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Development of a Realistic Gamma-ray Spectrum Database using Geant4 and Deep Learning-based Sim-to-Real Translation

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1. Introduction

In emerging nuclear applications such as disaster response and Small Modular Reactors (SMRs), the fast and accurate identification of radioisotopes is of paramount importance. To achieve reliable isotope identification, a robust measurement system grounded in a comprehensive database of actual measured data is essential. However, acquiring empirical data for specific accident-related isotopes-such as short-lived halogens (e.g., Iodine) or noble gases (e.g., Krypton, Xenon)-in standard laboratory settings is highly restricted due to safety regulations and their transient physical nature.

To overcome these limitations, Monte Carlo simulation toolkits like geant4 are widely utilized to generate synthetic gamma-ray spectra for such hard-to-measure isotopes. Nevertheless, a significant “Sim-to-Real gap” remains, preventing the direct application of simulated data. This gap inherently arises because ideal simulations often fail to perfectly model complex real-world phenomena, such as intrinsic background noise and non-linear spectral distortions. Specifically, variations in the light output of scintillators and the gain of photosensors (e.g., PMTs or SiPMs) lead to non-linear X-axis mismatches between the energy deposition and the actual detector channels.

To bridge this gap, we propose a deep learning-based, physics-aware Sim-to-Real translation framework. In this study, we enhance the physical fidelity of the simulation by applying energy resolution smearing prior to the model input. Furthermore, we integrate a Spatial Transformer Network (STN) into the U-Net architecture. The STN is designed to dynamically predict transformation parameters, such as gain and offset, automatically aligning the simulated X-axis with the measurement domain. The primary objective of this study is to train the deep learning model on these inherent detector response variations and evaluate whether it can enhance the generation of high-fidelity synthetic spectra, ultimately establishing a foundation for extending the model’s generalization capabilities to various unseen, accident-specific isotopes.

2. Methods

2.1. Data Acquisition and Pre-processing

Measured gamma-ray spectra were acquired using a scintillation detector system [1] consisting of a Ce:GPS crystal (3 × 3 × 5 mm³, OXIDE Corp.) scintillator with a PMT (R3991AH-07, Hamamatsu). To construct a robust dataset from a limited number of measured events, we employed a bootstrap resampling technique. For each of the six isotopes (^{133}Ba, ^{60}Co, ^{54}Mn, ^{152}Eu, ^{137}Cs, and ^{22}Na), 10,000 randomly selected events (with replacement) were grouped onto histograms (400 bins), generating 20,000 spectra per isotope. Corresponding simulated spectra were generated using Geant4. To enhance physical fidelity and minimize the initial Sim-to-Real gap, energy resolution smearing was applied to the ideal simulated energy-deposition events prior to network input.

2.2 Data preparation and augmentation

To evaluate the model’s robustness against calibration variations, we applied a broad range of channel-warping data augmentation to the simulated spectra. We utilized randomized gain (0.75-1.10) and offset (±15 channels) values. Furthermore, we expanded the assessment to a multi-isotope leave-one-out (LOO) cross-validation strategy. In each validation fold, a specific target isotope (e.g., ^{22}Na, ^{137}Cs, or ^{133}Ba) was entirely excluded from training and utilized exclusively as an unseen holdout dataset to evaluate generalization. All spectra were normalized to a range of 0-1.

2.3. STN-Integrated U-Net Architecture and Training

To address channel-axis misalignment, we integrated a Spatial Transformer Network (STN) into a 1D U-Net architecture. The STN's localization network predicts transformation parameters to automatically align the simulated ADC channels with the measurement domain before feature extraction. The network was optimized using a combined loss of Mean Absolute Error (MAE) and Spectral Angle Mapper (SAM) (0.6 x MAE + 0.4 x SAM) to preserve both peak localization and spectral integrity.

3. Results and Discussion

The proposed STN-Integrated U-NET Architecture model demonstrated the feasibility of transforming simulated spectra into distributions that reflect real-world detector responses. During the training phase on a five-isotope mixture, the model achieved a Mean Absolute Error (MAE) of 0.045214 and a total loss of 0.163651, indicating stable convergence.

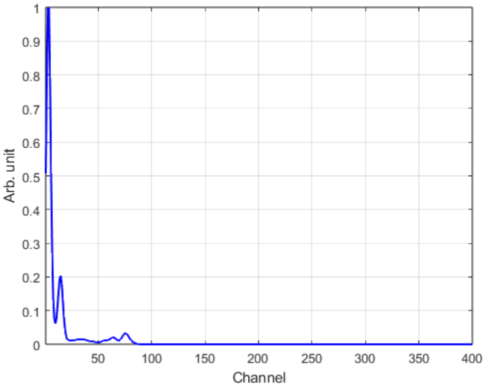

Fig. 1. Examples of input Simulation Spectrum for training & prediction (^{133}Ba).

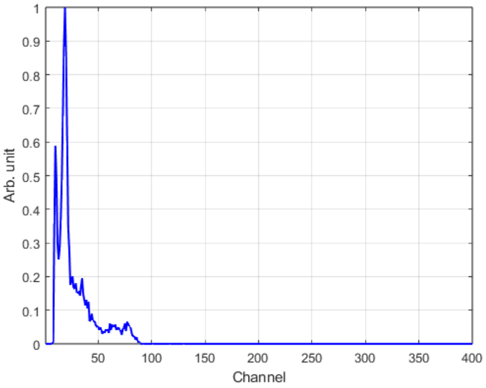

Fig. 2. Examples of input Real Spectrum for training & prediction (^{133}Ba).

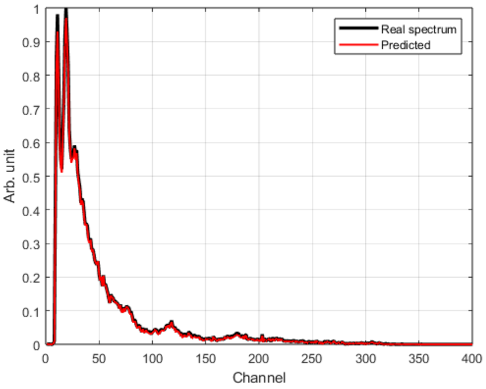

Fig. 3. Examples of Sim-to-Real transformation results for mixed-isotope spectra from training/validation datasets.

To evaluate the generalization capability of the model, Leave-One-Out (LOO) cross-validation was performed using hold-out datasets for ^{133}Ba, ^{152}Eu, ^{137}Cs, and ^{22}Na. In the validation for unseen ^{22}Na, the model recorded a loss of 0.253725 and MAE of 0.068125. For ^{137}Cs, the results showed a loss of 0.277803 and an MAE of 0.047816.

A qualitative fidelity analysis was conducted by randomly sampling 50 outputs from a total of 20,000 generated spectra to assess the model's ability to recover critical physical signatures. High-fidelity reconstruction was defined by a rigorous criterion: the error in both photopeak position and height must be within 20% of the experimental values (511keV for ^{122}Na and 662keV for ^{137}Cs) (with an absolute height difference of < 0.05 specifically for ^{137}Cs). Under this metric, the model achieved a success rate approximately 44% (22/50) for ^{22}Na and 24% (12/50) for ^{137}Cs.

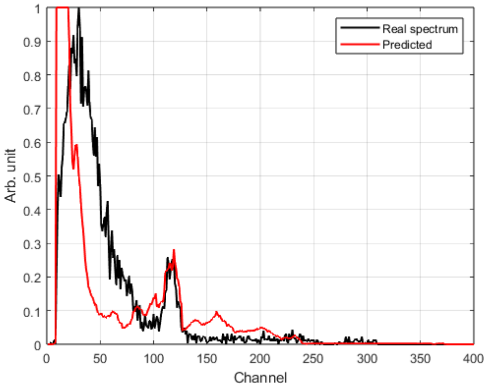

Fig. 4. Sim-to-Real transformation results for the isotope (^{22}Na).

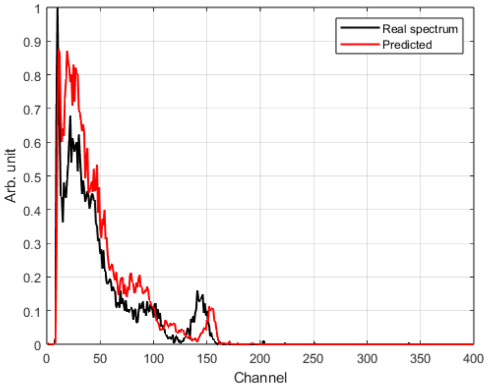

Fig. 5. Sim-to-Real transformation results for the isotope (^{137}Cs).

These results indicate that while the model effectively captures broad noise trends and gain/offset shifts, consistent reproduction of fine photopeak structures remains a significant challenge. The observed variation in performance across different nuclides suggests that the model is learning nuclide-specific energy profiles rather than applying a uniform transformation, which is a key step toward bridging the sim-to-real gap. However, the current loss function, which weighs all spectral channels equally, may lead to the underrepresentation of high-energy photopeak features compared to high-count low-energy noise. Future work will focus on analyzing these high-fidelity cases to develop a more robust precision model.

Specifically, we intend to implement a Weighted Loss Function that assigns higher priority to high-energy channels. By compelling the model to prioritize these physically significant regions, we aim to improve the consistency of peak reproduction and ensure the generated data can reliably support downstream radioisotope identification tasks in complex environments.

4. Conclusions

This study demonstrates that an STN-integrated U-Net architecture with a hybrid MAE-SAM loss function can effectively bridge the Sim-to-Real gap in gamma spectroscopy. By dynamically correcting physical detector responses, the model successfully reproduces key features such as photopeak and Compton regions, even for unseen radionuclides. While discrepancies remain in peak reproduction consistency (ranging from 24% to 44%), these results establish a rigorous foundation for generating high-fidelity virtual training data. Future research will focus on refining loss functions to prioritize high-energy features and expanding the model’s capability to account for environmental variables such as temperature and radiation dose rates, ultimately enhancing the reliability of AI-based isotope identification in real-world environments.

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