyticity. This strategy avoids reliance on model-specific dynamics, such as potentials, which are not directly observable in scattering experiments. Since the S-matrix encodes all information about asymptotically free initial and final states, this method provides a model-independent framework for interpreting experimental data. In this contribution, I summarize this method to highlight its potential in disentangling different interpretations of threshold effects in amplitude analysis.

2. Proof of principle

The early application of deep learning in this program (line shape analysis) began with a deceptively simple problem: distinguishing between a bound-state and a virtual-state enhancement in a single-channel system [13, 19]. Within the scattering-length approximation, this distinction is lost due to the modulus-squared nature of observables, which renders the sign of the scattering length inaccessible. To overcome this limitation, we introduced a specific amplitude parametrization that preserved a simple pole structure in the momentum variable while incorporating a unitary background. The physical motivation was that the true S-matrix likely includes background singularities beyond the simple pole, and these features may contain discriminative information. We adopted the following parametrization with a unitary background:

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

where k is the two-body center-of-mass momentum and α, β, γ are training parameters. The parameter γ determines the nature of the near-threshold enhancement, while the background singularities correspond to the two branch points located at $k = i \pm \beta$. The parameter β therefore controls how far the background singularities are from the threshold, and we restrict it to the range $\beta \in (400MeV, 700MeV)$. Using the parametrization in Eq. (1) with randomized background parameters and controlled γ, we trained a neural network and found that it could reliably identify the correct pole nature, as shown in Fig. 1. This success suggested that the background singularities might be playing a key role in the classification.

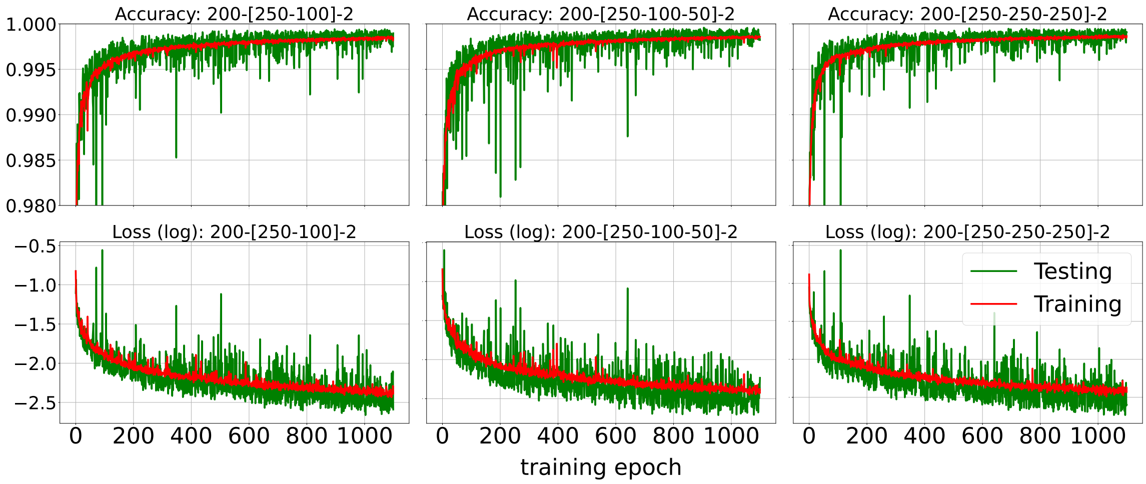

Figure 1: Sample training results of DNN classifiers developed to distinguish bound- versus virtual-state enhancements.

It is plausible that the background singularities affect the scattering region in ways that help the neural network distinguish the line shapes, even though the precise mechanism is not important for our purposes. To test the hypothesis that the background singularity assists the DNN in its classification task, we used two types of separable potential models that generate distinct pole structures:

$$v_{const}(p, p') = \lambda \frac{\Lambda^2}{p^2 + \Lambda^2} \frac{\Lambda^2}{p'^2 + \Lambda^2} \quad \text{and} \quad v_{Edep}(p, p') = \lambda(E - M_{sep}) \frac{\Lambda^2}{p^2 + \Lambda^2} \frac{\Lambda^2}{p'^2 + \Lambda^2} \tag{2}$$

where p, p' are the initial and final momenta, λ is the coupling constant, Λ is the cut-off parameter, and M_{sep} is some parameter in the energy-dependent part.

The separable potential with constant coupling produces a single near-threshold pole together with second-order poles at $k = \pm i\Lambda$ associated with the s-wave Yamaguchi form factor. In contrast, the energy-dependent coupling produces a near-threshold pole accompanied by a nearby background simple pole in addition to the form-factor poles. We generated two sets of partial cross sections from these potential models by solving the Lippmann-Schwinger equation and fed them to the trained

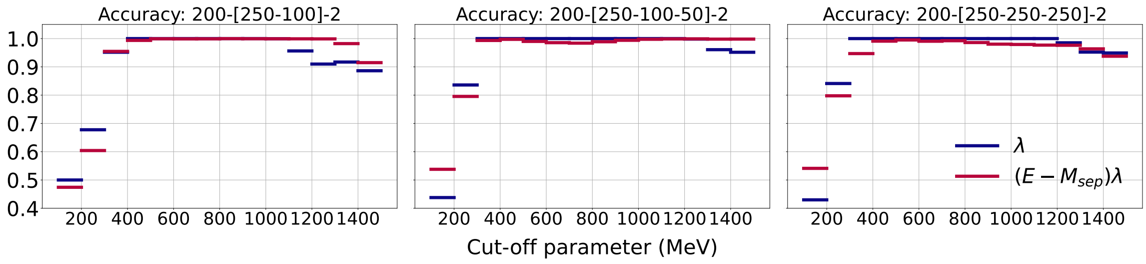

Figure 2: Validation of DNN accuracy using separable potentials with constant and with energy-dependent couplings.

DNN. The effect of the background singularity is determined by the cutoff parameter of the model. Figure 2 shows the prediction accuracy as a function of the cutoff parameter.

When the background singularity is too close to the threshold (i.e., small cutoff parameter), the trained DNN has difficulty classifying bound and virtual enhancements. This can be attributed to the fixed energy window of the scattering region: when all the singularities lie very close to the threshold, the resulting line shapes become nearly indistinguishable. For moderate and physically reasonable values of the cutoff parameter, the classification accuracy is very good. The most interesting behavior appears when the cutoff parameter lies outside the original range of β ($\Lambda > 700MeV$): the accuracy remains high. Moreover, in the energy-dependent case, the performance improves further, which we attribute to the presence of a nearby background simple pole.

The above demonstration for distinguishing bound- and virtual-state pole enhancements suggests that the analytic structure of the S-matrix is already useful in learning the line shape. Although the exact form of the S-matrix may not be accessible, its analytic properties should be sufficient to generate a large sample of possible amplitudes that can approximate the actual analytic structure. It is then the task of the DNN to exploit these subtle features and map the observed line shapes to their corresponding physical interpretations.

3. Conventional fitting and deep learning

The previous section demonstrated that the analytic structure of the S-matrix alone can already provide useful information for classifying line shapes. Prior to deep learning approaches, conventional fitting was the primary tool for discriminating among competing interpretations of observed near-threshold enhancements. In many cases, however, standard fits cannot deliver a definitive conclusion, often because of limited statistics or large systematic uncertainties in the data. This motivates the use of deep learning as a complementary tool rather than a replacement for established fitting strategies.

A representative comparison between conventional fitting and a deep learning approach appears in Ref. [12]. There, a DNN was trained to determine whether the $P_{c\bar{c}}(4312)^+$ corresponds to a bound or a virtual state of the $\Sigma_c\bar{D}$ channel. The network was trained on samples generated with the effective-range expansion [20],

$$T(s) = \frac{m_{22} - ik_2}{(m_{11} - ik_1)(m_{22} - ik_2) - m_{12}^2} \tag{3}$$

where k_1 and k_2 are the channel momenta for $J/\psi p$ and $\Sigma_c\bar{D}$, respectively, and m_{11}, m_{22}, and m_{12} are coupling parameters with m_{22} controlling whether the state is a bound or virtual state of $\Sigma_c\bar{D}$. The trained DNN reached the same physical interpretation as the conventional analysis in Ref. [21]. This result is a valuable validation, as the fitting function used in Ref. [21] shares the same effective-range parametrization as the training model, making the comparison between methods particularly transparent. In effect, the DNN served as a high-capacity surrogate operating within the same parametrization class, which offers a valuable cross-check and a demonstration that machine learning can reproduce established conclusions when trained consistently. Separately, recent work in Ref. [22] demonstrates that deep learning, within the framework of Simulation-Based Inference (SBI), can even outperform conventional fitting by being less sensitive to noise and misspecified data points.

While this validation is important, restricting machine-learning pipelines to a single preferred parametrization risks underutilizing their potential. If both the training generator and the downstream fit share the same functional form, the exercise primarily tests internal consistency within that form. A broader use case would be to train deep networks to recognize generic analytic features of amplitudes that are not tied to a particular model choice. In this contribution, I therefore propose an S-matrix-based learning framework. The networks are trained on synthetic amplitudes constructed from general S-matrix principles such as unitarity and analyticity, with controlled variations that include poles on different Riemann sheets, threshold cusps, coupled-channel effects, and triangle singularities. This design avoids reliance on potentials, which are physically motivated but not directly observable or uniquely constrained by scattering measurements. Since the S-matrix encodes the information accessible through asymptotically free initial and final states, the resulting training data remain as model-independent as possible. The trained network is then applied to experimental distributions to assess which analytic scenarios are most compatible with the data.

In this way, machine learning functions as a unified interpretation-selection layer that complements conventional fitting and helps disentangle bound- versus virtual-state behavior, coupled-channel distortions, and kinematic effects within a common, observable-anchored framework.

4. Interpretation-selection framework

It is well known that resonance-like enhancements in scattering amplitudes do not always signal the presence of a genuine unstable quantum state. Such ambiguities are particularly pronounced when the experimental data exhibit large uncertainties, making it difficult to unambiguously distinguish between enhancements generated by a nearby pole and those arising from kinematic effects. A prominent example of the latter is the triangle singularity, which can mimic the behavior of a resonance despite originating from a non-analytic feature of the amplitude that does not correspond to a pole in the complex energy plane. To benchmark our approach, we again consider the $P_{c\bar{c}}(4312)^+$ structure. Although initially considered as a possible manifestation of a triangle singularity, this interpretation has been ruled out by the LHCb analysis in Ref. [23].

Ref. [14] presents a machine-learning-based framework to distinguish between different physical mechanisms behind near-threshold enhancements, specifically focusing on whether an observed peak is generated by a pole (indicating a genuine resonance or bound state) or by a non-pole kinematic effect such as a triangle singularity. The approach involves generating synthetic data from amplitude models with known underlying structures, either containing a pole or a triangle singularity, and training deep neural networks (DNNs) to classify the origin of the enhancement based solely on the line shape. By using a classification-based approach rather than a direct fit to experimental data, the method avoids overfitting to statistical fluctuations and enables probabilistic interpretation of the results.

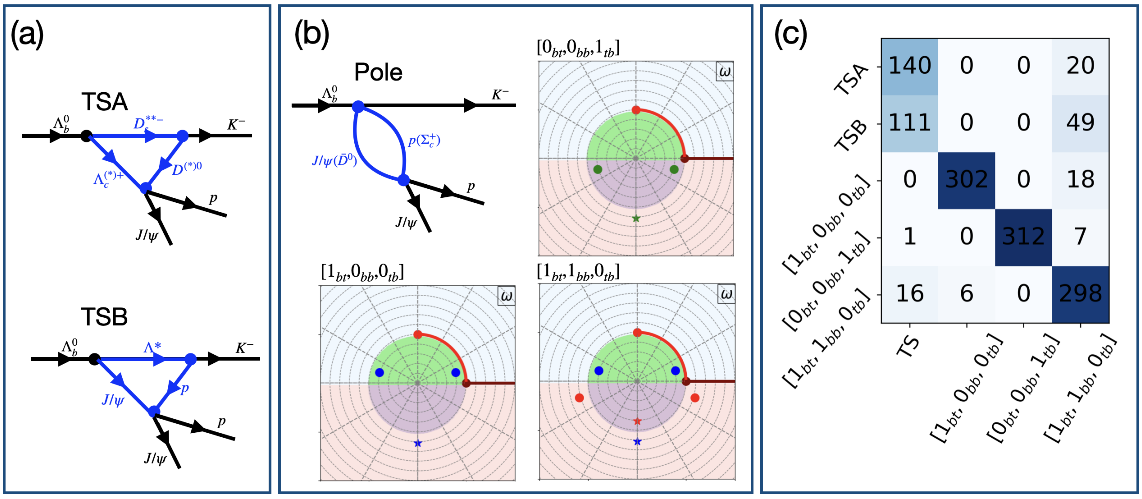

Figure 3: Different interpretations of $P_{c\bar{c}}(4312)^{+}$ from Ref. [14]. Panel (a) shows two triangle diagrams, (b) depicts the corresponding pole structures, and (c) presents the confusion matrix of one of the trained DNN trials.

Two triangle diagrams are considered in Ref.[14], as shown in Fig.3(a). The masses of the intermediate particles are varied to generate sizable training line shapes for each diagram. For the pole-based enhancement, independent S-matrix poles are introduced using the uniformization method developed in Refs.[24, 25], leading to the pole structures shown in Fig.3(b). The advantage of uniformized independent S-matrix pole is that it is no longer tied to any dynamical or potential model. A set of deep neural networks (DNNs) is trained on these data, achieving relatively high classification accuracy during the testing stage, although some signs of overfitting are observed in certain DNN configurations. Figure 3(c) shows the confusion matrix for one of the DNNs used in the study. Overall, the distinction between a kinematic enhancement and one caused by a pole is shown to be learnable by the network. The trained and validated DNNs are then applied to LHCb data, taking into account experimental uncertainties. The analysis favors the interpretation that the $P_{c\bar{c}}(4312)^{+}$ is an enhancement generated by a pole.

It is important to note that Ref.[14] considers only a limited subset of possible pole structures. As demonstrated in Ref.[26], extracting the precise pole configuration responsible for a given line shape is a nontrivial task. When using a standard deep learning pipeline, it was found that DNN models generally fail to learn and distinguish between different pole configurations based solely on the line shape. This difficulty arises from the analytic form of the S-matrix, which is expressed in terms of Jost-like functions used to generate the poles. In particular, it is possible for a zero of the S-matrix on one Riemann sheet to cancel a pole on another, effectively masking the presence of certain pole structures. This complexity motivates the simplified approach adopted in Ref. [14], which restricts the set of pole scenarios to those most relevant for isolating the main sources of ambiguity.

It is worth mentioning that Ref.[27] offers a potential solution to the challenges identified in Ref.[26] by incorporating predictive uncertainty estimation into the neural network framework. By allowing the model to express confidence (or lack thereof) in its predictions, this approach helps detect regions where distinct pole structures yield similar line shapes and are therefore difficult to separate. This added layer of uncertainty modeling enables a more nuanced interpretation of the DNN output and improves the reliability of pole structure classification in cases where traditional pipelines struggle.

Further investigation in Ref. [15] into the preferred pole structure of the $P_{c\bar{c}}(4312)^+$ suggests that the enhancement is most likely associated with a pole-shadow pair residing on the second and third Riemann sheets, along with an additional pole on the fourth sheet. This pattern of poles is consistent with a compact pentaquark interpretation, potentially contaminated by a virtual state associated with the $\Sigma_c\bar{D}$ channel. The identified pole structure aligns with the analysis in Ref.[28] and lends further support to the hybrid explanation proposed in Ref. [29].

5. Summary and Outlook

In this contribution, I discussed the potential of deep learning in interpreting line shapes in hadron spectroscopy. We examined the challenge of distinguishing between bound and virtual state enhancements using only the scattering region above the threshold. Despite the subtle influence of the analytic structure of the S-matrix in this region, a deep neural network (DNN) can successfully learn to identify the origin of the enhancement. This capability is further demonstrated in the benchmark task of separating kinematical enhancements from those caused by dynamical poles. In particular, we showed that a trained DNN can rule out the triangle singularity interpretation of the $P_{c\bar{c}}(4312)^+$, even when the physics constraints in the training dataset are relaxed.

There remain many opportunities for applying deep learning in hadron spectroscopy. A key consideration is that the training dataset should be generated using model-independent formulations. The S-matrix provides such a foundation, as it encodes only asymptotically observable features and avoids reliance on specific dynamical models. Since experimental data are expected to reflect the correct physics, the combination of the S-matrix and deep learning offers a promising framework for uncovering the underlying dynamics of hadronic states.

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