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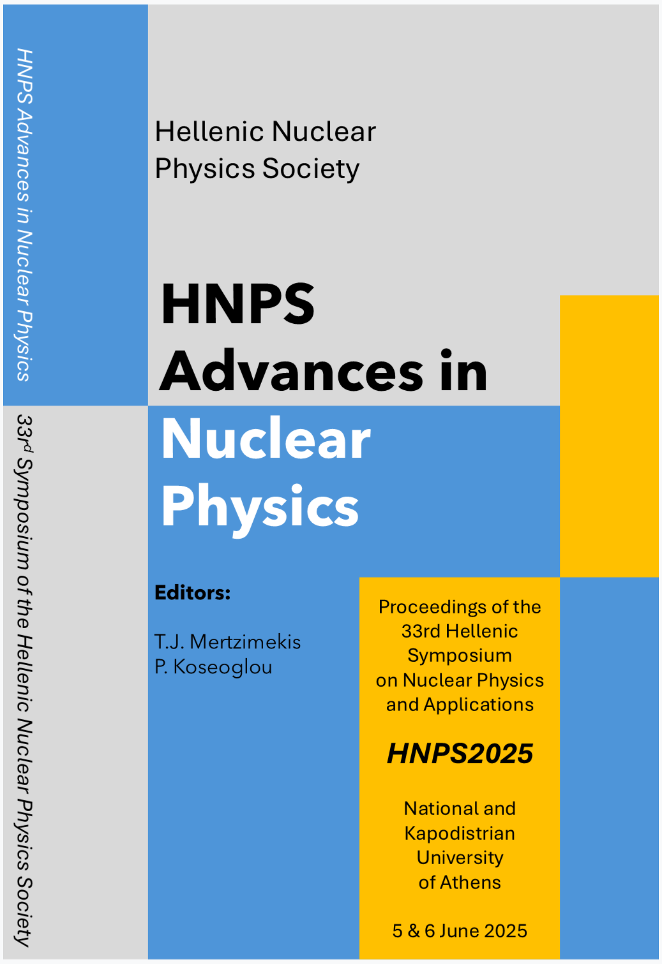

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ARTICLE

A Bayesian Network-Based Framework for Predicting Fission Charge Yields

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Abstract
Predicting neutron-induced fission charge yields is a long-standing challenge due to the complex, non-equilibrium nature of the fission process and the limited availability of experimental data across a broad range of neutron energies. This work presents a Bayesian machine learning framework that integrates Gaussian Process Regression (GPR), Bayesian Neural Networks (BNNs), and Mixture Density Network (MDN) outputs to address these challenges. The GPR component augments sparse datasets with synthetic samples and associated uncertainties, while BNN layers capture model uncertainty through variational inference. The MDN output models the multimodal nature of charge yields and accounts for data-driven (aleatoric) uncertainty. The proposed model accurately reproduces known features of fission yields, such as odd-even staggering and energy dependence, and generalizes well to isotopes not included in the training set. Its probabilistic predictions are consistent with experimental observations and semi-empirical models, offering a robust tool for fission yield modeling.

Keywords: fission charge yields; Bayesian neural networks; Gaussian process regression; mixture density networks; uncertainty quantification

1. Introduction

Nuclear fission remains one of the most intricate phenomena in low-energy nuclear physics, owing to its non-equilibrium nature and the interplay between collective and microscopic degrees of freedom. Accurate modeling of fission observables—particularly charge yields—is vital for applications in reactor engineering, isotope production, and astrophysical processes [1–4]. Despite decades of experimental and theoretical progress, evaluated libraries such as ENDF [5], JENDL [6], and JEFF [7] still provide limited energy-dependent charge-yield data. These gaps arise because charge-yield measurements are experimentally demanding, and theoretical approaches remain computationally expensive.

Recent experimental developments employing inverse kinematics and magnetic spectrometry [8–12] have improved yield resolution and clarified the role of shell and pairing effects, including the

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characteristic odd–even staggering. However, data coverage remains sparse across excitation energies, constraining the ability to generalize results or benchmark models.

Traditional frameworks such as macroscopic-microscopic models, the Brosa approach [13], and the GEneral description of Fission observables (GEF) model [14] successfully describe many average trends but often struggle when extrapolated beyond fitted regions. Fully microscopic methods, such as time-dependent density functional theory (TD-DFT) [15] or the time-dependent generator coordinate method (TD-GCM) [16–18], provide deep physical insight but remain computationally prohibitive for systematic evaluations.

Machine-learning (ML) approaches offer a complementary path to bridge these gaps. Bayesian Neural Networks (BNNs) [19] and Mixture Density Networks (MDNs) [20] have demonstrated their potential to represent nonlinear and multimodal nuclear observables [21–25]. Building on previous work applying Mixture Density Networks (MDNs) to fission-mass yields [25], the present proceedings summarize the results reported in [26], where a Bayesian Mixture Density Network (BMDN) unifying three probabilistic components was developed. (i) Gaussian Process Regression (GPR) for data augmentation and uncertainty-aware interpolation [27]; (ii) Bayesian Neural Network (BNN) layers for capturing epistemic uncertainty through variational inference [28, 29]; and (iii) a Mixture Density Network (MDN) output that models the multimodal character of charge yields and quantifies aleatoric uncertainty [20]. This hybrid framework captures essential nuclear-structure features, such as odd–even staggering and energy-dependent broadening, while quantifying model confidence across isotopes and incident-neutron energies. Section 2 details the model architecture, Section 3 presents the results and discussion, and Section 4 concludes with future perspectives.

2. Methodology

The Bayesian Mixture Density Network integrates three probabilistic components—Gaussian Process Regression, Bayesian Neural Network layers, and a Mixture Density Network output—each addressing a specific limitation in modeling neutron-induced fission yields.

2.1 Gaussian Process Regression

Gaussian Process Regression [27] augments the limited evaluated datasets from JENDL-5 [6] by generating smooth synthetic samples accompanied by predictive uncertainties. This non-parametric Bayesian approach assigns a prior over functions, updated with observed data to produce mean predictions and confidence intervals for new inputs. To model both global and local correlations, the GPR employs a composite kernel:

$$k(x, x') = k_{\mathrm{DP}} + k_{\mathrm{RQ}} + k_{\mathrm{WN}}, \tag{1}$$

where the Dot-Product term captures linear energy or charge trends, the Rational-Quadratic term introduces multi-scale correlations,

$$k_{\mathrm{RQ}}(x, x') = \left(1 + \frac{|x - x'|^2}{2\alpha l^2}\right)^{-\alpha}, \tag{2}$$

and the White-Noise term adds uncorrelated variance,

$$k_{\mathrm{WN}}(x, x') = \begin{cases} \sigma_n^2, & x = x', \\ 0, & x \neq x'. \end{cases} \tag{3}$$

The kernel parameters l, α, σ_n^2 are optimized for each isotope to balance smoothness and feature fidelity. The resulting synthetic data preserve the essential shape and staggering of evaluated distributions while filling sparsely sampled charge regions, forming the training input for the BMDN.

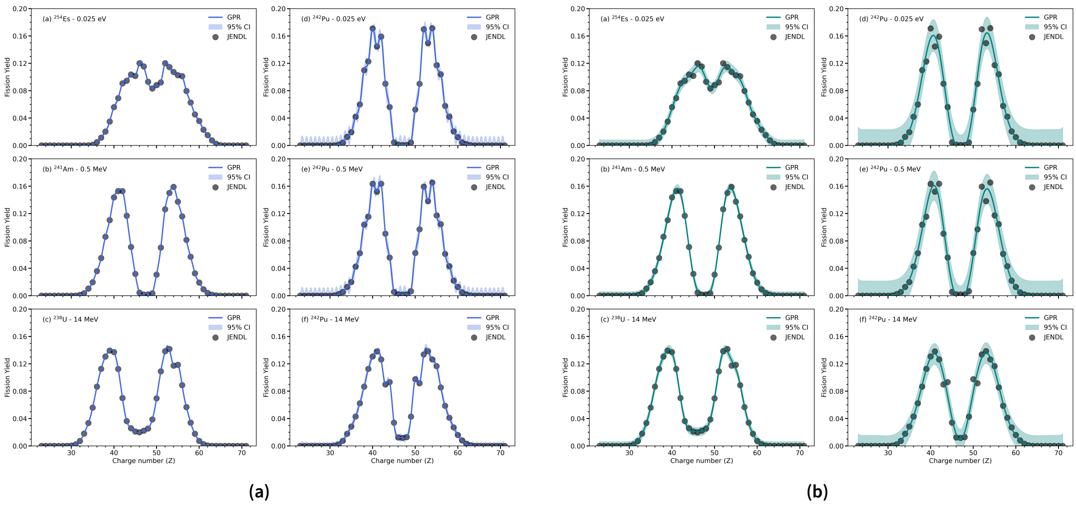


Figure 1. GPR-generated charge yield distributions without (left panel) and with (right panel) the WK for neutron-induced fission of (a) ^{254}Es at 0.025 eV, (b) ^{241}Am at 0.5 MeV, (c) ^{238}U at 14 MeV, (d) ^{242}Pu at 0.025 eV, (e) ^{242}Pu at 0.5 MeV, and (f) ^{242}Pu at 14 MeV. The shaded area corresponds to the 95% CIs. Evaluated data are taken from the JENDL-5 library [6].

2.2 Bayesian Neural Network Layers

The BNN layers model epistemic uncertainty by treating network weights ω as random variables governed by a posterior $p(\omega|X, Y) \propto p(Y|X, \omega)p(\omega)$. A variational approximation $q(\omega|\phi) = \mathcal{N}(\mu_\phi, \Sigma_\phi)$ is optimized by minimizing the Kullback–Leibler divergence between q and the prior $p(\omega)$:

$$\mathcal{L}_{\mathrm{KL}} = \int q(\omega|\phi) \log \frac{q(\omega|\phi)}{p(\omega)}\, d\omega. \tag{4}$$

Monte-Carlo sampling of the variational posterior during inference yields an ensemble of predictions whose variance reflects epistemic uncertainty.

Input features include the atomic and mass numbers of the fissioning system (Z_i, A_i), fragment charge Z_f, excitation energy $E=e+S_n$, and an odd–even indicator $\Delta=0.2$ (even) or -0.2 (odd). An attention layer assigns adaptive weights w_i to these features,

$$\mathbf{h}_{\mathrm{att}} = \sum_i w_i x_i + w_b, \tag{5}$$

allowing the network to emphasize physically relevant inputs dynamically.

The architecture comprises eight Bayesian dense layers of 64 neurons each with tanh activation. All Bayesian and attention components are implemented using TensorFlow-Keras [30].

2.3 Mixture Density Network Output

The MDN represents the conditional probability of charge yield y given features x as a weighted sum of M Gaussian components,

$$p(y|x) = \sum_{i=1}^{M} \pi_i(x)\, \mathcal{N}\big(y|\mu_i(x), \sigma_i^2(x)\big), \tag{6}$$

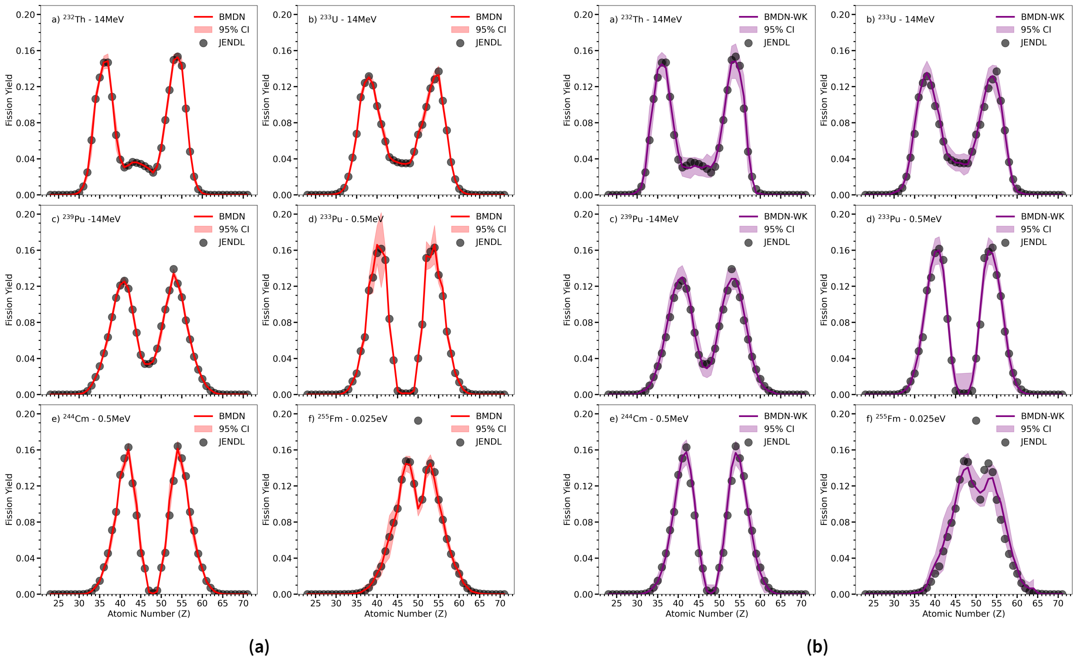


Figure 2. BMDN (left panel) and BMDN-WK (right panel) learning ability of neutron induced fission charge yields. The shaded region corresponds to the CIs estimated at 95%.

where $\pi_i(x)$ are normalized mixing coefficients. Training minimizes the negative log-likelihood over all samples:

$$\mathcal{L} = -\sum_n \log\left[\sum_i \pi_i(x_n)\mathcal{N}(y_n|\mu_i, \sigma_i^2)\right]. \tag{7}$$

In this study $M = 4$, enabling multimodal charge-yield representation and direct modeling of aleatoric uncertainty through $\sigma_i^2(x)$.

2.4 Uncertainty Quantification

Epistemic uncertainty σ^2_{epi} is estimated from prediction variance over multiple posterior samples,

$$\sigma^2_{\text{epi}} = \frac{1}{N}\sum_i (\hat{y}_i - \bar{y})^2, \tag{8}$$

while aleatoric uncertainty σ^2_{ale} arises from the MDN variance,

$$\sigma^2_{\text{ale}} = \sum_i \pi_i(x)\sigma_i^2(x). \tag{9}$$

The total predictive uncertainty combines both terms, $\sigma^2_{\text{tot}} = \sigma^2_{\text{epi}} + \sigma^2_{\text{ale}}$, and the corresponding 95% confidence interval is $\bar{y} \pm 1.96\sigma_{\text{tot}}$.

3. Results and Discussion

The Bayesian Mixture Density Network was trained using GPR-generated synthetic charge-yield data for 46 neutron-induced fissioning systems across thermal, intermediate, and fast neutron energies,

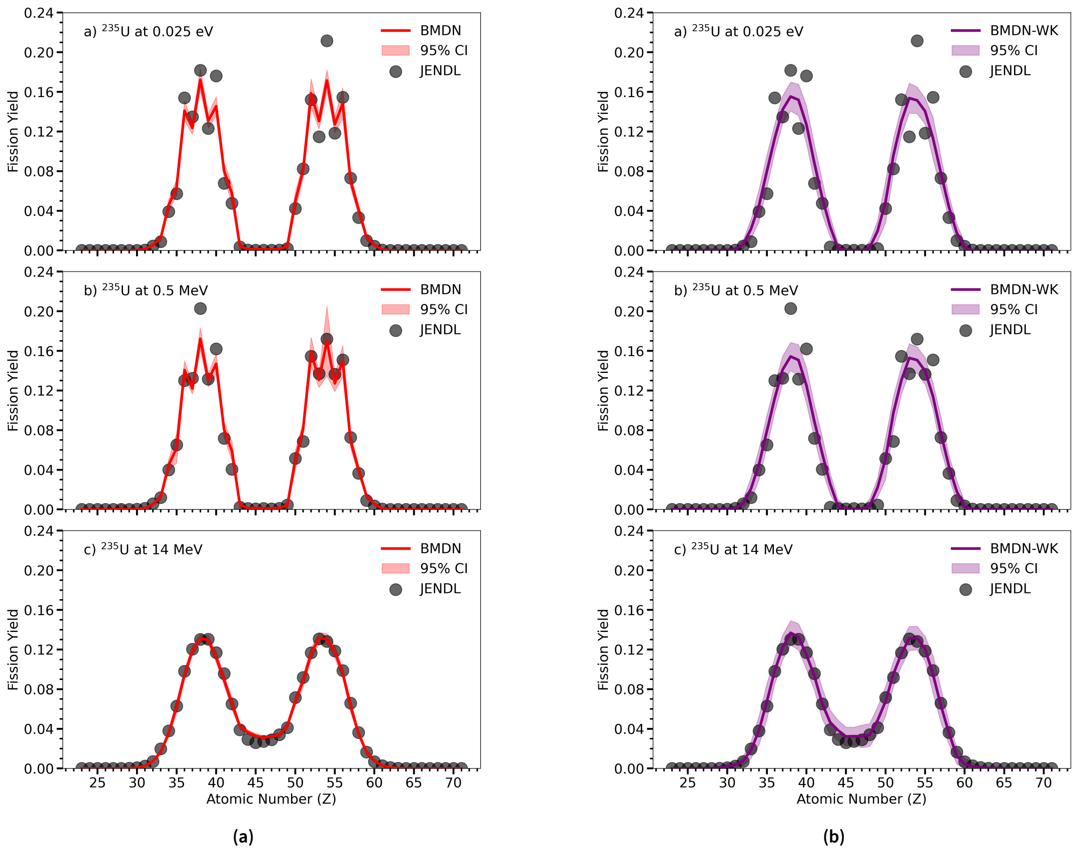


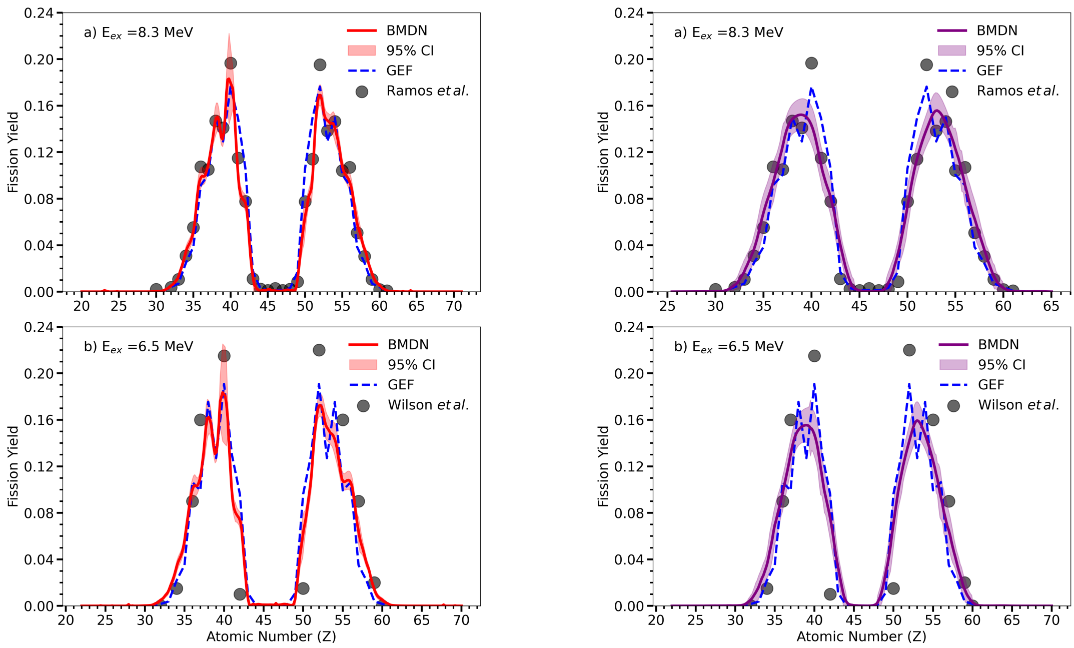
Figure 3. BMDN (left panel) and BMDN-WK (right panel) predictions of fission yields of $n + ^{235}$ U compared with JENDL-5 evaluations, with neutron incident energies at (a) 0.025 eV, (b) 0.5 MeV, and (c) 14 MeV. The shaded region corresponds to the CIs estimated at 95%.

excluding ^{235}U for validation. The model demonstrates accurate learning of both smooth trends and structural effects, with uncertainty bands reflecting data density and model confidence.

Synthetic data generation. The composite GPR kernel $k = k_{\mathrm{DP}} + k_{\mathrm{RQ}} + k_{\mathrm{WN}}$ preserves global and local patterns across isotopes, Fig. 1. Without the noise term, GPR reproduces narrow confidence intervals consistent with evaluated JENDL-5 data, whereas the addition of the White-Noise kernel broadens these intervals and suppresses fine staggering. This trade-off illustrates the sensitivity of fission-yield reconstruction to the noise model.

Model learning and kernel sensitivity. The BMDN achieves excellent agreement with evaluated data ($\chi^2 = 4.7 \times 10^{-5}$), reproducing both yield shapes and odd–even staggering, Fig. 2. The White-Kernel version (BMDN-WK) attains a similar average error but produces wider confidence intervals and weaker staggering contrast. Thus, while adding noise enhances generalization, excessive smoothing erodes structural fidelity.

Validation on unseen nucleus. For ^{235}U, excluded from training, the BMDN reproduces the energy-dependent evolution of charge yields with pronounced odd–even effects at low energy that



(a) **(b)**

Figure 4. BMDN (left panel) and BMDN-WK (right panel) predictions of fission yields for the compound nucleus ^{239}U are compared with experimental data and semiempirical models. Panel (a) shows results at an excitation energy of 8.3 MeV, with experimental data (Ramos *et al.*) from [12], while panel (b) presents results at 6.5 MeV, with experimental data (Wilson *et al.*) from [10]. The shaded regions represent the 95% CIs of the BMDN predictions. For reference, GEF results [14] are also included.

gradually fade with increasing excitation energy, as seen in Fig. 3. Uncertainty decomposition shows nearly equal contributions of aleatoric (51%) and epistemic (49%) components, confirming balanced modeling of intrinsic and data-driven variability. In contrast, the BMDN-WK variant displays larger epistemic fractions (≈52%) and broader bands, indicating that injected noise transfers variance from the data level to the model level.

Cross-isotope validation and discussion. For the compound nucleus ^{239}U, BMDN predictions align closely with both experimental data and GEF calculations (see Fig. 4). At 8.3 MeV the model reproduces the measured asymmetric peaks, while at 6.5 MeV it yields smoother distributions that challenge reported anomalies. Compared with BNN models employing MCMC sampling [22], the BMDN attains similar accuracy at a fraction of the computational cost, as both epistemic and aleatoric uncertainties are captured within a unified probabilistic framework.

Overall assessment. The chosen kernel combination (DotProduct + RationalQuadratic + WhiteKernel) provides optimal flexibility, capturing multiscale correlations while maintaining stability. The model's uncertainty intervals remain well-calibrated across datasets, widening only in poorly constrained regions. These results demonstrate that the BMDN framework yields physically interpretable charge-yield predictions with meaningful confidence intervals and improved computational efficiency for large-scale fission evaluations.

4. Conclusions

A Bayesian Mixture Density Network framework has been developed to predict fission charge yields under data-sparse conditions. By combining GPR data augmentation, Bayesian neural inference, and MDN outputs, the approach provides accurate, uncertainty-aware predictions that capture key physical features such as odd–even staggering and energy dependence. The framework yields realistic confidence intervals distinguishing between data and model uncertainty, making it a powerful and interpretable tool for future fission yield evaluations, isotope production studies, and reactor design applications.

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