Neutron spectrum unfolding using deep learning models for tabular data

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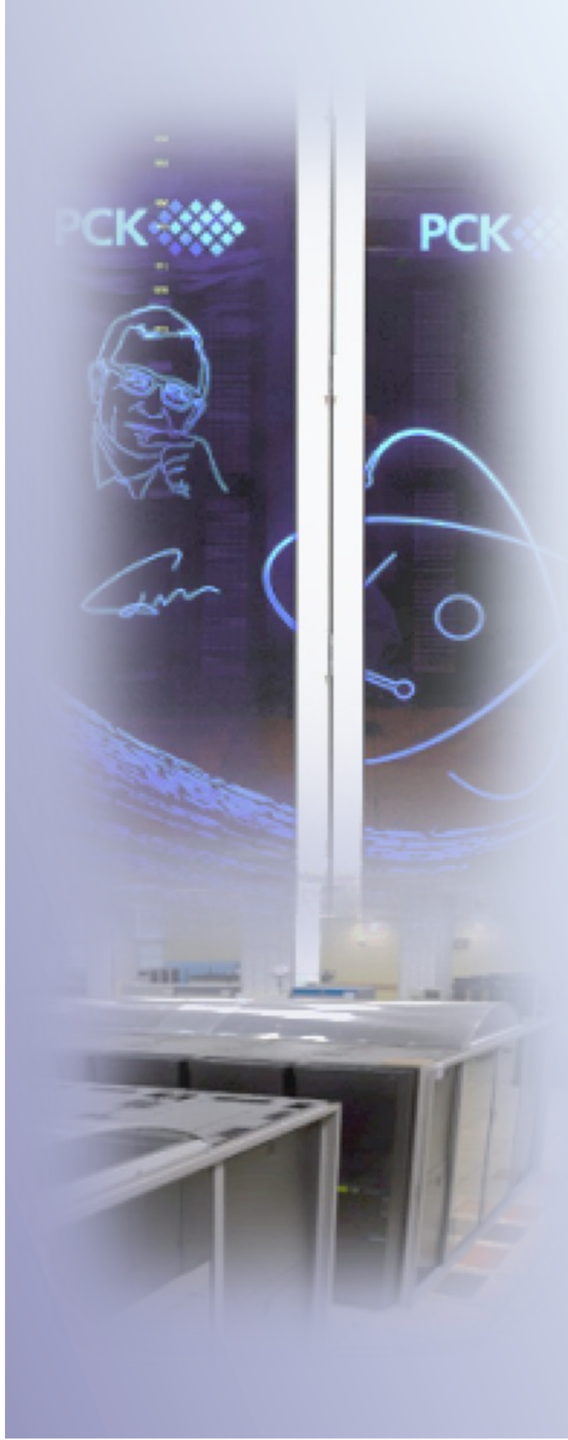
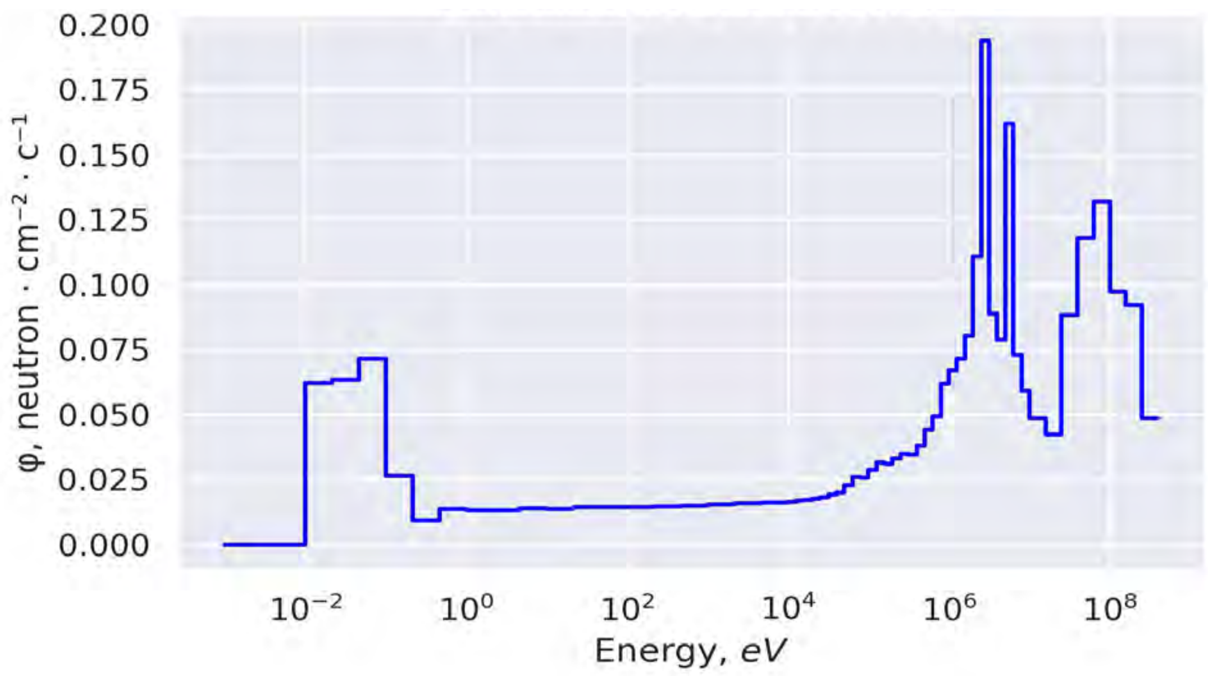
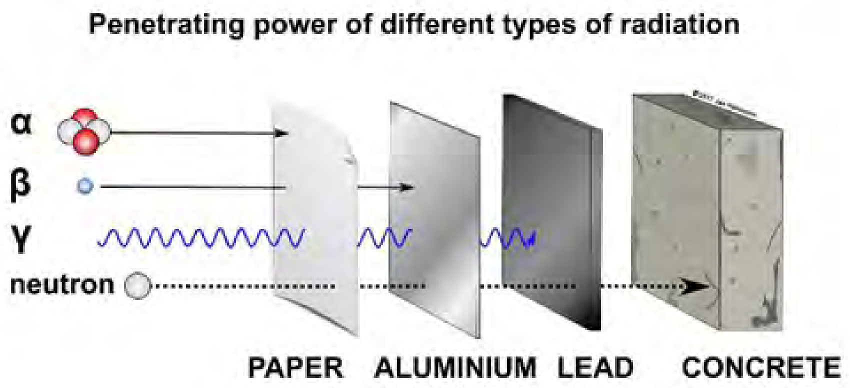


Introduction

Radiation fields behind the protective shields of nuclear physics facilities (particle accelerators, nuclear reactors) are formed mainly by *neutrons* of a wide energy spectrum.





Neutron energy range

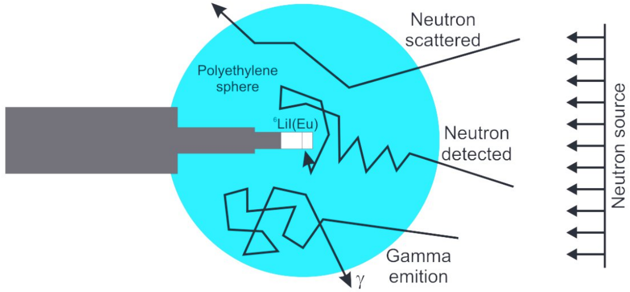
- Nuclear power plants, E ≈ 10^{-9} – 20.5 MeV
- Particle accelerators, E ≈ 10^{-9} – 10^{3} MeV
- Cosmic radiation, E ≈ 10^{-9} – 10^{4} MeV

Personal dosimeter
0.025 eV - 20 MeV

https://www.doza.ru

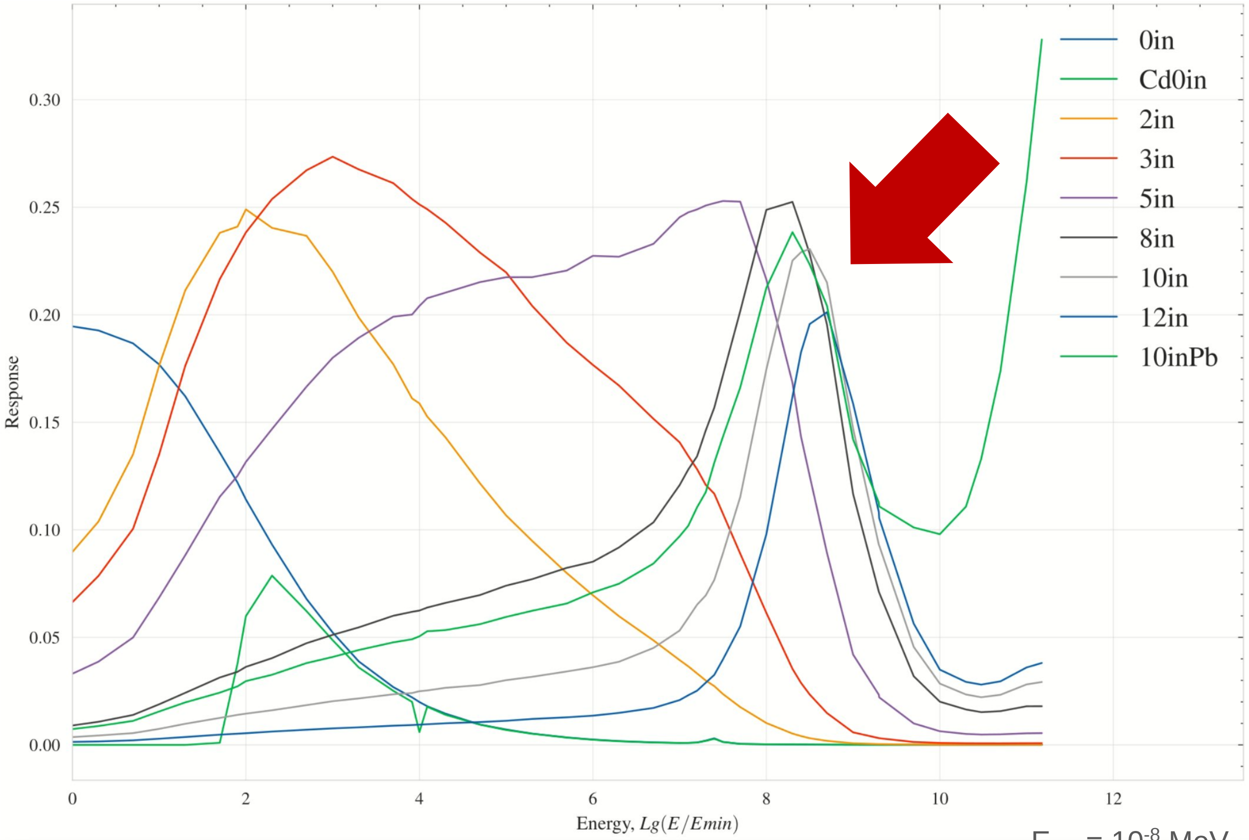
Bonner Multi-sphere Spectrometer

https://atomtex.com/

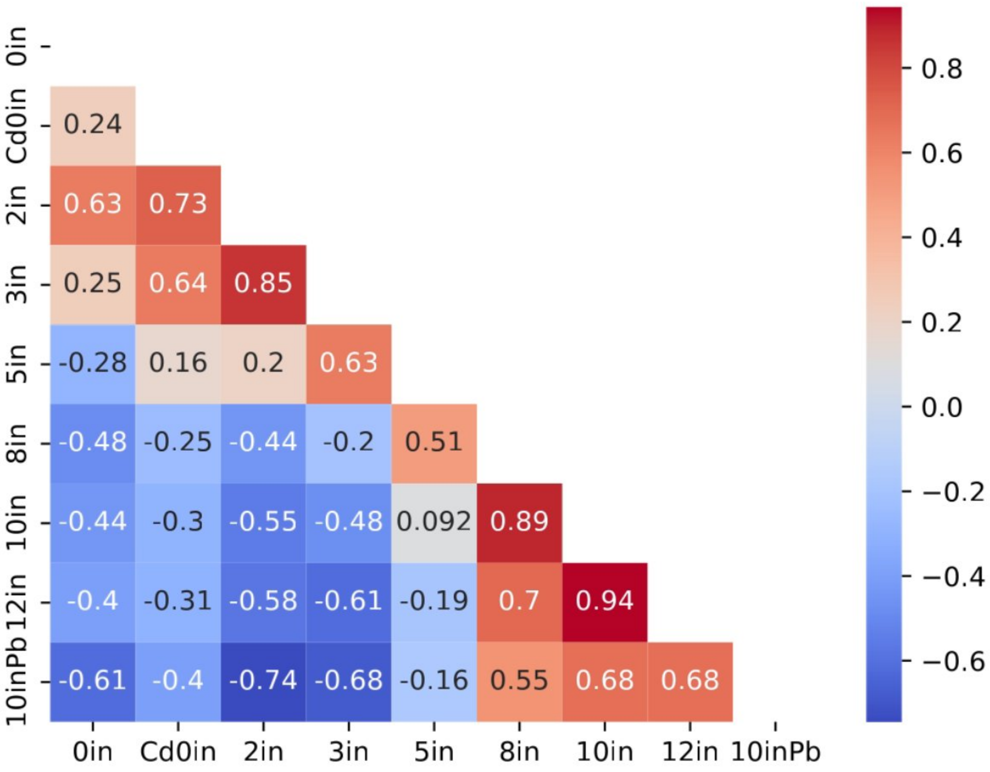


http://dx.doi.org/10.5772/51274

Response functions of moderator spheres



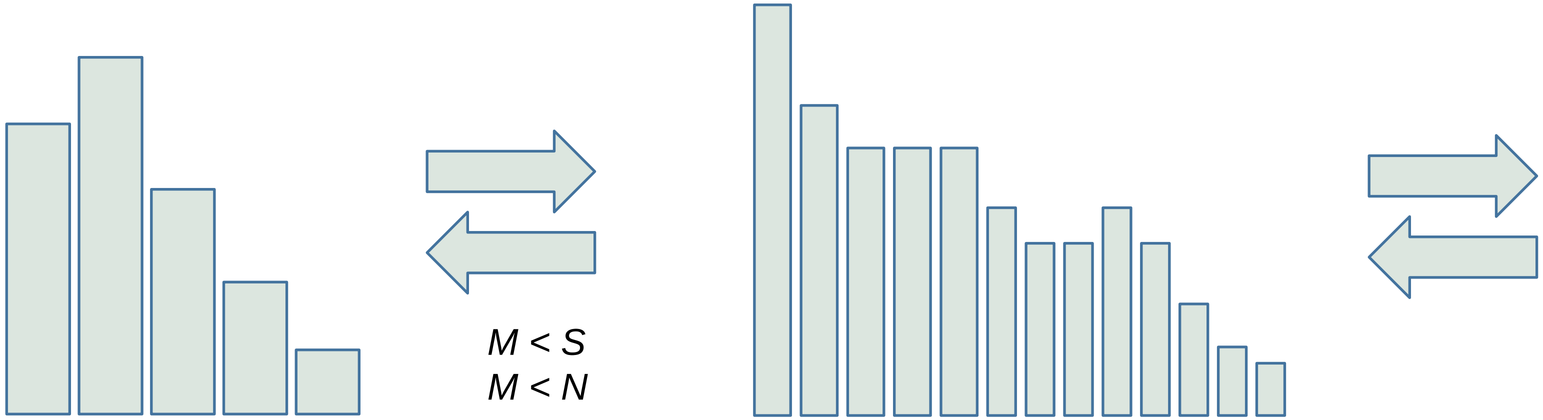
$E_{min} = 10^{-8}$ MeV

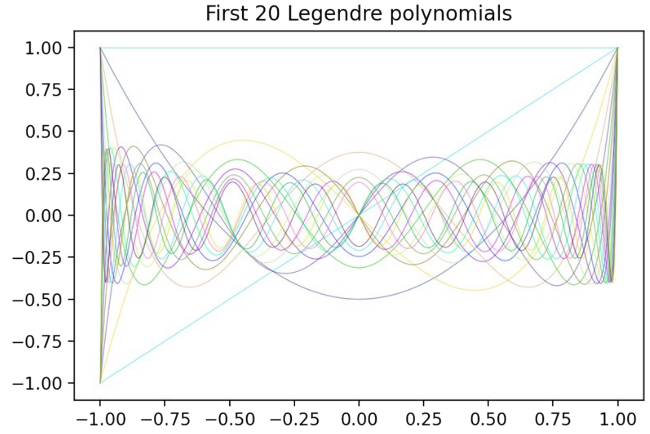


Martinkovic, J., and G. N. Timoshenko. *Calculation of multisphere neutron spectrometer response functions in energy range up to 20 MeV*. No. JINR-R--16-2005-105. Division of Radiation and Radiobiological Research, 2005.

Direct and inverse problems of spectrum unfolding

- Direct task: to obtain “effective” readings of the Bonner spectrometer (BSS) based on the given spectra.
- Inverse task: to obtain the initial spectra based on the measurements.





$Q_1 \dots Q_M$ $E_1 \dots E_S$ $C_1 \dots C_N$

$$Q_j \approx \sum_{i=1}^{S} K_{ji} \Phi(\mathrm{E}_i) \Delta E, \quad j = 1,\dots,M$$

$$\Phi = \sum_{i=1}^{N} C_i \, P_{i-1}$$

$$P_n(x) = \frac{1}{2^n n!} \cdot \frac{d^n}{dx^n} \left(x^2 - 1\right)^n$$

$$\begin{cases} \int_{E_{\min}}^{E_{\max}} K_1(E)\,\varphi(E)\,dE = Q_1 + \xi, \\ \vdots \\ \int_{E_{\min}}^{E_{\max}} K_M(E)\,\varphi(E)\,dE = Q_M + \xi, \end{cases}$$

- Q_j is the BSS reading for the j-th sphere,
- ξ - error of measurement,
- $\varphi(E)$ - neutron spectrum,
- $K_j(E)$ is a response function of the detector to neutrons,
- M is the number of spheres used,
- The integration limits $E_{\min}$ and $E_{\max}$.

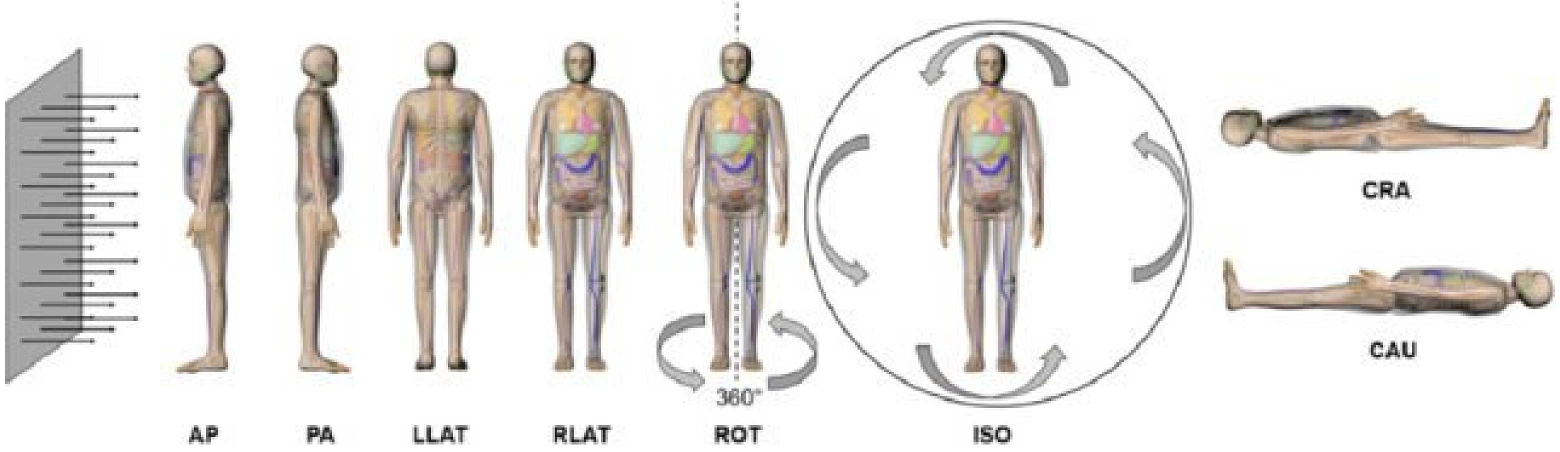
Dose estimation for spectrum

The Bonner multi-sphere spectrometer is used to measure neutron spectra in stationary fields to assess irradiation of personnel.

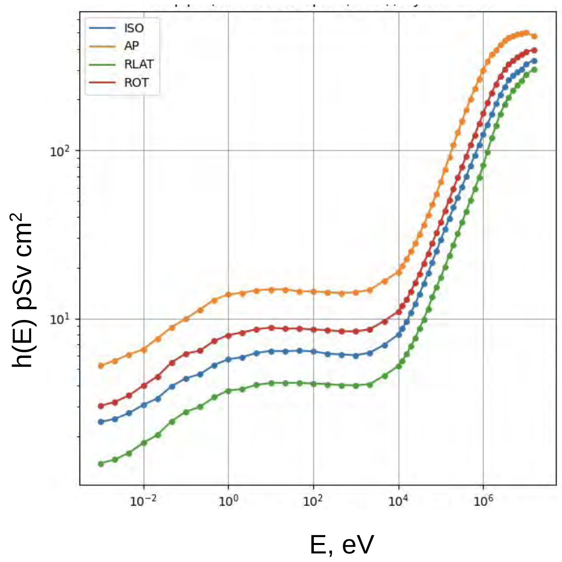
$$\dot{H} = \int_{Emin}^{Emax} \varphi(E) \cdot h(E) dE$$

$\dot{H}$ – dose rate ($\dot{H}_{eff\_AP}$,$\dot{H}_{eff\_ISO}$, $\dot{H}^*(10)$, $\dot{H}_p(10,0^\circ)$)

h(w) – corresponding conversion factor [pSv·cm^2] for monoenergetic particles in different irradiation geometries, ICRP Publication 116[1].



https://dceg.cancer.gov/tools/radiation-dosimetry-tools/phantoms-library

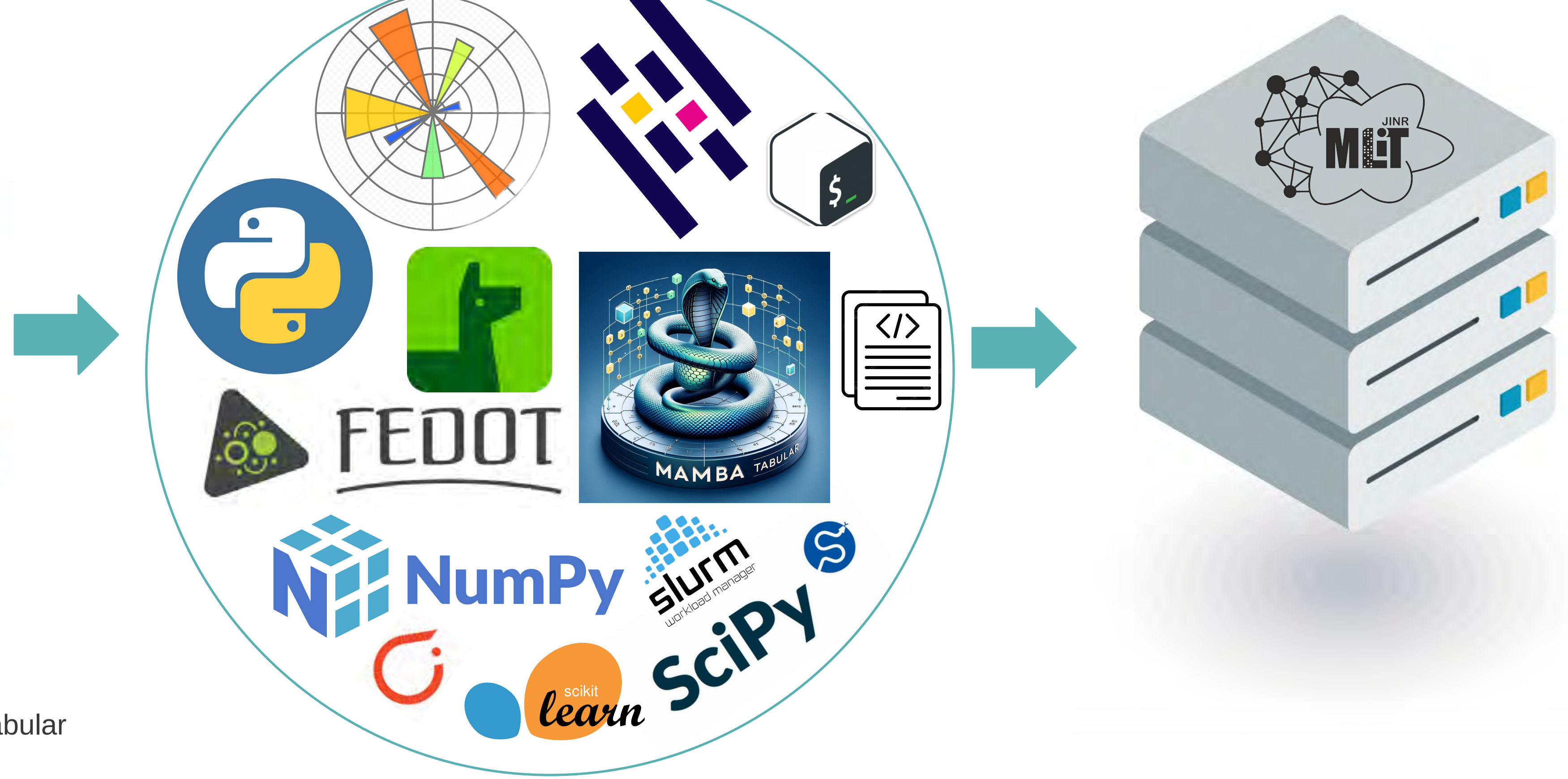


1. Petoussi-Henss, Nina, et al. "ICRP Publication 116—the first ICRP/ICRU application of the male and female adult reference computational phantoms." *Physics in Medicine & Biology* 59.18 (2014): 5209.

ML method & implementation

- Calculations on the multifunctional information and computing complex of the Joint Institute for Nuclear Research (JINR) Information Technology Laboratory.
- Deep learning (DL) framework: Mambular.
- Automated machine learning (AutoML) frameworks: Fedot, LightAutoML.

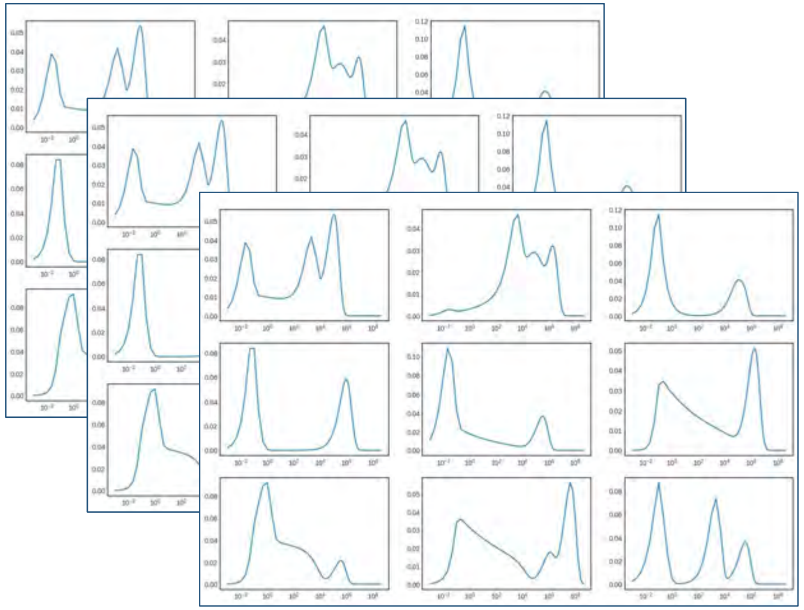
8 x GPU CUDA A100



1. http://hlit.jinr.ru/
2. https://github.com/OpenTabular/DeepTabular
3. https://github.com/aimclub/FEDOT
4. https://github.com/sb-ai-lab/LightAutoML

Dataset

- **Synthetic based on FRUIT[1] method ($5 \cdot 10^5$ spectra) for training**
  1. Input features: numerical: 10 measurements.
  2. Output target: Spectre values for 60 energy bins (10^{-9} - $6.3 \cdot 10^2$ MeV, log scale).
  3. 80% — training, 20% — validation.



- **Spectra from the literature (375 spectra) for testing**

IAEA dataset[2] (251 spectra) + 124 spectra from open access papers (manually digitized by our group).

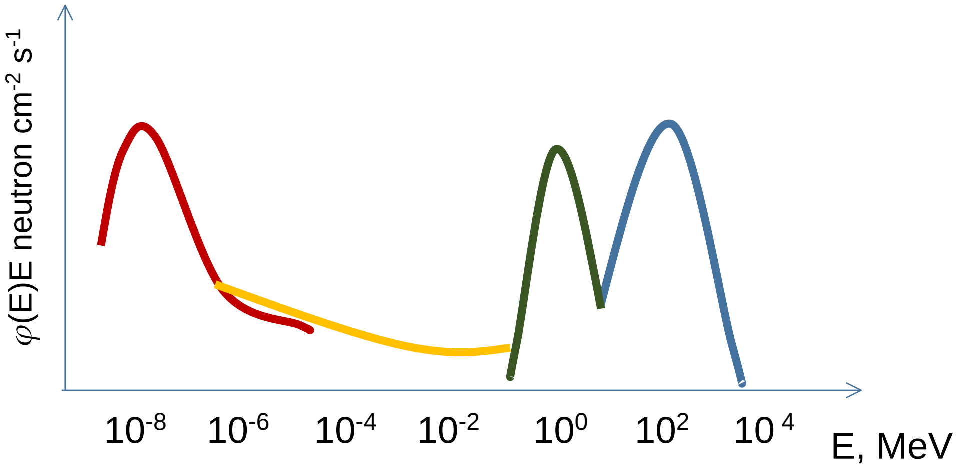
1. Input features: numerical: 10 measurements.
2. Output target: Spectre values for 60 energy bins (10^{-9} — $6.3 \cdot 10^2$ MeV, log scale).

Monte-Carlo simulation, regularization (Tikhonov, statistical, ...), Maximum entropy principle, Maximum likehood, Genetic, Iterative, Parametric, Bayesian, ...[3]

1. Frascati Unfolding Interactive Tool, doi: 10.1016/J.NIMA.2007.07.033
2. *Compendium of Neutron Spectra and Detector Response for Radiation Protection Purposes: Technical Report Series. Vienna: IAEA, 2001. No. 403.*
3. Gómez-Ros J. M. et al. Results of the EURADOS international comparison exercise on neutron spectra unfolding in Bonner spheres spectrometry. *Radiation Measurements* 153 (2022): 106755.

Synthetic dataset

Model	Thermal $\phi_{\mathrm{th}}\,(E,...)$	Epithermal $\phi_e\,(E,...)$	Fast $\phi_f\,(E,...)$	High Energy $\phi_{\mathrm{hi}}\,(E,...)$
Fission	$\left(\frac{E}{T_0^2}\right)e^{-E/T_0}$	$\left[1-e^{-(E/E_d)^2}\right]E^{b-1}e^{-E/\beta'}$	$E^{\alpha}e^{-E/\beta}$	0
Evaporation	↓	↓	$\left(\frac{E}{T_{ev}^2}\right)e^{-E/T_{ev}}$	0
Gaussian	↓	↓	$exp\left(-\frac{1}{2}\left(\frac{E-E_m}{\sigma E_m}\right)\right)$	0
High Energy	↓	↓	$\left(\frac{E}{T_{ev}^2}\right)e^{-E/T_{ev}}$	$\left(\frac{E}{T_{hi}^2}\right)e^{-E/T_{hi}}$



- φ_{th} — thermal (0.025 eV – 0.04 eV)
- φ_e — epitermal (0.04 eV – 100 keV)
- φ_f — fast (0.2 – 10 MeV)
- φ_{hi} — high-energy (> 10 MeV)

The tunable parameters for each model are:

Fission: $P_{th},P_e,P_f,b,\beta',\alpha,\beta$Pth,Pe,Pf,b,β′,α,β
Evaporation: $P_{th},P_e,P_f,b,\beta',T_{ev}$Pth,Pe,Pf,b,β′,Tev
Gaussian: $P_{th},P_e,P_f,b,\beta',E_m,\sigma$Pth,Pe,Pf,b,β′,Em,σ
High Energy: $P_{th},P_e,P_f,P_{hi},b,\beta',T_{ev},T_h$

$$\varphi(E) = P_{th}\varphi_{th}(E) + P_e\varphi_e(E) + P_f\varphi_f(E) + P_{hi}\varphi_{hi}(E),$$

$$P_{th} + P_e + P_f + P_{hi} = 1$$

Type	Energy	Velocity (m/s)	Wavelength (nm)	Temperature (K)
ultracold	$< 0.2\ \mu$eV	< 6	> 64	< 0.002
very cold	$0.2 \le E < 50\ \mu$eV	$6 \le v < 100$	$4 < \lambda \le 64$	$0.002 \le T < 0.6$
cold	$0.05 < E \le 3$ meV	$100 < v \le 760$	$0.5 \le \lambda < 4$	$0.6 < T \le 34$
thermal	$0.003 \le E < 0.04$ eV	$760 < v \le 2760$	$0.14 \le \lambda < 0.5$	$34 < T \le 0.46$
epithermal	0.04 eV$< E \le 100$ keV	$2760 < v \le 4.3 \cdot 10^6$	$92 \cdot 10^{-6} \le \lambda < 0.14$	$(0.46 < T \le 1.2) \cdot 10^6$
intermediate	$100 < E \le 200$ keV	$(4.3 < v \le 6.2) \cdot 10^6$	$(64 \le \lambda < 92) \cdot 10^{-6}$	$(1.2 < T \le 2.3) \cdot 10^6$
fast	$0.2 < E \le 10$ MeV	$(6.2 < v \le 43) \cdot 10^6$	$(9.2 \le \lambda < 64) \cdot 10^{-6}$	$(0.002 < T \le 120) \cdot 10^9$
high-energy	> 10 MeV	$> 4.3 \cdot 10^7$	$< 9.2 \cdot 10^{-6}$	$> 120 \cdot 10^9$

1. *McGreivy J., Manfredi J.J., Siefman D. Data Augmentation for Neutron Spectrum Unfolding with Neural Networks. Journal of Nuclear Engineering 4(1)): 77–95. 2023. (For neutron energy range from* 0.001 eV to 15.8 MeV)
2. Frascati Unfolding Interactive Tool, doi: 10.1016/J.NIMA.2007.07.033
3. Nico S., Snow W. M. Fundamental Neutron Physics. Annu. Rev. Nuc.Part. Sci., 55:27–69, 2005.

IAEA dataset

- Database of 251 spectra.
- Spectra normalized to 1.
- The database may contain errors due to the use of different methods. For example, non-physical waves on the graph due to solution of the inverse problem with choosed regularization parameter.

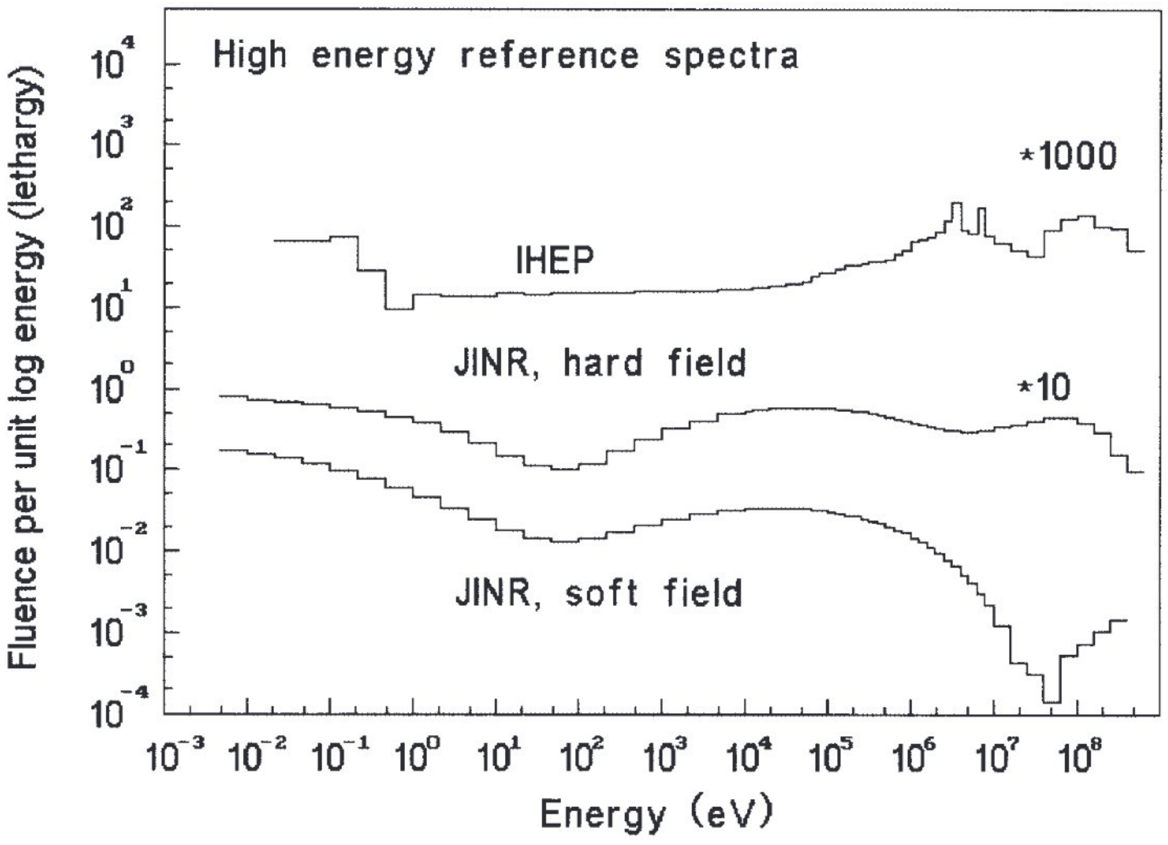
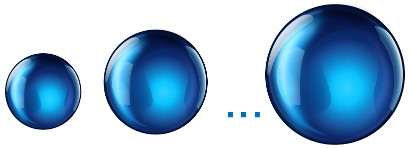


FIG. 4.21. High energy reference spectra (JINR and IHEP).

1. Compendium of Neutron Spectra and Detector Response for Radiation Protection Purposes: Technical Report Series. Vienna: IAEA, 2001. No. 403.
2. Aleinikov, V. E., et al. "Reference neutron fields for metrology of radiation monitoring." Radiation Protection Dosimetry 54.1 (1994): 57-59.

Advanced deep learning architecture for tabular data

10 Measurements

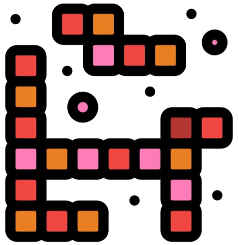


D = 0, 2, 3, 5, 6, 8, 10, 12, 15, 18 inch

^{6}LiI(Eu) detector GSF[1]

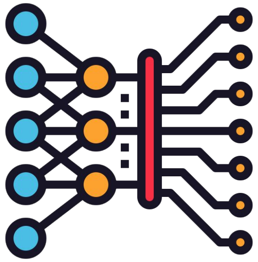
Feature Transformations

~10^5 - 10^6 parameters



min-max scaler, peicewise linear encoding (PLE)[2], dimensions d = 20

Estimator

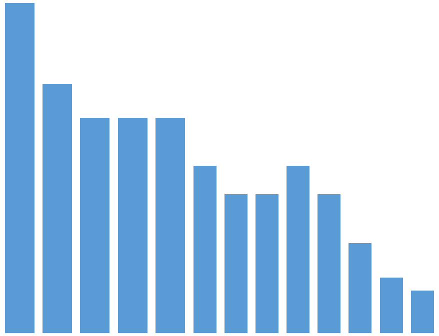


Mambular, TabM, ResNet, FTTransformer, MLP, SAINT, TabulaRNN, NDTF, NODE[2]...

	Name	Type	Params	Mode
0	loss_fct	MSELoss	0	train
1	estimator	Mambular	315 K	train
2	estimator.embedding_layer	EmbeddingLayer	12.8 K	train
3	estimator.mamba	Mamba	302 K	train
4	estimator.tabular_head	MLPhead	65	train

315 K Trainable params
0 Non-trainable params
315 K Total params
1.261 Total estimated model params size (MB)
69 Modules in train mode
0 Modules in eval mode

60 Targets



$E_1 \ldots E_S$
S = 60

Energy bins in logarithmic scale from 10^{-9} to $6.3 \cdot 10^2$ MeV

1.INTERNATIONAL ATOMIC ENERGY AGENCY, Compendium of Neutron Spectra and Detector Responses for Radiation Protection Purposes, Technical Reports Series No. 403, IAEA, Vienna (2002)

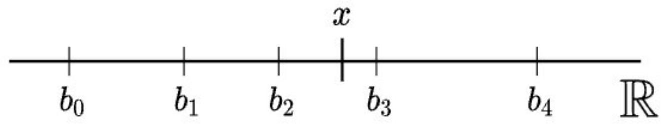
2. Thielmann A. F., et al. "Mambular: A sequential model for tabular deep learning." *arXiv preprint arXiv:2408.06291* (2024).

Feature transformations and processing in Mambular

- Each numerical feature (*x*) is encoded with *PLE* before being passed through the linear layer for rescaling.
- *Decision trees* are used for detecting the bin boundaries, b_t,
- *Embeddings* (e_t) are passed jointly through a stack of *Mamba layers*.

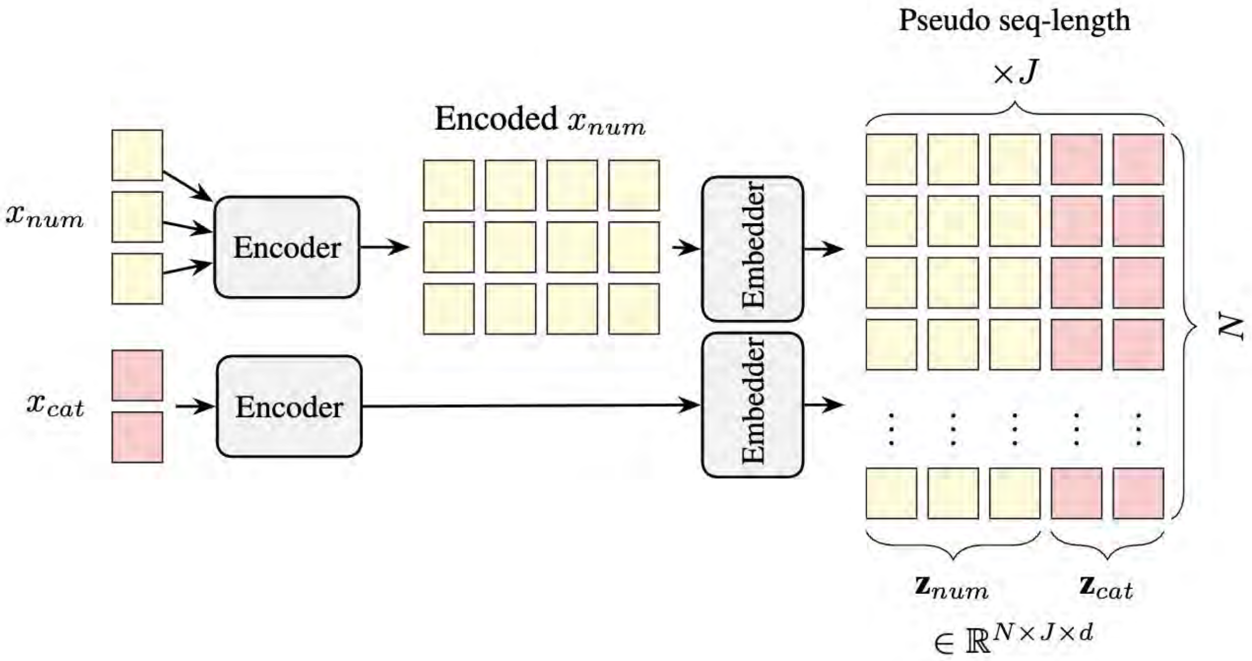
$$\mathtt{PLE}(x) = [e_1, \ldots, e_T] \in \mathbb{R}^T$$

$$e_t = \begin{cases} 0, & x < b_{t-1} \ \mathtt{AND} \ t > 1 \\ 1, & x \geq b_t \ \mathtt{AND} \ t < T \\ \frac{x - b_{t-1}}{b_t - b_{t-1}}, & \text{otherwise} \end{cases}$$



$$\Downarrow$$

$$\mathtt{PLE}(x) = \Big[\underbrace{1}_{e_1} \;\Big|\; \underbrace{1}_{e_2} \;\Big|\; \underbrace{\tfrac{x-b_2}{b_3-b_2}}_{e_3} \;\Big|\; \underbrace{0}_{e_4}\Big]$$



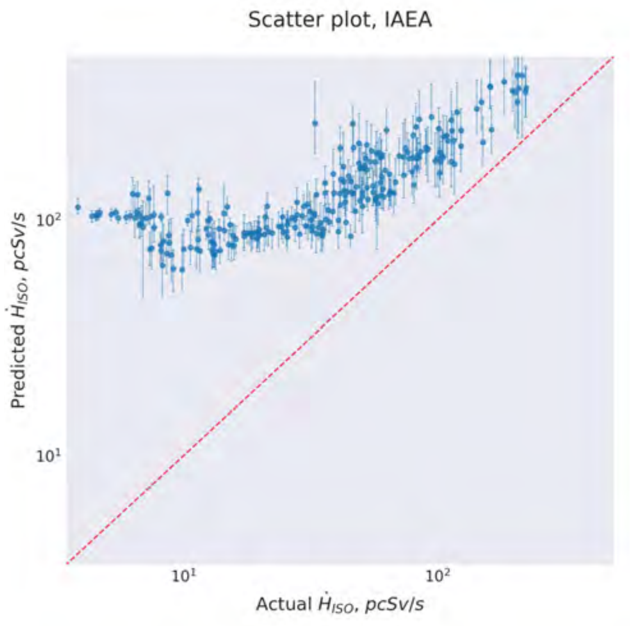
Gorishniy, Y., Rubachev, I., and Babenko, A. (2022). On embeddings for numerical features in tabular deep learning. Advances in Neural Information Processing Systems, 35:24991–25004.

Tabular deep learning in Mambular framework

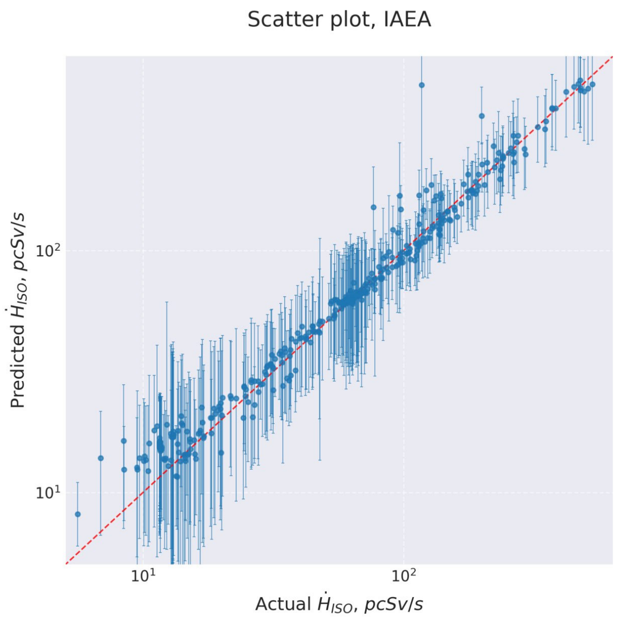
Model	Description
Mambular	A sequential model using Mamba blocks specifically designed for various tabular data tasks (arXiv:2408.06291).
TabM	Batch Ensembling for a MLP(Gorishniy et al.).
MLP	A classical Multi-Layer Perceptron (MLP) model for handling tabular data tasks (arXiv:2408.06291).
FTTransformer	Feature Tokenizer + Transformer. A model leveraging transformer encoders for tabular data (Gorishniy et al.).
NODE	Neural Oblivious Decision Ensembles (Popov et al.).
ResNet	An adaptation of the ResNet architecture for tabular data applications (Gorishniy et al 2021).
TabTransformer	A transformer-based model for tabular data, enhancing feature learning capabilities (Huang et al.).
MambaTab	A tabular model using a Mamba-Block on a joint input representation. Not a sequential model. (arXiv:2401.08867).
TabulaRNN	A Recurrent Neural Network for Tabular data (arXiv:2411.17207v).
MambAttention	A combination between Mamba and Transformers (arXiv:2411.17207v1).
NDTF	A neural decision forest using soft decision trees (Kontschieder et al.)
SAINT	Improve neural networks via Row Attention and Contrastive Pre-Training (arXiv:2106.01342v1).

Sufficiency of the training dataset

Dataset optimization



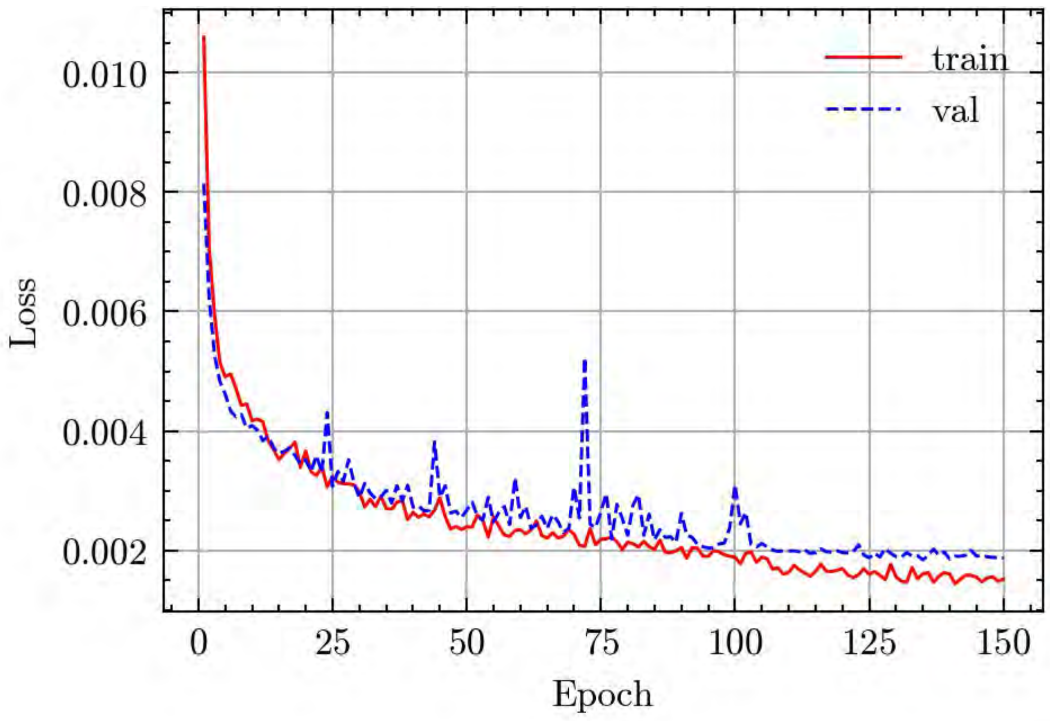
Training dataset
of 10^4 samples



Training dataset
of 5×10^5 samples

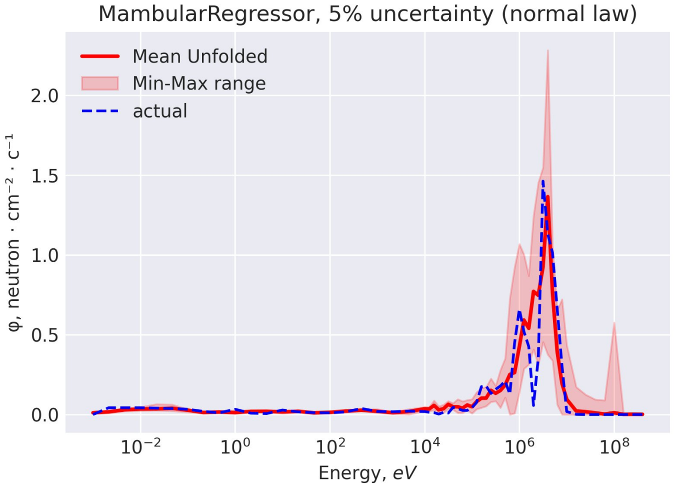
Difference in effective dose rate estimation
on predicted spectra

Model Optimization
Training and Validation Loss

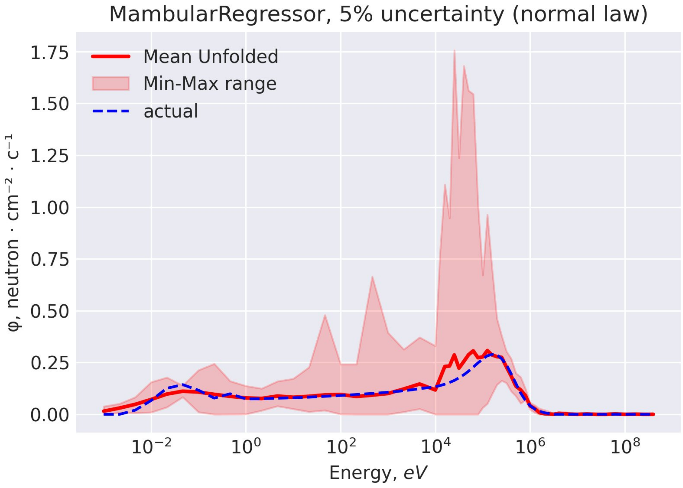


Learning rate = 10^{-4}

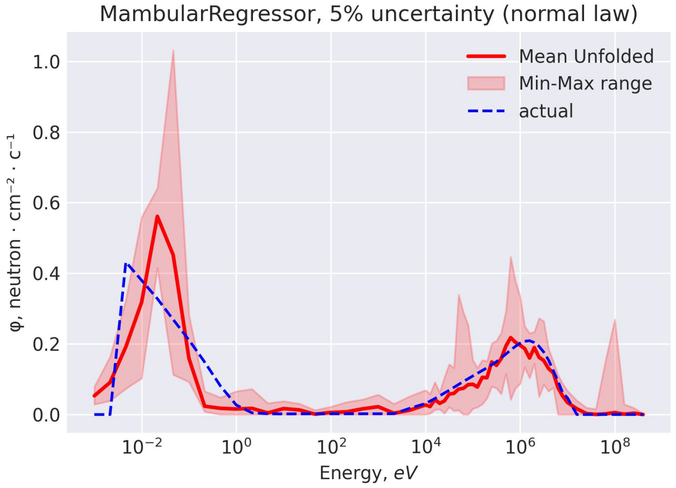
Mambular results. Spectra comparison for 375 real cases



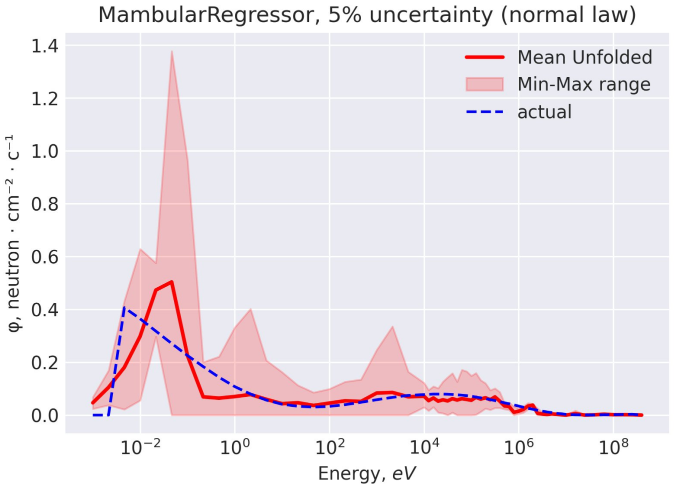
Spectra №0



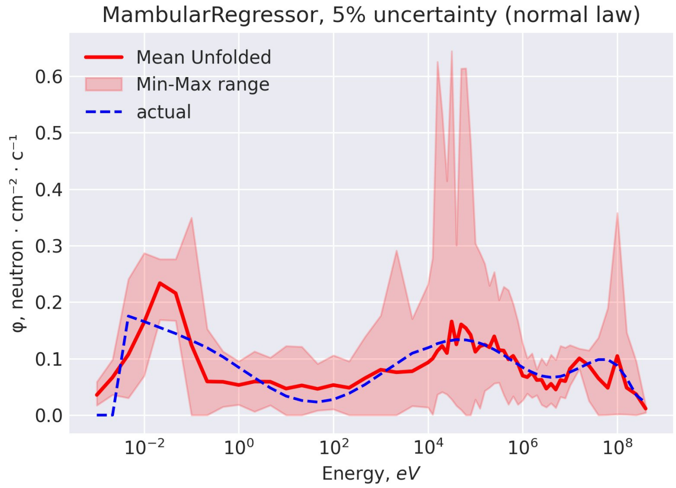
Spectra №102



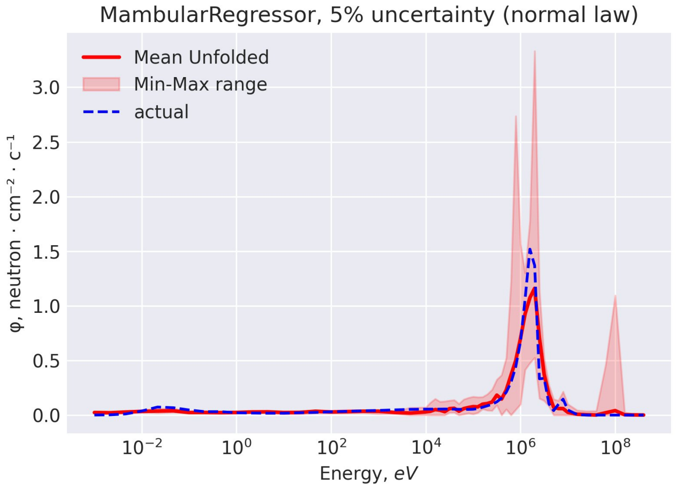
Spectra №83



Spectra №67 (soft field)



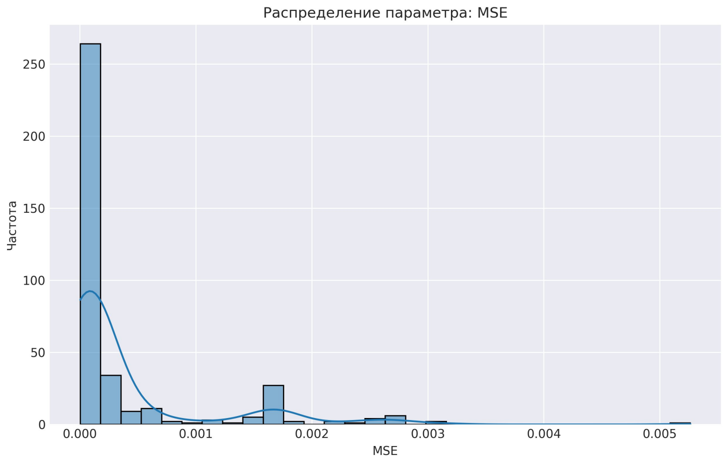
Spectra №68 (hard field)



Spectra №226

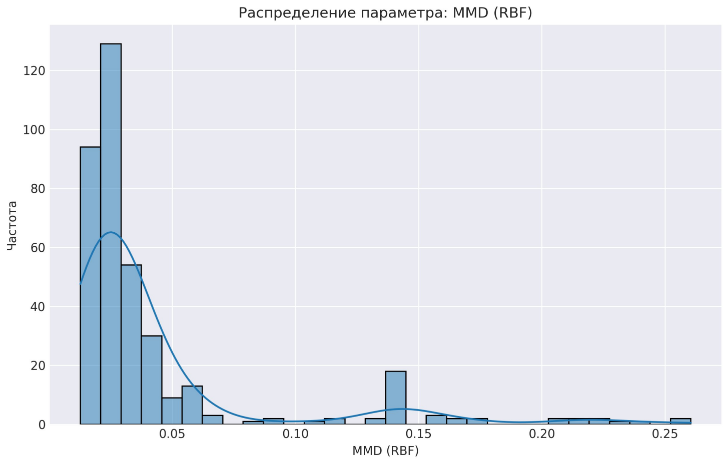
The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data.

Mambular results. Spectra comparison for 375 real cases



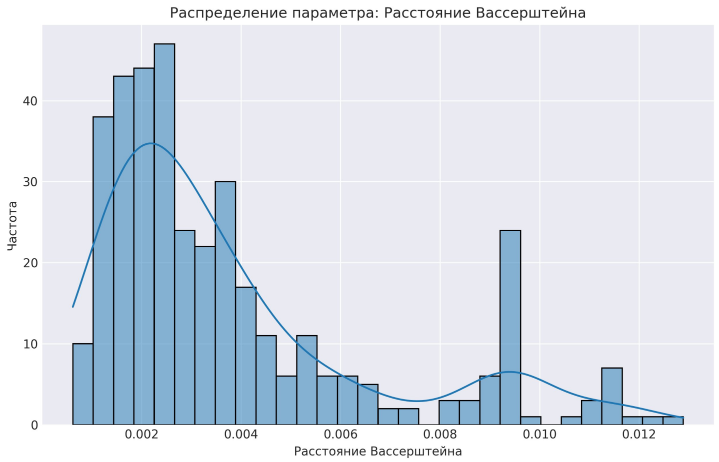
MSE

Mean squared error



MMD

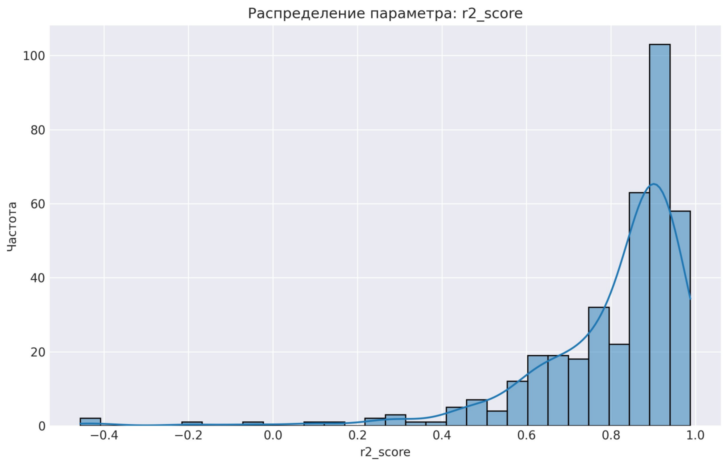
Maximum mean discrepancy



Wasserstein distance

Pearson correlation

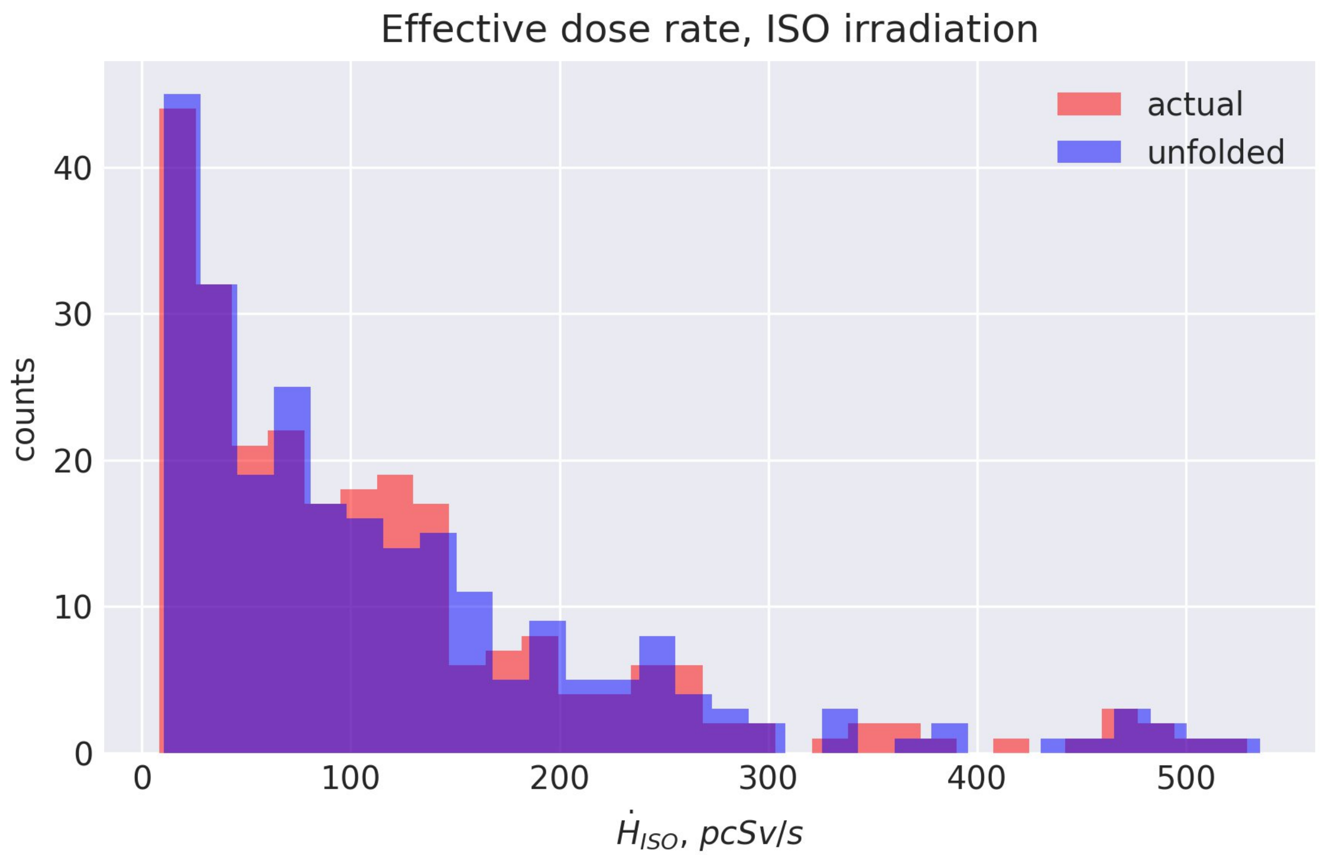
Cosine similarity

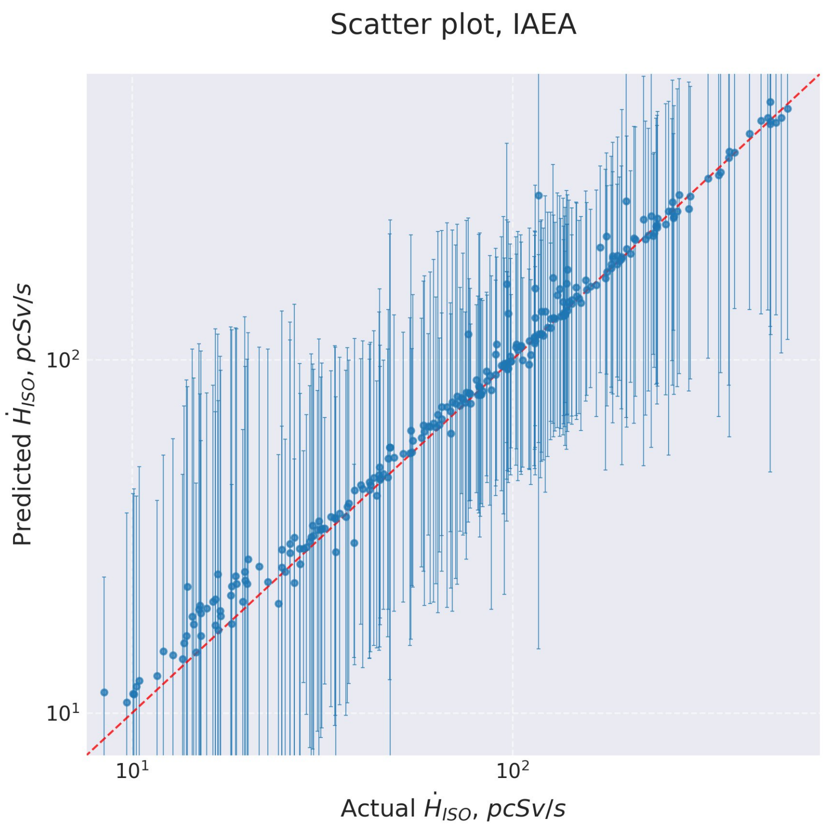


R^2

Coefficient of determination

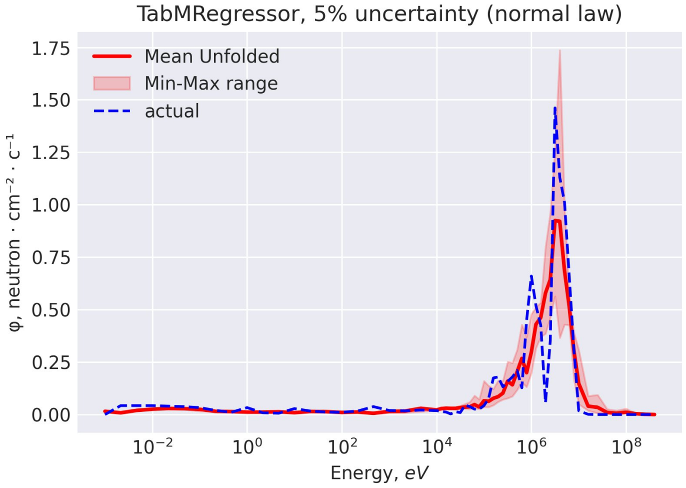
Mambular results. Dose assessment for 375 real cases



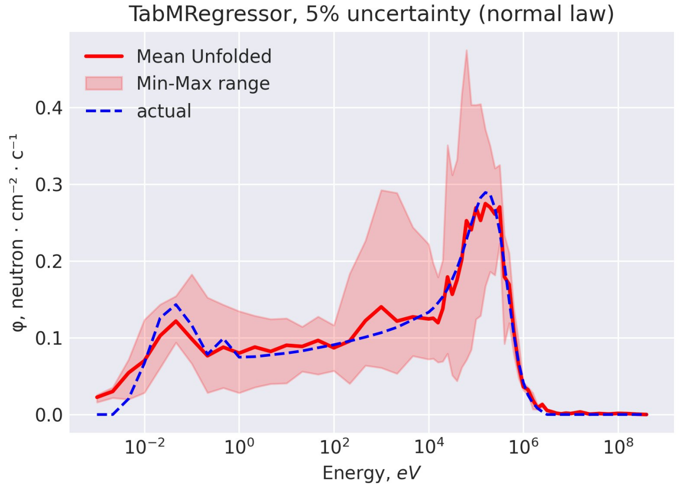


The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data (measurements error = 5%).

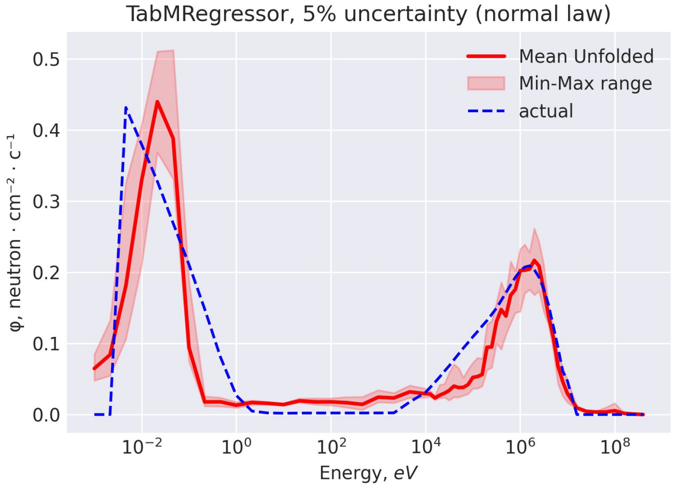
TabM results. Spectra comparison for 375 real cases



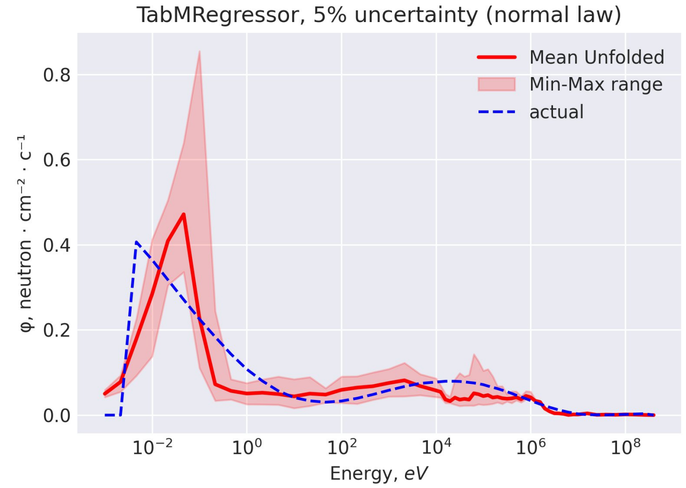
Spectra №0



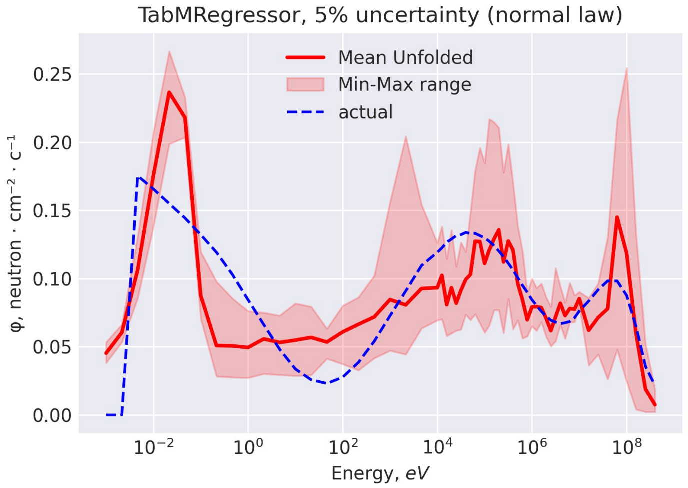
Spectra №102



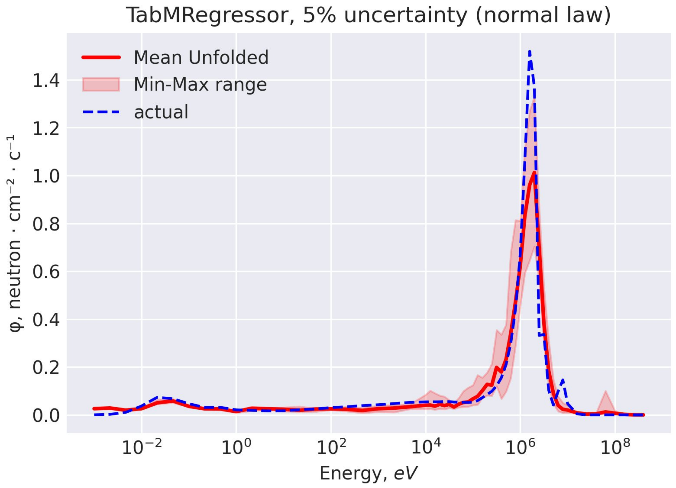
Spectra №83



Spectra №67 (soft field)



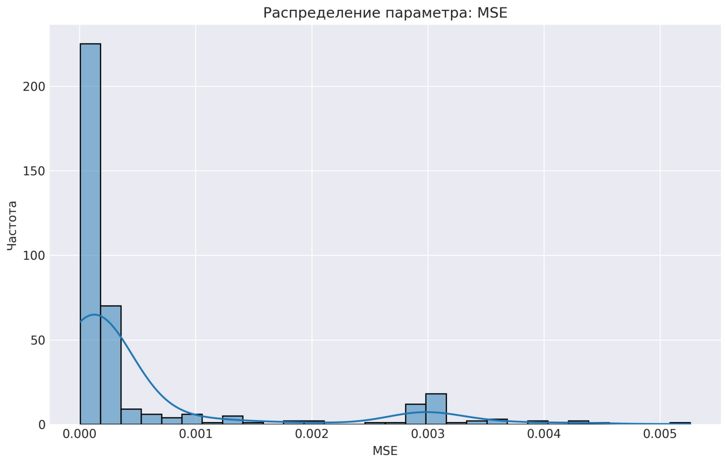
Spectra №68 (hard field)



Spectra №226

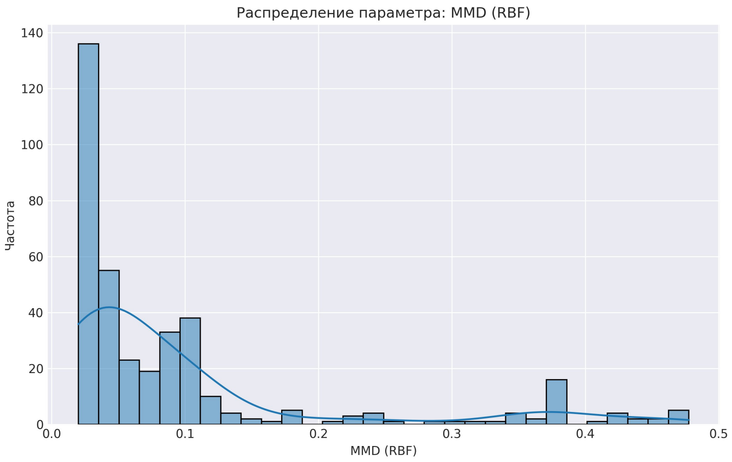
The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data.

TabM results. Spectra comparison for 375 real cases



MSE

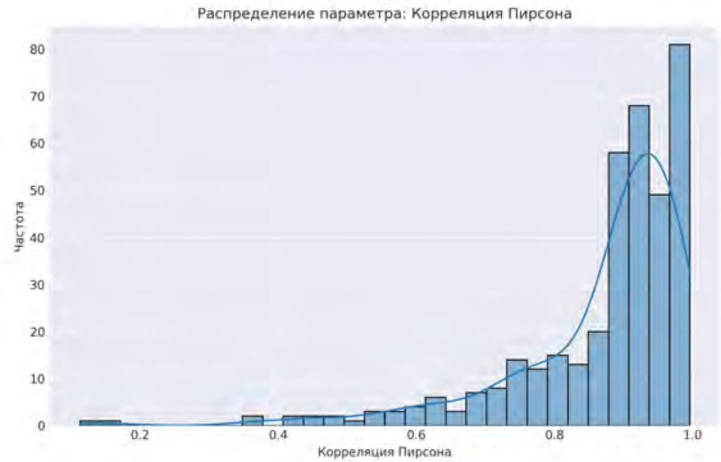
Mean squared error



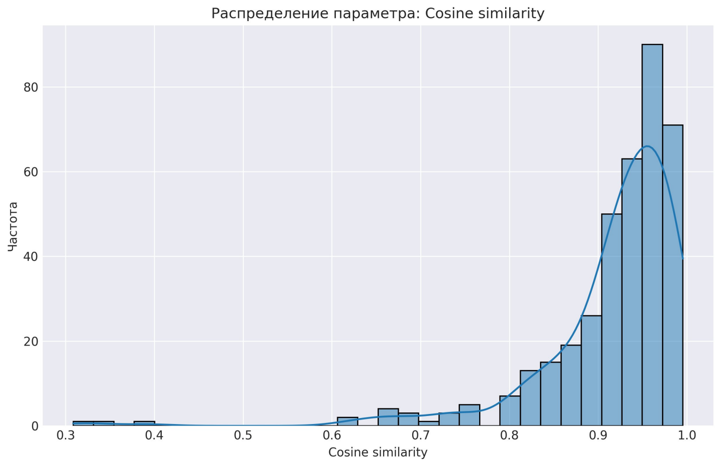
MMD

Maximum mean discrepancy

Wasserstein distance



Pearson correlation

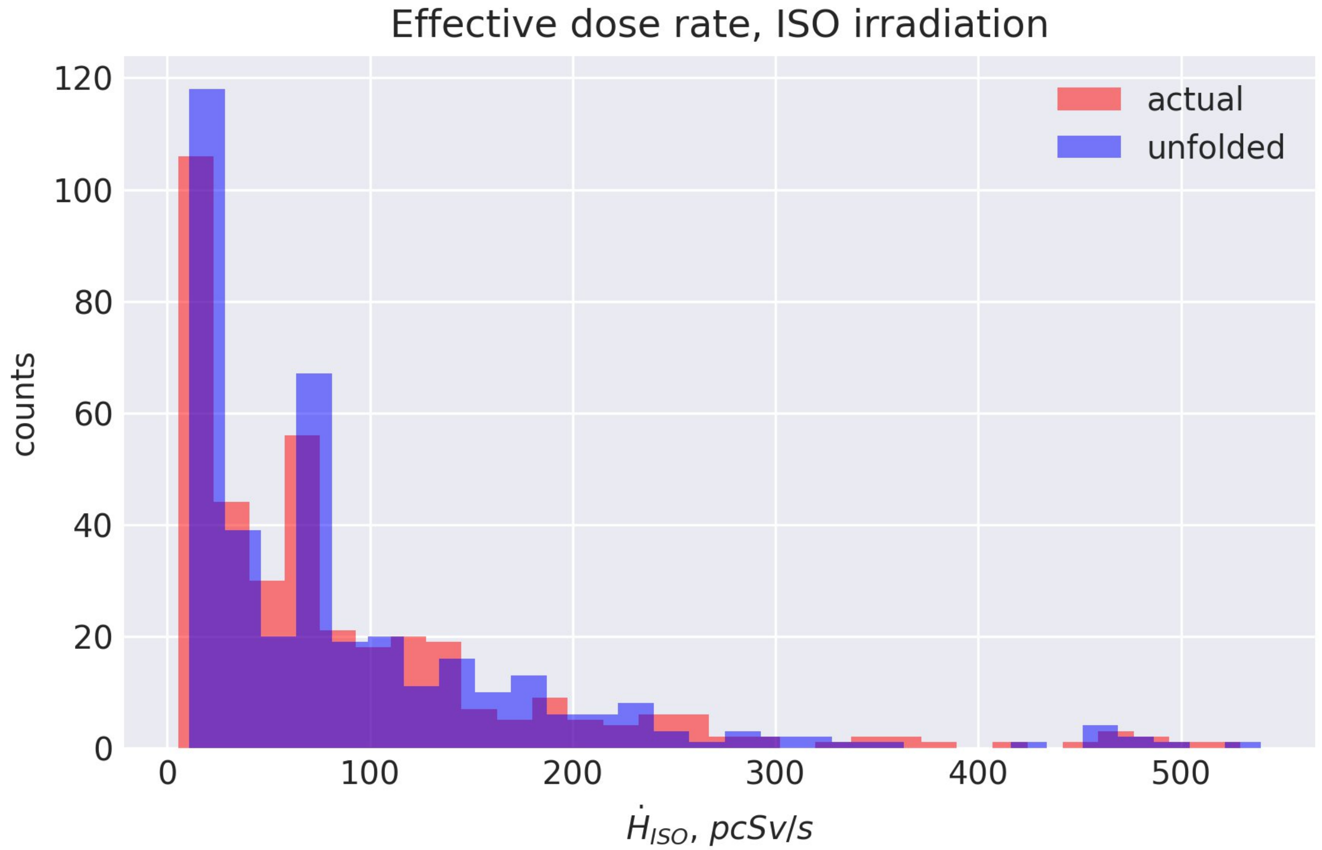


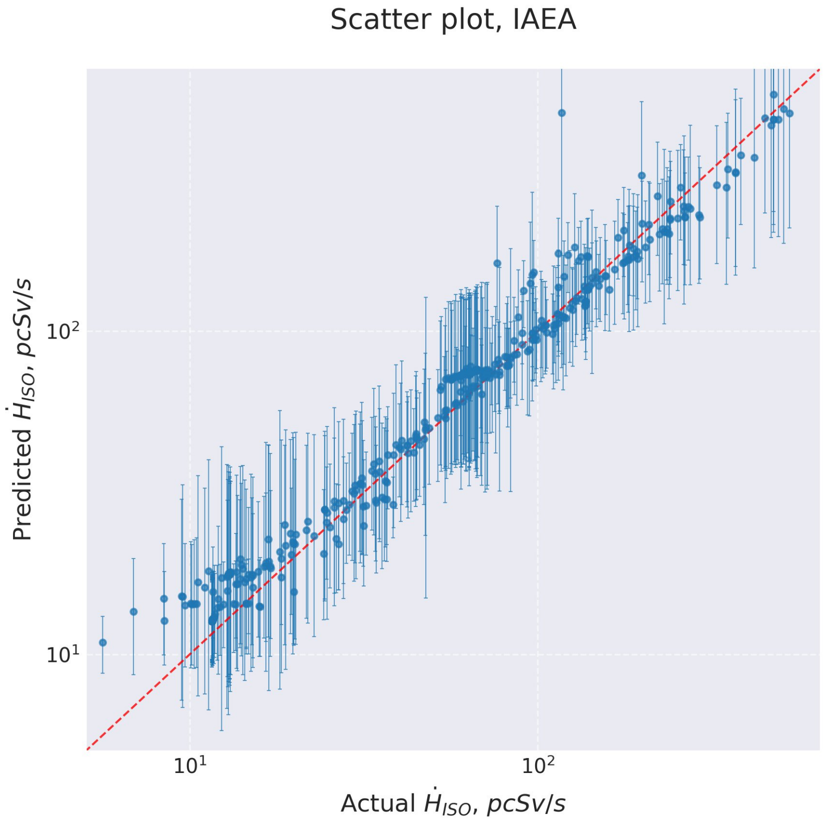
Cosine similarity

R^2

Coefficient of determination

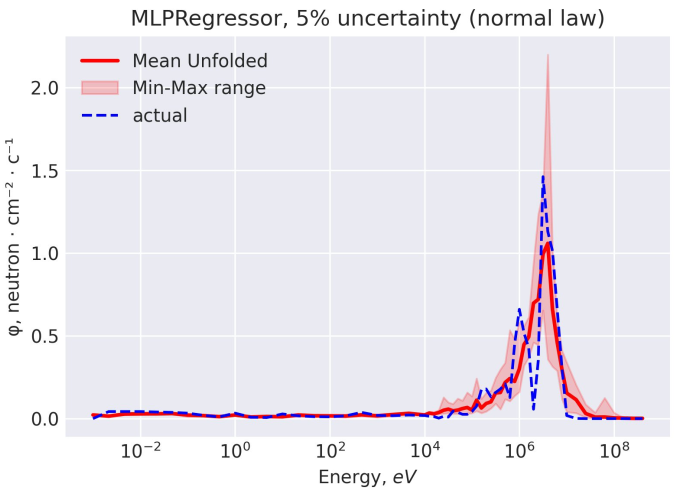
TabM results. Dose assessment for 375 real cases



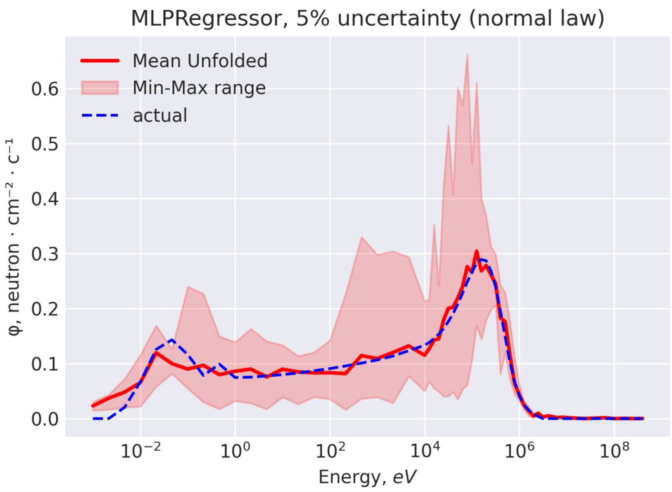


The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data (measurements error = 5%).

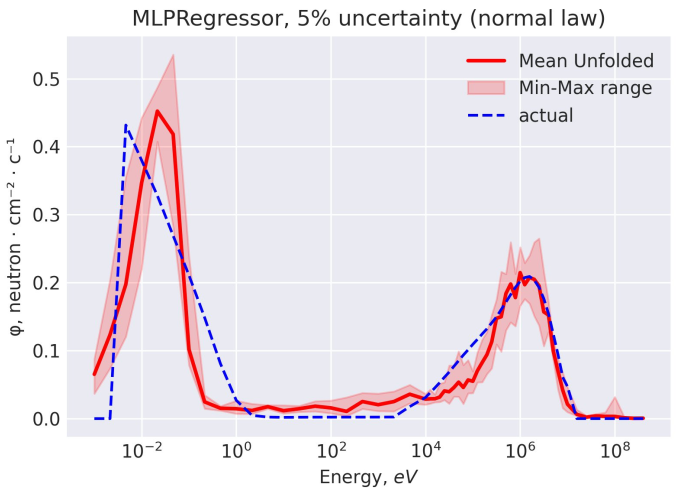
MLP results. Spectra comparison for 375 real cases



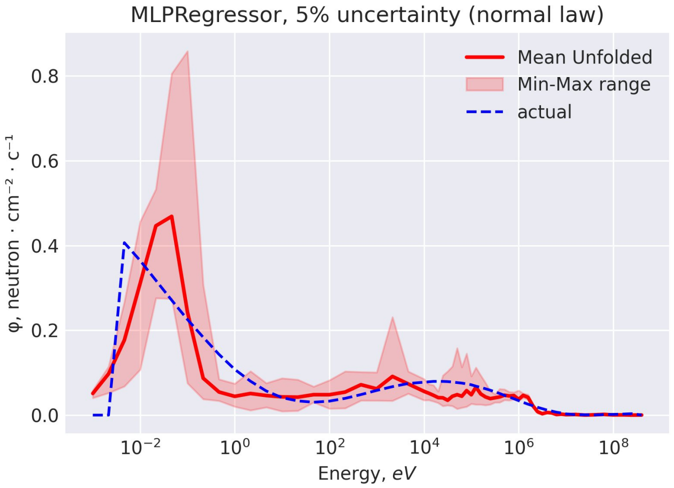
Spectra №0



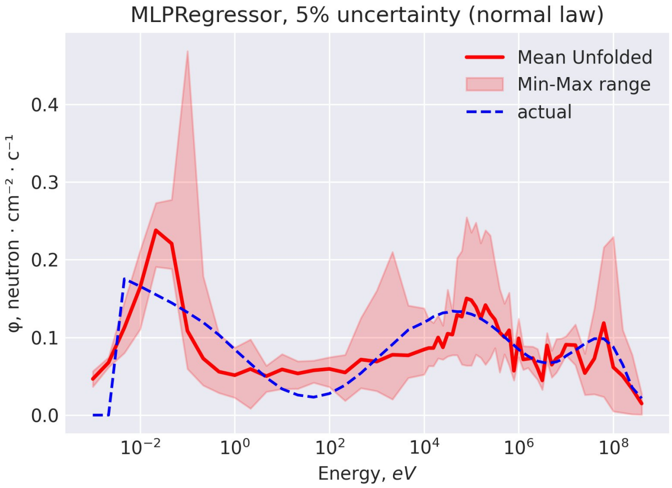
Spectra №102



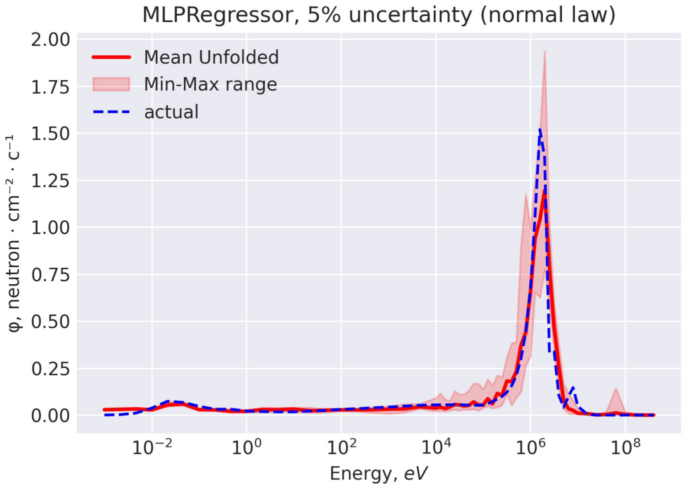
Spectra №83



Spectra №67 (soft field)



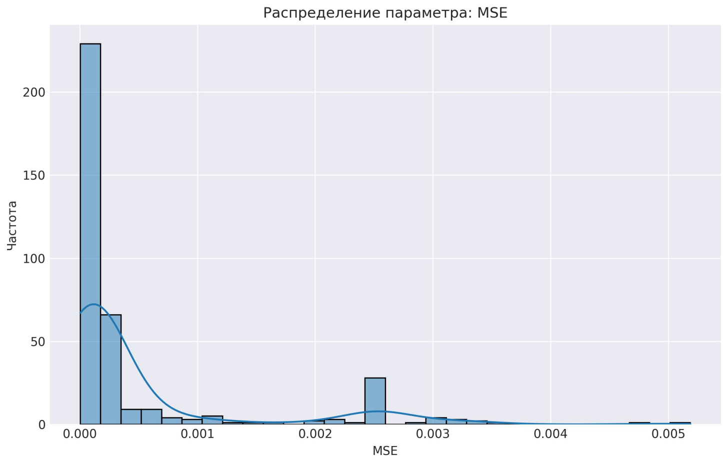
Spectra №68 (hard field)



Spectra №226

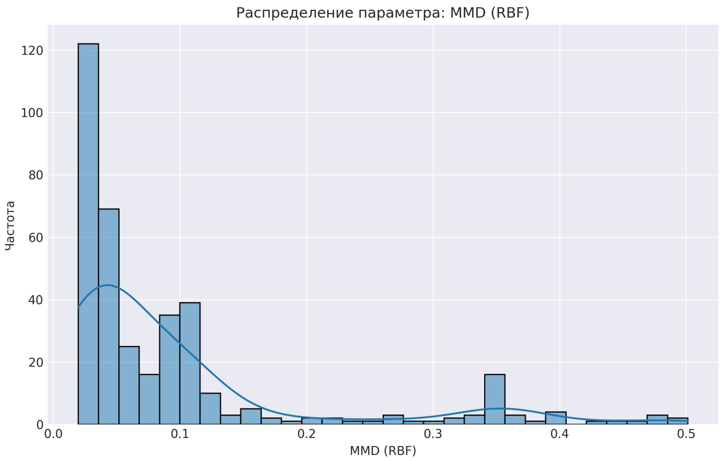
The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data.

MLP results. Spectra comparison for 375 real cases



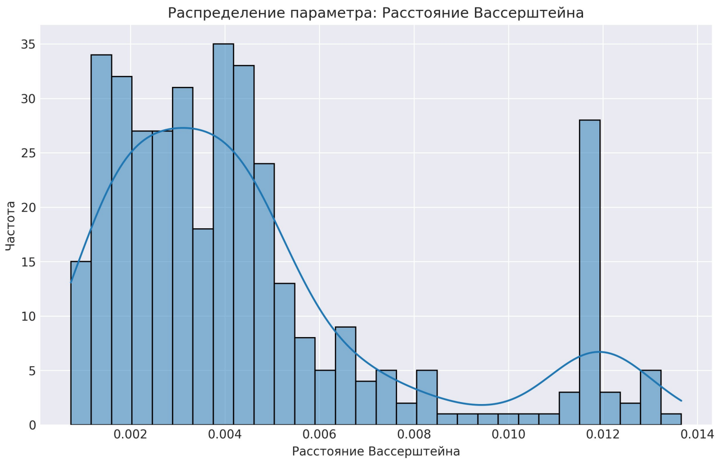
MSE

Mean squared error



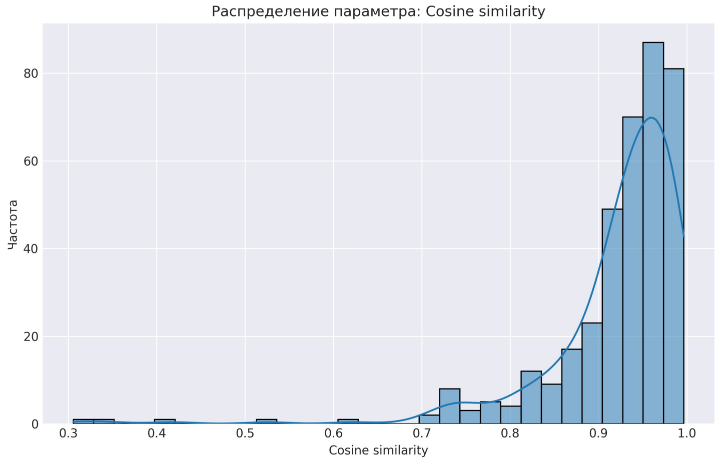
MMD

Maximum mean discrepancy

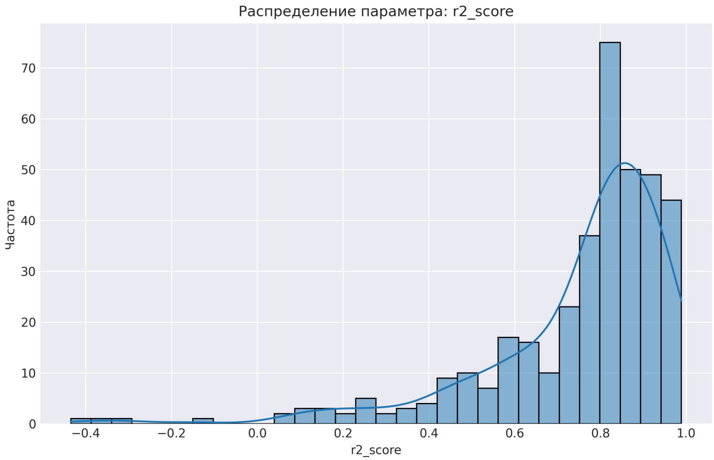


Wasserstein distance

Pearson correlation



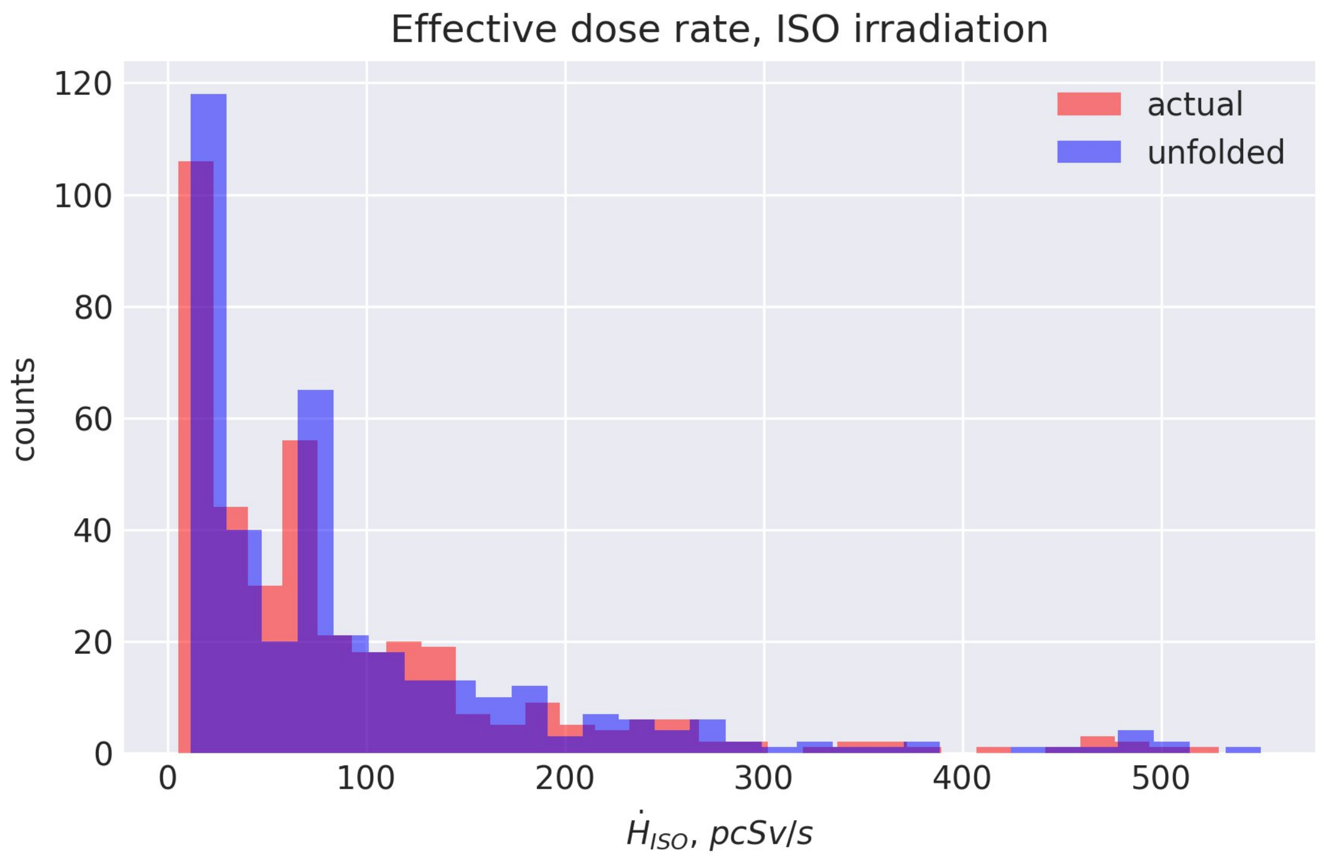
Cosine similarity

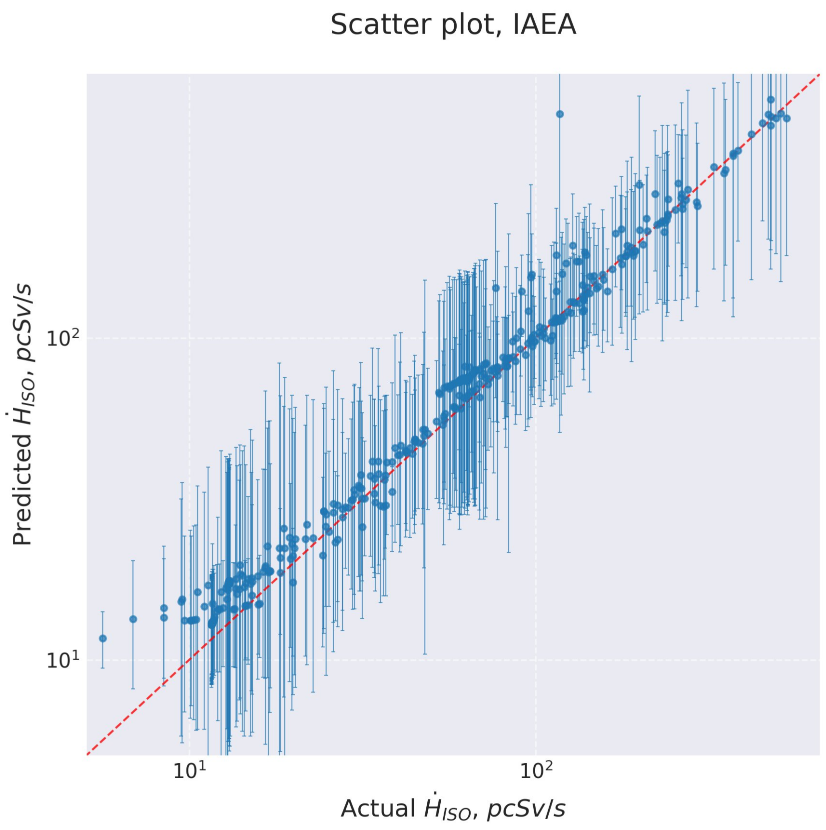


R^2

Coefficient of determination

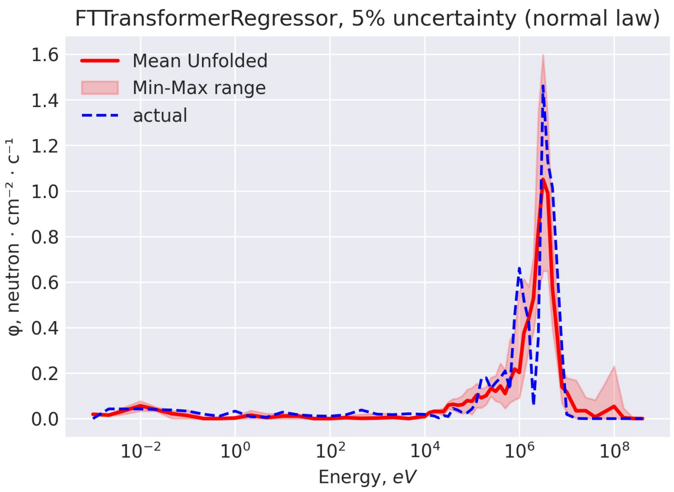
MLP results. Dose assessment for 375 real cases



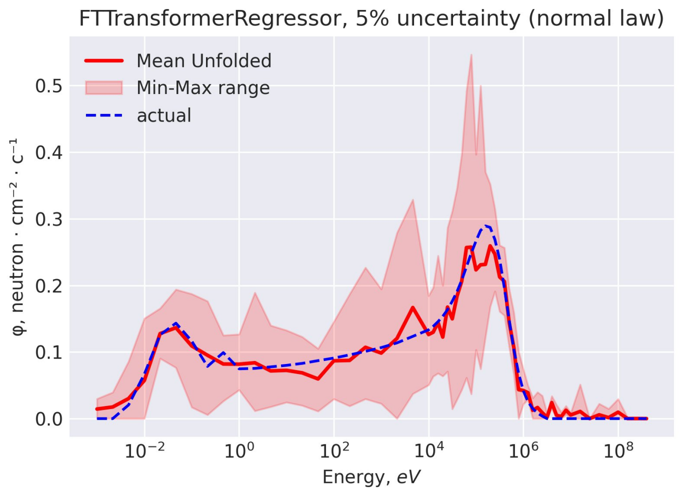


The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data (measurements error = 5%).

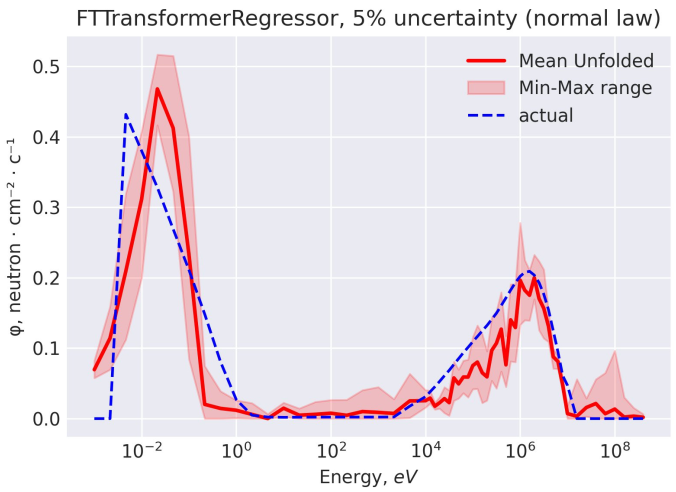
FTTransformer results. Spectra comparison for 375 real cases



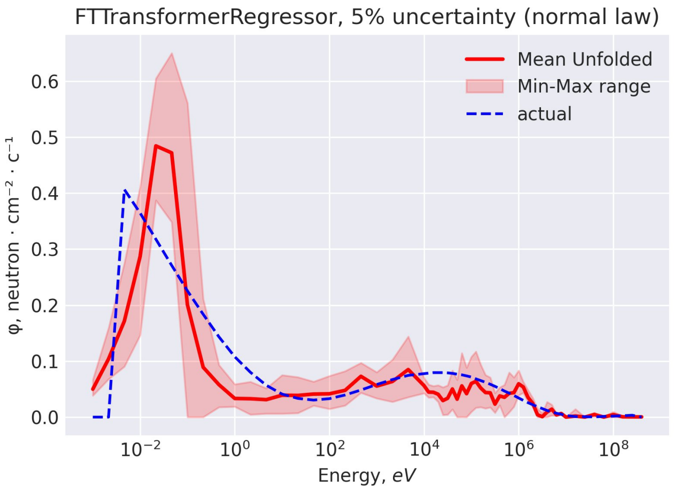
Spectra №0



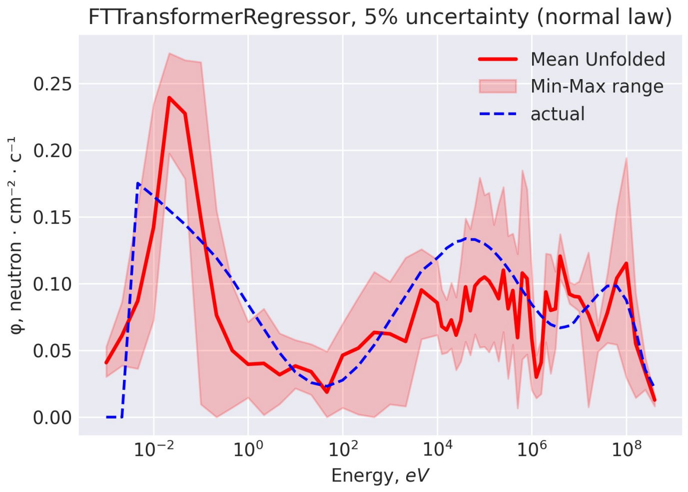
Spectra №102



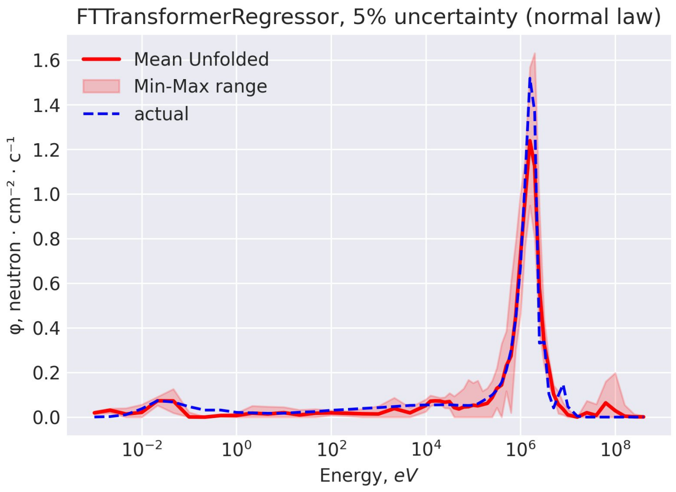
Spectra №83



Spectra №67 (soft field)



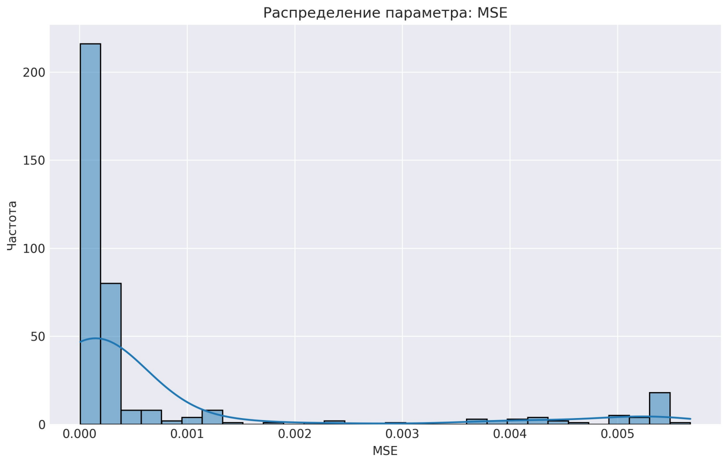
Spectra №68 (hard field)



Spectra №226

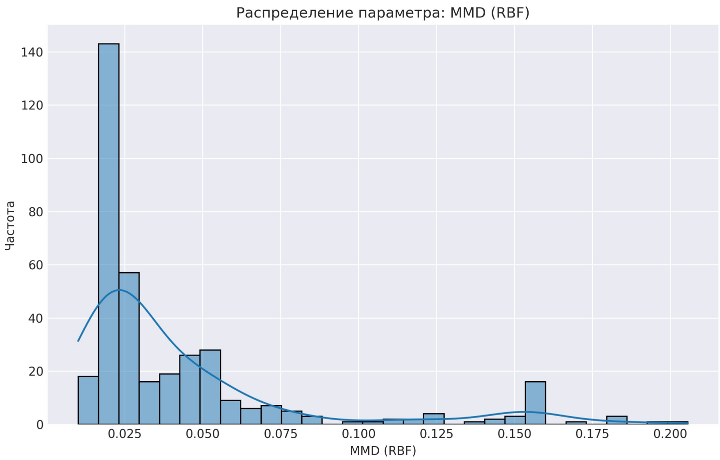
The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data.

FTTransformer results. Spectra comparison for 375 real cases



MSE

Mean squared error

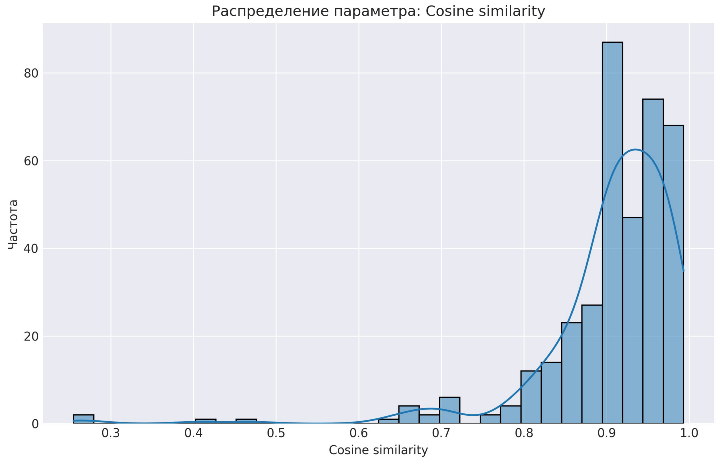


MMD

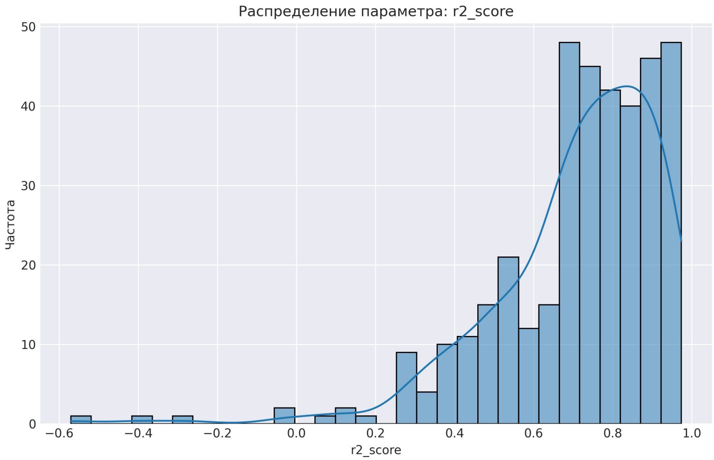
Maximum mean discrepancy

Wasserstein distance

Pearson correlation



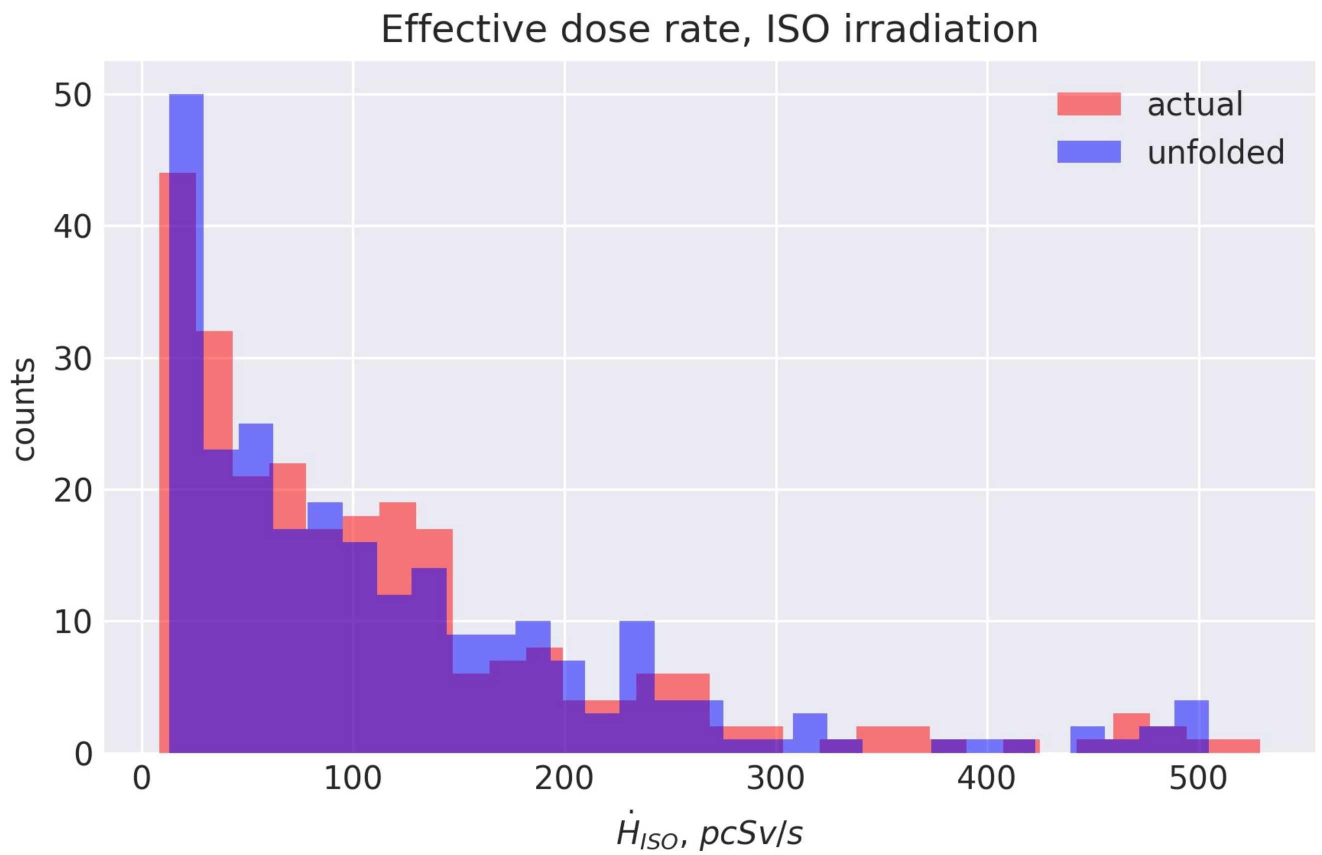
Cosine similarity



R^2

Coefficient of determination

FTTransformer results. Dose assessment for 375 real cases



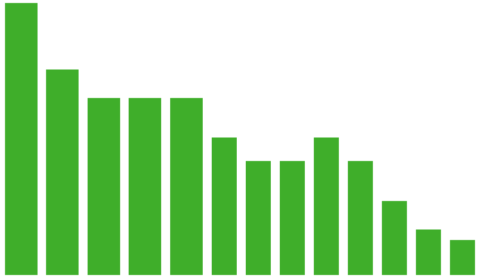
The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data (measurements error = 5%).

AutoML

AutoML solutions automatically develop ML-based models. AutoML provides automatic fine-tuning of the model hyperparameters and blending of different models:

Measurements

Composite model

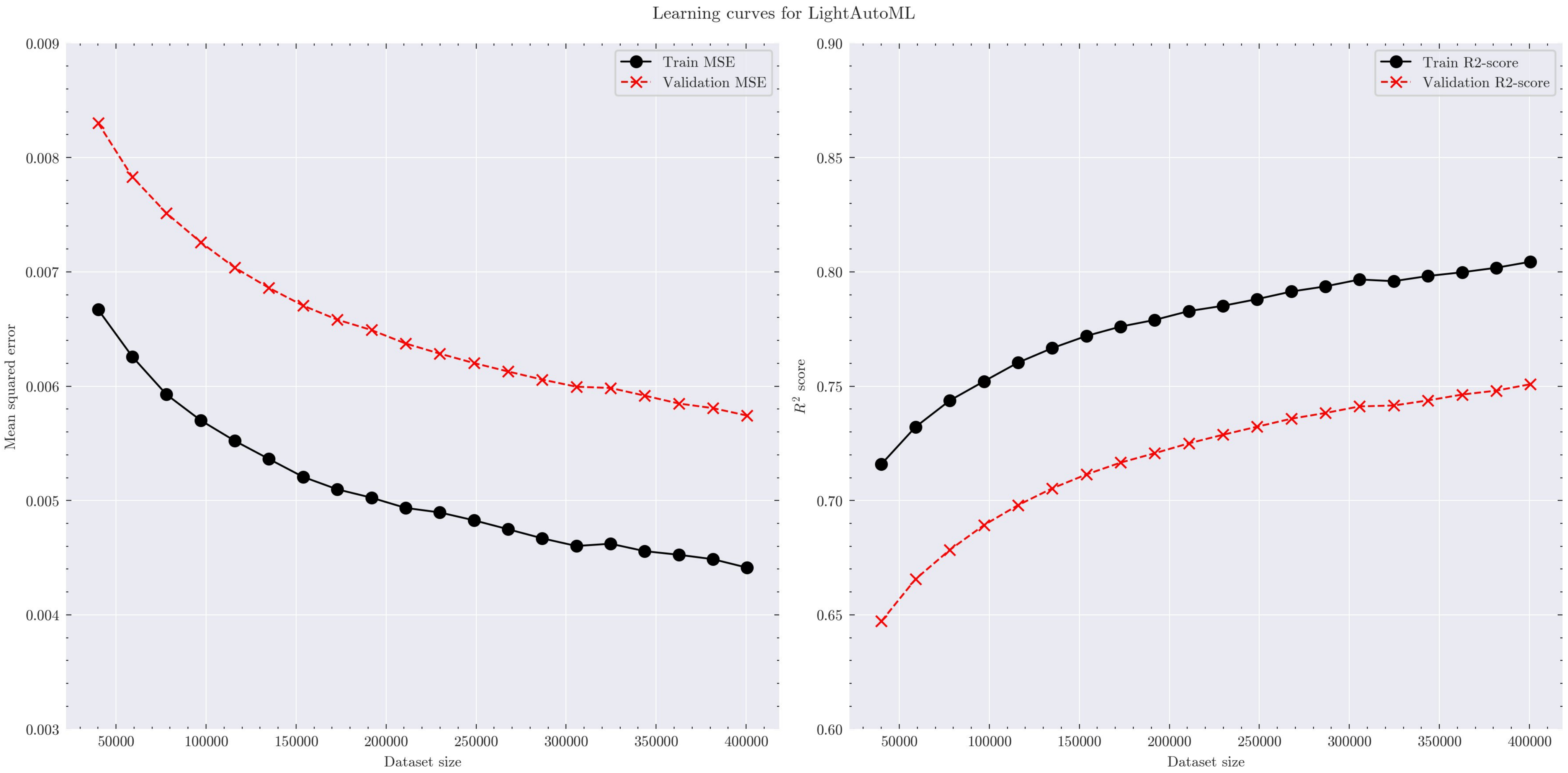


$E_1 \dots E_S$

1. LightAutoML
2. FEDOT

1. Vakhrushev, Anton, et al. "Lightautoml: Automl solution for a large financial services ecosystem", *arXiv preprint arXiv:2109.01528* (2021).
2. https://doi.org/10.1016/j.future.2021.08.022

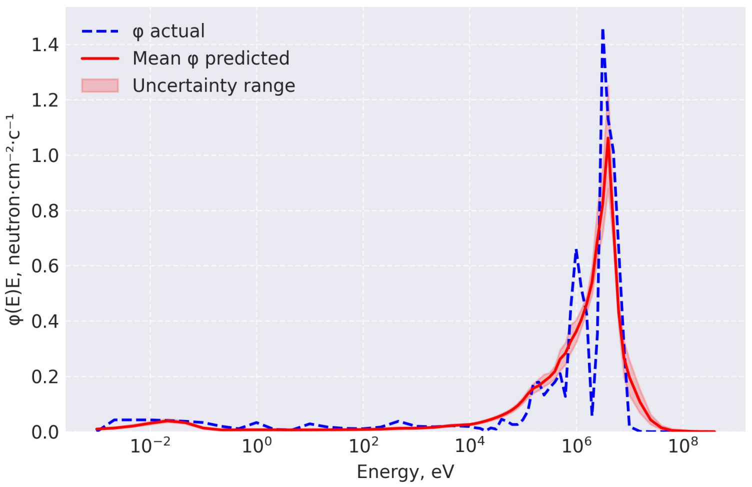
LightAutoML. Learning curve



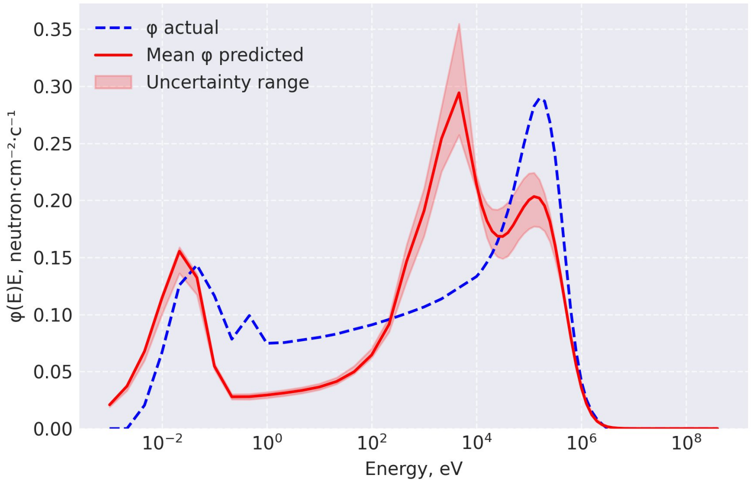
Loss = MAE (mean absolute error),
Metric = MSE.

Final model: Random forest.

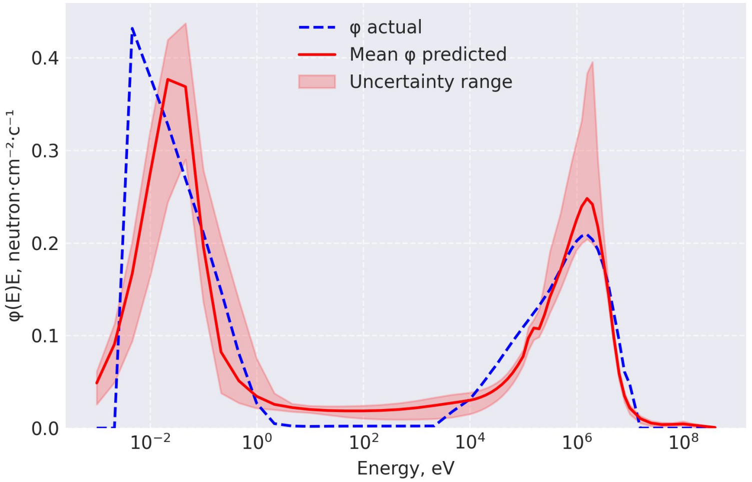
LightAutoML results. Spectra comparison for 375 real spectra



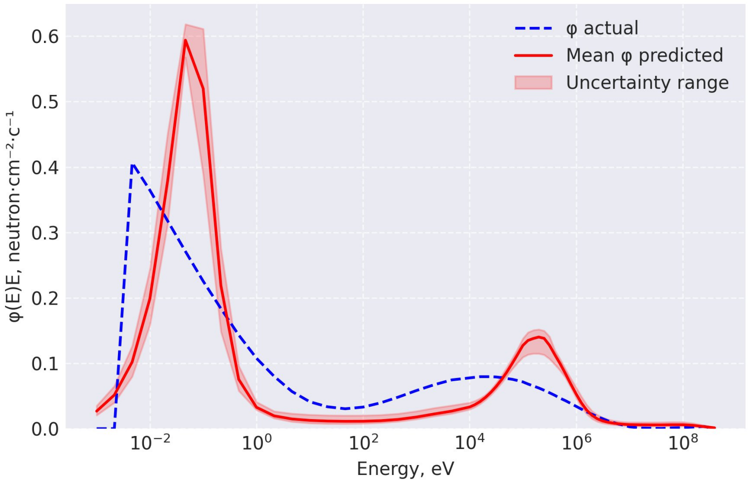
Spectra №0



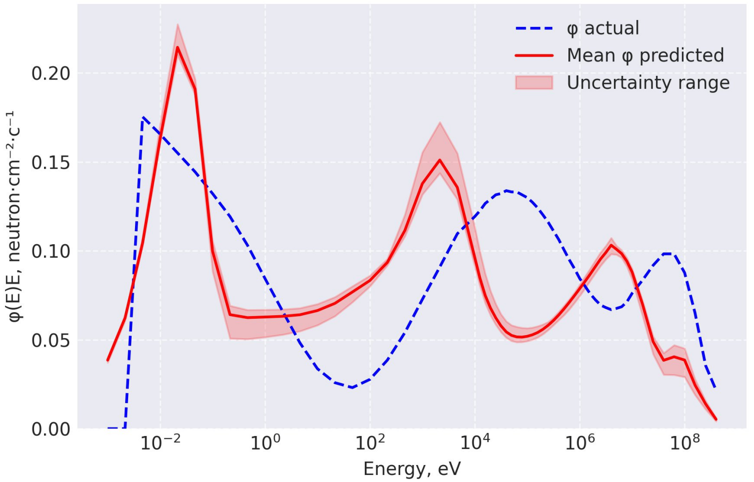
Spectra №102



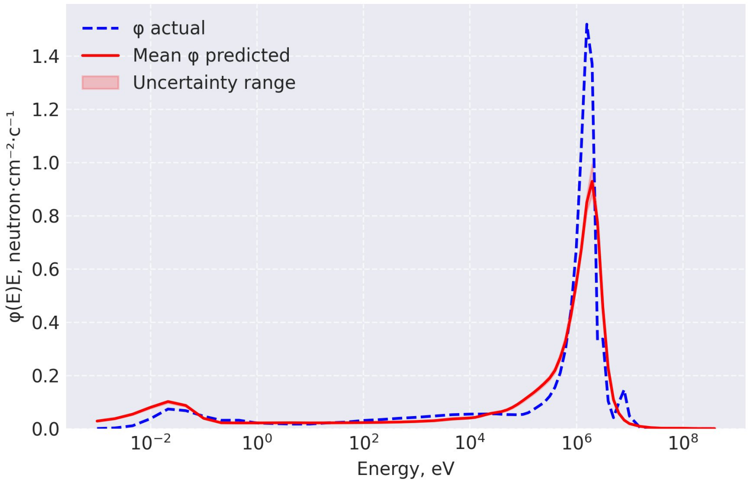
Spectra №83



Spectra №67 (soft field)



Spectra №68 (hard field)

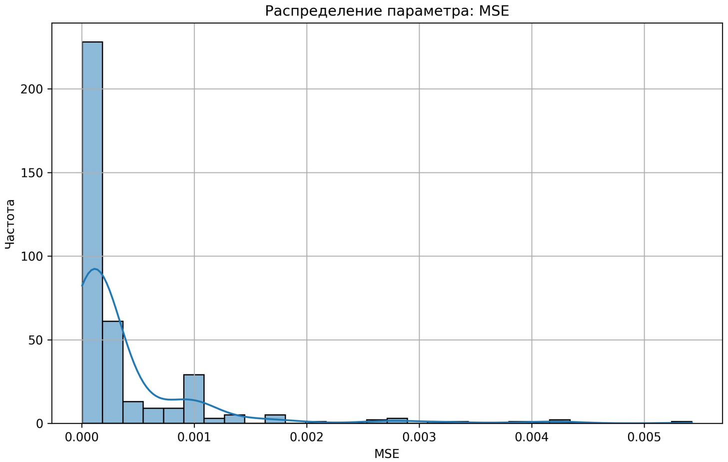


Spectra №226

The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations (1%) were introduced into the input data.

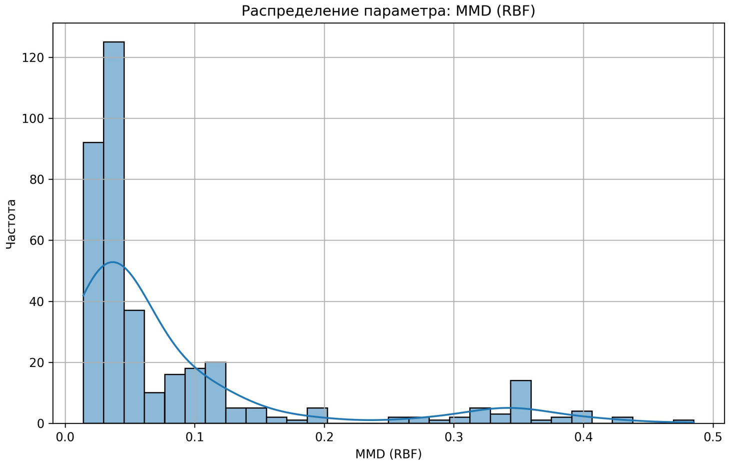
Timeout = 720 minutes

LightAutoML results. Spectra comparison for 375 real cases



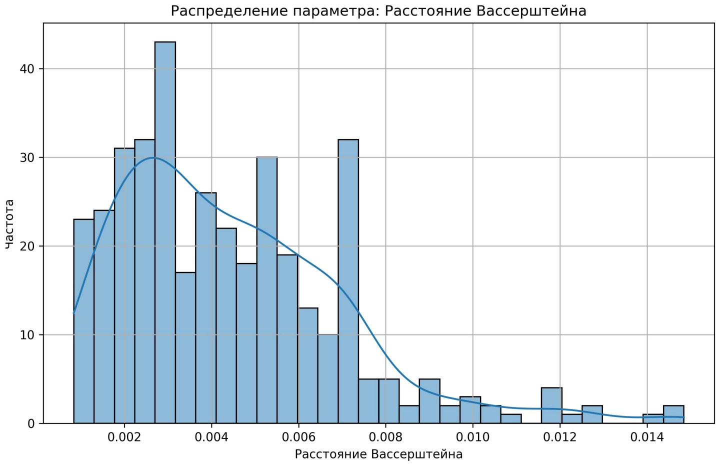
MSE

Mean squared error

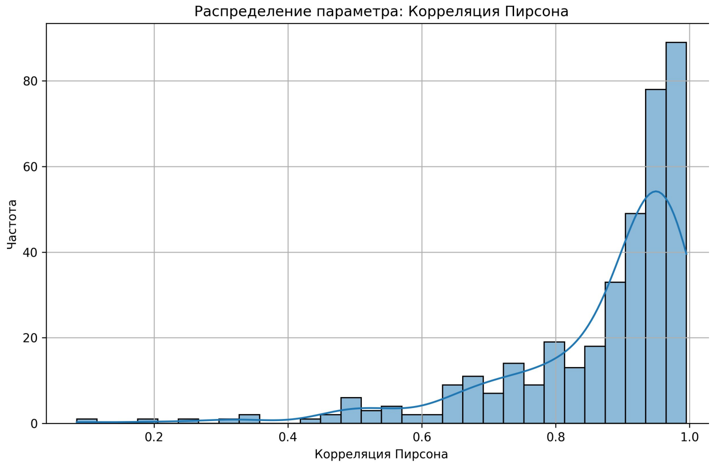


MMD

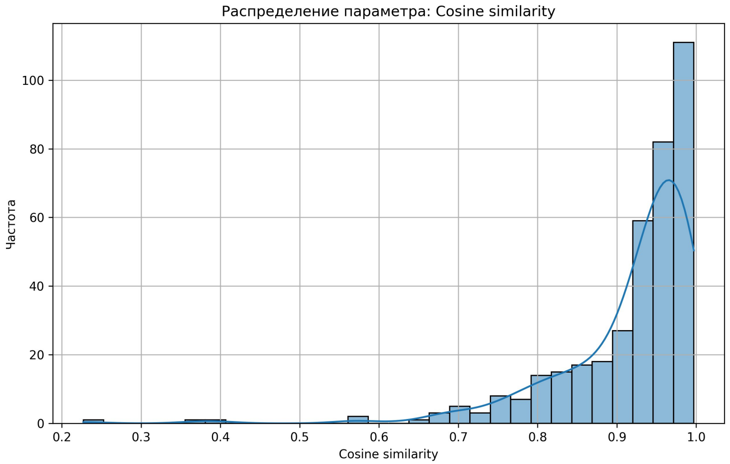
Maximum mean discrepancy



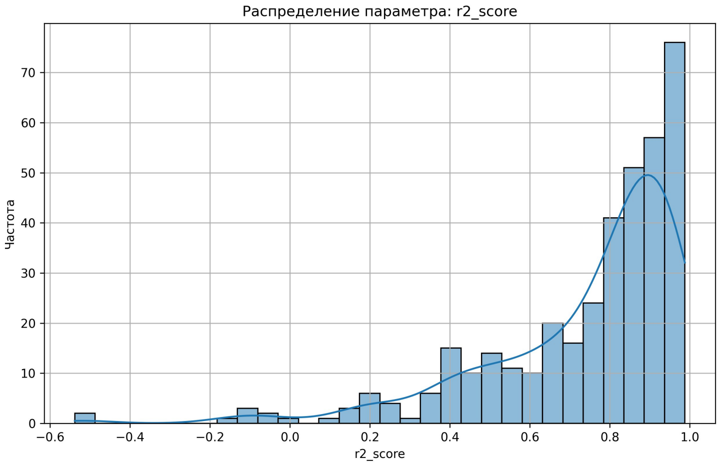
Wasserstein distance



Pearson correlation



Cosine similarity

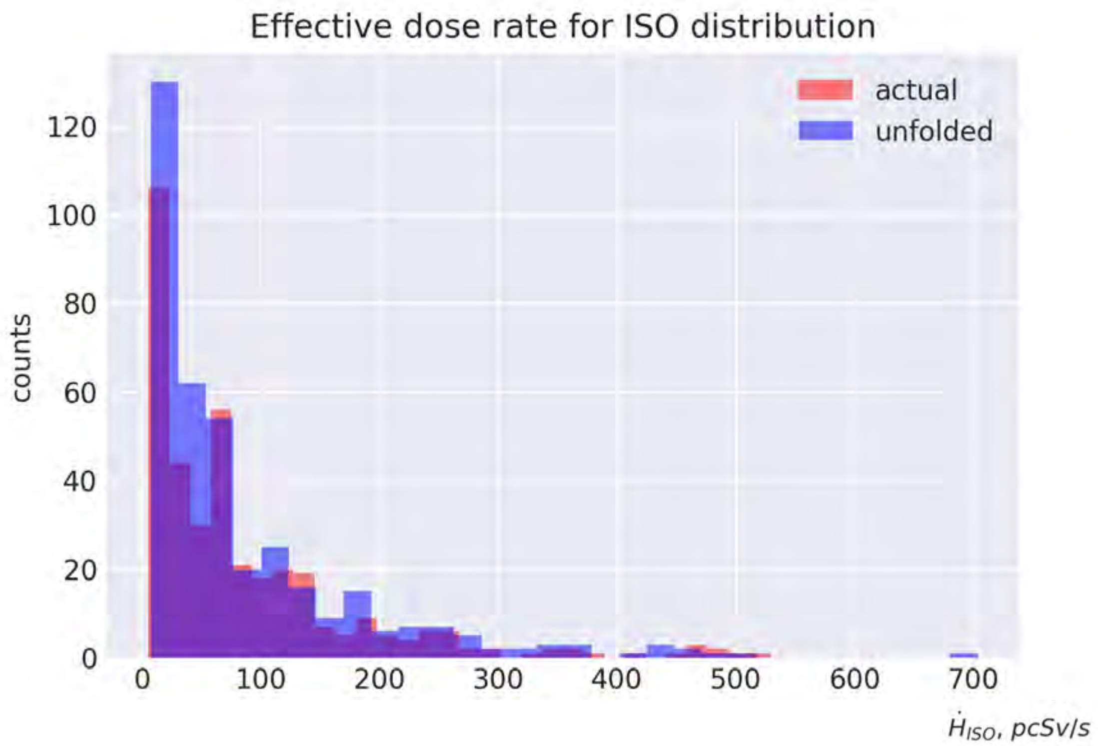


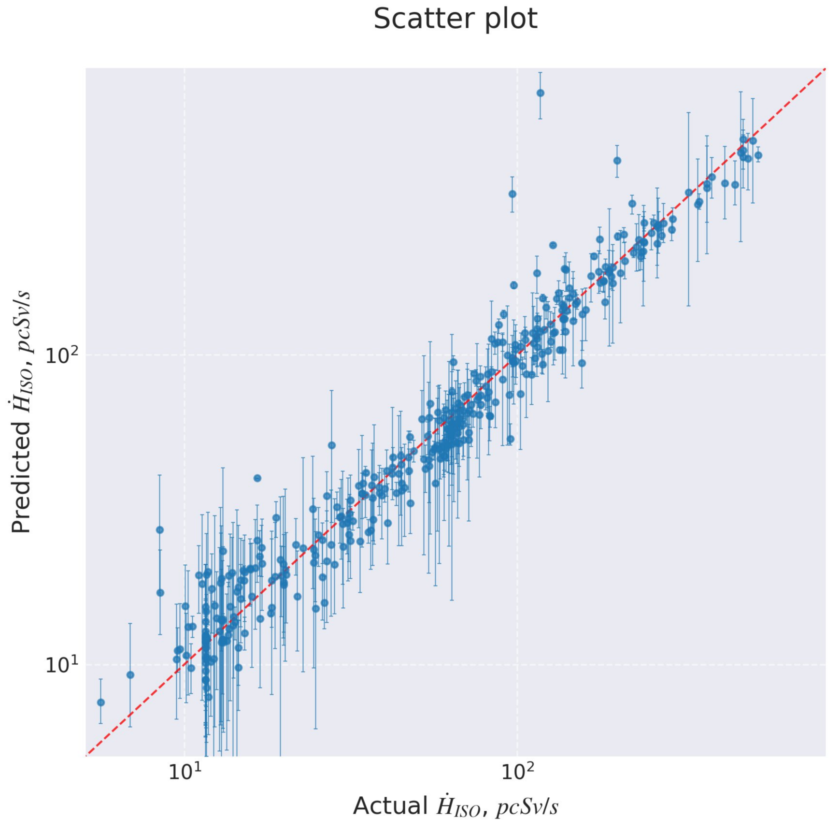
R^2

Coefficient of determination

LightAutoML results. Dose assessment for 375 real spectra

The best model selected: *Random forest regressor.*

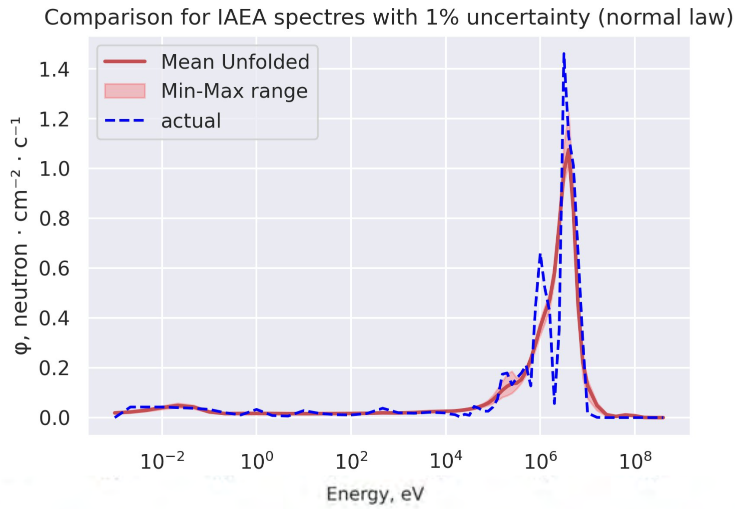




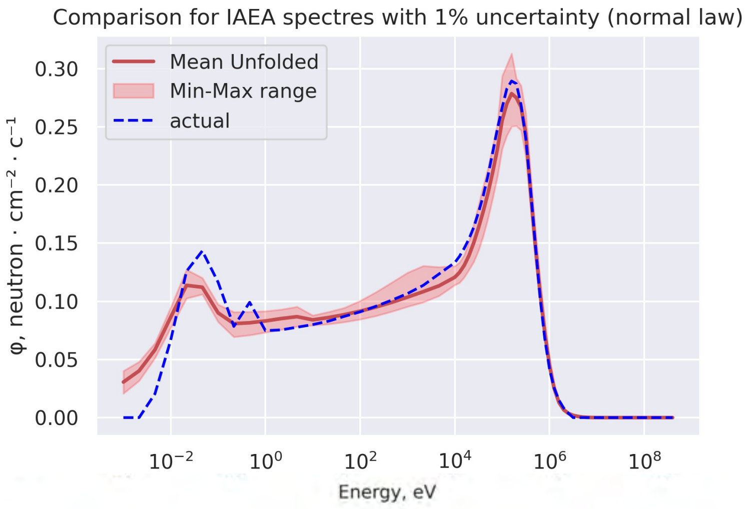
Timeout = 24 hours

The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data (measurements error = 5%).

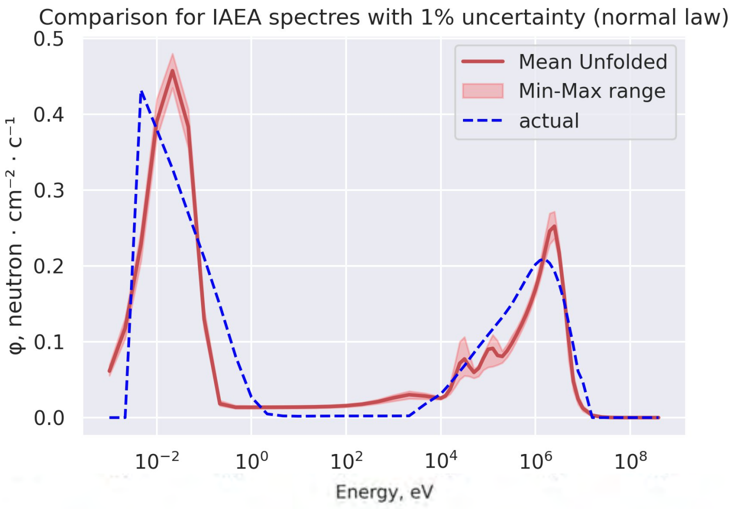
FEDOT results. Spectra comparison for 375 real cases



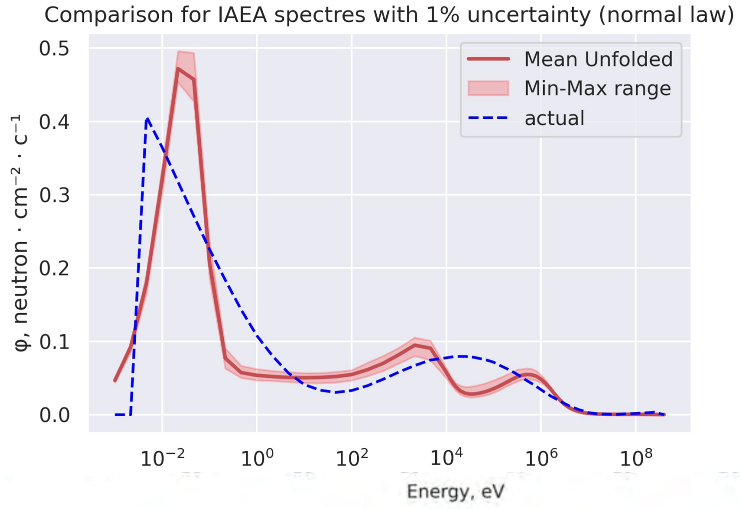
Spectra №0



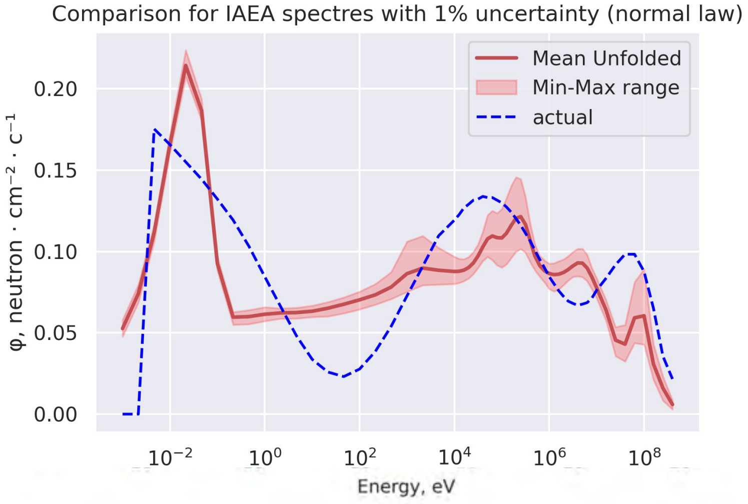
Spectra №102



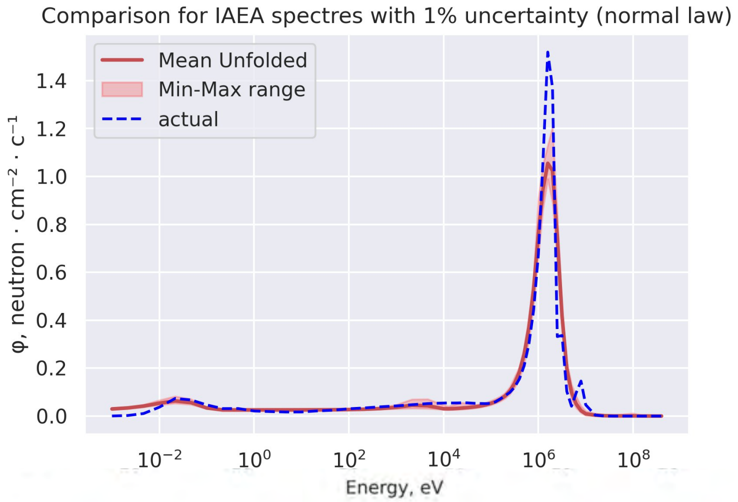
Spectra №83



Spectra №67 (soft field)



Spectra №68 (hard field)

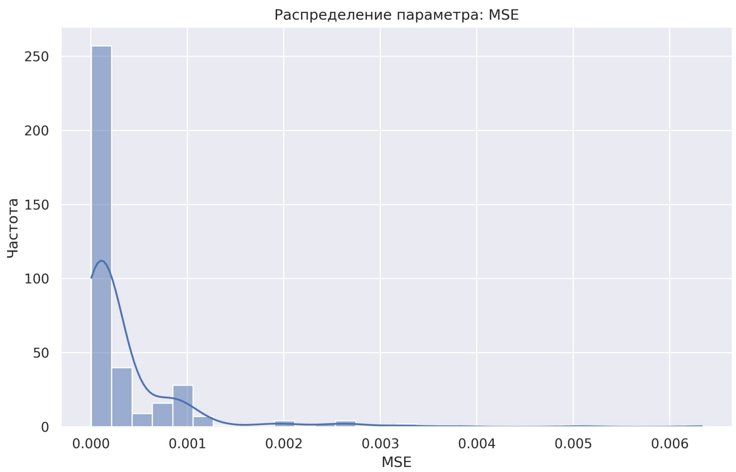


Spectra №226

The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations (1%) were introduced into the input data.

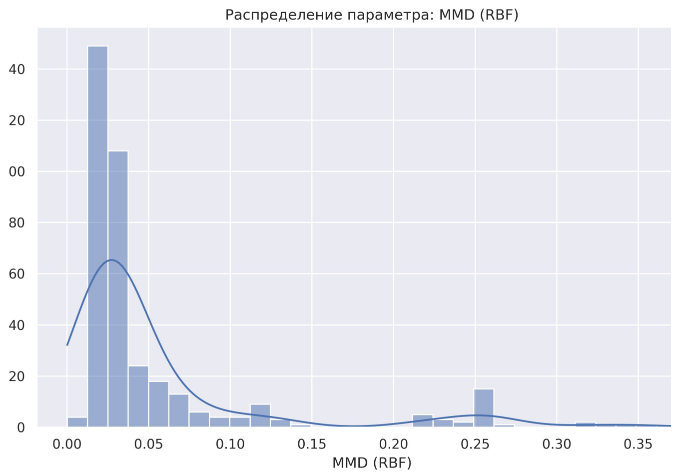
Timeout = 720 minutes

FEDOT results. Spectra comparison for 375 real cases



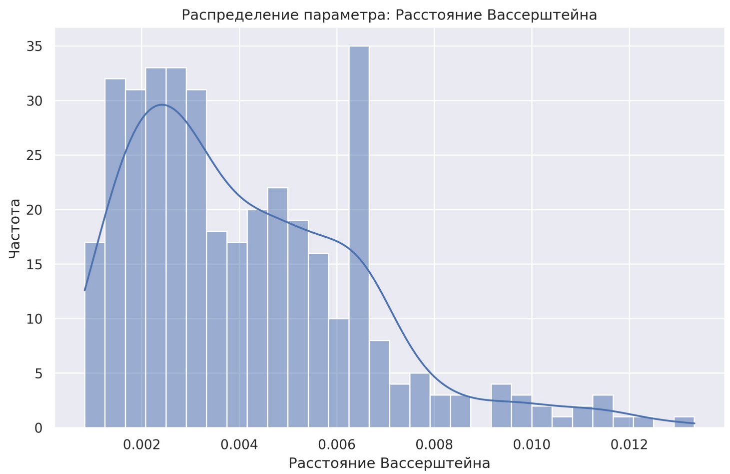
MSE

Mean squared error



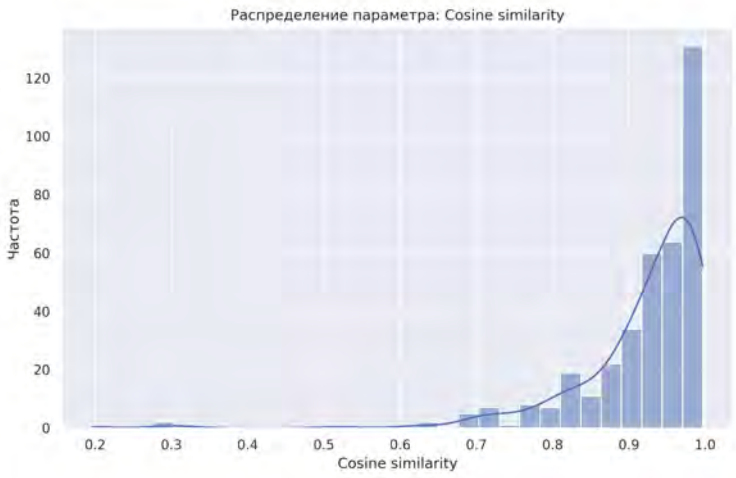
MMD

Maximum mean discrepancy

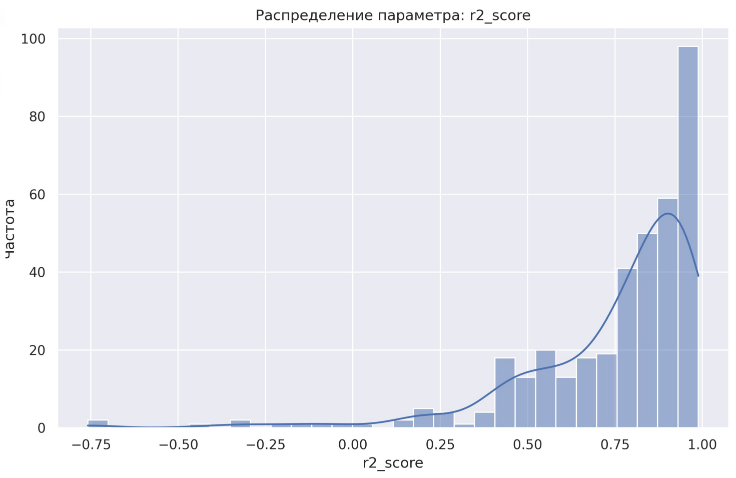


Wasserstein distance

Pearson correlation



Cosine similarity

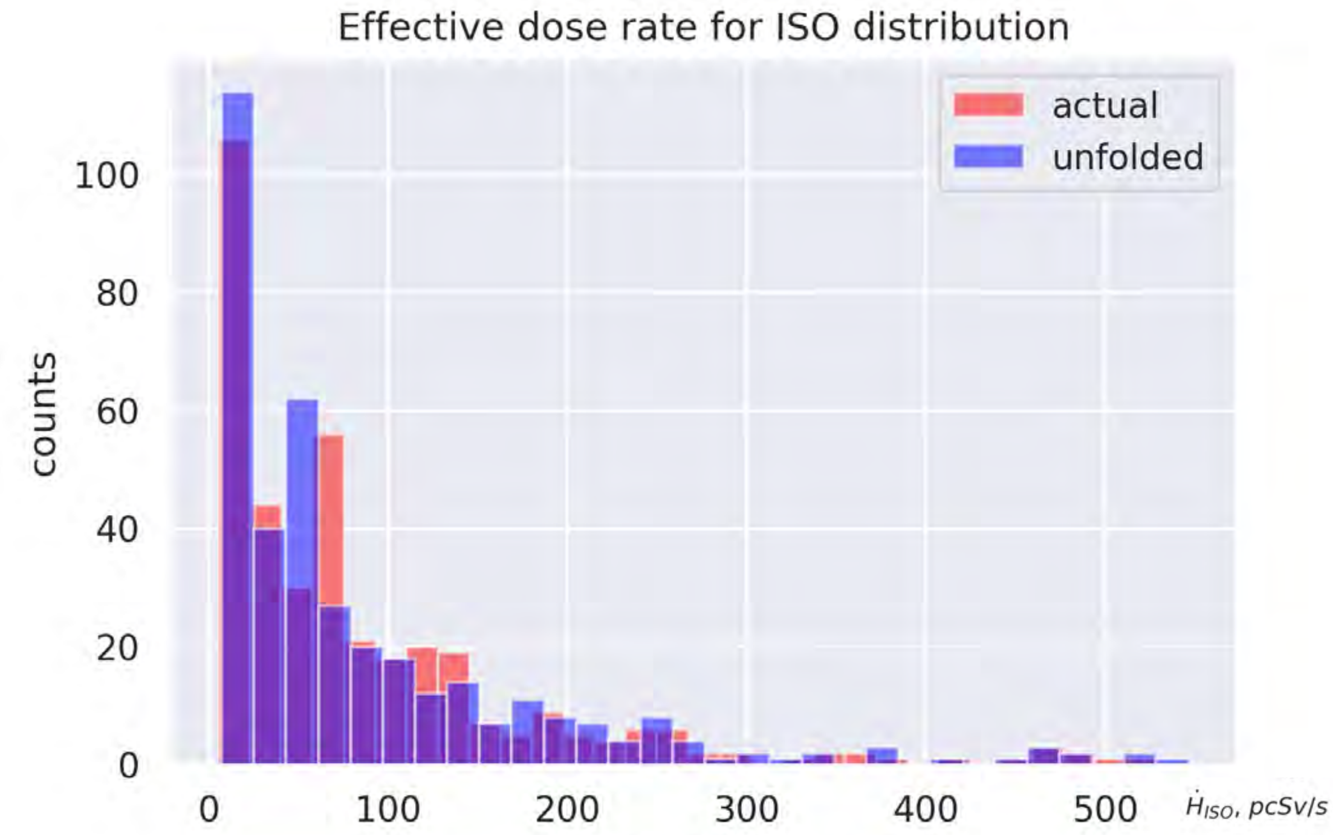


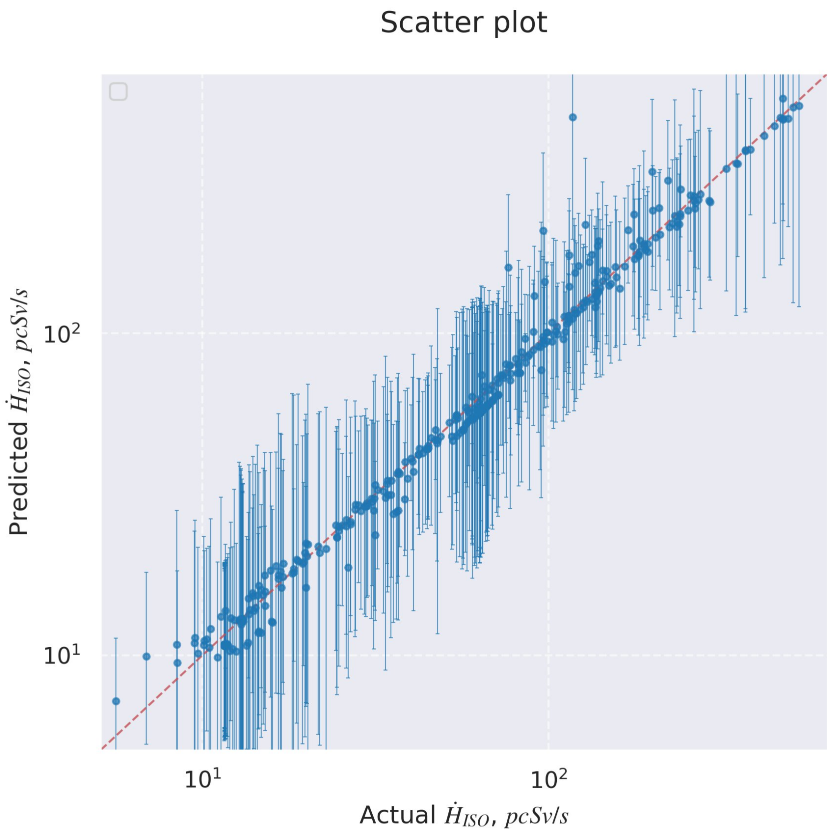
R^2

Coefficient of determination

FEDOT results. Dose assessment for 375 real spectra

The best model selected: *Scaling + Random forest regressor.*

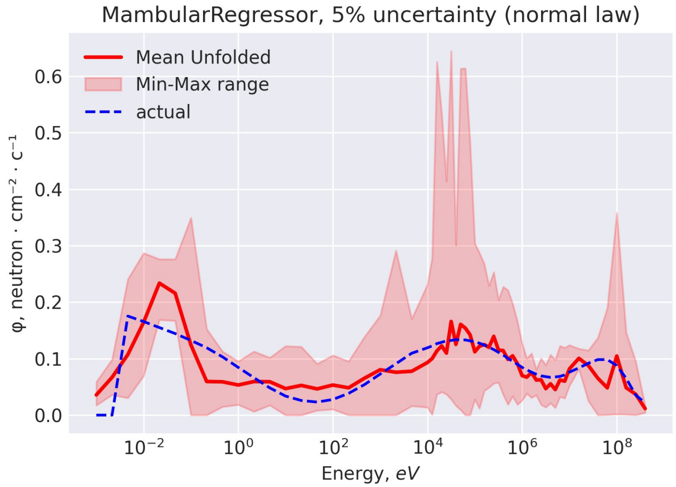




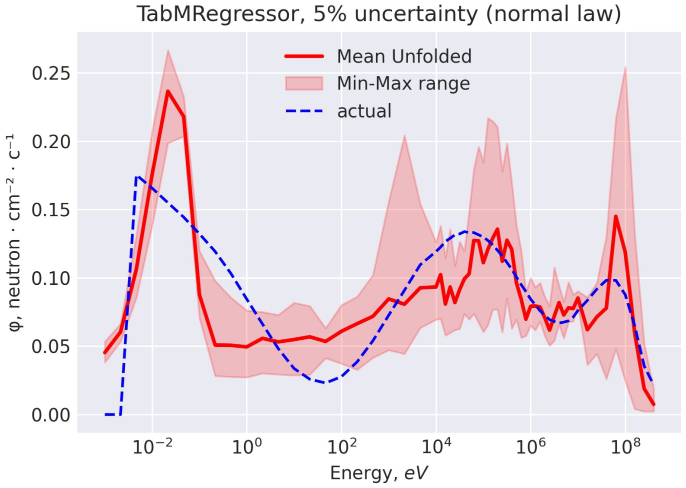
Timeout = 720 minutes

The uncertainty of the spectra unfolding was estimated using the Monte Carlo method, in which random perturbations were introduced into the input data (measurements error = 1%).

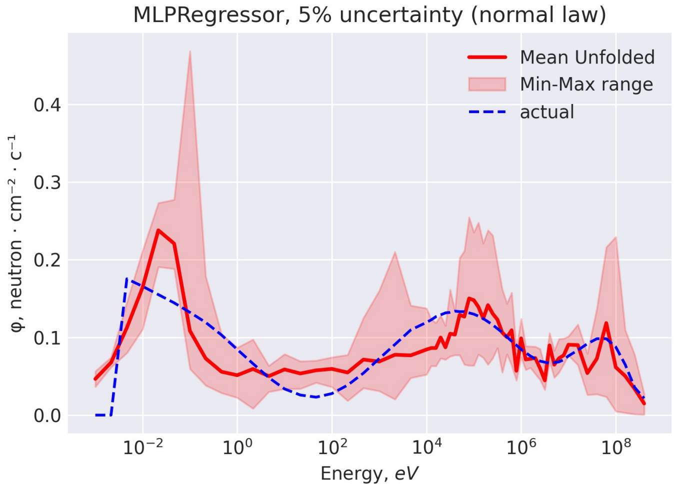
Comparison of models for JINR phasotron hard field



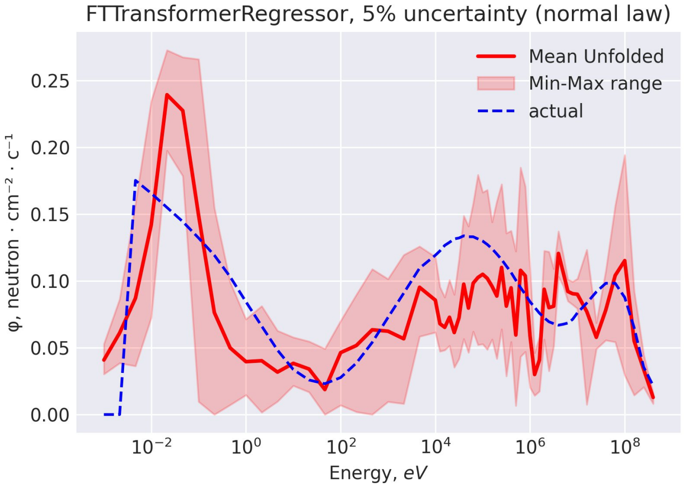
Mambular



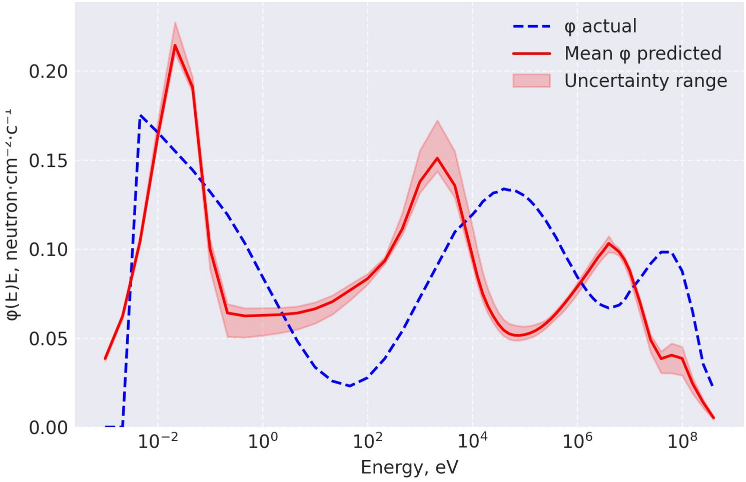
TabM



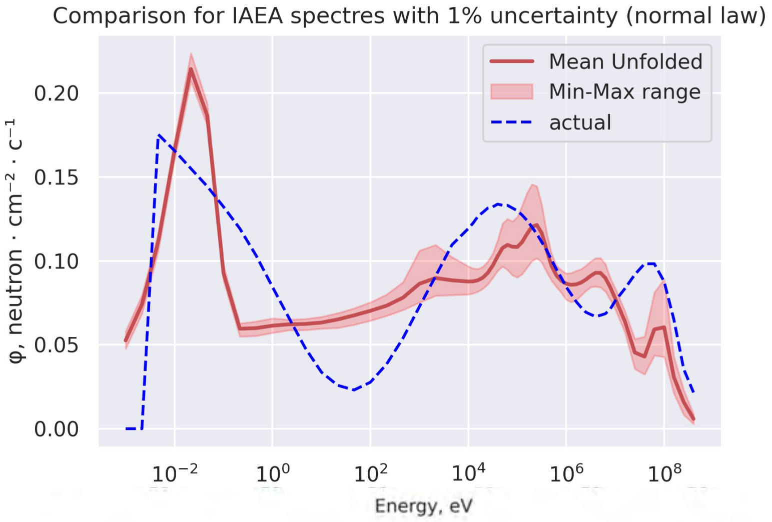
MLP



FTTransformer



LightAutoML



FEDOT

Comparison of models

Mean metrics for the test dataset.

	№	Model name	R^2	MSE	MAE	Cosine similarity	Pearson correlation	MMD	Wasserstein distance	MAPE for dose rate, %
DL	1	Mambular	0,803	3,88E-04	5,84E-03	0,937	0,903	0,043	3,80E-03	9,42
	2	FT Transformer	0,713	7,58E-04	7,94E-03	0,908	0,858	0,043	5,11E-03	14
	3	TabM	0,742	5,60E-04	7,05E-03	0,917	0,871	0,097	4,77E-03	15,1
	4	MLP	0,755	4,98E-04	6,67E-03	0,923	0,879	0,097	4,53E-03	14,54
	5	ResNet	0,755	5,86E-04	7,00E-03	0,921	0,881	0,045	4,71E-03	13,41
	6	TabulaRNN	0,779	3,66E-04	6,14E-03	0,929	0,892	0,043	4,03E-03	12,27
	7	NODE	0,779	5,04E-04	6,36E-03	0,930	0,893	0,034	4,18E-03	9,5
	8	SAINT	0,683	8,31E-04	7,81E-03	0,896	0,848	0,930	5,22E-03	132,2
	9	NDTF	0,711	0,001	0,008	0,909	0,859	0,052	4,90E-03	11
AutoML	10	LightAutoML	0,740	3,95E-04	6,76E-03	0,916	0,866	0,087	4,51E-03	14
	11	FEDOT	0,750	3,55E-04	6,34E-03	0,920	0,873	0,055	4,13E-03	9,15

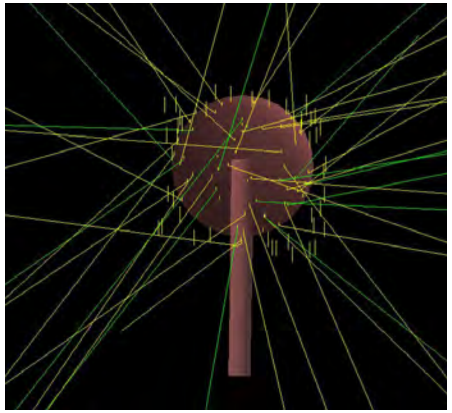
MAPE is the mean absolute percentage error.

On a regular basis, the capabilities of nuclear enterprises around the world are tested through international exercises and must achieve within 30% error for neutron dose measurements, https://doi.org/10.1080/00295639.2025.2458437.

Discussion

Improvements of the experiment setup:

- Development of a training set using Monte Carlo[1] simulations (Geant4)[2].
- Improving the set of moderator spheres in the **high-energy region** (composite spheres with lead and other materials).
- Models for other BSS with different response functions.
- Optimal set of spheres[3,4].



Geant4 simulation

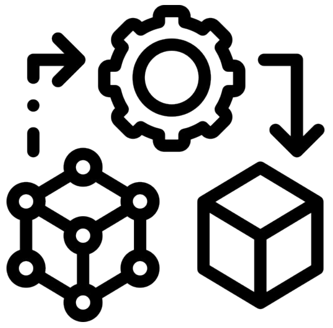
Improvements of the spectra unfolding:

- Combination of methods to improve accuracy.
- Interpretation of the results and selecting input features with explainable Artificial Intelligence (XAI) methods[5].
- Other types of feature transformations[6].
- Penalty for $\varphi<0$ during training, other limitations based on the physics of neutrons.

1. Bouhadida, M. et al, Neutron Spectrum Unfolding Using Two Architectures of Convolutional Neural Networks». Nuclear Engineering and Technology 55(6),2023, 2276–82. (CNN, range 10^{-9} - 20 MeV).
2. Agostinelli S., et al. GEANT4—a simulation toolkit.*Nuclear instruments and methods in physics research section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 506.3,2003: 250-303.
3. Chizhov, K., Chizhov, A. Optimization of the Neutron Spectrum Unfolding Algorithm Based on Tikhonov Regularization and Shifted Legendre Polynomials. *MMCP 2024*, 74.
4. Chizhov A., Chizhov K., Unfolding of the spectra of reference neutron fields at the Phazotron (JINR) based on readings of the Bonner multi-sphere spectrometer using the truncated singular value decomposition method // LXI All-Russian Conference on Problems of Dynamics, Particle Physics, Plasma Physics and Optoelectronics, RUDN University, 2025 (in Russian).
5. Chizhov K. "Random forest regression and Shapley additive explanation for effective dose rate estimation in high-energy neutron fields based on Bonner spectrometer measurements." First Conference of Mathematics of AI, 2025, Sirius, Sochi.
6. Song W et al. Autoint: Automatic feature interaction learning via self-attentive neural networks. Proceedings of the 28th ACM international conference on information and knowledge management. 2019.

Implementation of other DL and AutoML algorithms

- **NAMformer**, a fully connected tabular deep learning architecture that combines a tabular transformer with interpretable feature networks (*arXiv:2504.08712v*).
- **Gradient Boosting Neural Networks: GrowNet** (*arXiv:2002.07971v2*).
- **TabDDPM** (*arXiv:2209.15421*).
- **TabR** (*arXiv:2307.14338*).



Implementation of models from pytorch Tabular[1]

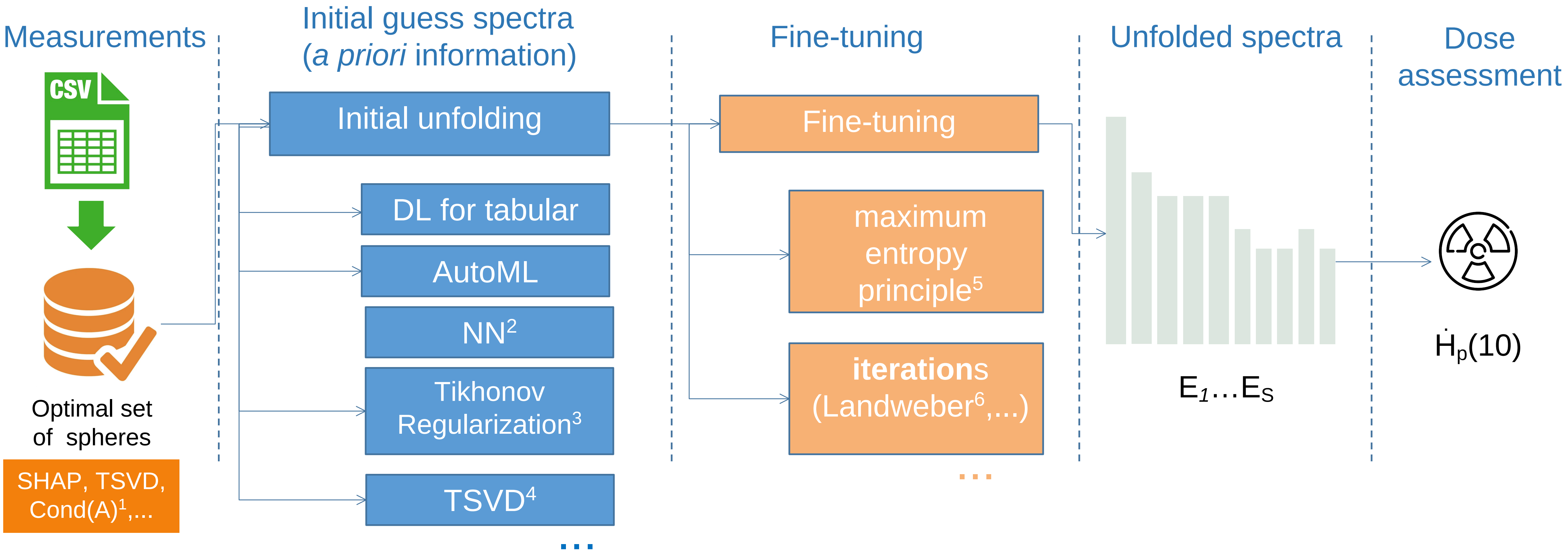
- Feed Forward Network with Category Embedding.
- Neural Oblivious Decision Ensembles for Deep Learning on Tabular Data.
- TabNet: Attentive Interpretable Tabular Learning (Sparse Attention).
- Mixture Density Networks (uses Gaussian components to approximate the target function).
- AutoInt: Automatic Feature Interaction Learning via Self-Attentive Neural Networks.
- FTTransformer from Revisiting Deep Learning Models for Tabular Data.
- Gated Additive Tree Ensemble (GATE).
- Gated Adaptive Network for Deep Automated Learning of Features (GANDALF).
- DANETs: Deep Abstract Networks for Tabular Data Classification and Regression (AbsLay).

Large language models (LLM) + AutoML

1. **FEDOT.LLM[3]**: combines the power of Large Language Models with automated machine learning techniques to enhance data analysis and pipeline building processes (*https://github.com/aimclub/FEDOT.LLM.git*).

[1] Joseph, Manu. "Pytorch tabular: A framework for deep learning with tabular data." *arXiv preprint arXiv:2104.13638* (2021).

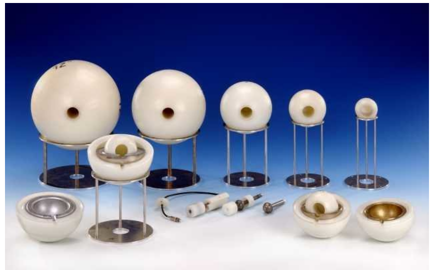
App

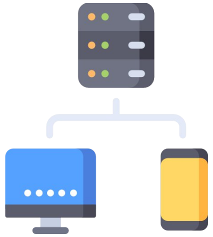


1. Chizhov, K., Chizhov, A. Optimization of the Neutron Spectrum Unfolding Algorithm Based on Tikhonov Regularization and Shifted Legendre Polynomials. *MMCP 2024*, 74.
2. Bely A.A., Chizhov K.A. Development of a web application for an experiment on unfolding neutron spectra using a neural network algorithm, XXX All-Russian scientific and practical conference of students, graduate students and young specialists, “Dubna” University, Dubna, 2025 (in Russian).
3. Chizhov, K., Beskrovnaya, L., Chizhov, A. Neutron Spectra Unfolding from Bonner Spectrometer Readings by the Regularization Method Using the Legendre Polynomials, *Phys. Part. Nuclei*, 55: 532–534, 2024.
4. Chizhov A., Chizhov K., Unfolding of the spectra of reference neutron fields at the Phazotron (JINR) based on readings of the Bonner multi-sphere spectrometer using the truncated singular value decomposition method // LXI All-Russian Conference on Problems of Dynamics, Particle Physics, Plasma Physics and Optoelectronics, RUDN University, 2025 (in Russian).
5. Reginatto M., Goldhagen P. MAXED, a computer code for maximum entropy deconvolution of multisphere neutron spectrometer data. *Health Physics* 77.5 (1999): 579-583.
6. Landweber L.,An iteration, formula for Fredholm integral equations of the first kind. *Amer. J. Math.*73, 615–624, 1951.

Implementation & restrictions

- The method is suitable for unfolding spectra in stationary neutron fields.
- It is necessary to prepare a model for each BSS detector and set of moderator spheres. Trained models could take up a lot of disk space.
- Used set of Bonner spectrometer spheres limits the energy range of unfolded spectrum.
- The uncertainty of sensitivity functions is not taken into account. It is usually ~ 2% because it's calculated by the Monte Carlo Method with sufficient statistics[1].
- The app uses many dependencies, it is necessary to run in a virtual environment or container.
- The client-server implementation will allow access to spectrum analysis from any device, even a portable one.



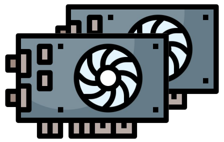


[1] DOI: 10.1088/1009-0630/17/1/15

Neutron spektrometer NEMUS, https://www.ptb.de/cms/en/ptb/fachabteilungen/abt6/fb-64/643-neutron-spectrometry/nemus/neutron-spektrometer-nemus-neutron-multisphere-spectrometer.html

Conclusions

1. Transformations of original scalar continuous features (readings of the Bonner spectrometer) into vectors were used for training of deep neural networks. This allowed us to expand the set of input features, since due to the limited set of spheres and correlations in it sensitivity functions, the number of input measurements is limited.
2. Neutron spectra were unfolded using deep learning regressor models included in the Mambular framework. The results are compared with the spectra unfolded using the AutoML frameworks: LightAutoML and FEDOT. Metrics R^2, MSE, cosine similarity, Wasserstein distance, Pearson correlation coefficient and MMD were assessed. The effective dose rate estimated from unfolded spectra showed good agreement with the actual ones, the estimation error does not exceed 15%, except SAINT method.
3. Comparison of algorithms showed that Mambular has the best metrics for R^2 = 0.80, Pearson correlation coefficient = 0.90, cosine similarity = 0.94 and Wasserstein distance = 3.8E-3. Mambular, ResNet, FTTransformer has the best metric for MMD = 4.5E-2. The smallest MSE = 3.55E-4 is for FEDOT.
4. The conditional stability of models to uncertainty in input data was investigated, MLP showed the best results.
5. The proposed method could be used for improving radiation protection in high-energy neutron fields.



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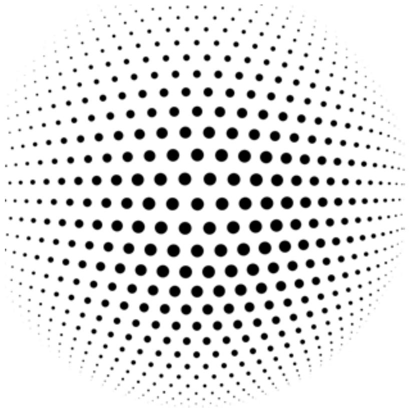
Thank you!



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1. Chizhov K.A. et al. Unfolding of the energy spectrum of the neutron radiation flux using the random forest machine learning algorithm. *Modern information technologies and IT education*, 20, 4 (Dec. 2024). ISSN 2411-1473 (in Russian).
2. Chizhov, K., Beskrovnaya, L. & Chizhov, A. Neutron Spectrum Unfolding Method Based on Shifted Legendre Polynomials, Its Application to the IREN Facility. *Phys. Part. Nuclei Lett.* 22, 337–340 (2025). https://doi.org/10.1134/S154747712470239X
3. Chizhov, K., L. Beskrovnaya, and A. Chizhov. "Neutron Spectra Unfolding from Bonner Spectrometer Readings by the Regularization Method Using the Legendre Polynomials." *Physics of Particles and Nuclei* 55.3 (2024): 532-534.
4. Chizhov K, Chizhov A. Dose assessment of personnel neutron irradiation on high-energy accelerators using a multi-sphere Bonner spectrometer. *Mathematical Modeling* 7 (2), 63-64 (2023).

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