

## **FhyMetric-Net: Interpretable mixed radioisotope identification model integrating prior characteristic peak physical information and feature metric constraints**

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### **Abstract**

The automatic identification of radionuclides is essential for remote, unmanned monitoring and the rapid detection of radioactive contamination. While deep learning techniques have significantly enhanced recognition accuracy, their “black-box” nature and reliance on large-scale datasets pose challenges. These issues include poor interpretability, high overfitting risk, and uncontrollable errors, all of which limit their use in high-reliability fields such as the nuclear industry. This paper introduces FhyMetric-Net, a novel interpretable model for mixed radionuclide identification that integrates physical priors and feature metric constraints. The core innovations of this work include: (1) Embedding radionuclide characteristic peak physical information into neural networks in a differentiable manner, for the first time. This technique constrains the feature optimization space, enhancing both the reliability and interpretability of the model. (2) Proposing a feature space metric constraint method for mixed radionuclide samples to improve the model’s ability to extract discriminative features. During training, we used only 1% of the sample size compared to the test dataset. In extensive performance tests, involving various detector types and more complex radionuclide mixtures, FhyMetric-Net achieved a 97.589% F1 Score comprehensive performance. This result places it at the forefront of the field, with a parameter count of just 0.051032M—only 1.316% of ResNet-18. Ablation studies revealed that the physical prior constraints and feature metric constraints played a significant role in improving Precision and Recall, respectively. Qualitative analysis of the model’s weights further confirmed that the model advances the application of automated mixed radionuclide identification in high-reliability scenarios within the nuclear industry.

## Full Text

### Preamble

#### **FhyMetric-Net: Interpretable mixed radioisotope identification model integrating prior characteristic peak physical information and feature metric constraints**

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The automatic identification of radionuclides is essential for remote, unmanned monitoring and the rapid detection of radioactive contamination. While deep learning techniques have significantly enhanced recognition accuracy, their “black-box” nature and reliance on large-scale datasets pose challenges. These issues include poor interpretability, high overfitting risk, and uncontrollable errors, all of which limit their use in high-reliability fields such as the nuclear industry. This paper introduces FhyMetric-Net, a novel interpretable model for mixed radionuclide identification that integrates physical priors and feature metric constraints. The core innovations of this work include: (1) Embedding radionuclide characteristic peak physical information into neural networks in a differentiable manner, for the first time. This technique constrains the feature optimization space, enhancing both the reliability and interpretability of the model. (2) Proposing a feature space metric constraint method for mixed radionuclide samples to improve the model’s ability to extract discriminative features. During training, we used only 1% of the sample size compared to the test dataset. In extensive performance tests involving various detector types and more complex radionuclide mixtures, FhyMetric-Net achieved a 97.589% F1 Score comprehensive performance. This result places it at the forefront of the field, with a parameter count of just 0.051032M—only 1.316% of ResNet-18. Ablation studies revealed that the physical prior constraints and feature metric constraints played a significant role in improving Precision and Recall, respectively. Qualitative analysis of the model’s weights further confirmed advances in the application of automated mixed radionuclide identification in high-reliability scenarios within the nuclear industry.

**Keywords:** Radioisotope Identification, Deep Learning, Physical Interpretability, Feature Metric Constraints, Interdisciplinary

### Introduction

Radioisotope identification (RIID) is a key technology for detecting radioactive contamination and identifying radioactive sources, which plays a crucial role in nuclear safety and environmental protection [1-5]. Traditional RIID methods

mainly search for characteristic peaks based on derivative, Fourier transform, or wavelet analysis techniques, and match them with a predefined nuclide library (containing key information such as energy and branching ratio) to determine the type of nuclide [6-10]. However, due to factors such as statistical fluctuations and peak overlapping, these methods typically require manual iterative adjustment of parameters to achieve optimal noise smoothing and peak finding performance. This process is not only cumbersome but also susceptible to human factors, which limits the efficiency and accuracy of identification [11].

In recent years, methods based on Deep Learning (DL), which can automatically adjust parameters to extract deep features from energy spectra, have been widely studied. Existing research results generally indicate that DL models have significant advantages in achieving high identification accuracy when facing challenges such as low count rates and low SNR [12-16]. The mainstream DL methods rely on large-scale training data and deep neural networks (NN) to create an end-to-end mapping between input energy spectra and output probabilities, achieving high recognition accuracy. In other words, the performance of these methods is typically determined by the scale of the training data [17]. However, the shape of radioactive nuclide energy spectra is influenced by random factors, such as environmental background and noise, making it challenging to obtain large-scale real energy spectra samples. RIID tasks clearly exhibit the characteristics of “Few-shot + multi-label” problems.

So far, purely data-driven methods have faced challenges in other fields, including high data acquisition costs, poor interpretability, and susceptibility to noise, as seen in cancer, fusion plasma, earthquakes, weather, and climate change. The key challenge lies in the fact that, without appropriate constraints, the high dimensionality of the data leads to an excessively large model search space [18]. Due to the black-box nature of NN models, issues such as poor interpretability, high overfitting risk, and uncontrollable errors are inevitable. These issues limit the widespread application of such methods in the nuclear industry, particularly in high-reliability scenarios.

A key issue that needs to be addressed is how to enable NNs to learn in a way that aligns with human expert knowledge and exhibits strong generalization ability, even with insufficient data samples. The data-knowledge dual-driven methods have brought transformative innovations in DL [19]. These methods integrate domain-specific prior knowledge into the learning process, effectively constraining the model’s hypothesis space [20]. Research shows that this method can reduce data requirements, improve generalization capabilities [21], and enhance interpretability [22].

For recent studies, we will discuss categorizing them into two main areas: the exploration of model interpretability and methods for enhancing model reliability. Researchers have studied the interpretability of NN models to understand the reasons behind their high identification accuracy. Mario Gomez-Fernandez et al. showed the connection between the region of interest (ROI) and physical characteristics (e.g., photoelectric peaks) using thermal vector maps. Yu Wang

et al. [24] used Class Activation Mapping (CAM) to visualize and explain the key regions learned by the model. Findings from these studies suggest that effective classification models tend to concentrate their learning on physically meaningful regions of the gamma-ray spectrum—such as characteristic photopeaks—rather than on irrelevant areas like background noise. This observation underscores the necessity of establishing explicit constraints between model predictions and spectral regions that embody physical characteristics. For instance, the presence of a full-energy peak at 661.7 keV is a strong indicator of the radionuclide  $^{137}\text{Cs}$ . Embedding such relationships into model training has the potential to simultaneously enhance both the reliability and physical interpretability of NNs.

Some researchers have worked to improve the robustness of the model. Zakariya Chaouai et al. [25] improved the robustness of the model by using adversarial learning techniques to reduce the likelihood of NN misguidance. Hao-Lin Liu et al. [26] performed classification by integrating local and global characteristics of a deep convolutional neural network (CNN), enhancing intraclass similarity and differences between classes. For RIID in urban environments [27], a detection model based on a weighted k-nearest neighbors (KNN) framework was developed to extract discriminative features from energy spectra and minimize inter-class similarity for the same radioactive material. Nevertheless, current approaches remain largely data-driven, with limited incorporation of domain-specific physical knowledge. In particular, these methods often overlook the probabilistic constraints that link the presence of radionuclides with specific spectral features, resulting in a lack of intuitive physical explainability.

Attention has become a key concept in the rapidly advancing field of DL. In computer vision, salient visual attention models have been shown to extract low-level visual features to identify potential key regions [28, 29]. In multi-label image classification tasks, it has been proven to effectively capture semantic and spatial relationships between labels in images [30, 31]. These studies align with RIID, as each category of radionuclide is associated with specific characteristics of the energy spectrum region, such as the energy and intensity of full-energy peaks. Jiaqian Sun et al. [32] presented a NN model that combines convolution and self-attention mechanisms. Wang et al. [33] proposed a DL-based method for recognizing multiple radioactive nuclides using a channel attention module. This model explains how it utilizes feature information from the photopeak and Compton edge by interpreting spectral features. However, existing methods are purely data-driven and do not incorporate prior physical information to establish constraints between prediction results and the physical characteristic regions in the energy spectrum.

To address these issues, we have developed a novel model that combines physical constraints with data-driven approaches for mixed RIID. The model integrates prior physical information about radionuclide characteristic peaks with feature space metric constraints and can effectively capture the latent relationship between radionuclide presence probabilities and characteristic peaks through a learnable convolutional network, offering intuitive physical interpretability. The

specific contributions are outlined as follows: (1) A residual network incorporating multi-scale dilated convolutions was utilized for energy spectrum feature extraction, allowing the model to efficiently integrate both local details and global spatial semantic features. (2) The optimization space of NN weights was constrained by prior information on radionuclide physical characteristic peaks, thereby enhancing the reliability and interpretability of the model. (3) A feature metric constraint method tailored for the multi-label classification (MLC) of mixed radionuclides was proposed, constructing a discriminative feature space. (4) A clear and intuitive computational process was established that links radionuclide prediction probabilities with feature weights, enhancing the causal logic and physical interpretability of the model inference.

## II. Materials and Methods

### A. Backbone Network

The overall architecture of the proposed model, shown in Fig. 1 [Figure 1: see original paper], consists of four components: the backbone network, prior physical constraints, feature metric constraints, and MLC. Deep features of the energy spectrum were extracted using a one-dimensional CNN. Delicate local features need to be extracted for stacked, narrow, or weak peaks. However, some radionuclide characteristic peaks, such as those of  $^{129}\text{I}$ , are distributed across multiple energy ranges, necessitating the extraction of global spatial semantic features.

A novel NN architecture called Multi-Scale Dilated Residual Network (MSDR-Net) was proposed. This architecture integrates local detail features and global spatial semantic features in the energy spectrum, effectively addressing the vanishing gradient problem while maintaining a lightweight structure. The model input is a one-dimensional vector of the gamma energy spectrum,  $X \in \mathbb{R}^{(1 \times 1024)}$ . Each radionuclide category was labeled with a binary sequence  $P = (cid : 2)P_1, P_2, \dots, P_C(cid : 3)^T \in \mathbb{R}^C$ , where  $P_i = 1$  if category  $i$  is present, and 0 otherwise. Additionally, each energy spectrum sample was normalized to a maximum value of 1 to ensure consistent scaling across the dataset. Three parallel residual modules then process the input features at multiple scales using different dilation rates. Dilated convolutions expand the receptive field by inserting gaps between kernel elements without increasing the number of parameters.

The output of the dilated convolution can be expressed as:  $(cid : 88)Y[i] = (W[k] \cdot X[i + r \cdot (k - \lfloor K/2 \rfloor)]) + b$ . The receptive field is defined by the following formula: *Receptive Field* =  $(K - 1) \times r + 1$ , where  $Y[i]$  is the output feature,  $X[i]$  is the input feature,  $W[k]$  is the convolution kernel,  $b$  is the bias,  $K = 3$  is the kernel size, and  $r = 4, 6, 8$  are the dilation rates. Each module captured contextual information from distinct energy ranges using two layers of dilated convolution and adjusted the channel dimension with a  $1 \times 1$  convolution.

The Leaky ReLU activation function was applied in the paper, which is defined as follows:  $\sigma(x) = (cid : 40)x \geq 0; kx, x < 0$ , where  $k$  is a small constant

(0.15 in this study) that allows a small gradient to flow through negative inputs, preventing neurons from becoming inactive. It preserves the nonlinear activation characteristics and enhances the stability of gradient propagation.

To accelerate model convergence and reduce overfitting, a Batch Normalization layer was applied after each convolutional layer, as expressed by the following formula:  $x - E[x]/\sqrt{Var[x] + \epsilon \cdot \gamma_{bn} + \beta_{bn}}$ , where  $E[x]$  denotes the mean of the input data,  $Var[x]$  represents the variance, and  $\epsilon = 1e - 5$  is introduced to prevent division by zero. The learnable parameters  $\gamma_{bn}$  and  $\beta_{bn}$  are introduced to restore the representational capacity of the model, allowing flexible adjustments to the output distribution of each layer.

Each branch output was padded to a fixed length of 1024 using dilated convolutions. The outputs were then concatenated along the channel dimension into 384-dimensional features, which were assigned to the number of classes by a  $1 \times 1$  convolutional layer, resulting in a class feature  $F_{MSDR} \in \mathbb{R}^{(C \times 1024)}$ .

$$F_{MSDR} = f_{MSDR}(X; \theta_{MSDR}), F_{MSDR} \in \mathbb{R}^{(C \times 1024)}$$

where  $f_{MSDR}(\cdot)$  represents the parametric function of the backbone network, while  $\theta_{MSDR}$  refers to the learned parameters, including the convolutional kernel weights  $w$  and biases  $b$ . In general, the input energy spectrum samples undergo feature decomposition for each class using MSDR-Net, facilitating subsequent physical information processing and feature space constraints.

## B. Prior Physical Constraints

The characteristic peak energy of gamma radionuclides and the associated Full Width at Half Maximum (FWHM) is a function of energy. To constrain the model to focus on these physically significant regions, we introduce a constant gamma characteristic peaks prior information matrix  $M_{PhyPeak} \in \mathbb{R}^{C \times N}$ , where  $C$  is the number of nuclide categories and  $N = 1024$  is the number of channels. For each characteristic peak of a radionuclide, the corresponding channel addresses within the FWHM range are assigned a weight of 1, while the remaining channels are assigned a weight of  $\alpha$  ( $\alpha \in [0, 1]$ ). Based on the energy calibration, the matrix  $M_{PhyPeak}$  indexed by channels was obtained:

$$M_{PhyPeak} = [V_{rad1}, V_{rad2}, \dots, V_{radC}]^T$$

In the above equation,  $V_{radn} = [w_1, w_2, \dots, w_N]$  is the weight mask for the  $n$ -th radionuclide, with  $w_i = 1$  if channel  $i$  is within a characteristic peak region, and  $w_i = \alpha$  otherwise. This matrix is applied to the features  $F_{MSDR}$  extracted by the backbone network via element-wise multiplication to obtain physically-attentive features:

$$\tilde{F}_{PhyAtt} = M_{PhyPeak} \times F_{MSDR}, \tilde{F}_{PhyAtt} \in \mathbb{R}^{(C \times N)}$$

Subsequent adaptive average pooling and a  $1 \times 1$  convolution layer are applied for dimensionality reduction and fine-tuning, yielding the final physical attention features  $F_{PhyAtt}$ . During training,  $M_{PhyPeak}$  is a constant attention weight

matrix derived from physical prior information. Traditional data-driven methods rely on weakly supervised learning to generate attention weights adaptively. Therefore, the method proposed in this paper imposes stronger constraints.

Adaptive Average Pooling was applied to reduce feature dimensionality from 1024 to 128 and smooth weights. Additionally, a  $1 \times 1$  convolution operation was employed for further weight fine-tuning:

$$F_{PhyAtt} = Conv_{1 \times 1}(AdaAvg_{128}(\tilde{F}_{PhyAtt})), F_{PhyAtt} \in \mathbb{R}^{(C \times 128)}$$

### C. Feature Metric Constraints

Implementing feature space metric constraints to separate dissimilar classes and group similar ones aids the model in extracting discriminative features, thereby improving model reliability, as shown in previous studies [27, 34–36]. However, in MLC tasks involving mixed radionuclides, sample labels often overlap, making it challenging to apply metric constraints at the sample level. In this study, we proposed a novel feature space metric constraint method specifically designed for mixed RIID tasks.

For a training batch, the model outputs a feature tensor  $F_{Batch} \in \mathbb{R}^{(B \times C \times D)}$ , where  $B$  is the batch size,  $C$  the number of categories, and  $D$  the feature dimension (e.g., 128). Based on the multi-label ground truth  $y \in \{0, 1\}^{B \times C}$ , we construct the following sets for each nuclide category  $i$ :

**Presence Feature Set  $E_i$ :**  $E_i = \{f_i^b | y_i^b = 1\}$ , containing the feature vectors for nuclide  $i$  from all samples in the batch where it is present. Here,  $f_i^b$  denotes the feature vector for the  $i$ -th nuclide from the  $b$ -th sample.

**Absent Feature Set  $A_i$ :**  $A_i = \{f_i^b | y_i^b = 0\}$ , containing the feature vectors for nuclide  $i$  from all samples where it is absent.

The distance metric  $d(a, b)$  is defined using cosine distance, which focuses on the angular difference between vectors and is less sensitive to absolute magnitudes, making it suitable for comparing weight distributions:

$$d(a, b) = 1 - \frac{a \cdot b}{\|a\|_2 \|b\|_2}$$

**Presence Constraint (Triplet Loss):** For each nuclide  $i$  present in the batch, we aim to pull features of the same nuclide closer and push features of different nuclides apart. The triplet loss for nuclide  $i$  is:

$$L_{triplet}^i = \max(0, d(f_i^a, f_i^p) - d(f_i^a, f_j^n) + \gamma)$$

where  $f_i^a$  is the anchor point. The  $f_i^p$  is the eigenvector of the same nuclide as anchor  $f_i^a$  (both being nuclide  $i$ ) but farthest from it, representing the difficult positive sample. Similarly,  $f_j^n$  is the eigenvector of a different nuclide (not nuclide  $i$ ) but closest to the anchor, representing the difficult negative sample. The  $\gamma$  is a margin that enforces a minimum distance between positive and negative pairs, ensuring that the model learns to distinguish between them effectively.

The overall presence constraint loss is the average over all present nuclides in the batch:

$$L_{triplet} = \frac{1}{|I|} \sum_{i \in I} L_{triplet}^i$$

where  $I$  is the set of indices for nuclides present in the batch, and  $|I|$  is the size of this set  $I$ .

**Absence Constraint (Contrastive Loss):** This constraint ensures that features for an absent nuclide are distant from all features of present nuclides. For each feature  $f_i^a \in A_i$  of an absent nuclide  $i$ , we calculate its minimum distance to any feature of any present nuclide:

$$d_{min}(f_i^a) = \min_{j \in I, f_j \in E_j} d(f_i^a, f_j)$$

The absence constraint loss is:

$$L_{contrastive} = \frac{1}{A} \sum_{i \notin I} \sum_{f_i^a \in A_i} \max(0, \gamma - d_{min}(f_i^a))$$

where  $A$  is the total number of absent nuclide features in the batch. The loss penalizes absent nuclide features that are too close to any present nuclide features, pushing them apart by at least the margin  $\gamma$ .

The total feature metric loss is the sum of the two constraints:

$$L_{Metric} = L_{triplet} + L_{contrastive}$$

#### D. Multi-Label Classification and Total Loss Function

The multi-label classification head processes the feature  $F_{PhyAtt} \in \mathbb{R}^{(C \times D)}$  to produce the predicted probability  $\hat{P}_i$  for each nuclide category  $i$  using global sum pooling followed by a sigmoid function:

$$S_i = \sum_{k=1}^D F_{PhyAtt}(i, k)$$

$$\hat{P}_i = \text{Sigmoid}(S_i)$$

This linear-additive process enhances the causal interpretability between the feature weights and the final prediction. The classification loss is the Binary Cross-Entropy (BCE) loss:

$$L_{BCE} = - \sum_{j=1}^C [P_j \log(\hat{P}_j) + (1 - P_j) \log(1 - \hat{P}_j)]$$

The total loss function for training is a weighted sum of the classification loss and the feature metric loss:

$$L_{Total} = L_{BCE} + \lambda L_{Metric}$$

where  $\lambda$  is a hyperparameter controlling the weight of the metric constraint. The values of  $\gamma$  and  $\lambda$  were determined via grid search, as detailed in Section IV.A.

### III. Data Preparation

#### A. Monte Carlo Simulation

To quantitatively assess the generalizability of the model, a particle transport model based on Geant4-11.1.3 [37] was developed. This allows us to accurately control multiple variables for quantitative analysis. In this study, two scintillators were considered: a 3-inch NaI(Tl) and a 1-inch CeBr, as shown in Fig. 2 [Figure 2: see original paper]. The detectors consist of a 2-mm-thick stainless steel shell containing Fe, Cr, Ni, and C, a 0.3-mm-thick MgO reflective layer, and a SiPM photoelectric converter. The NaI detector is widely used due to its low cost and ease of processing into larger sizes. In contrast, CeBr has emerged as an alternative to traditional NaI(Tl) and LaBr:Ce crystals due to its excellent energy resolution, negligible background, and increasing application in environmental monitoring [41–43].

The simulated gamma-ray energy response range spans from 30 to 3000 keV, with 100 million photons simulated per calculation. The statistical uncertainty of the simulated results ranged from 0.0002 to 0.0017. The energy deposition spectrum of gamma photons in the detector was obtained by inputting the target radionuclide energy and branching ratio. To simulate the finite energy resolution of real detectors, we apply Gaussian broadening to the simulated energy deposition values  $E_0$ . Specifically, for each energy deposition event, a broadened energy  $E$  is generated according to Equation 20, which is then used as the pulse height recorded in the final simulated spectrum. The FWHM in the equation is calculated using Equation 19, modeling the intrinsic resolution of the detection system at energy  $E_0$ .

$$FWHM(E_0) = C_1 + C_2\sqrt{E_0} + C_3E_0$$

$$FWHM_g + E_0$$

We considered eight artificial radioactive nuclides ( $^{241}\text{Am}$ ,  $^{133}\text{Ba}$ ,  $^{60}\text{Co}$ ,  $^{131}\text{I}$ ,  $^{60}\text{Co}$ ,  $^{137}\text{Cs}$ ,  $^{134}\text{Cs}$ ,  $^{152}\text{Eu}$ ). These include common emission contaminants after nuclear accidents [38–40] and present challenges such as low-energy Compton plateau interference and peak overlapping.

#### B. Data Augmentation

Data augmentation was conducted by controlling the gross count, SNR, and radionuclide mixing ratio. These methods have been widely used in previous research and proven to effectively simulate the random noise in measured energy spectra [12, 15, 24]. The parameters to be adjusted and their corresponding ranges are listed in Table 1. Specifically, the SNR is defined as  $N_{nu}/N_{bg}$ , where  $N_{nu}$  is the counts of photon events emitted by the nuclides, and  $N_{bg}$  is the number of photon events from the background. The background spectrum was experimentally measured with a NaI(Tl) or CeBr detector in a lead shielding environment over 3600 seconds. To generate a mixed energy spectrum, we

randomly selected  $k$  radionuclides from the eight candidates and combined their individual spectra, weighted by randomly assigned activity levels.

### C. Dataset Splitting

To rigorously evaluate the model's generalization ability under controlled distribution shifts, as shown in Table 2, we quantitatively assess performance by adjusting multiple parameters. The training set is only 1% of the sample size of each subgroup in the test set, to simulate the scenario of Few-shot training. The primary approach involves intentionally introducing discrepancies between the training and test data using the "hold-out method." This allows us to assess the model's ability to handle complex, unseen scenarios. Specifically, the training set NaI-Train uses a NaI(Tl) detector with a limited number of mixed radionuclides ( $k_{train} \leq 2$ ), creating a simpler environment for model learning. In contrast, the test set introduces new challenges that the model has not encountered during training: (1) Increased number of mixed radionuclides: Test sets with  $k_{test} = 3$  or 4 require the model to predict new spectral patterns and radionuclide combinations, going beyond the training set's scope. (2) Variation in Gaussian broadening coefficients: Altering these parameters simulates different detector responses, introducing instrumental uncertainties.

This strategy ensures that no radionuclide combinations from the test set appear in the training set. As a result, the model faces more demanding generalization requirements than models evaluated using conventional partitioning methods (e.g., randomly splitting all data into 70% and 30% for training and testing). Importantly, this design exposes the model to entirely new data distributions during testing, providing a more rigorous challenge to its robustness.

### D. Evaluation Metrics

In this study, we use Precision, Recall, and F1 Score as the key evaluation metrics to assess the performance of our multi-label classification model. To handle the multi-label nature of the problem, we compute these metrics using Micro-Averaging, which aggregates the performance across all labels by treating the problem as a single binary classification task. This approach ensures a balanced evaluation. Micro-Averaging combines the predictions for all labels by summing the true positives, false positives, and false negatives across all labels. The overall Precision, Recall, and F1 Score are then computed based on these aggregated counts, providing a comprehensive measure of model performance. The formulas for Micro-averaged Precision, Recall, and F1 Score are as follows:

$$Precision_{micro} = \frac{\sum_{i=1}^N TP_i}{\sum_{i=1}^N (TP_i + FP_i)}$$

$$Recall_{micro} = \frac{\sum_{i=1}^N TP_i}{\sum_{i=1}^N (TP_i + FN_i)}$$

$$F1_{micro} = 2 \times \frac{Precision_{micro} \times Recall_{micro}}{Precision_{micro} + Recall_{micro}}$$

In these equations,  $TP_i$ ,  $FP_i$ , and  $FN_i$  represent the true positives, false positives, and false negatives for the  $i$ -th label, respectively. The final Micro-averaged metrics are computed by summing over all labels, providing a global evaluation of the model's performance across all labels.

## E. Compared Methods

To evaluate the recognition performance of the proposed method, we considered three classic CNN models: AlexNet [44], VGG-16 [45], and ResNet-18 [46]. VGG-16 is a representative of dense and deep CNNs, while ResNet-18 represents the residual network structure. These models were originally designed for 2D CNNs in image recognition tasks but have been adapted to 1D in this paper based on their original architecture.

## F. Model Training

During training, the Train dataset was split into an 8:2 ratio for training and validation. During each data reading step in training, Gaussian random noise with a mean of 0.1 and variance of 0.04 was added to augment the training dataset. The initial learning rate was set to  $1e-4$ , and parameter optimization was performed using the Adam optimizer. All compared models were trained from scratch with random initialization. All layers of the networks were updated during training to ensure a fair comparison.

# IV. Quantitative Analysis

## A. Parameter Sensitivity Analysis

**Determination of Parameter  $\alpha$**  : The ratio between the characteristic peak region and the non-characteristic peak region ( $1 : \alpha$ ) is a critical hyperparameter of the model. To determine its optimal value without relying on empirical settings, we conducted a systematic sensitivity analysis. We fixed the weight of the characteristic peak region to 1 and tested multiple values of  $\alpha$  within the interval  $[0.01, 1.0]$  (specifically  $\alpha = 0.01, 0.03, 0.05, 0.07, 0.1, 0.3, 0.5, 0.7, 0.9, 1.0$ ). For each value of  $\alpha$ , the model was trained from scratch and evaluated on a unified comprehensive test set, with the primary evaluation metric being the micro-average F1 Score. The experimental results are shown in Fig. 4 [Figure 4: see original paper].

The analysis revealed that while the model achieved the optimal F1 Score (95.61%) with ( $\alpha = 0.7$ ) (ratio 1:0.7), a slightly lower performance (94.81%) was observed at ( $\alpha = 0.05$ ) (ratio 1:0.05), which was only about 0.8% lower but still superior to most configurations. After considering the trade-off between performance and physical interpretability, we chose ( $\alpha = 0.05$ ) as the default parameter. This decision was based on two factors: first, a smaller  $\alpha$  enhances physical interpretability by concentrating the model's feature weight around the characteristic peak region, which strengthens the physical transparency of

the model's decision-making; second, the performance cost of a 0.8% drop in F1 Score is minimal compared to the substantial benefits in model reliability and physical consistency, aligning with the study's focus on embedding physical priors for improved interpretability.

**Determination of Parameter  $\gamma$  and  $\lambda$ :** A comprehensive grid search was performed to determine the optimal values for the margin  $\gamma$  in the triplet loss and the weight  $\lambda$  for the metric loss in Eq. 14. The search space was  $\gamma \in [0.1, 0.3, 0.5, 0.7, 0.9]$  and  $\lambda \in [0.001, 0.003, 0.005, 0.007, 0.009, 0.01, 0.03, 0.05, 0.07, 0.09]$ . The model was evaluated using the micro-averaged F1 Score. The optimal performance was achieved with  $\gamma = 0.3$  and  $\lambda = 0.005$ , as shown in Fig. 5 [Figure 5: see original paper].

## B. Comprehensive Performance

To comprehensively evaluate the performance of the FhyMetric-Net model, we compared it with several benchmark models and conducted ablation experiments to verify the effectiveness of its core components. All experiments were conducted on the Test-ALL dataset, with the results shown in Table 3.

**Comparison with Traditional Models:** We first compared FhyMetric-Net with several classic deep learning models, including AlexNet, VGG-16, and ResNet-18. The results clearly demonstrate that FhyMetric-Net significantly outperforms these models in key performance metrics. FhyMetric-Net achieved an F1 Score of 97.589%, outperforming ResNet-18, VGG-16, and AlexNet by 3.999%, 5.812%, and 5.846%, respectively. This advantage is primarily attributed to its excellent recall rate of 95.304%, which, while maintaining a high precision of 99.986%, enables the model to more comprehensively identify existent isotopes and effectively reduce false negatives. In contrast, although traditional models also exhibit high precision, their relatively lower recall rates indicate issues with missed detections in complex mixed energy spectrum scenarios. Notably, FhyMetric-Net not only leads in performance but also has a significantly smaller parameter count (0.051032 M), just 1.316% of the next-best ResNet-18 and only 0.057% of VGG-16. This highlights the efficiency of the lightweight network structure designed specifically for gamma energy spectrum characteristics, effectively capturing key features while avoiding the substantial parameter redundancy present in traditional general-purpose architectures.

**Ablation Experiments:** To analyze the contribution of each innovative component in FhyMetric-Net, we conducted a series of systematic ablation experiments. - **Baseline Model (CLS):** The model trained using only binary cross-entropy loss (BCE Loss) performed poorly, achieving an F1 Score of 87.707%. - **Incorporating Physical Priors (CLS+PHY):** After applying prior physical constraints to the baseline model, the performance improved dramatically. The F1 Score increased from 87.707% to 94.812%, and the recall rate rose from 82.924% to 91.634%. This strong improvement convincingly demonstrates that incorporating physical prior information provides crucial inductive bias and op-

timization guidance for model training. It helps the model focus on physically meaningful regions, such as characteristic peaks, greatly alleviating training difficulties and enhancing both the reliability of features and the model's generalization ability. - **Introducing Feature Metric Constraints (FhyMetric-Net)**: By further adding feature metric constraints on top of CLS+PHY, forming the complete FhyMetric-Net model, the performance received a final boost. The F1 Score reached 97.589%, and the recall rate improved to 95.304%. This indicates that the feature metric constraint, by imposing intra-class compactness and inter-class separation in the high-dimensional feature space, sharpened the model's decision boundary. It guided the model to learn feature representations that are more robust to complex situations like background fluctuations and peak overlaps, thereby optimizing recall rate on top of the already high precision.

Based on the above results, we can conclude that the introduction of physical prior constraints is key to the model's success. It addresses the core issue of insufficient data-driven model training in Few-shot scenarios, providing a reliable initial optimization direction. Metric learning further refines the decision boundary, and the feature metric constraint fine-tunes it by improving the distribution quality in feature space, thus enhancing the model's discriminative power, especially on difficult samples (e.g., low activity, complex mixtures). There is a clear synergistic effect between physical and metric constraints. The physical constraints provide a solid starting point for feature learning, while the metric constraints "refine" it, leading to FhyMetric-Net achieving exceptional classification performance while maintaining high efficiency.

### C. Control Variables

To further investigate the effects of physical prior constraints and feature metric constraints, we conducted quantitative tests on four different datasets, including those with varying detector types, mixed isotopes, low gross counts, and low SNR, as shown in Table 2. As shown in Fig. 6-9 [FIGURE:6-9], the results demonstrate that the proposed method achieves state-of-the-art (SOTA) F1 Score performance across all tests.

As shown in Fig. 6 [Figure 6: see original paper], the F1 Score of the model fluctuates between 94.597% and 96.329% when facing different detector types with varying energy resolution, demonstrating strong overall performance. The performance of CLS+PHY is generally superior to other methods, indicating that incorporating prior physical information to optimize constraint weights effectively enhances the utilization of limited parameters. The precision performance of CLS+PHY is comparable to that of FhyMetric-Net, with the primary improvement in performance due to the increased Recall. This suggests that presence constraints enhance the discriminative power of features to ensure recognition precision, while the absence constraints reduce the false positive rate.

As shown in Fig. 7 [Figure 7: see original paper], when faced with mixed isotopic spectra (containing more than three isotopes) not encountered during training, FhyMetric-Net outperforms other methods. The performance gap primarily stems from Recall. When the number of isotopes in the mixture is less than three, all methods achieve an F1 Score greater than 95%. This indicates that methods based on deep learning perform well on test data from the same distribution as the training set. When the isotope mixture contains three isotopes, FhyMetric-Net maintains an F1 Score above 95%. However, when the mixture includes four isotopes, its performance drops to 87.599%, though it still outperforms other methods. CLS+PHY shows a more significant performance improvement over CLS, demonstrating that the physical prior constraints contribute to the model's generalization ability.

In Fig. 8 [Figure 8: see original paper] and 9 [Figure 9: see original paper], we evaluate the model's performance on low-count and low-SNR spectra. As with the previous analysis, CLS+PHY and FhyMetric-Net exhibit comparable precision performance. The primary improvement with the inclusion of feature metric constraints is observed in Recall, further confirming the role of feature metric constraints. In Fig. 9 [Figure 9: see original paper], the F1 Score of CLS+PHY is on par with that of ResNet-18. In extreme low-SNR conditions (0.1-0.2), ResNet-18 outperforms CLS+PHY in F1 Score, likely due to its innovative residual network structure and larger parameter count. However, overall, ResNet-18 has lower precision than CLS+PHY, indicating that the incorporation of physical prior information helps the model focus on key regions with physical characteristics, enhancing precision.

Overall, all methods maintain high recognition precision, with performance differences primarily in Recall. Notably, CLS+PHY and FhyMetric-Net show comparable precision, and FhyMetric-Net with feature metric constraints further improves Recall, consistent with the overall performance evaluation in Table 3. Physical priors (such as the information of characteristic peaks in this paper) can be regarded as domain knowledge independent of detector types when energy resolution fluctuations are minimal. By implementing necessary constraints, the features learned by the model will inherently focus on the "identity" of the nuclide rather than specific data distributions. Through the application of feature metric constraints and limited weight fine-tuning, the model's recall rate can be further improved, thereby enhancing its overall generalization capability.

#### D. Feature Metrics Analysis

To better demonstrate the effectiveness of the measurement constraints in the feature space, we visualized the  $F_{PhyAtt}$  weights distribution in the feature space using t-distributed Stochastic Neighbor Embedding (t-SNE) [47] on the Test-ALL dataset. The t-SNE visualization of the  $F_{PhyAtt}$  features (Fig. 10 [Figure 10: see original paper]) reveals that after training with metric constraints, the feature distributions for different nuclides become more separable in the embedding space. Features of the same nuclide form compact clusters, while features

of absent nuclides are well separated from those of existent nuclides, validating the effectiveness of the proposed metric learning approach.

For quantitative analysis, we computed the average loss values of the model for presence and absence constraints separately, using Equation 11 and Equation 13. The results are presented in Table 4. After applying the feature metric constraints, the loss associated with the presence constraint decreased from 0.013368 to 0.011823. This suggests a reduction in intra-class distance and an increase in inter-class distance, indicating improved feature separation. The absence constraint loss also decreased from 0.001707 to 0.000958, demonstrating that the feature metric constraints effectively adjust feature weights to maximize the distance between spectra with and without nuclides, which will significantly reduce the false alarm rate and further improve recall.

## V. Explainable Analysis

To investigate the impact of feature metric constraints on the model's discriminative mechanism, we performed a visual analysis of its  $F_{PhyAtt}$  feature weight distribution using the same test spectrum (containing four nuclides:  $^{131}\text{I}$ ,  $^{60}\text{Co}$ ,  $^{137}\text{Cs}$ , and  $^{134}\text{Cs}$ ), as shown in Fig. 11 [Figure 11: see original paper]. By comparing the model's weights before and after applying the constraints, we uncover the mechanism that enhances decision reliability.

As shown in Fig. 11 [Figure 11: see original paper], the 604.721 keV characteristic peak of  $^{137}\text{Cs}$  has a relatively low count and overlaps with the 661.7 keV peak of  $^{60}\text{Co}$ . This presents a challenge for the model, as it must effectively handle low gross count spectra with low SNR levels. In contrast, the 364.489 keV peak of  $^{131}\text{I}$  has a significantly higher count, which may interfere with the model's ability to correctly assign weights to key regions of other nuclides, such as the 1173.2 keV and 1332.5 keV peaks of  $^{60}\text{Co}$ . It is important to note that the feature weights output by the model include both positive and negative values. In the visualization, negative weights are represented by darker colors, while positive weights (bright colors) indicate areas the model is emphasizing. Negative weights (dark colors) reflect the model's active suppression of certain regions. This suppression mechanism is vital for excluding irrelevant features or background interference, which enhances the model's discriminative precision.

Without feature metric constraints (CLS+PHY), the model mistakenly assigned high weights to the non-existent  $^{133}\text{Ba}$  feature peak at 356.013 keV, leading to false positives. This suggests that relying solely on physical prior constraints may still cause the model to overfit to noise or spectral similarities that occasionally appear in the training data. However, after introducing feature metric constraints (FhyMetric-Net), the model completely suppressed the response to  $^{133}\text{Ba}$ . The underlying mechanism is the absence constraint (Equation 13), which forces the model to learn that "the absence feature representation of  $^{133}\text{Ba}$  must remain distinct from those of existing nuclides," thus eliminating false positives in the feature space and improving specificity.

For  $^{60}\text{Co}$ , which was present but missed by the CLS+PHY model, the weight distribution provides further insight. Although CLS+PHY assigned strong weights to the 1173.2 keV and 1332.5 keV peaks of  $^{60}\text{Co}$ , it failed to suppress weights in other regions. As a result, the SNR of the feature was insufficient, and classification confidence fell below the required threshold (the sum of weights is -50.51763170245655). In contrast, FhyMetric-Net exhibited global optimization: it maintained moderate weights at key characteristic peaks while applying significant negative weight suppression in other regions, thus improving the discriminative power of the target features.

At the 604.721 keV feature peak of  $^{13}\text{Cs}$ , the CLS+PHY weight distribution was skewed to the right, while FhyMetric-Net's weights were shifted left, aligning more accurately with the actual peak position. This subtle shift suggests that the feature metric constraint guides the model to avoid potential overlap interference with the 661.7 keV peak of  $^{13}\text{Cs}$ , further refining feature localization and enhancing the ability to distinguish complex spectral shapes. This pattern results from the joint optimization of intra-class feature compactness and inter-class feature separation, achieved by the presence constraint. This strategy successfully prevents missed detection of  $^{60}\text{Co}$  and fine-tunes the weight distribution of  $^{13}\text{Cs}$ , improving feature discriminability.

The visual analysis above demonstrates that feature metric constraints optimize decision-making by guiding the model to learn globally discriminative feature distribution patterns. The core mechanism involves the synergistic optimization of positive and negative weights—positive weights reinforce key features, while negative weights suppress interference. This dual mechanism enables more reliable identification in complex spectral backgrounds.

## VI. Conclusions

This paper introduces FhyMetric-Net, a lightweight and interpretable hybrid RIID model. By deeply integrating domain knowledge (physical priors of characteristic peaks) with data-driven approaches (feature metric learning), the model effectively addresses key challenges in Few-shot, multi-label scenarios, such as poor interpretability, weak generalization, and low reliability in traditional deep learning models. The main contributions of this work can be summarized as follows:

1. A novel NN paradigm, **Physical Constraint-Driven Metric Learning Sharpening**, is proposed. By constructing a physical prior constraint matrix, the model receives high-value initialization guidance, significantly reducing reliance on large datasets and mitigating overfitting risks.
2. A feature space metric constraint method for mixed radionuclide recognition tasks is designed. By enforcing intra-class compactness and inter-class separation in the feature space, the model is compelled to learn more discriminative feature representations, achieving SOTA performance in complex scenarios such as low gross count, low SNR levels, and multi-nuclide

mixtures.

3. The model achieves both lightweight design (with only 0.051M parameters) and high accuracy (comprehensive F1 Score performance > 95%), while providing intuitive weight visualizations. This creates a clear causal link between predicted results and physical features, laying a solid foundation for its deployment in high-reliability nuclear industry applications.

**Current Issues:** - The proposed method requires tuning several hyperparameters during the training process, which presents a challenge. - There is room for further improvement in the model's performance for spectra with more mixed radionuclides.

**Future Works:** - Explore dynamic or adaptive physical constraint strengths (e.g., parameter  $\alpha$ ) and metric constraint boundaries (e.g., parameter  $\gamma$ ) to allow the model to intelligently adapt to data of varying quality. - Investigate more elegant feature metric constraint methods to better balance the geometric structure of the feature space with the final classification objective, further enhancing the model's generalization ability. - Explore how to incorporate richer physical information (e.g., Compton plateau profiles, Peak-to-Compton ratios) in a differentiable manner, leveraging techniques such as transfer learning to address challenges in broader detector applications, including CdTe and HPGe detectors. - Address the critical issue of how to systematically and fairly evaluate the model's generalization ability. Designing appropriate test datasets will be key to moving the model toward practical applications. - Systematically evaluate various noise models, including Poisson noise, and explore the correlation between their parameters and the noise characteristics of real gamma spectrometers, aiming to obtain better and more targeted data augmentation solutions.

We believe that FhyMetric-Net offers a promising solution to the common challenges of “Few-shot, High-reliability, Interpretable” scientific computing, and its core ideas may serve as a reference for future radionuclide automatic identification methods.

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