Isotope Stability Classifier

Nicholas March

4/24/2024

Rensselaer200

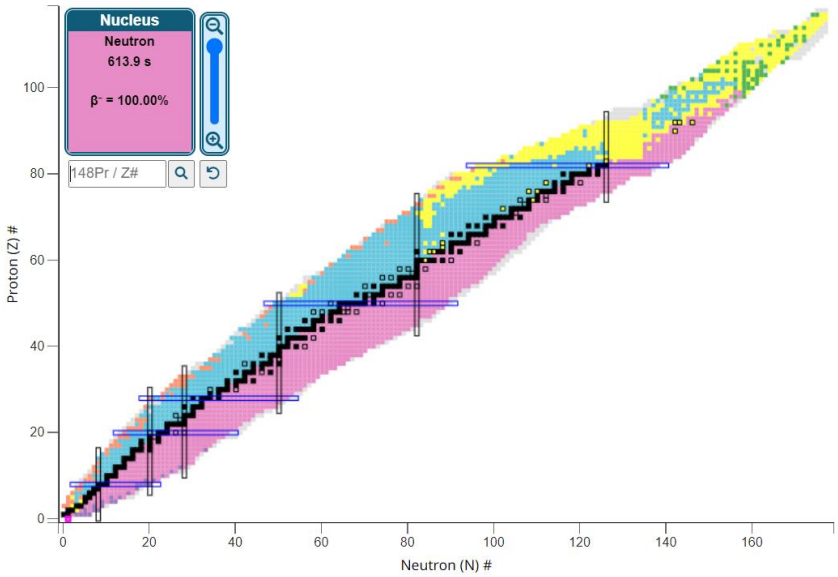
Agenda

- Background and Objective
- Feature and Class Selection
- Data Preprocessing and Visualization
- Classification Scheme
- Results and Analysis

Background

NuDat 3.0 and the Chart of Nuclides

- Comprehensive online database containing up-to-date properties for the entire Chart of Nuclides.
- Maintained by National Nuclear Data Center at Brookhaven National Lab.
- Provides information about atomic structure, stability and radioactivity, nuclear reactions, etc..



Objective: Produce a classification model capable of predicting decay type.

Feature and Class Selection

Features:

- Proton number (Z)
- Mass number (A)
- Neutron to Proton Ratio (N/Z)
- Mass defect (M - A)

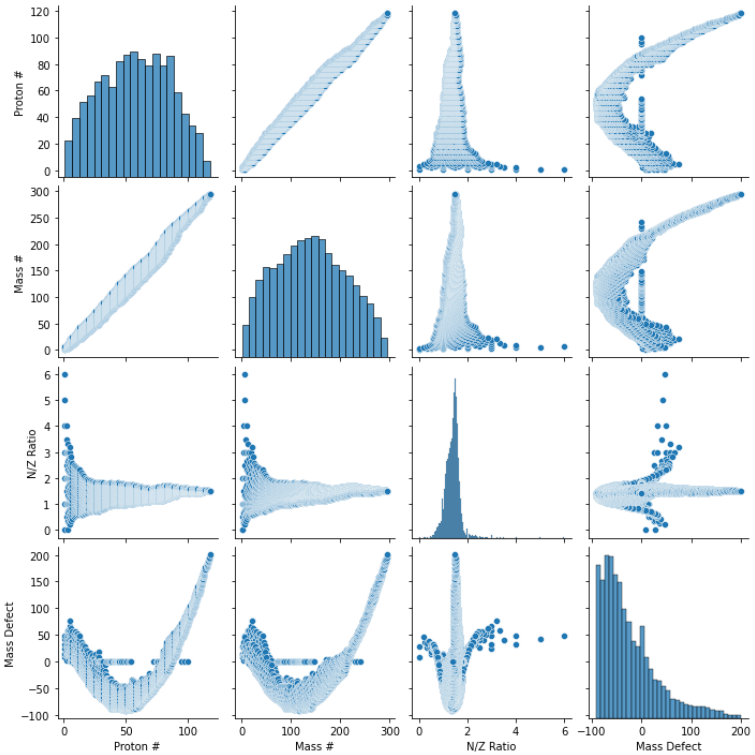
Classes:

- Stable
- Beta minus decay (B^-)
- Neutron decay (N)
- Alpha decay (A)
- Proton emission (P)
- Electron Capture (EC)
- Spontaneous Fission (SF)
- Other

Data Preprocessing

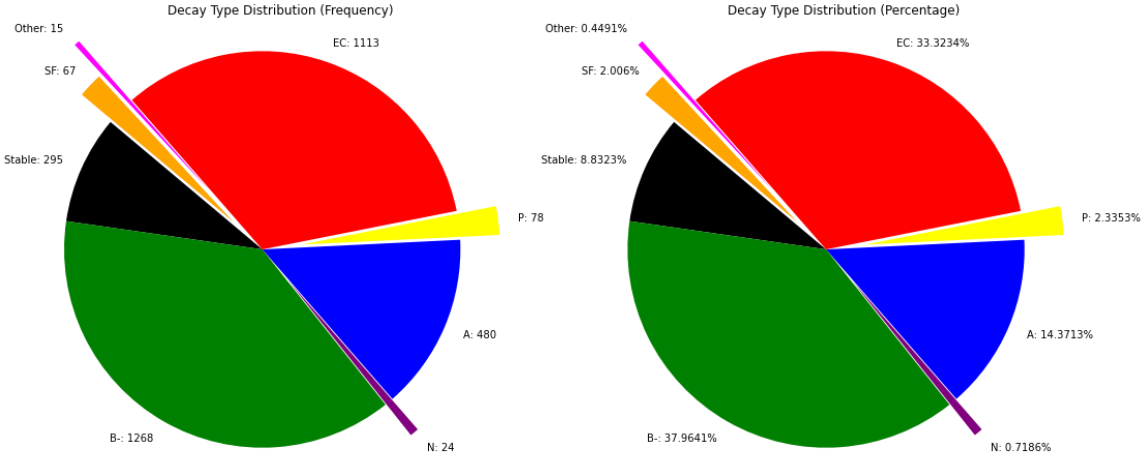
1. Feature and label data extracted from nuclear_data package as two lists.
2. Decays besides primary are removed from label data.
3. Multi-emissions/rare labels consolidated.
4. LabelEncoder() applied to label data.
5. All data recast as numpy arrays.
6. Data split into training and testing arrays.
7. Model weighting set to “balanced” when applicable to account for label imbalance.

Data Visualization



Feature Pair Plot

Feature Training Data Shape: (2338, 4)
Feature Testing Data Shape: (1002, 4)
Target Training Data Shape: (2338,)
Target Testing Data Shape: (1002,)

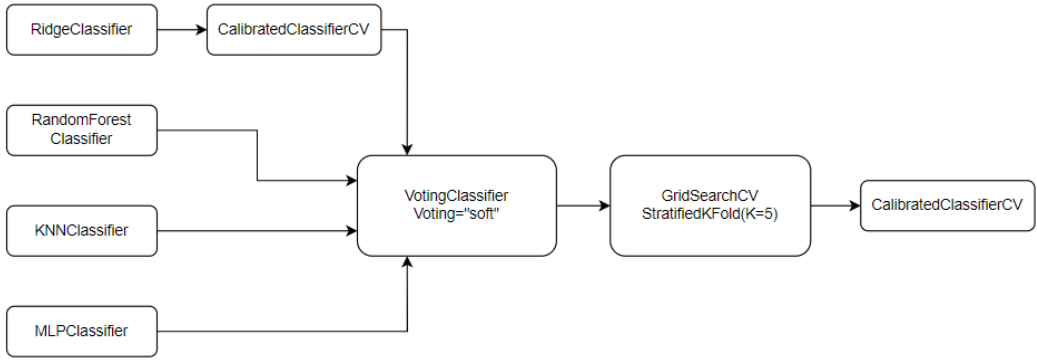


Class Distribution

Classification Scheme

Parameter Space:

- Ridge: alpha [0.1, 1.0, 10.0]
- RF: n_estimators [50, 100, 200]
- RF: max_depth [None, 10, 20, 30]
- KNN: n_neighbors [3, 5, 7, 10]
- MLP: lr_init [0.001, 0.01, 0.1]
- MLP: hidden_layers [(64,), (128,), (128, 64), (256, 128, 64)]



Best Model:

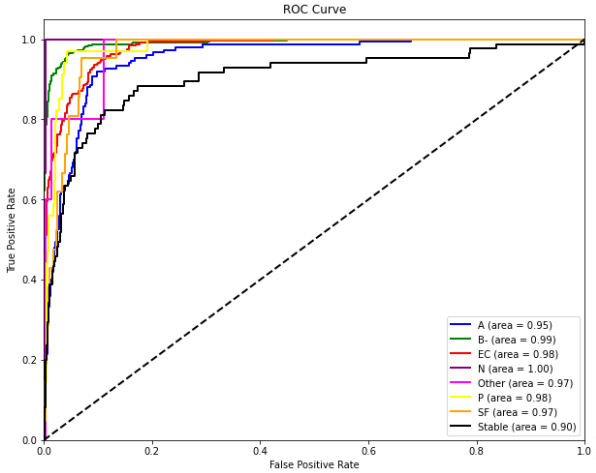
Ridge(alpha=10), RandomForest(max_depth=10, n_estimators=50)

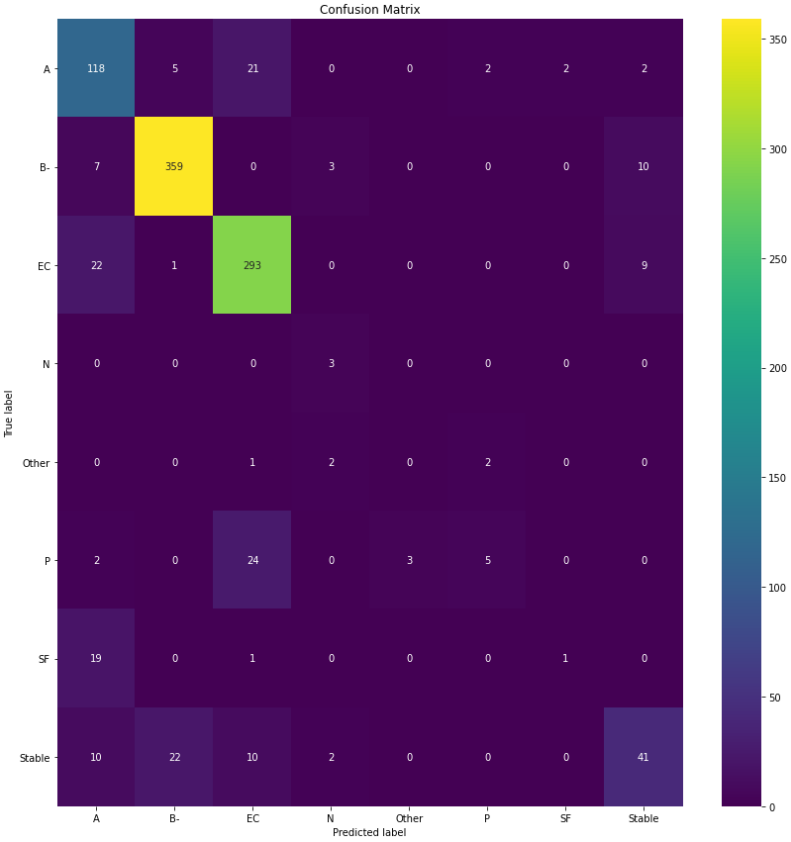
KNN(n_neighbors=7), MLP(lr_init=0.001, hidden_layers=(256, 128,64))

Results and Analysis

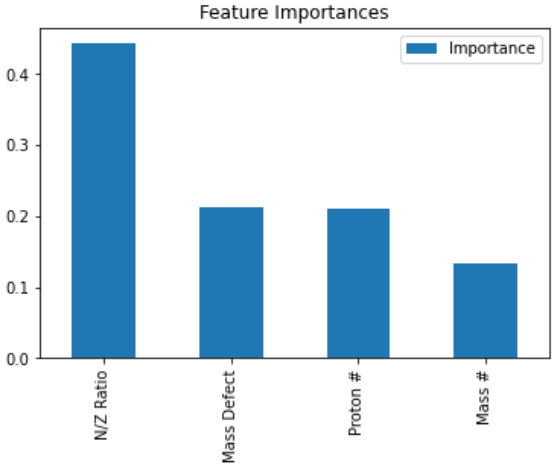
Log Loss: 0.50228

Mean Brier Score: 0.03086

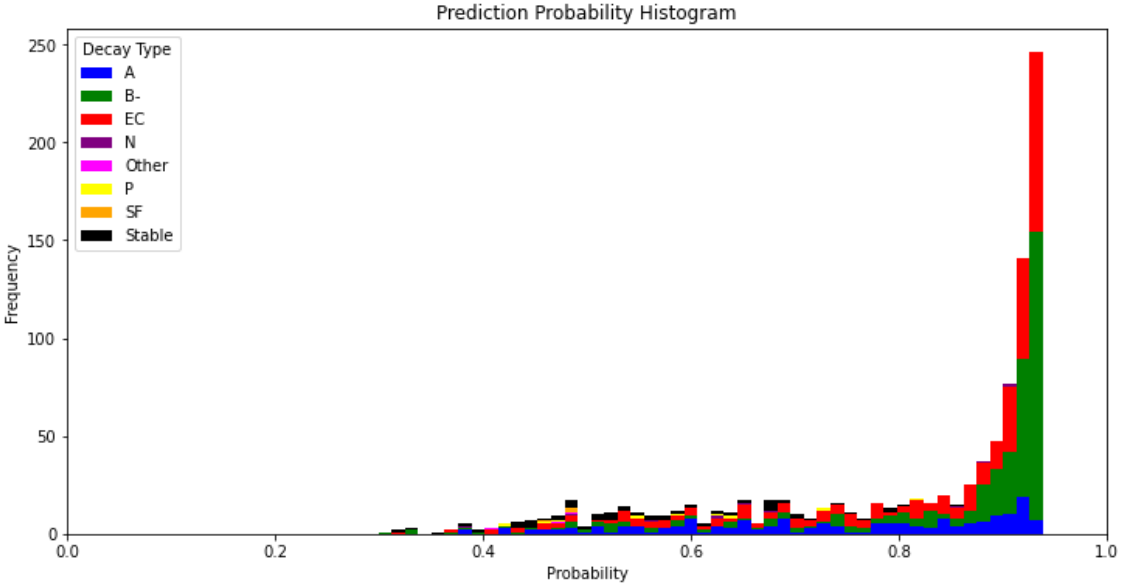


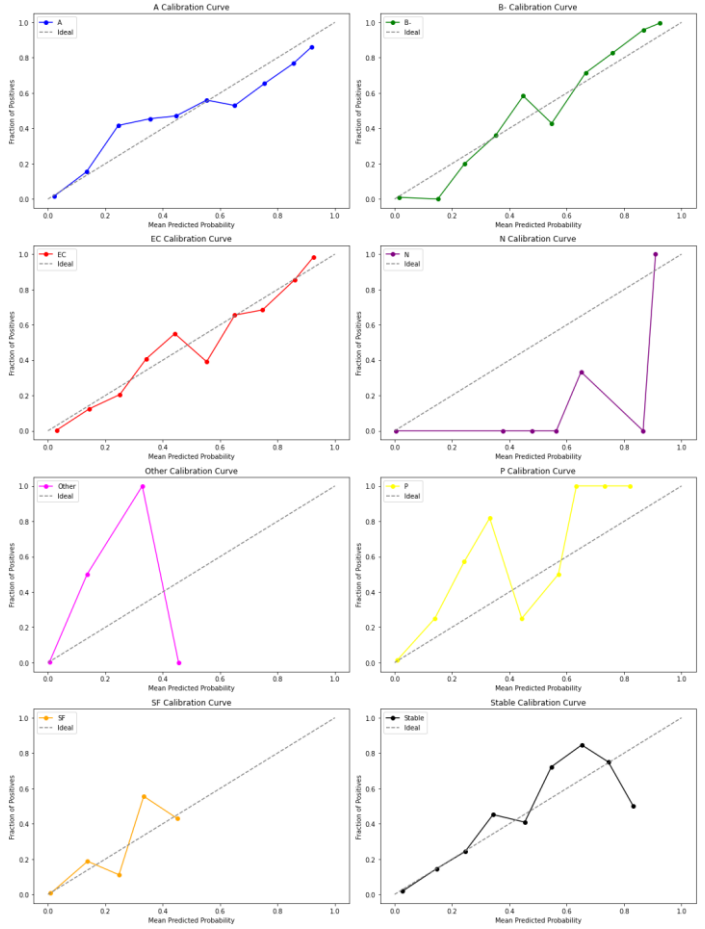


	precision	recall	f1-score	support
A	0.66	0.79	0.72	150
B-	0.93	0.95	0.94	379
EC	0.84	0.90	0.87	325
N	0.30	1.00	0.46	3
Other	0.00	0.00	0.00	5
P	0.56	0.15	0.23	34
SF	0.33	0.05	0.08	21
Stable	0.66	0.48	0.56	85
accuracy			0.82	1002
macro avg	0.53	0.54	0.48	1002
weighted avg	0.80	0.82	0.80	1002

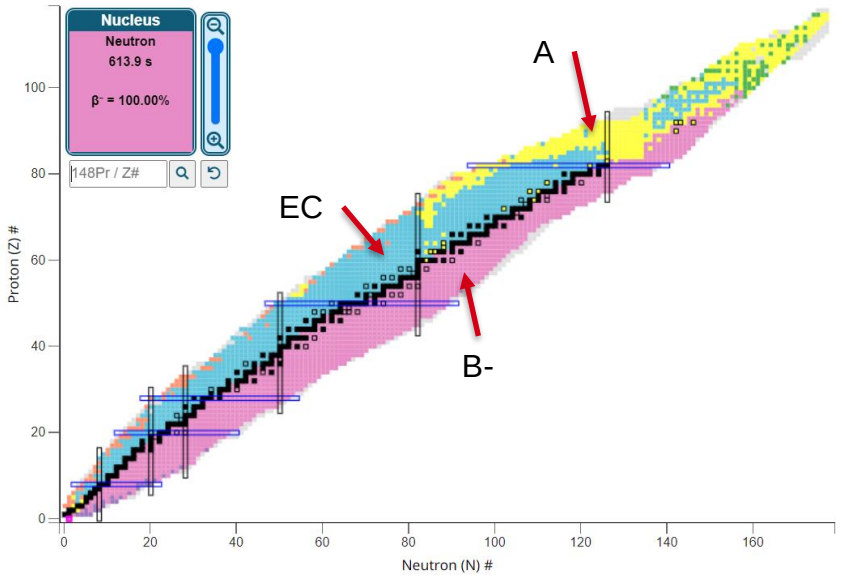


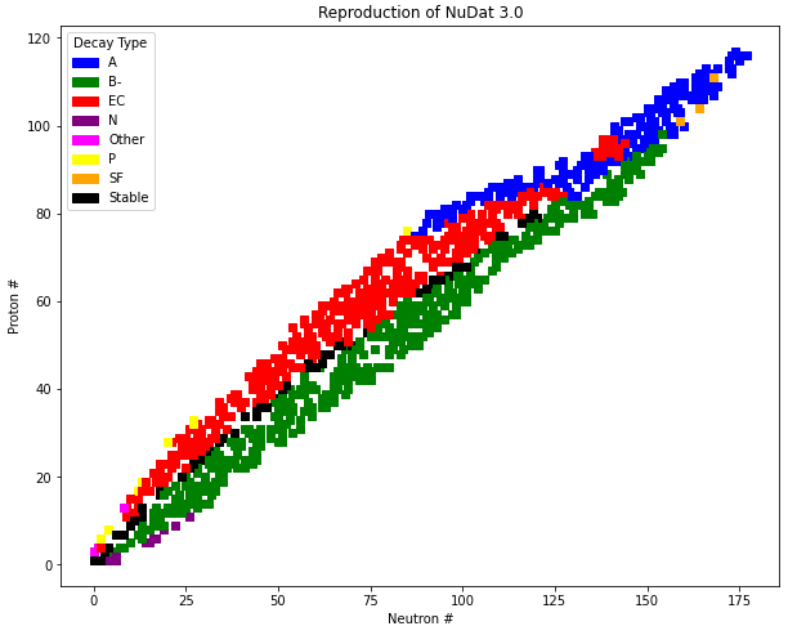
Results and Analysis





NuDat 3.0 Reproduction





References

- NuDat 3, Brookhaven National Lab, https://www.nndc.bnl.gov/nudat3/
- A. Boehnlein et al., “Colloquium: Machine learning in nuclear physics,” Reviews of Modern Physics, vol. 94, no. 3, Sep. 2022. doi:10.1103/revmodphys.94.031003
- L. Neufcourt, Y. Cao, W. Nazarewicz, and F. Viens, “Bayesian approach to model-based extrapolation of nuclear observables,” Physical Review C, vol. 98, no. 3, Sep. 2018. doi:10.1103/physrevc.98.034318
- Z. M. Niu, H. Z. Liang, B. H. Sun, W. H. Long, and Y. F. Niu, “Predictions of nuclear β-Decay Half-Lives with Machine Learning and Their Impact on r-process Nucleosynthesis,” Physical Review C, vol. 99, no. 6, Jun. 2019. doi:10.1103/physrevc.99.064307
- U. B. Rodríguez, C. Z. Vargas, M. Gonçalves, S. B. Duarte, and F. Guzmán, “Alpha half-lives calculation of superheavy nuclei with q α -value predictions based on the Bayesian neural network approach,” Journal of Physics G: Nuclear and Particle Physics, vol. 46, no. 11, p. 115109, Oct. 2019. doi:10.1088/1361-6471/ab2c86
- Morgan, Dane, et al. “Machine Learning in Nuclear Materials Research.” arXiv.Org, 16 Nov. 2022, arxiv.org/abs/2211.09239.
- “Scientific Machine Learning for Nuclear Engineering.” American Nuclear Society, www.ans.org/meetings/mc2021/session/view-793/.

Rensselaer200