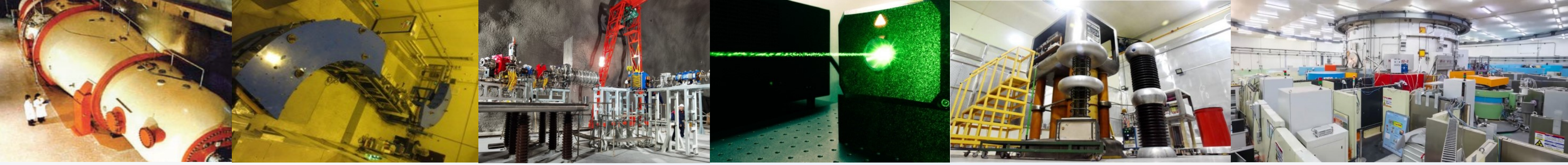


International Nuclear Data Evaluation Network (INDEN) Evaluated Nuclear Data of the Structural Materials, December 16-20, 2024, IAEA, Vienna

Research on Machine Learning Methods for Nuclear Reaction Cross Section Data of Structural Materials

Speaker: Xiaodong SUN

China Nuclear Data Center, China Institute of Atomic Energy

Nuclear Data Section, International Atomic Energy Agency

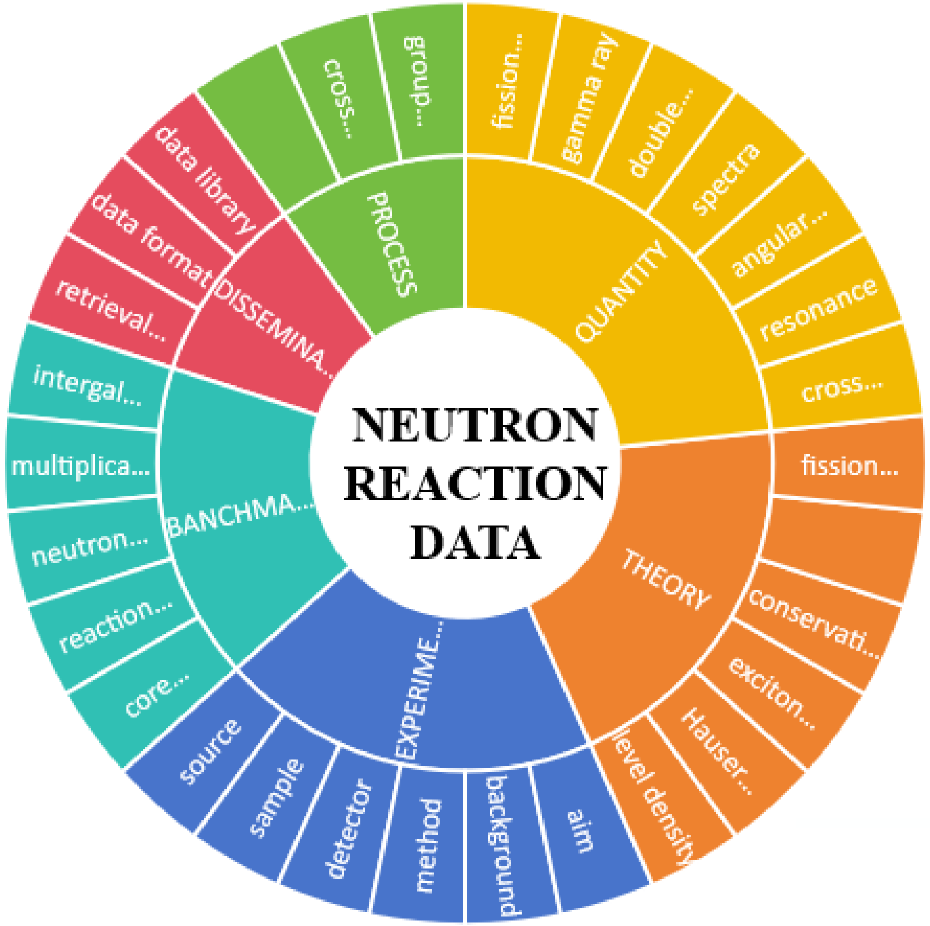
中国原子能科学研究院 CHINA INSTITUTE OF ATOMIC ENERGY 中核集团 CNNC

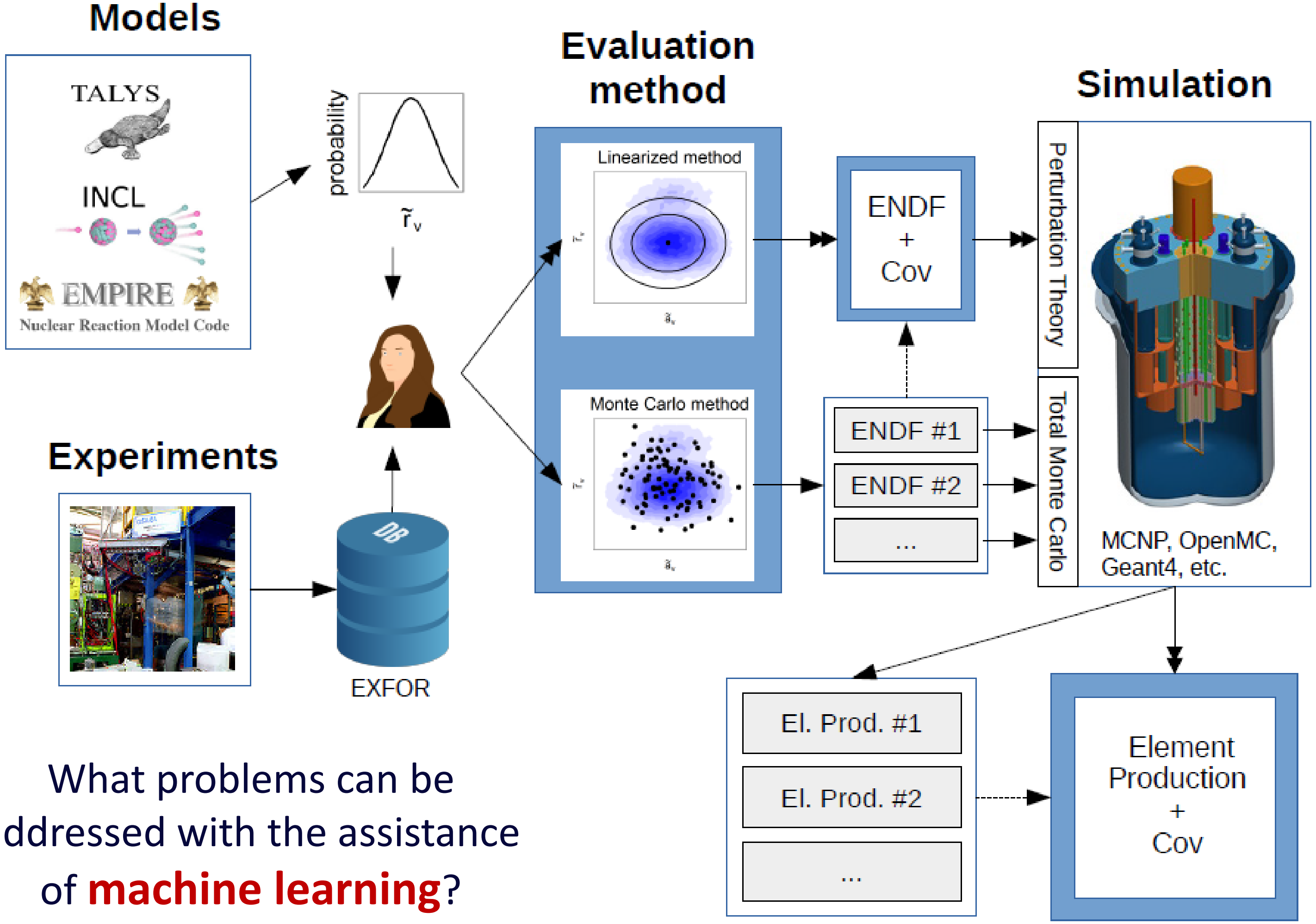
CNDC CHINA NUCLEAR DATA CENTER

IAEA International Atomic Energy Agency

Nuclear data, which encompasses experimental measurements, theoretical models, evaluation, processing, validation, as well as database management and dissemination, necessitates highly specialized expertise.

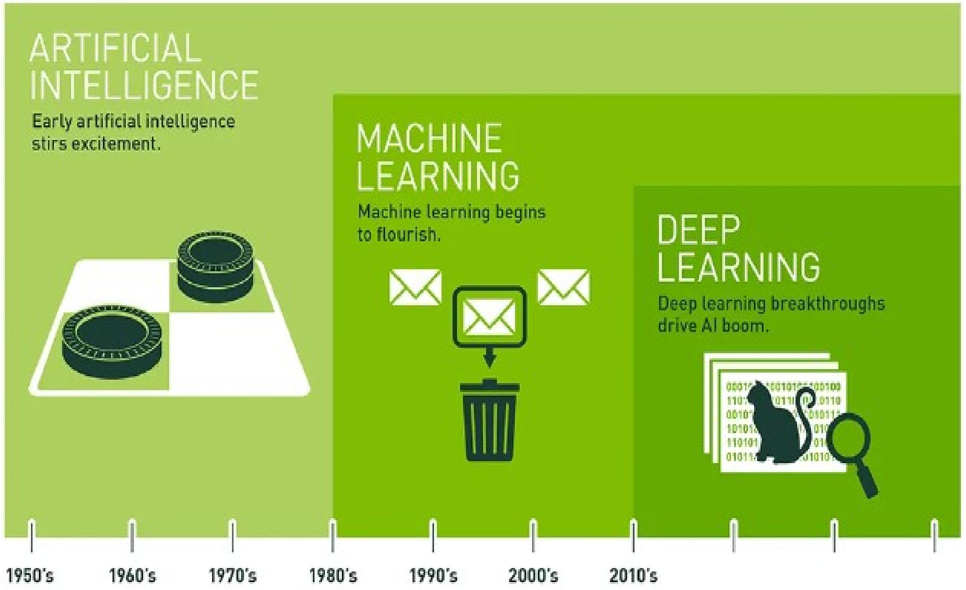
Theory + Experiment + Statistics = evaluation



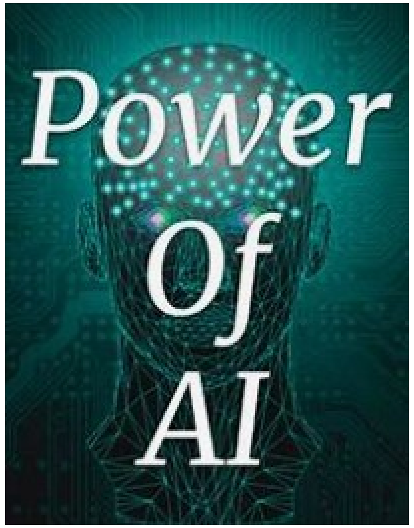


What problems can be addressed with the assistance of **machine learning**?

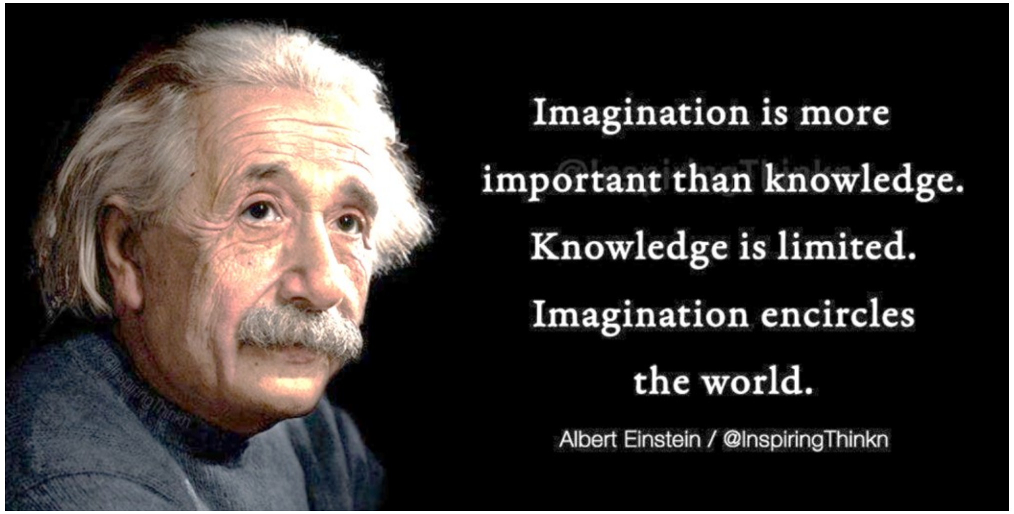
MOTIVATION

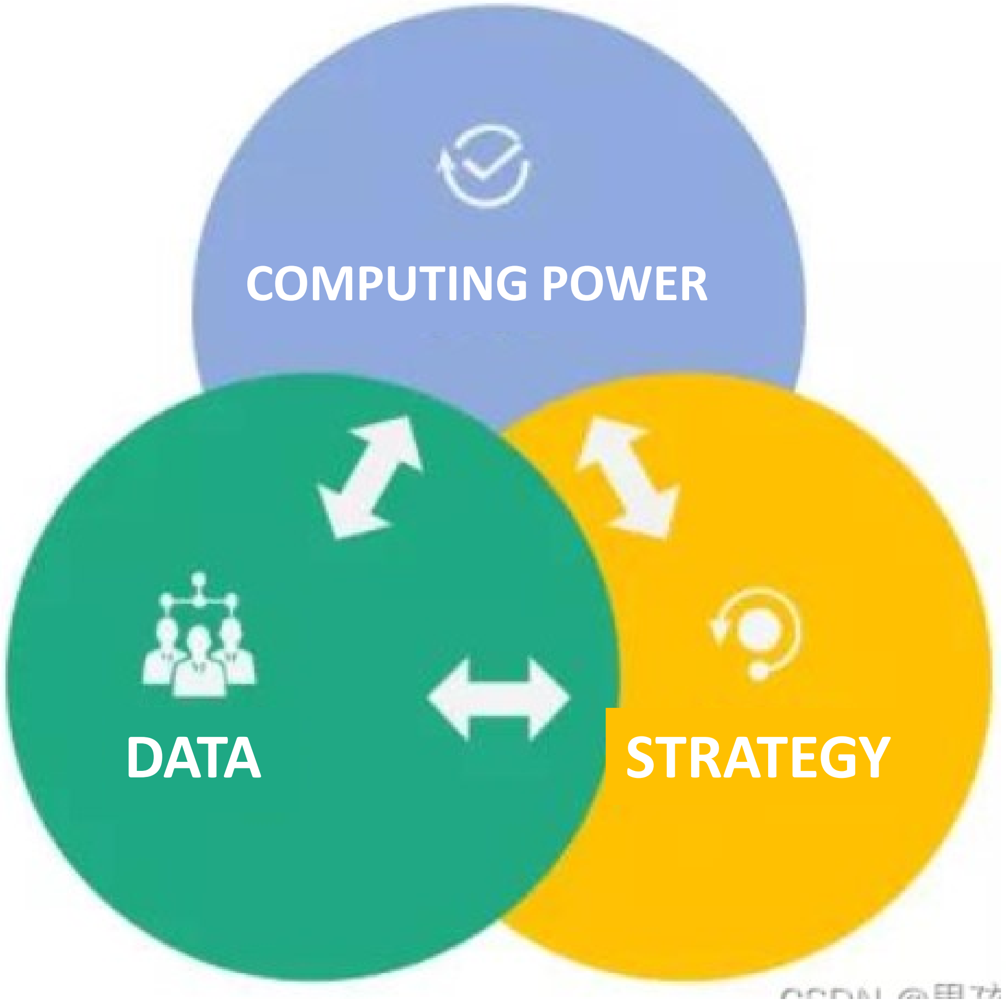


- AI has witnessed remarkable success in recent years.
- While AI systems are essentially responsive to input data, lacking the autonomy and depth of human cognition.



- In the realm of nuclear data evaluation, established theoretical models and data processing techniques currently hold sway. These methods, grounded in rigorous scientific principles, are not readily displaceable by AI.
- Now we will discuss the way of integrating AI-related algorithms and data processing approaches to enhance the efficiency and quality of nuclear data evaluation.



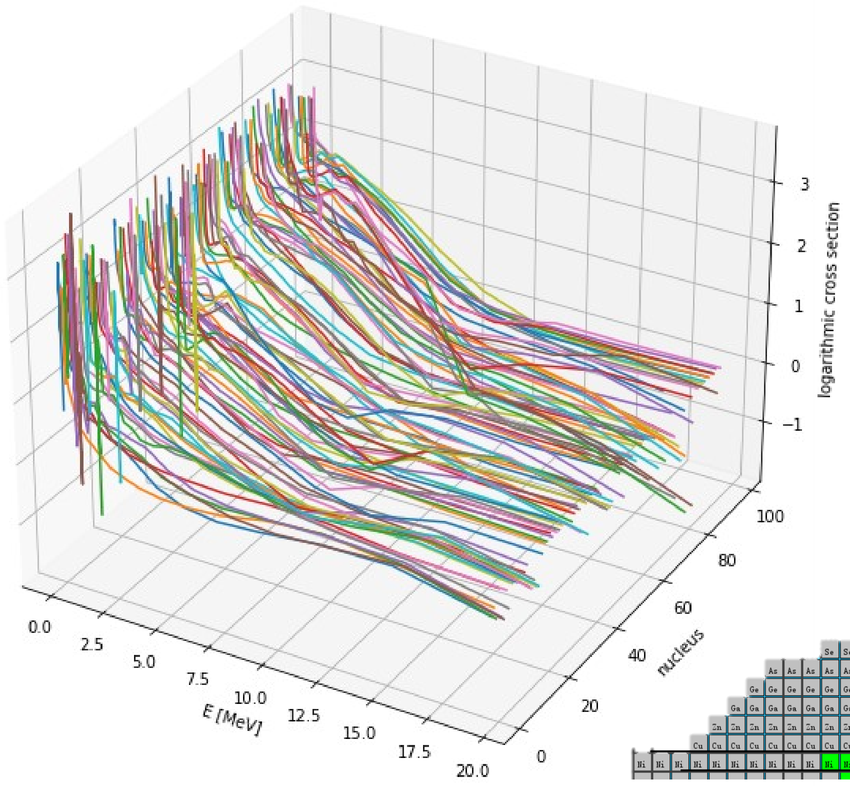


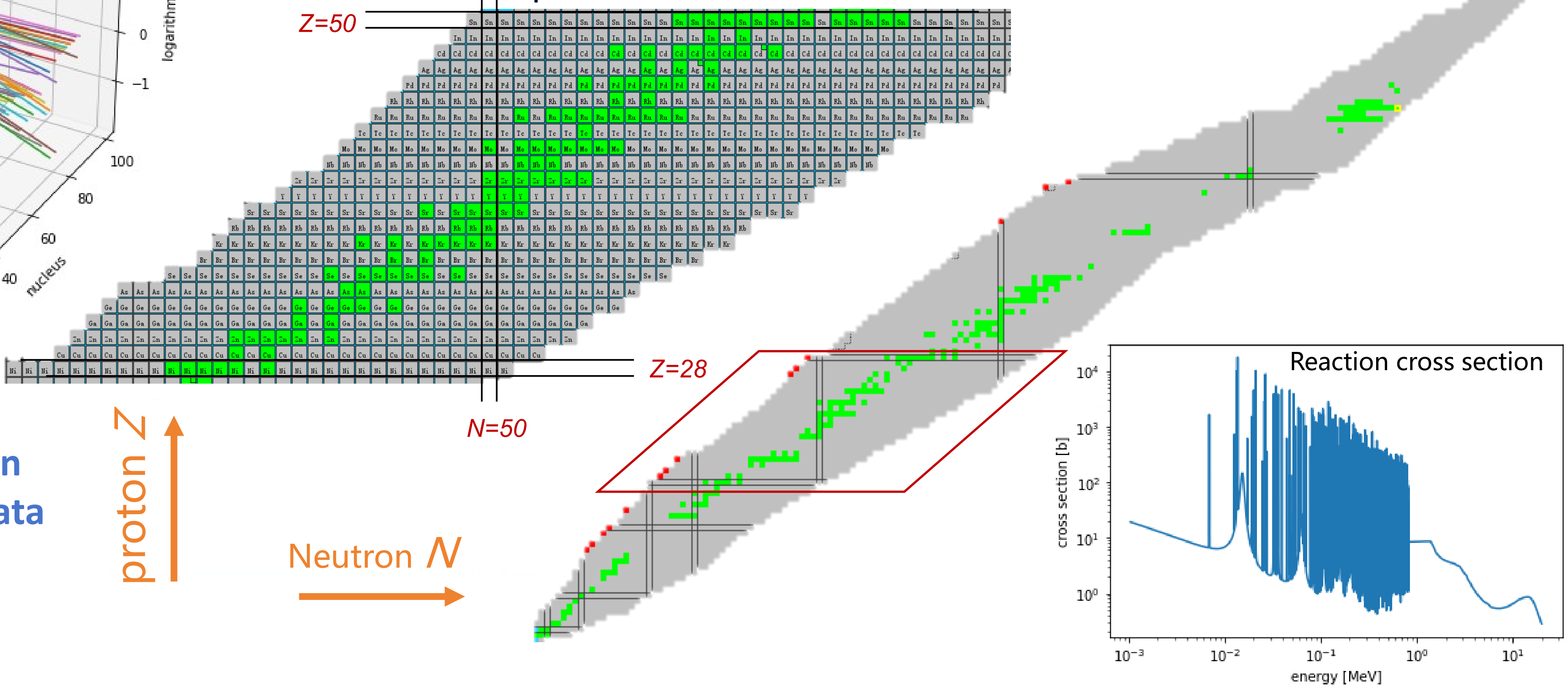
Three elements of machine learning

CONTENT

DATA for training neural network

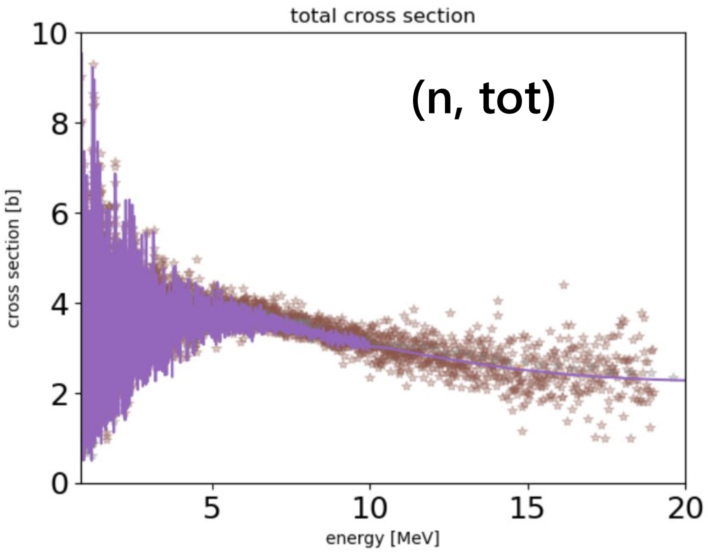
- The relationship between reaction cross section and the properties of the target nucleus is intricate.
- The number of neutrons and protons is the fundamental feature of atomic nuclei.
- Creating a dataset for training a neural network allows for the automatic identification of patterns.

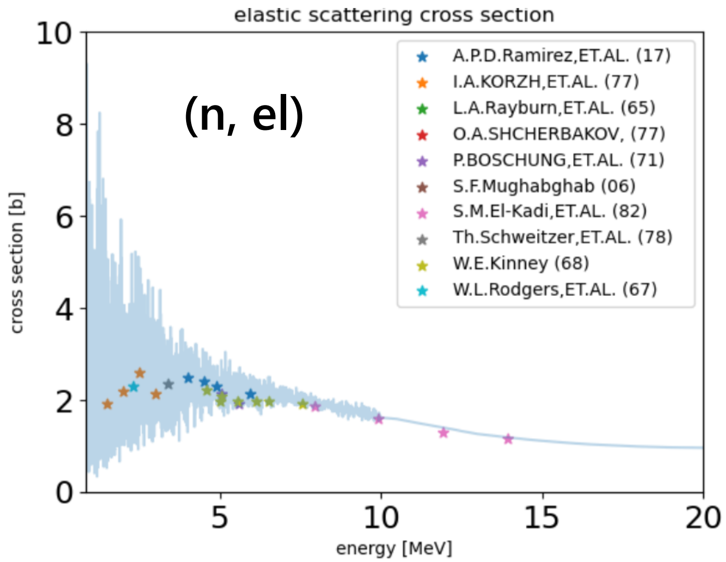


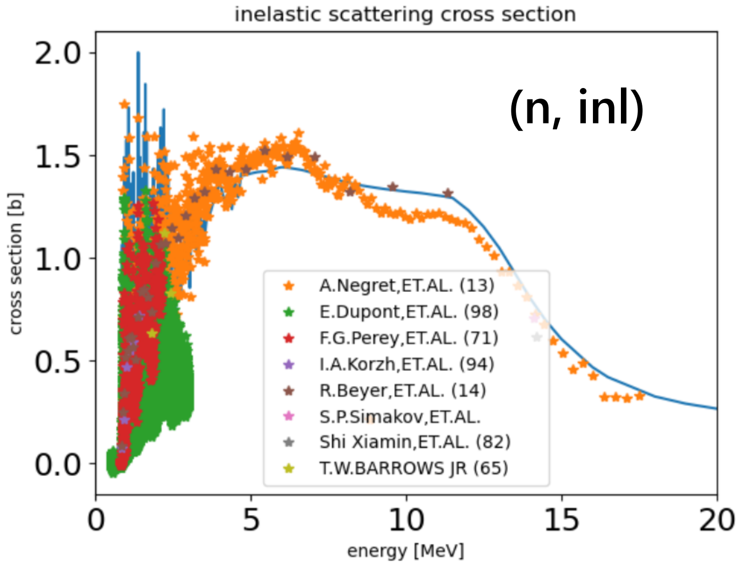


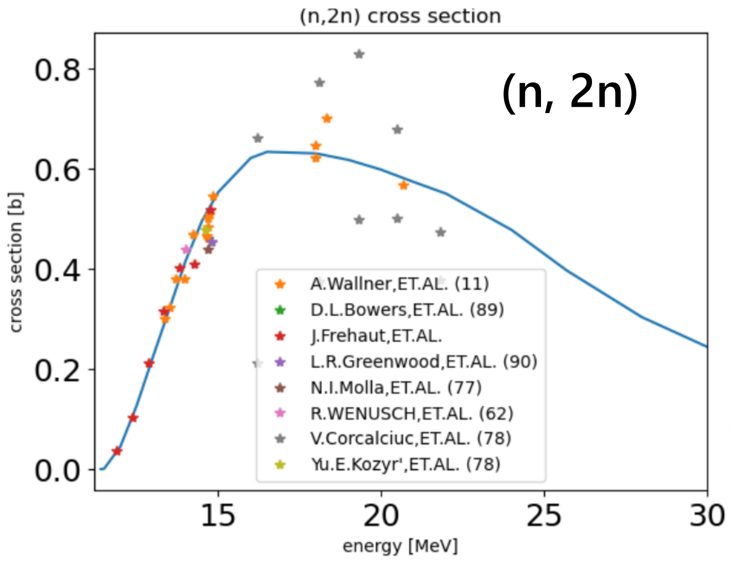
Is there any underlying pattern present in the cross section data of numerous target nucleus within a specified range?

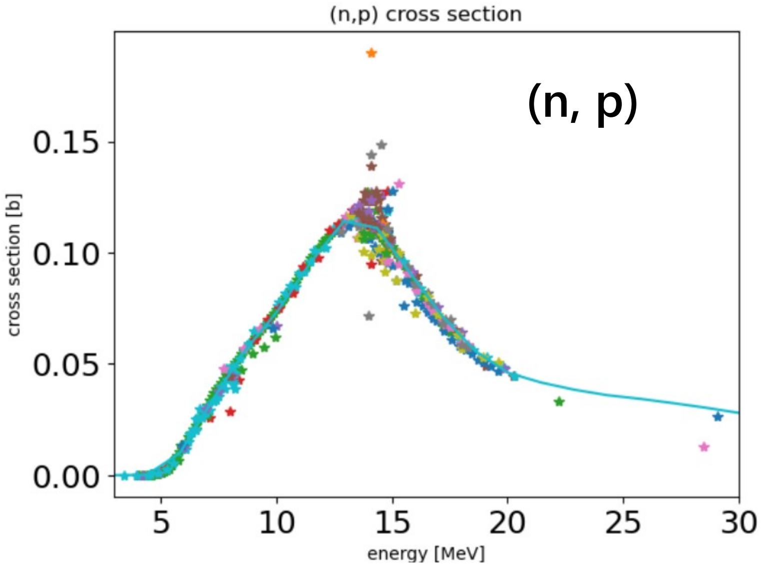
DATA for Bayesian inference graph

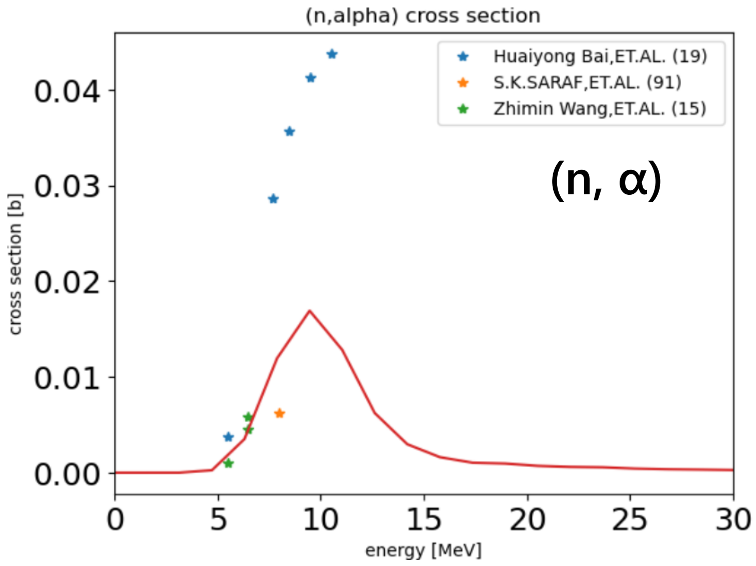












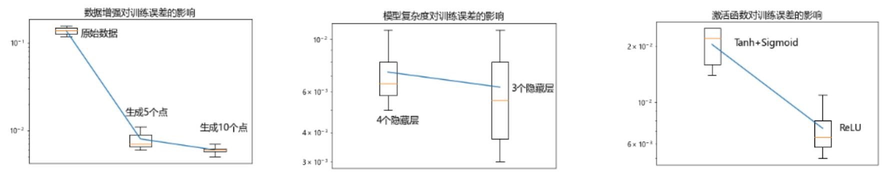
II. Strategy

STRATEGY for training neural network

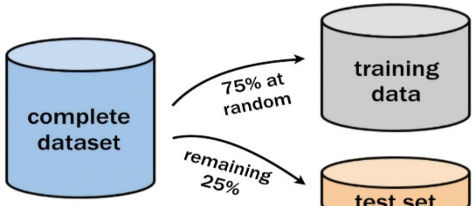
Data augmentation LANSAAR RESEARCH

Noise injection

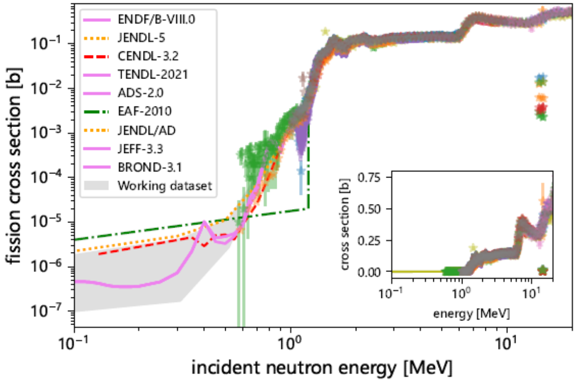
Data preprocessing



Training Machine Learning Models



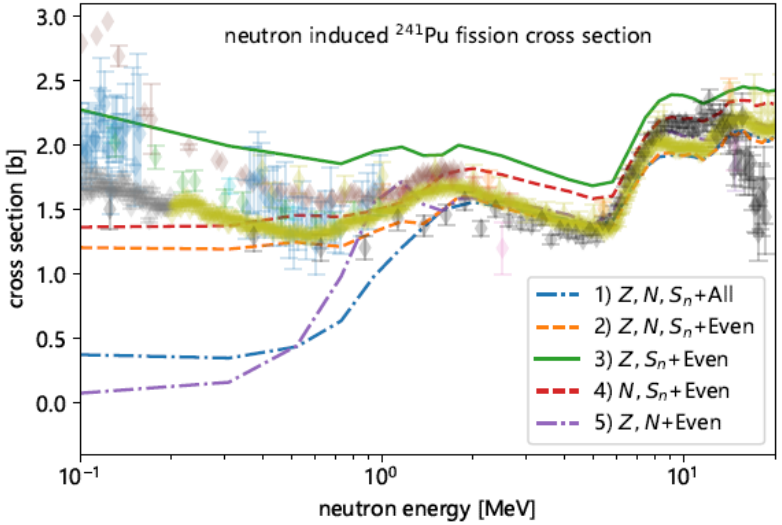
Data comparison and analysis



- EXFOR dataset
- ENDF library
- Data retrieval visualization
- Processing

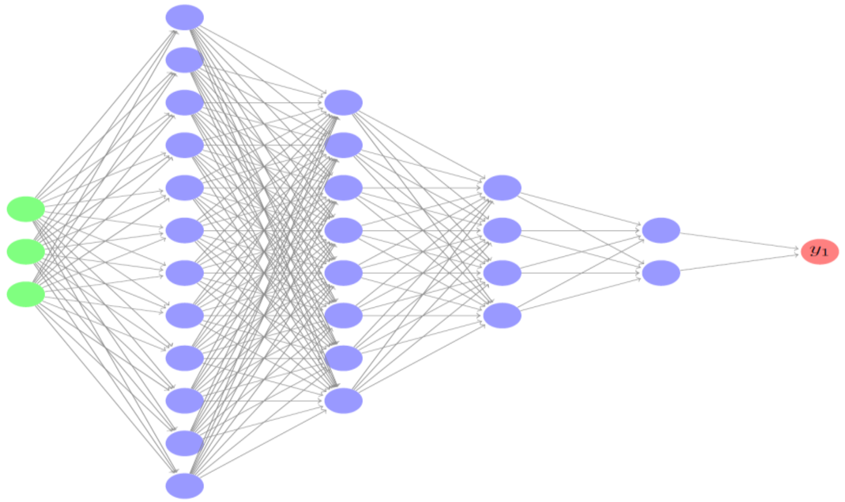
Physical law

- Asymmetry role of neutron and proton numbers
- Fission potential surface and barrier, level density above hump



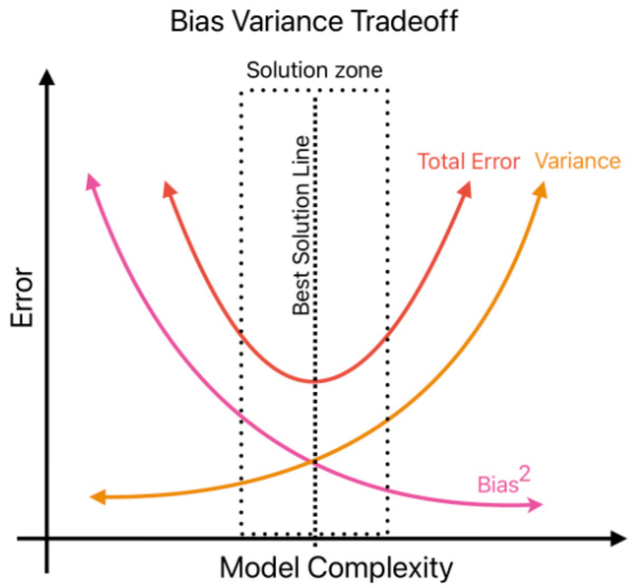
STRATEGY for training neural network

1. Neural network

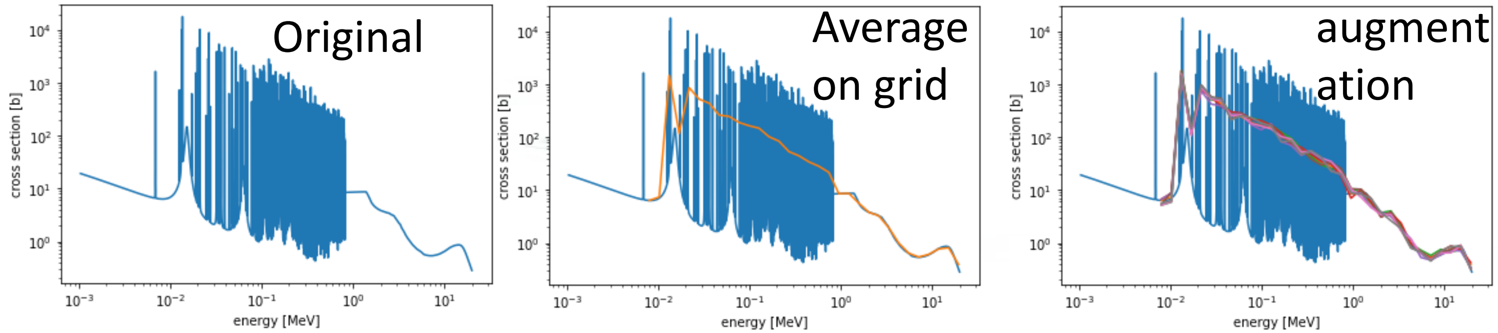


2. Dataset process

- Pre-process
- Data augmentation
- Energy grid
- Normalization



3. Iterative training

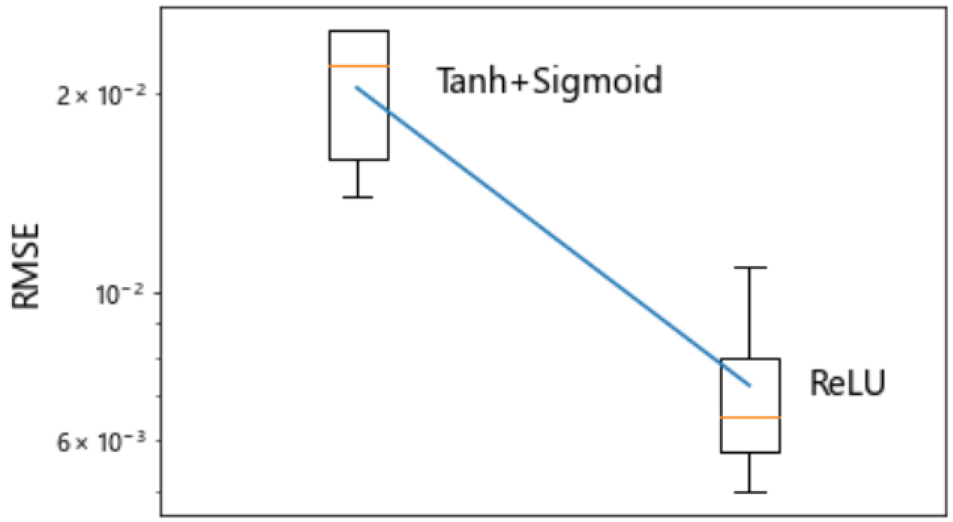


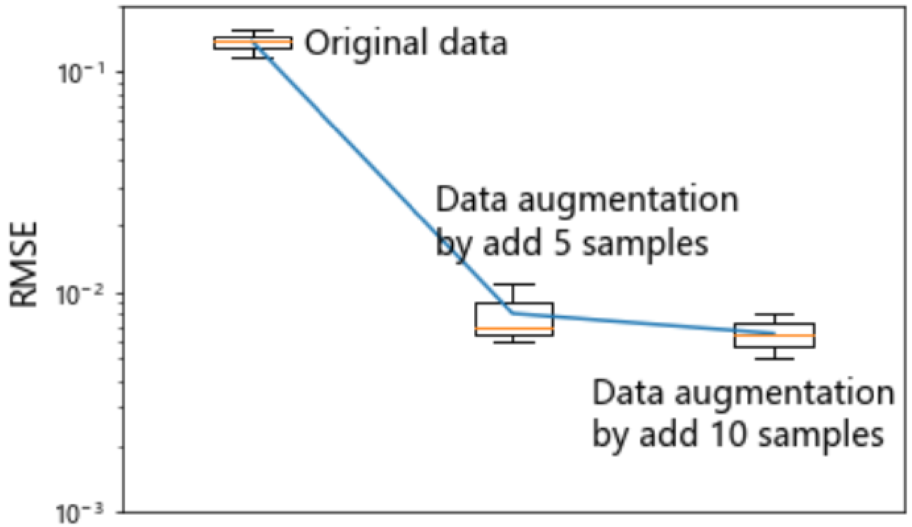
- Cross validation
- Regularization
- Model hyper-parameters
- Early stop
- ……

$$\text{MSE loss} = \frac{1}{n}\sum_{i=1}^{N}\sum_{t=1}^{M}(y_t^i - \hat{y}_t^i)^2$$

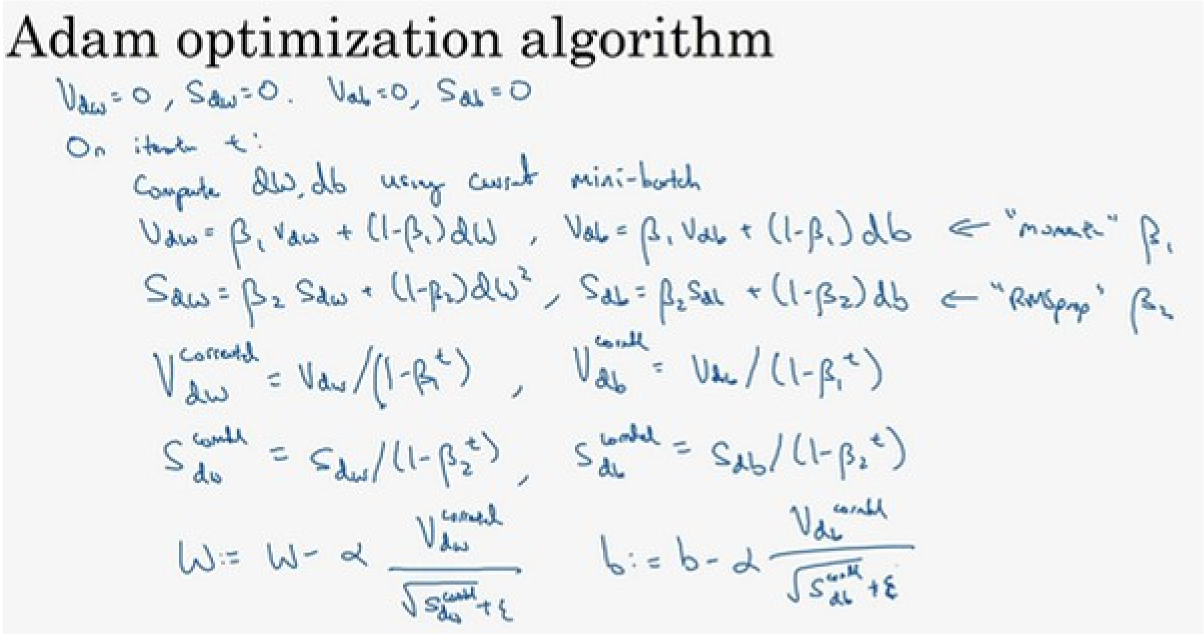
Effective strategies avoiding overfit:

- Early stopping: halt the training iteration if the loss of validation set begins to increase.
- L2 Regularization: smooth prediction of cross section
- Dataset splitting: the training and validation sets are randomly selected.
- Neural network structure: only ReLU activation for hidden layer can reduce the loss.



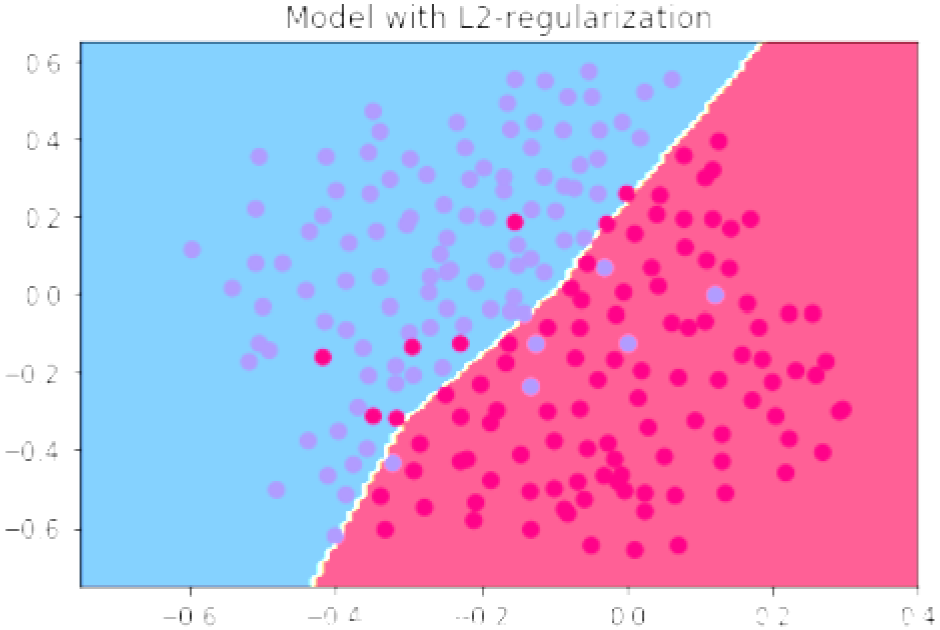


Adaptive Moment Estimation

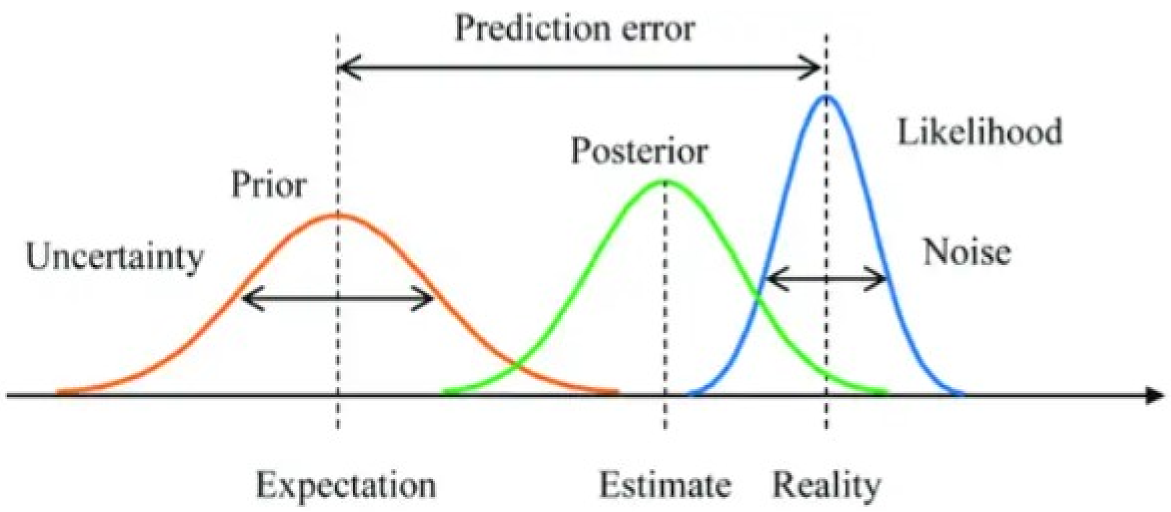


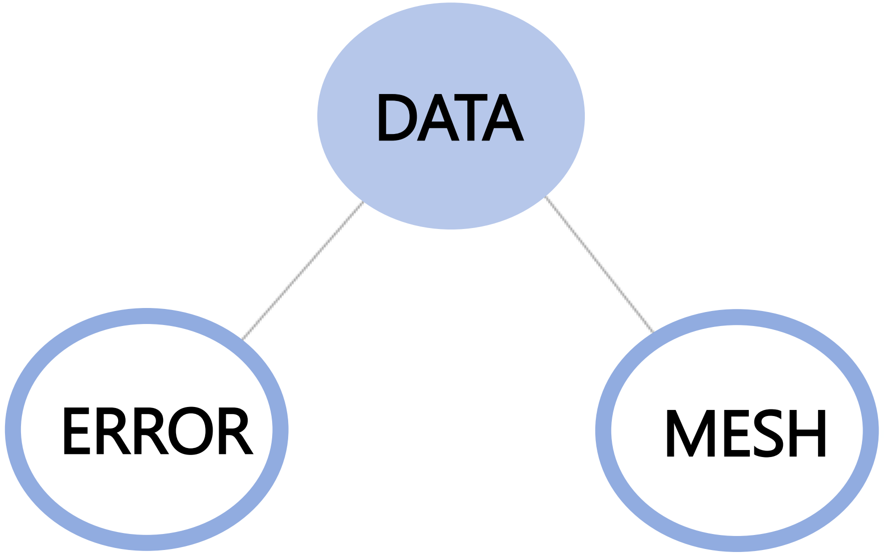
Weight decay (Regularization) is considered

$$C = C_0 + \frac{\lambda}{2n}\sum_w w^2$$



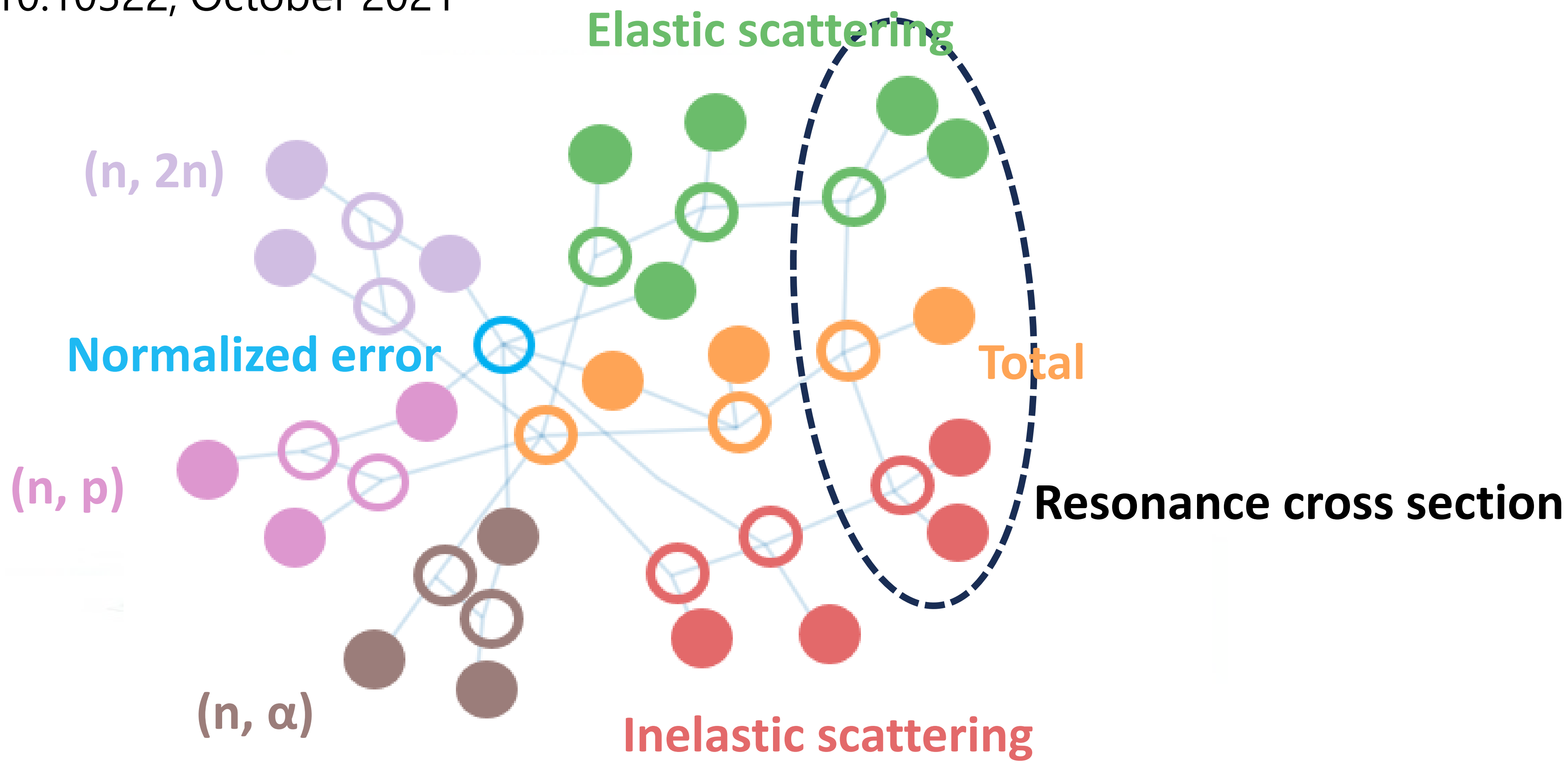
STRATEGY for Bayesian inference graph



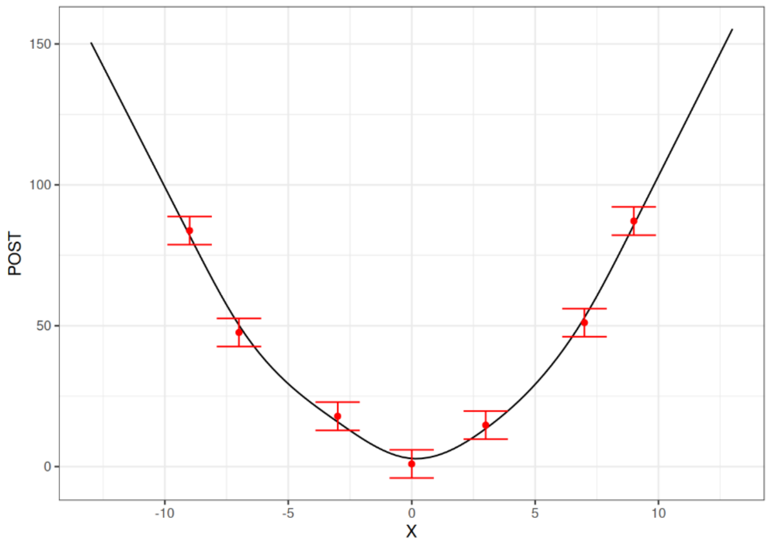


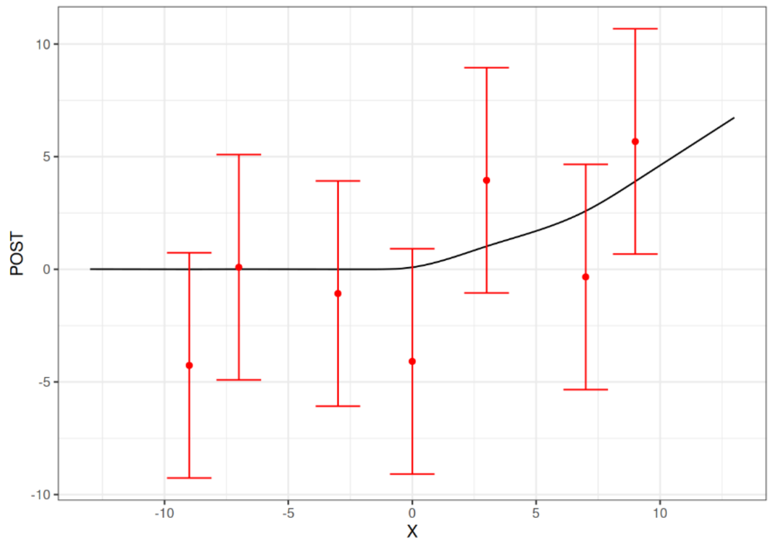
- Bayesian Inference allowing us to iteratively incorporate new data, thereby refining our estimates of the true value.
- The graph offers a clear reflection of the relationships among various quantities.
- Fill nodes denote data or physical constraints, whereas open nodes represent the outputs of our interest

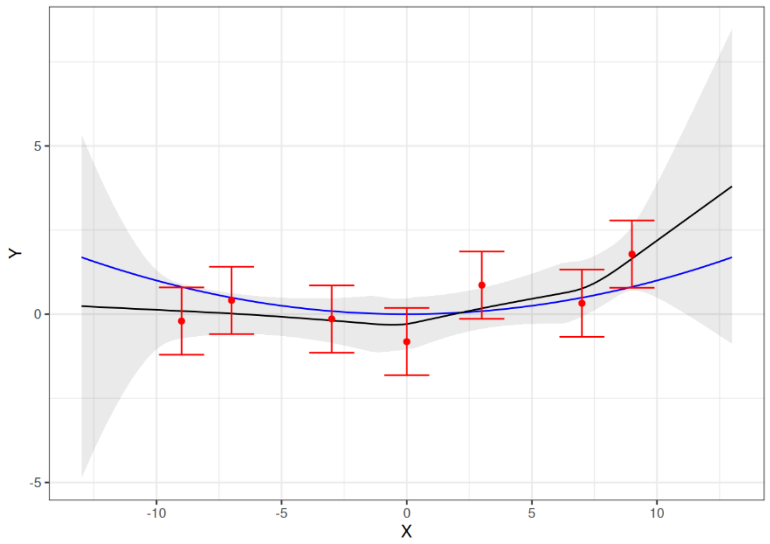
nucdataBaynet: Bayesian networks for nuclear data evaluation - v0.2.0.
G. Schnabel, R. Capote, A.J. Koning, D.A. Brown, "Nuclear data evaluation with Bayesian networks", preprint, arXiv:2110.10322, October 2021



STRATEGY for Bayesian inference graph







Smooth constraint

Positivity constraint

convexity constraint

nucdataBaynet: Bayesian networks for nuclear data evaluation - v0.2.0.

Solve nonlinear least square optimization efficiently

4 The Levenberg-Marquardt Method

The Levenberg-Marquardt algorithm adaptively varies the coefficient updates between the gradient descent update and the Gauss-Newton update,

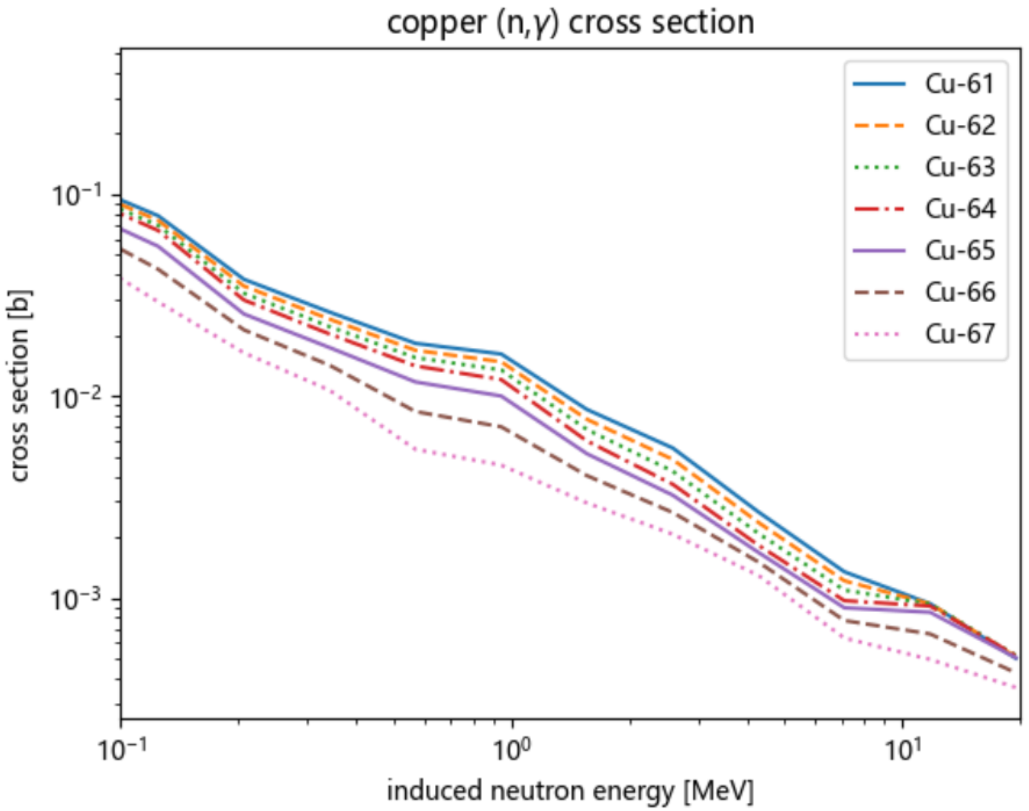
$$\left[\boldsymbol{J}^{\mathsf{T}}\boldsymbol{W}\boldsymbol{J} + \lambda \boldsymbol{I}\right] \boldsymbol{h}_{\mathsf{lm}} = \boldsymbol{J}^{\mathsf{T}}\boldsymbol{W}(\boldsymbol{y} - \hat{\boldsymbol{y}}) \ , \tag{12}$$

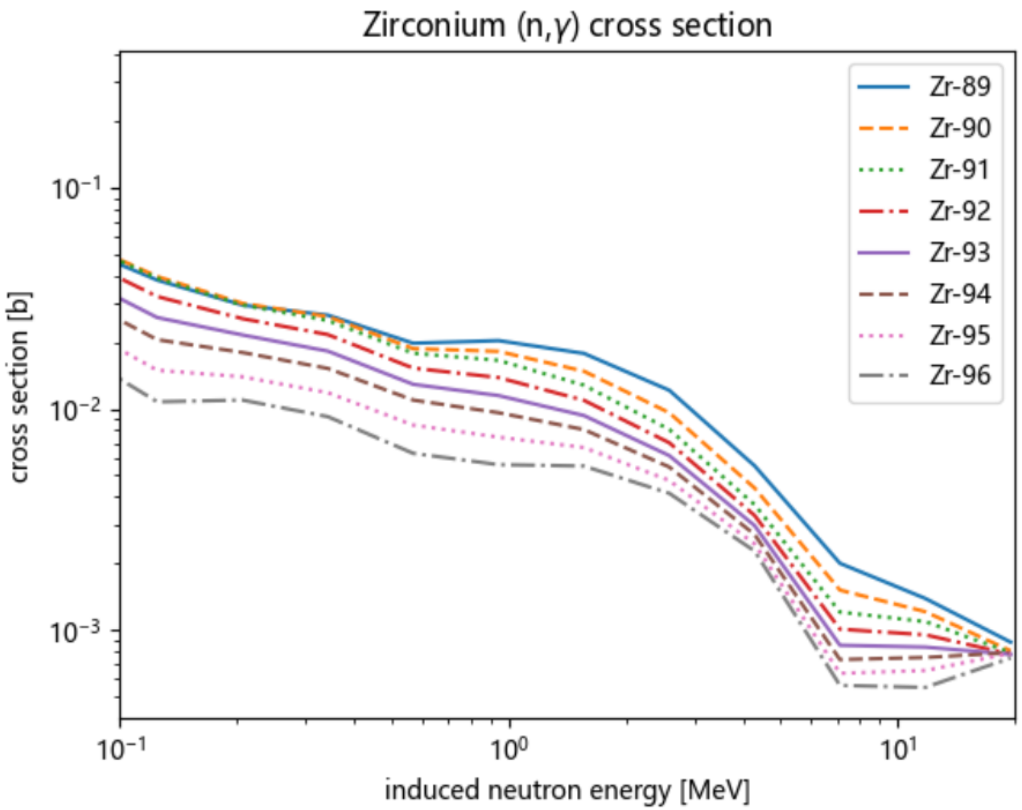
where small values of the *damping coefficient* λ result in a Gauss-Newton update and large values of λ result in a gradient descent update. The damping coefficient λ is initialized to be large so that first updates are small steps in the steepest-descent direction. If any iteration happens to result in a worse approximation ($\chi^2(\boldsymbol{a} + \boldsymbol{h}_{\mathsf{lm}}) > \chi^2(\boldsymbol{a})$), then λ is increased. Otherwise, as the solution improves, λ is decreased, the Levenberg-Marquardt method approaches the Gauss-Newton method, and the solution typically accelerates to the local minimum [8, 9, 10].

In Marquardt's update relationship [10], the damping coefficient λ is scaled by the diagonal of the Hessian $\boldsymbol{J}^{\mathsf{T}}\boldsymbol{W}\boldsymbol{J}$ for each coefficient.

$$\left[\boldsymbol{J}^{\mathsf{T}}\boldsymbol{W}\boldsymbol{J} + \lambda \, \mathsf{diag}(\boldsymbol{J}^{\mathsf{T}}\boldsymbol{W}\boldsymbol{J})\right] \boldsymbol{h}_{\mathsf{lm}} = \boldsymbol{J}^{\mathsf{T}}\boldsymbol{W}(\boldsymbol{y} - \hat{\boldsymbol{y}}) \ , \tag{13}$$

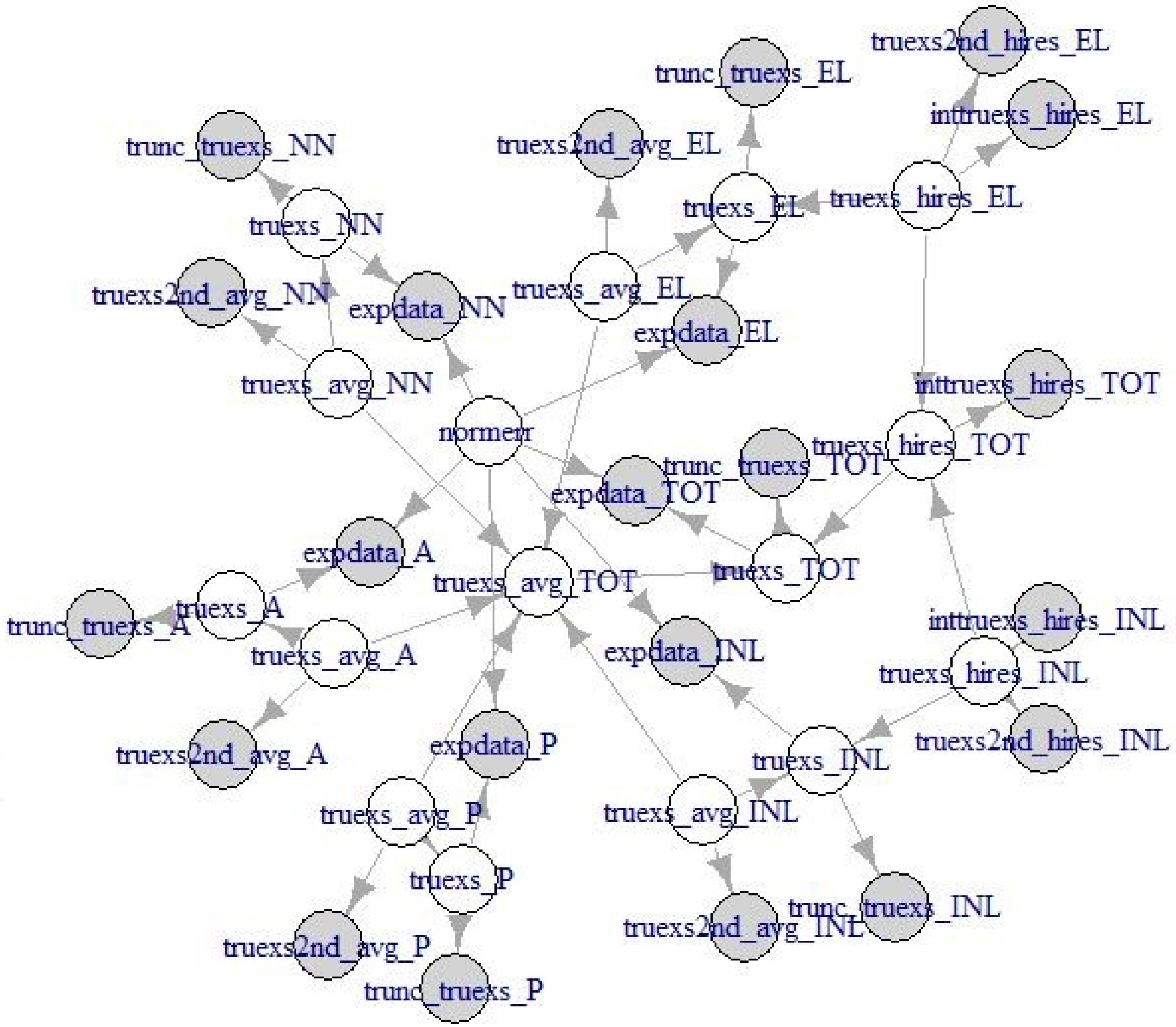
III. Results





Advantage: cross section predictions for nuclei lacking experimental measurements

Limitation: angular distributions and other quantities are beyond the capability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truexs2nd_avg_NN
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truexs_avg_NN
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normerr
truexs_hires_TOT
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expdata_INL
truexs_hires_INL
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expdata_P
truexs2nd_hires_INL
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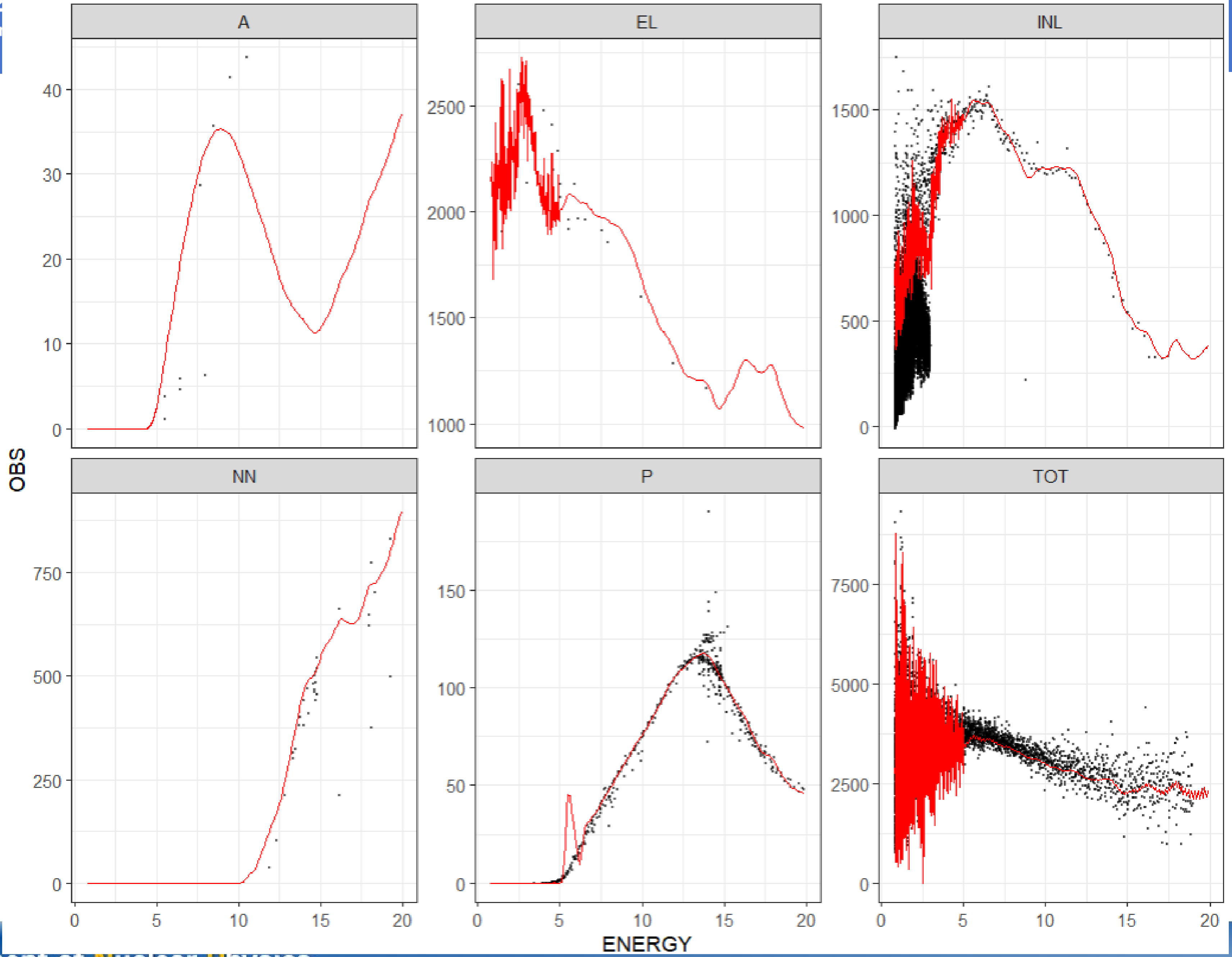
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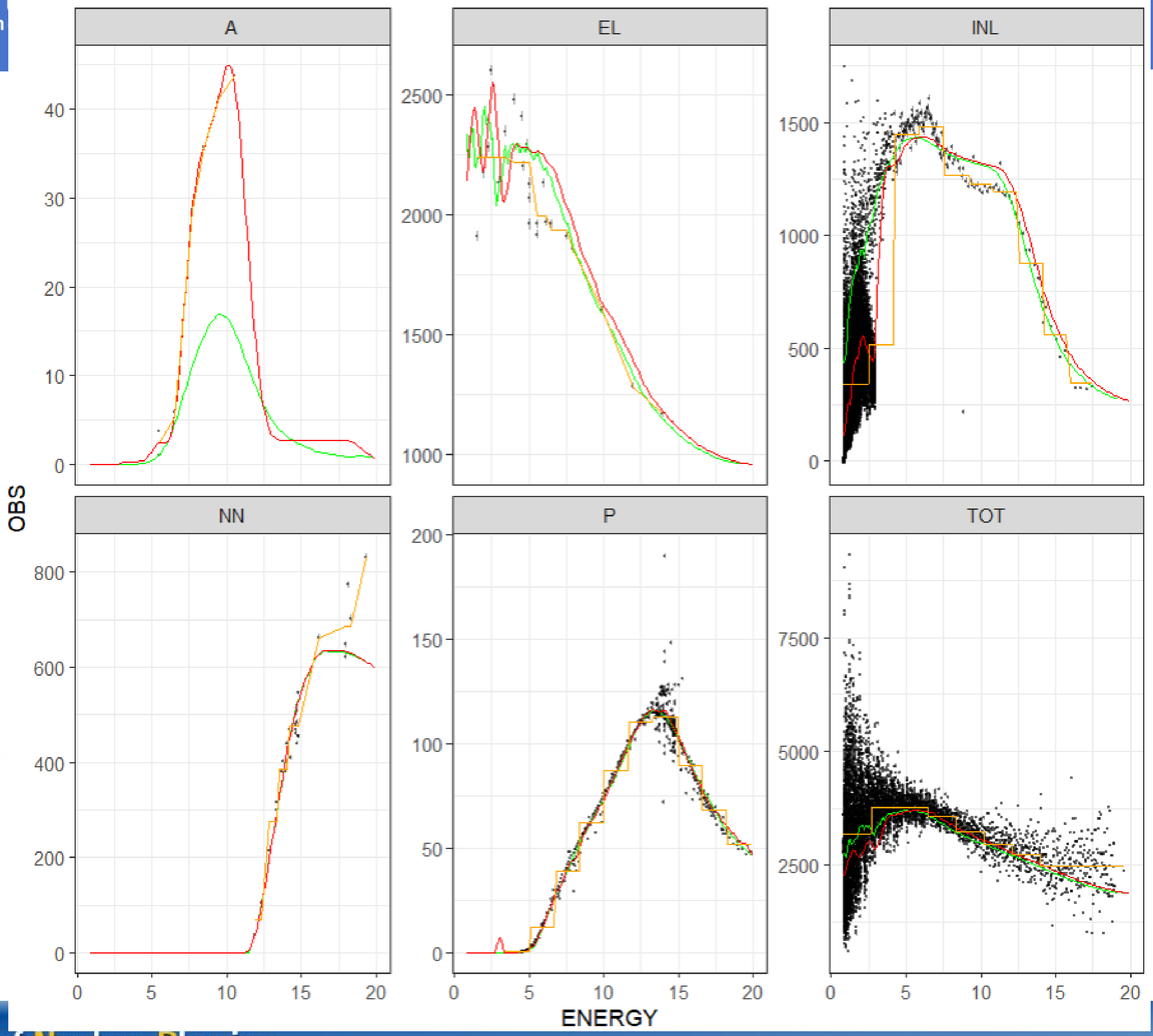
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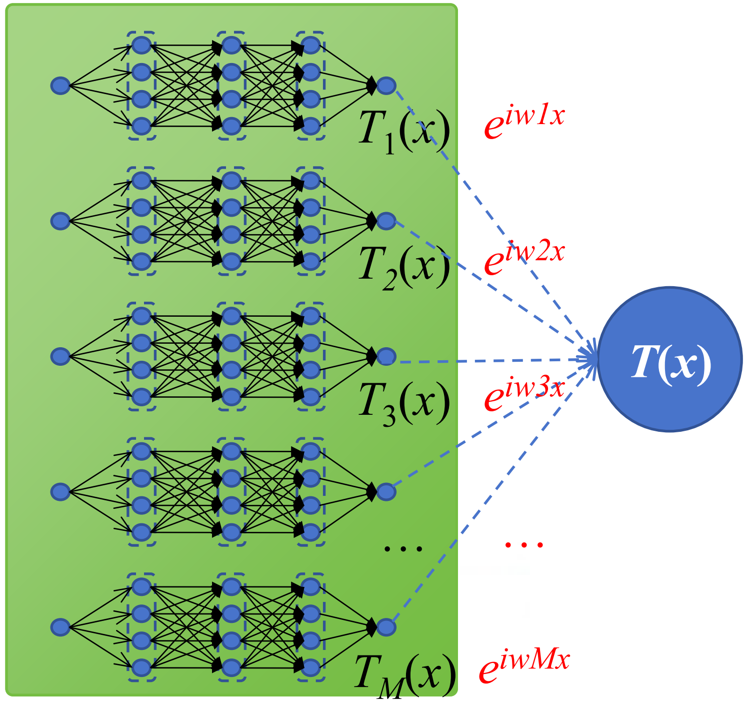
Summary

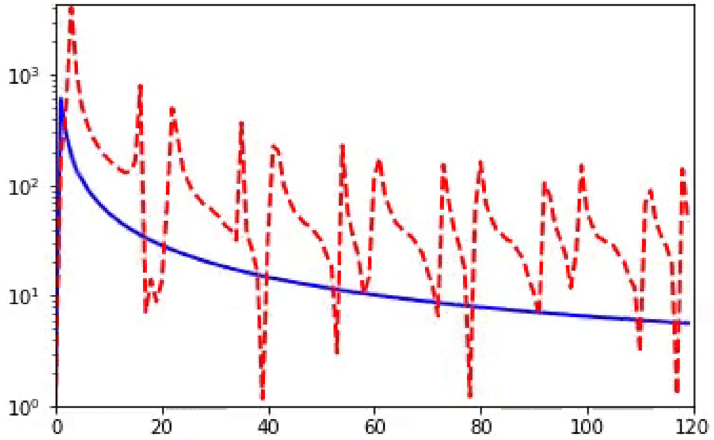
- Machine learning methods helps nuclear data research evolve.
- Machine learning offers practical tools for data processing and optimization algorithms.
- Our current neural network primarily focuses on cross section, but we plan to encompass other types of data in the future.
- Bayesian inference hold promise for studying uncertainties and covariances in nuclear data, warranting further attention.

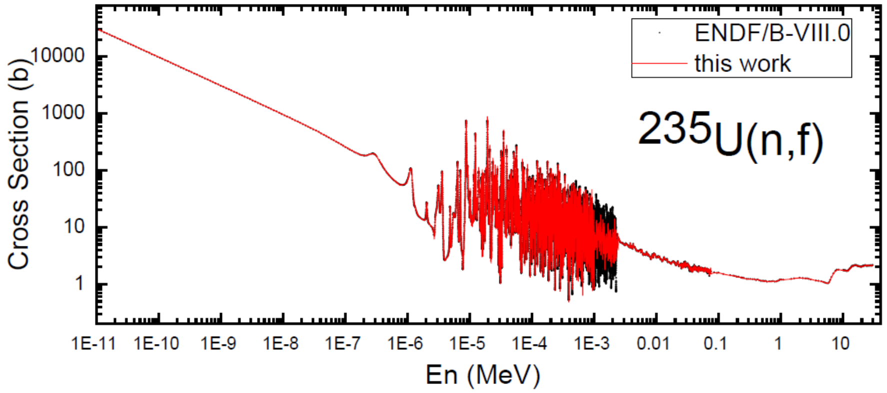
Phase Shift Deep Neural Network (PSDNN)

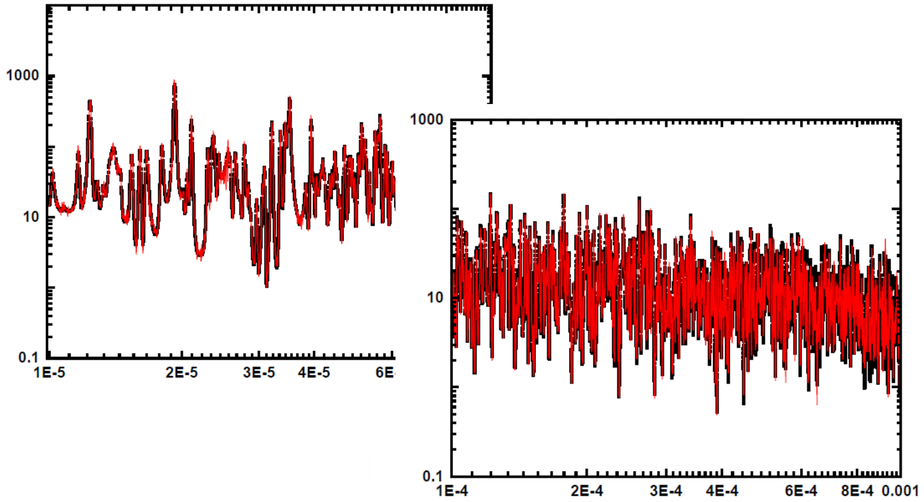
CHINA NUCLEAR DATA CENTER   GXNU   北京应用物理与计算数学研究所 Institute of Applied Physics and Computational Mathematics



Frequency principle: Deep learning tends to prioritize fitting the low-frequency component of the objective function.







Physics Letters B, 855 138825, 857 138978.

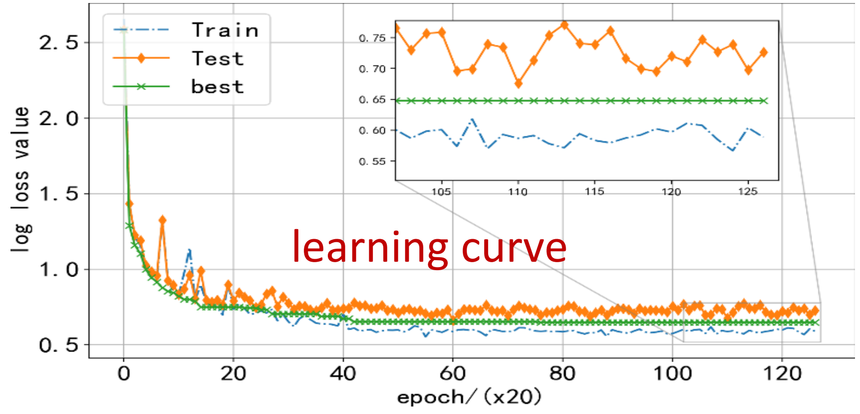
The neural network acquires the capability to learn the resonance cross section of rapid oscillations, thereby enriching the investigative techniques employed in nuclear data.

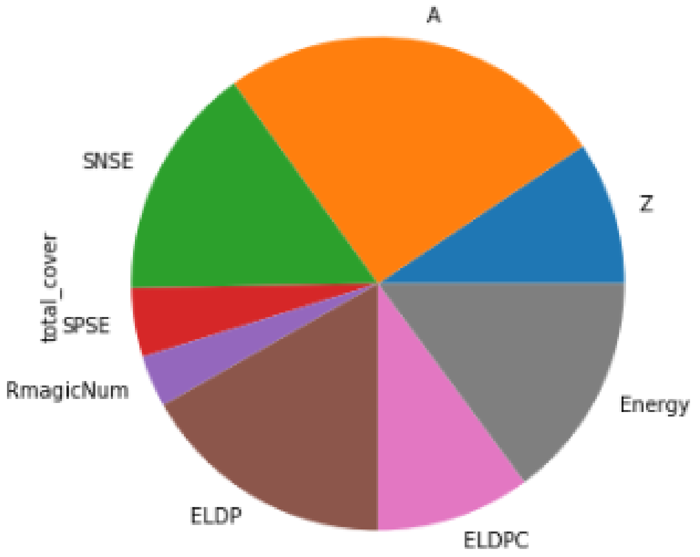
Systematic study of (n,2n) cross section adopting ANN and DT

CHINA NUCLEAR DATA CENTER

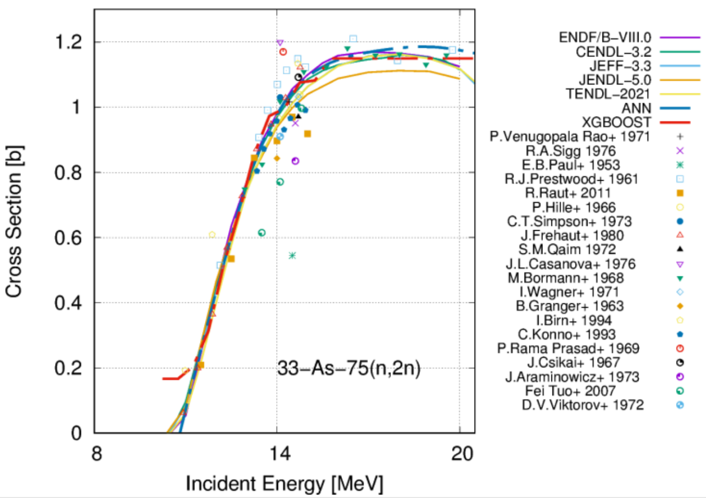
China nuclear industry college

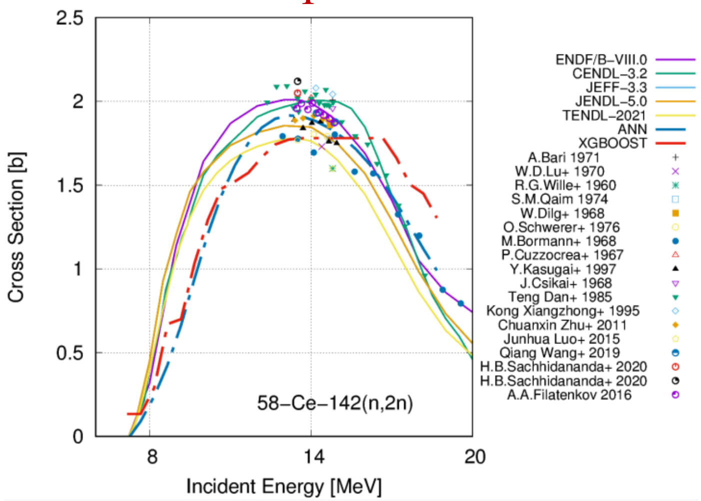
The proportion of data exhibiting a prediction deviation of less than 10% surpasses 85%, enabling the successful calculation of covariance for cross-sectional data predictions across various energy levels.





Comparison of ML results, evaluation and experimental data





EPJ Conferences, 294, 04008 (2024)

Machine learning techniques uncover systematic patterns within nuclear reaction cross sections.

THANK YOU!