Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

Automating neutron resonances classification with Machine Learning

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[7]Georgia Institute of Technology, School of Physics

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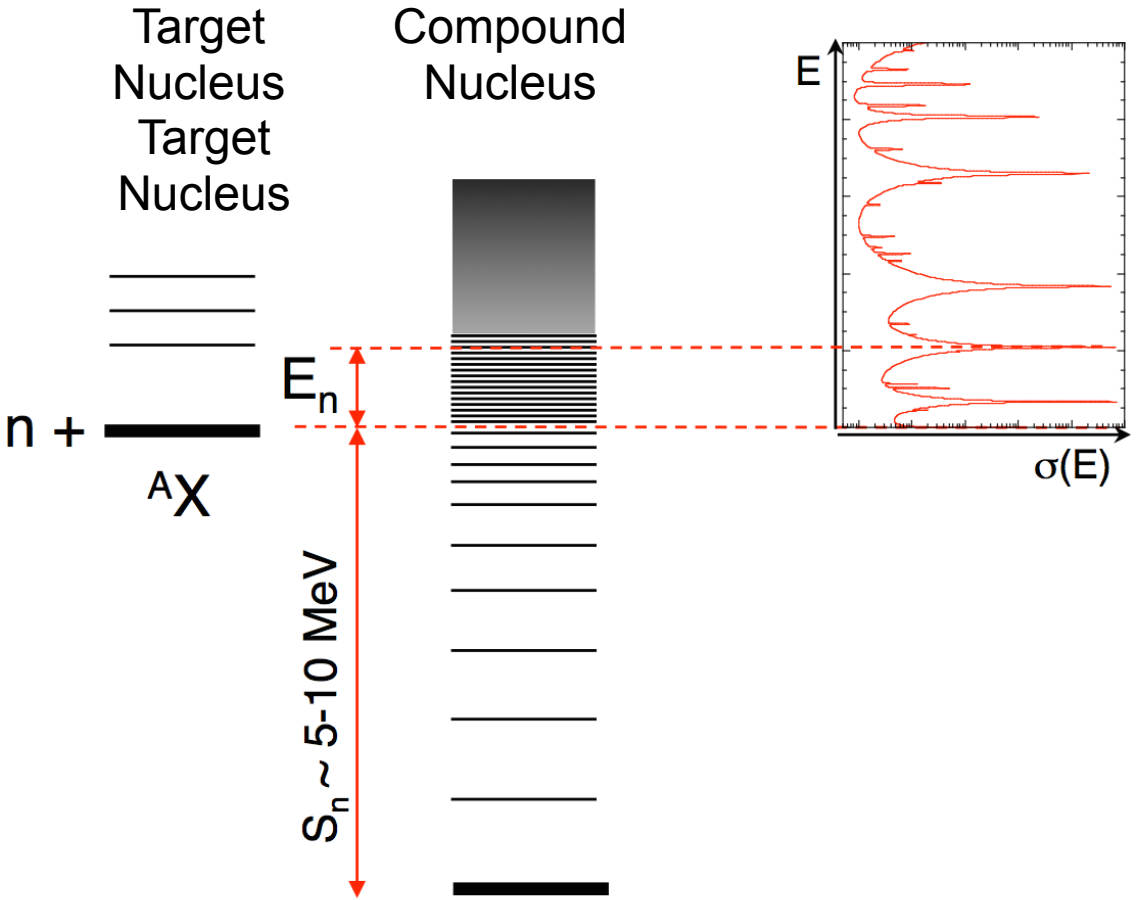
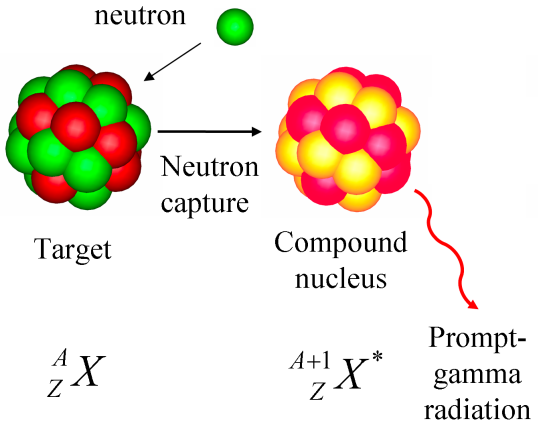
Nuclear Criticality Safety Program (NCSP)
Technical Program Review, February 15-17, 2022

Neutron Resonances





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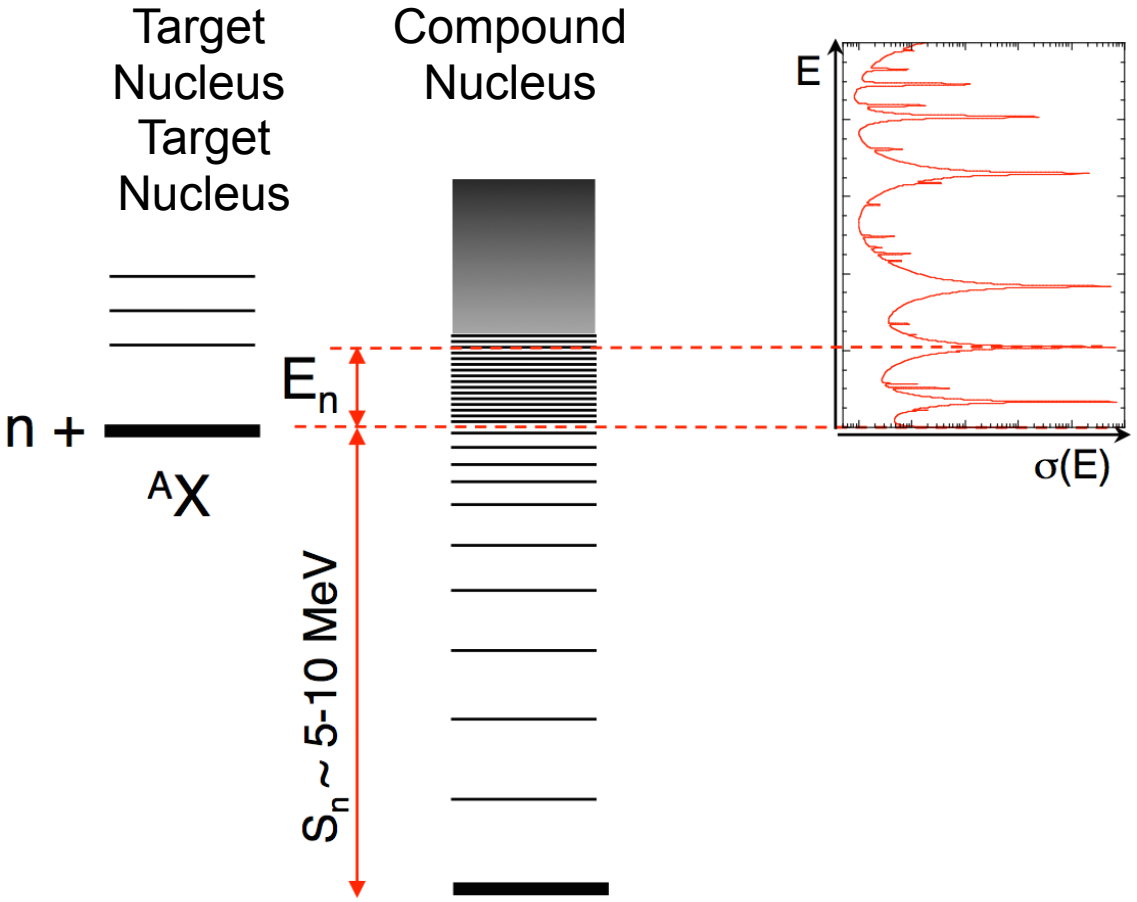

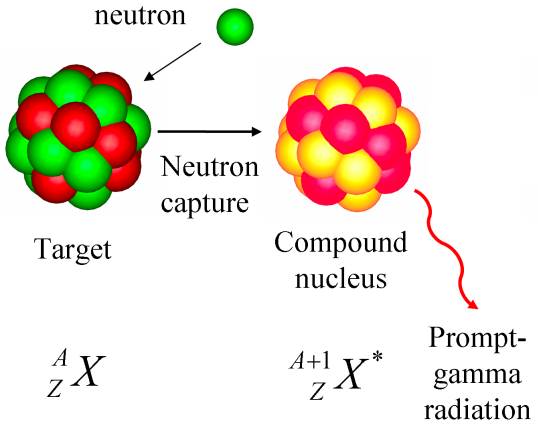

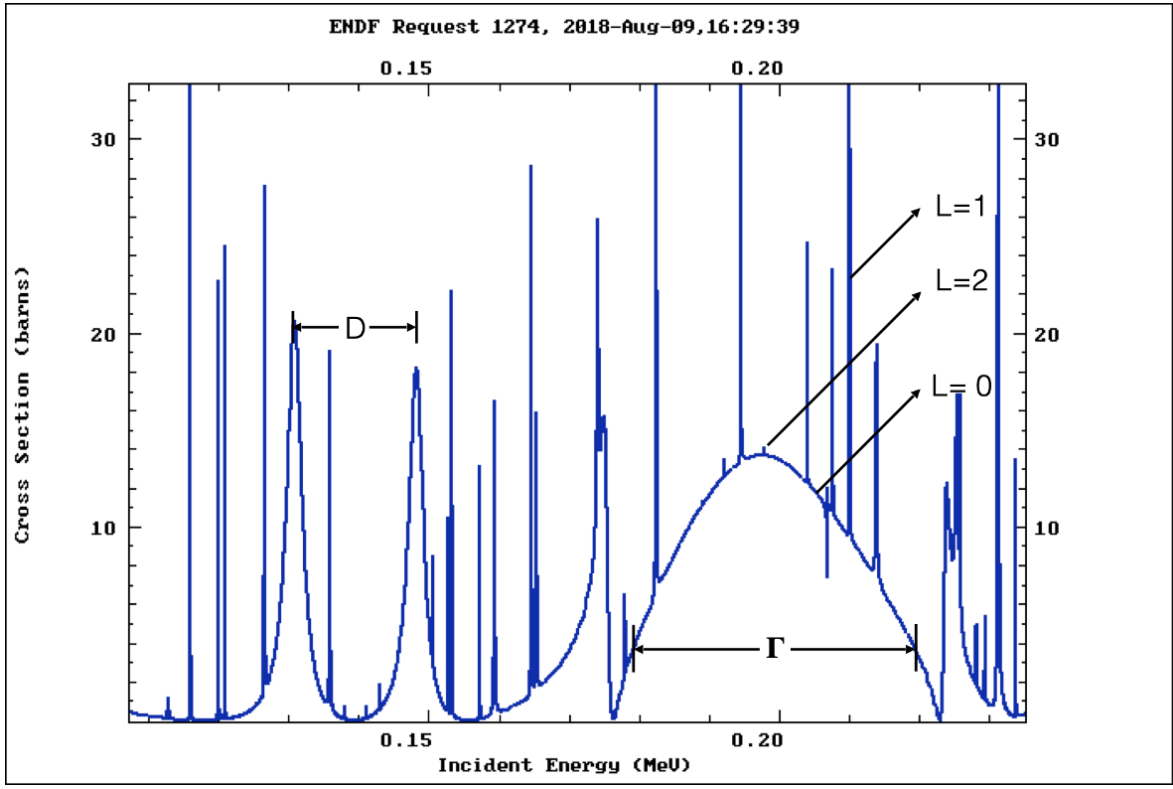

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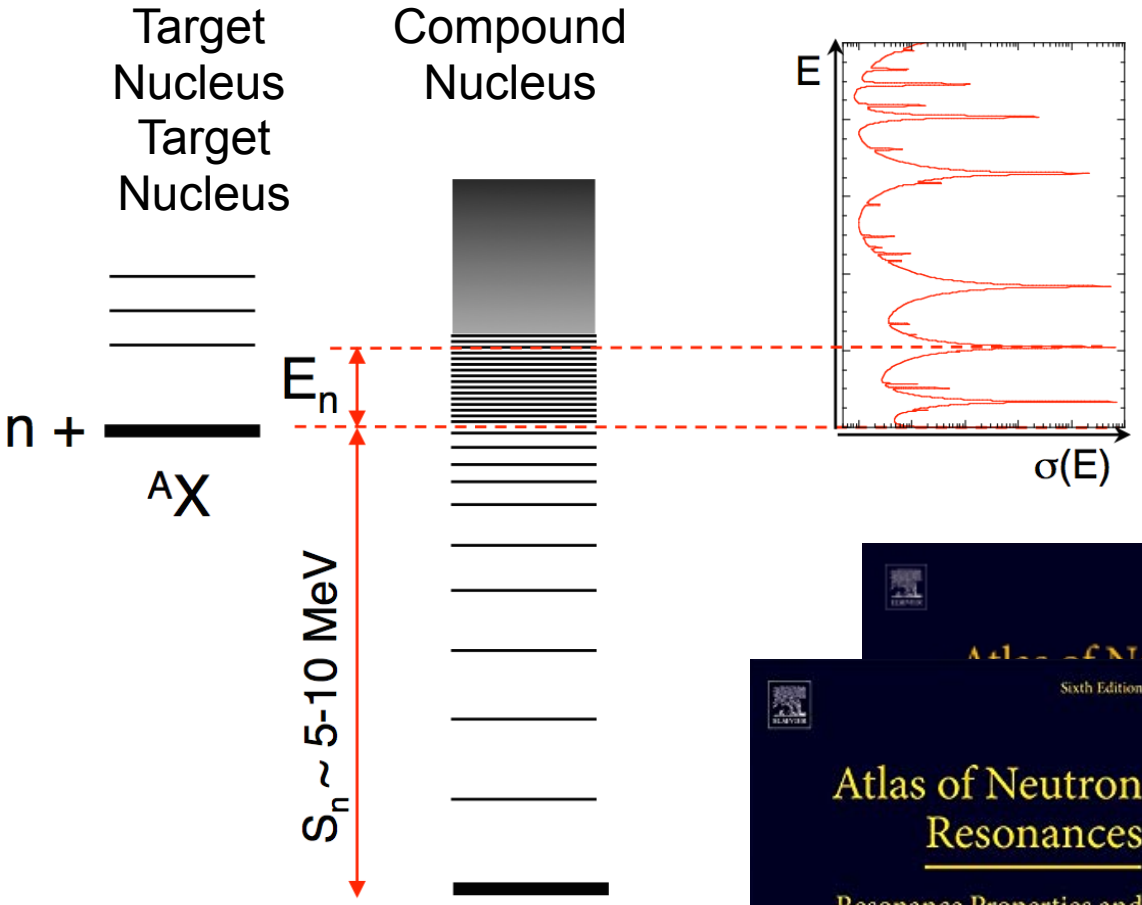
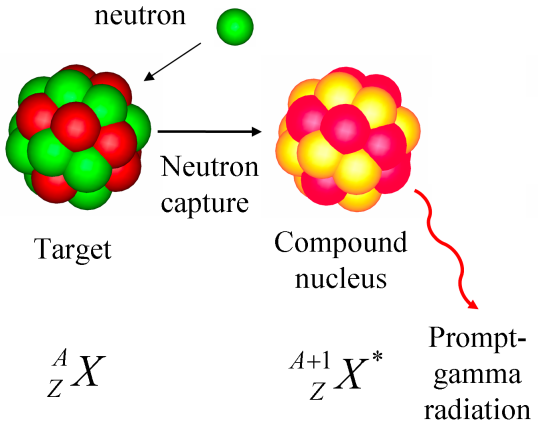
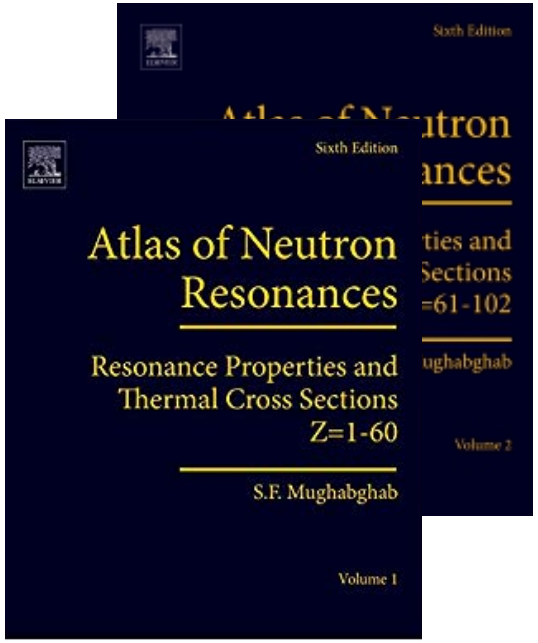
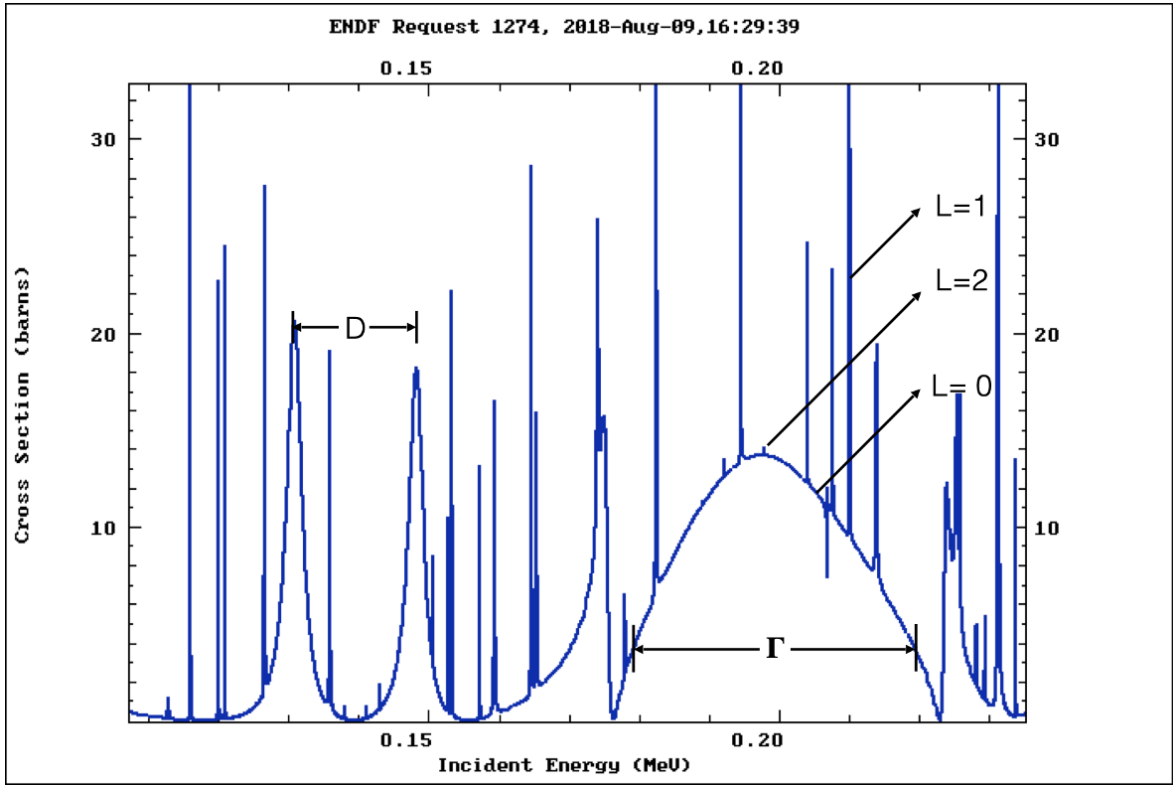






Published by Elsevier in 2018



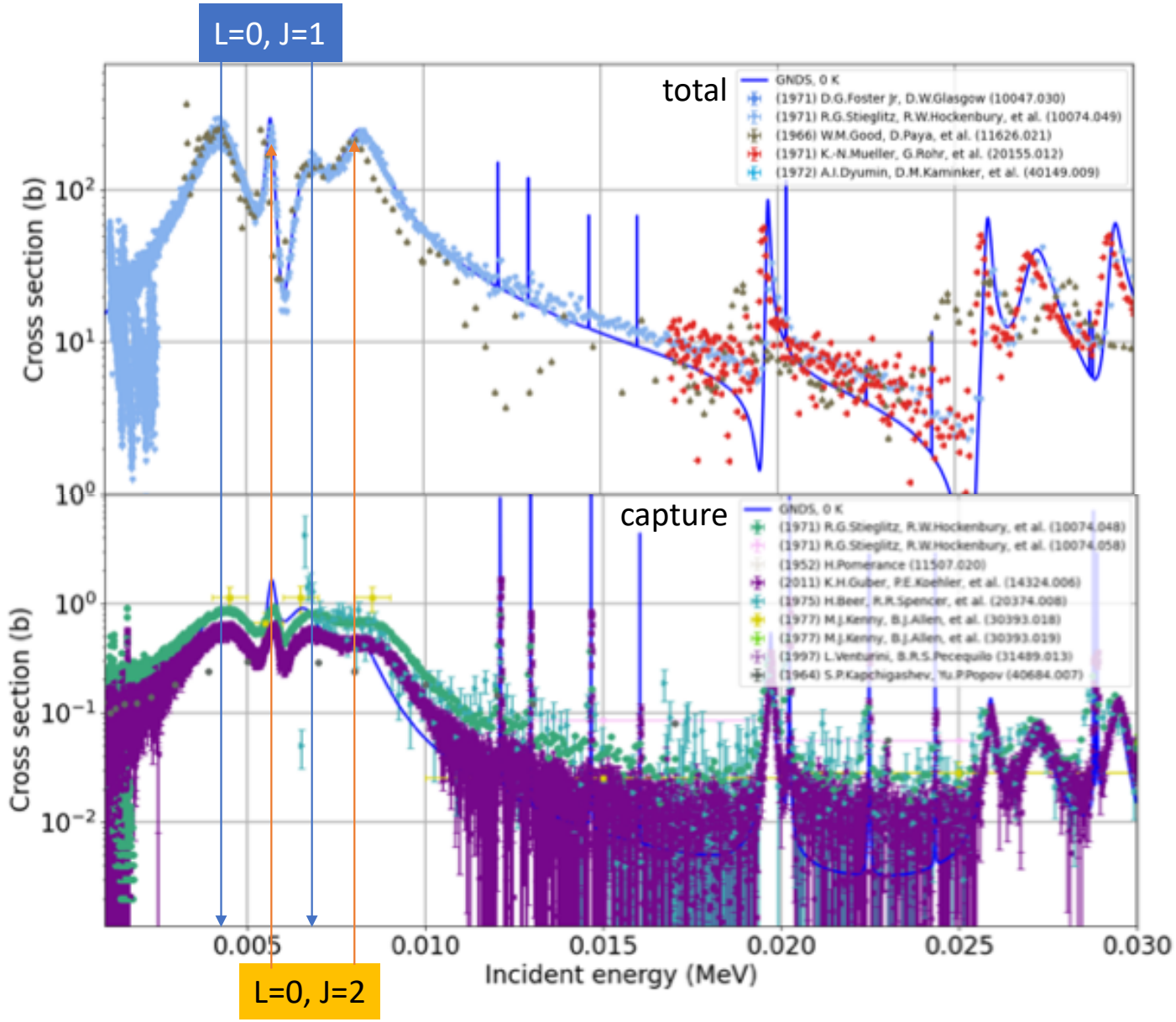
Traditional approach is to do a shape analysis

Near separation energy, use shape analysis to determine L

- Big resonances must be S-wave
- Interference helps

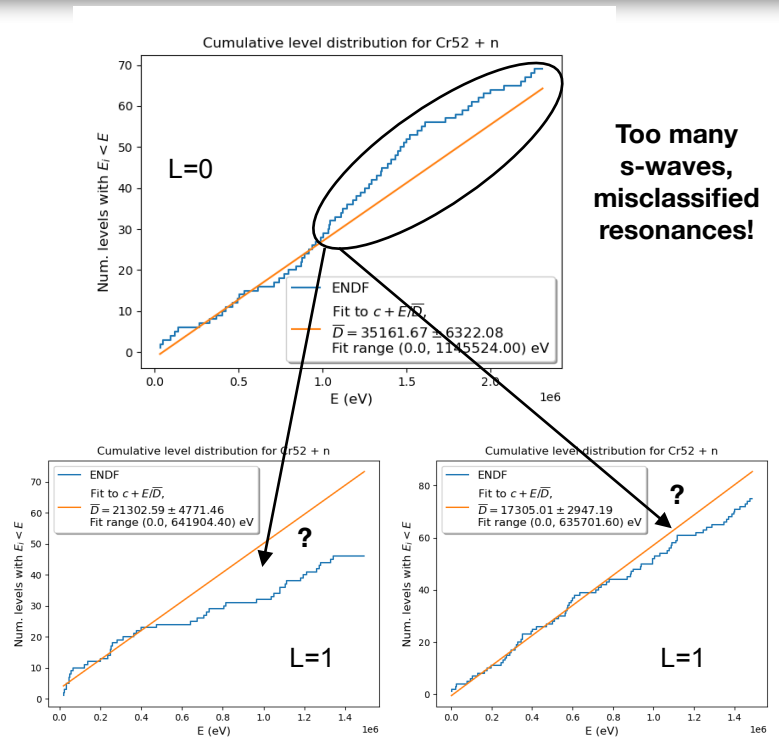
For J, need more information

- Angular distributions (n or γ)
- Gamma coincidences
- Polarization



Identifying resonance spin assignments is tricky

- Process of fitting R-matrix to data can be difficult, time consuming and may not be reproducible
- The Atlas is rife with misclassified resonances!
- Often done with trial, error and significant human intervention



Too many s-waves, misclassified resonances!

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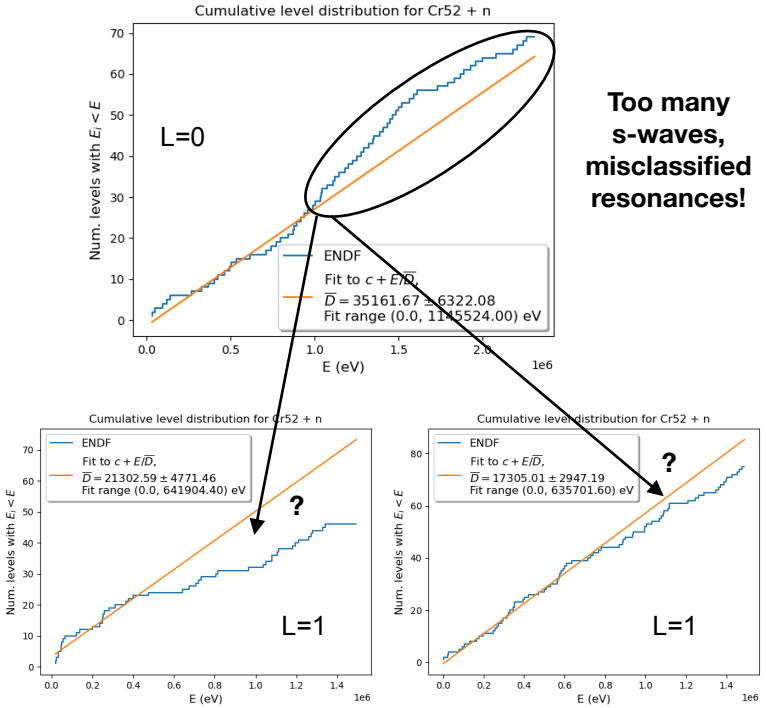

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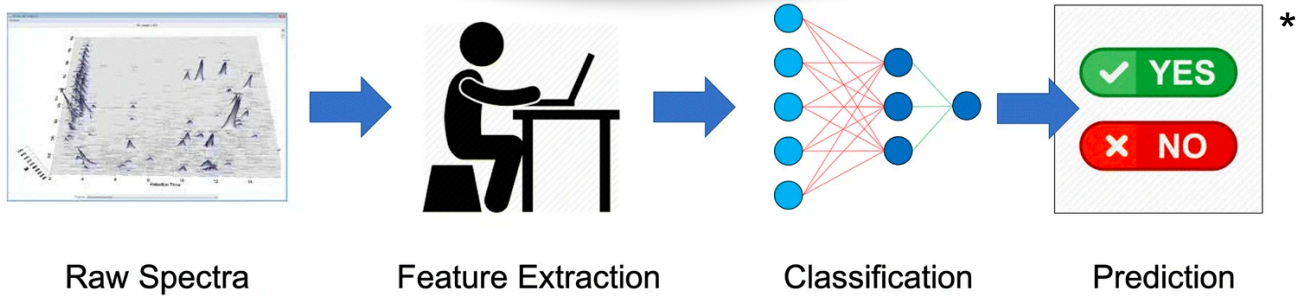
Machine Learning approach



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* Fig. taken from K.M. Mendez et al. *Metabolomics* **15,** 142 (2019) https://doi.org/10.1007/s11306-019-1608-0

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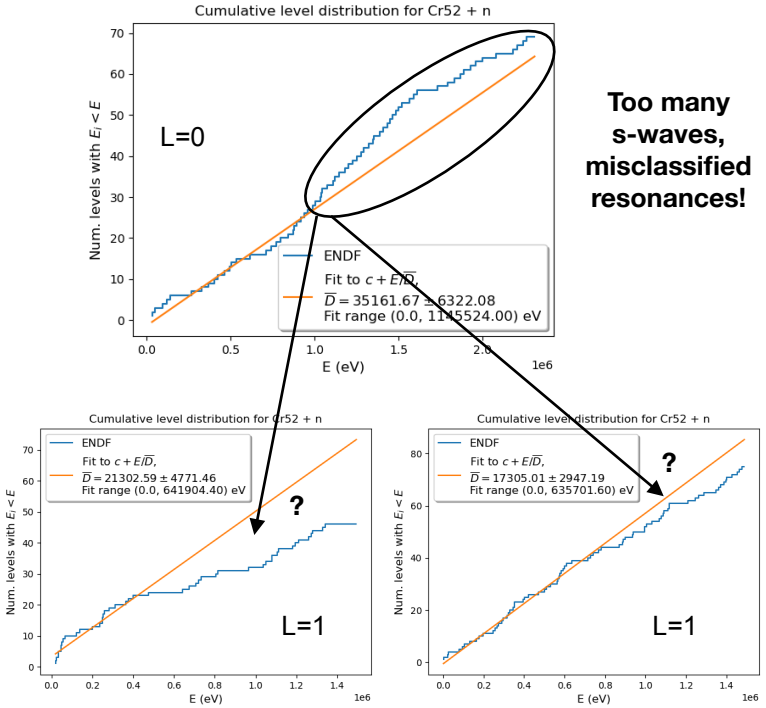

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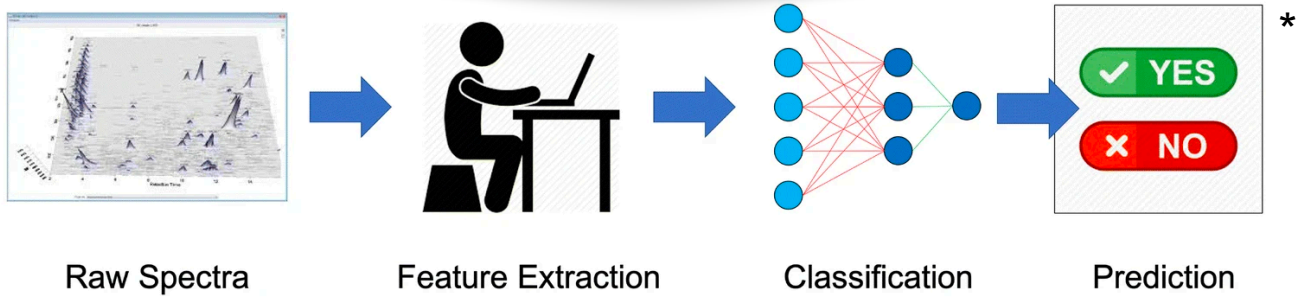

Lightweight scikit-learn classifiers + clever problem design may do the trick!

- **Simple and robust method**
- **Convert resonances into features**
- **Cannot train and test on real data:**
  - **Synthetic resonances based on the statistical properties of real nuclei**
  - **"Jumble" these sequences to mimic mis-assignments**
  - **Split jumbled data into training and test sets**
  - **Assess accuracy of predictions**
- **Apply trained algorithm to sequence of real experimental data**

* Fig. taken from K.M. Mendez et al. *Metabolomics* **15,** 142 (2019) https://doi.org/10.1007/s11306-019-1608-0

Progress in this past year

- We expanded this project in 5 (more or less) independent approaches, with intense collaboration from undergrad students:
  - **Feature impact**: Applied an additive metric to quantify the impact of features in the final classification decision (SHAP).
  - **Integration with the Atlas**: Integrated the evaluated resonance data from the Atlas with the data objects used by our code to process sequences of resonances.
  - **Training optimization**: Performed grid search of the hyperparameters associated with the different machine-learning classifiers.
  - **Spacings systematics**: Investigated the use running averages of resonance spacings to identify missing resonances.
  - **Validation with polarized data**: Used resonance data obtained from polarized neutron experiments for validation of the machine-learning method.
- BNL lab report: **BNL-222202-2021-INRE**

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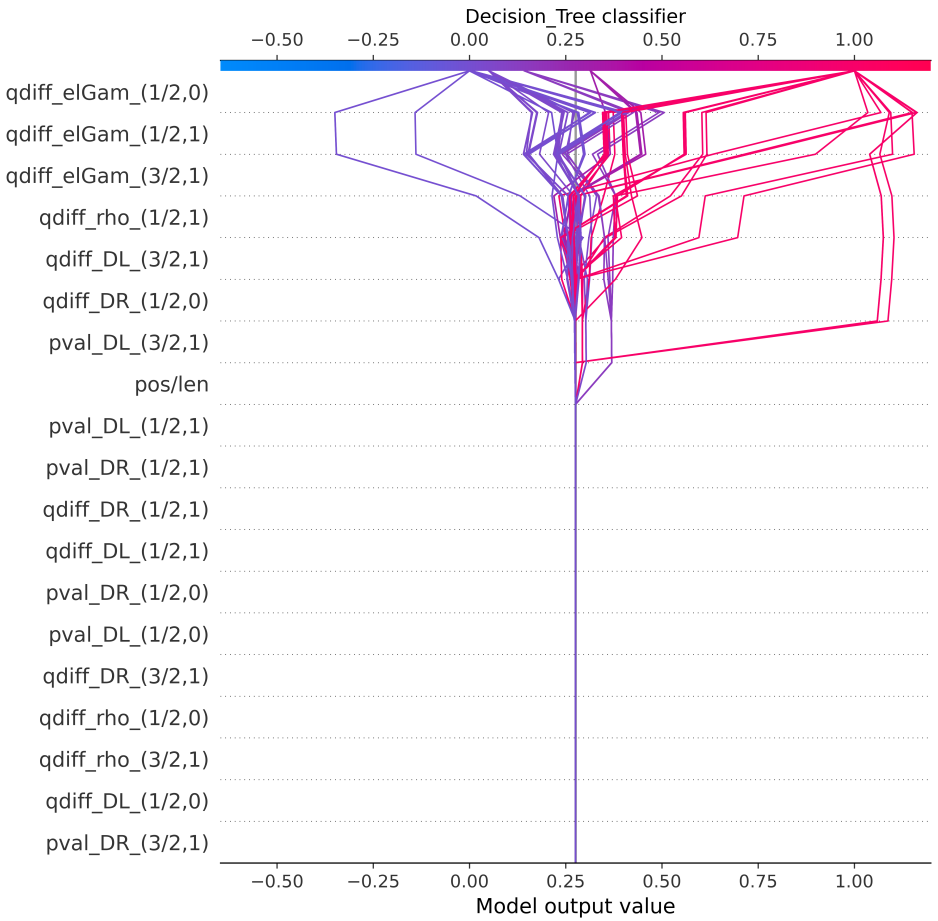
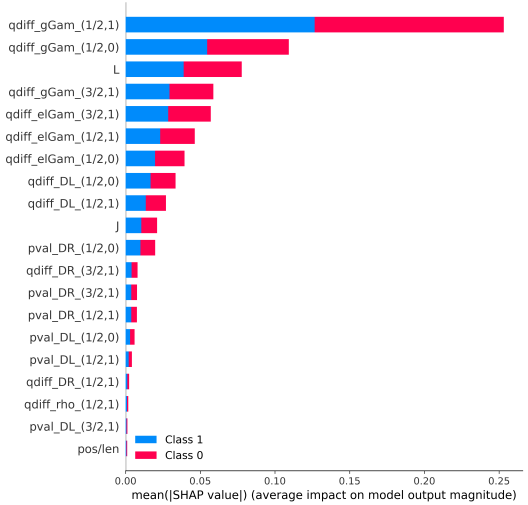
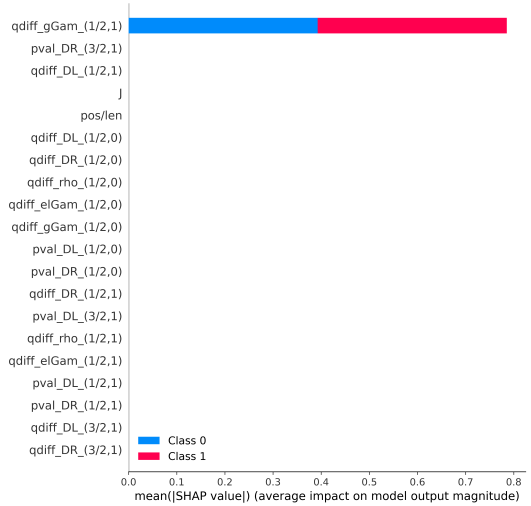
Analysis of feature impact in classification

- Preliminary tests with an initial set of features using Decision Trees and Random Forests have shown signs of overfitting
- Used SHapley Additive exPlanations (SHAP) to quantify this
- Identified many unimportant features and an over-reliance on features related to Γ_γ
- <u>Redefined set of features and implemented option to turn on and off Γ_γ</u>







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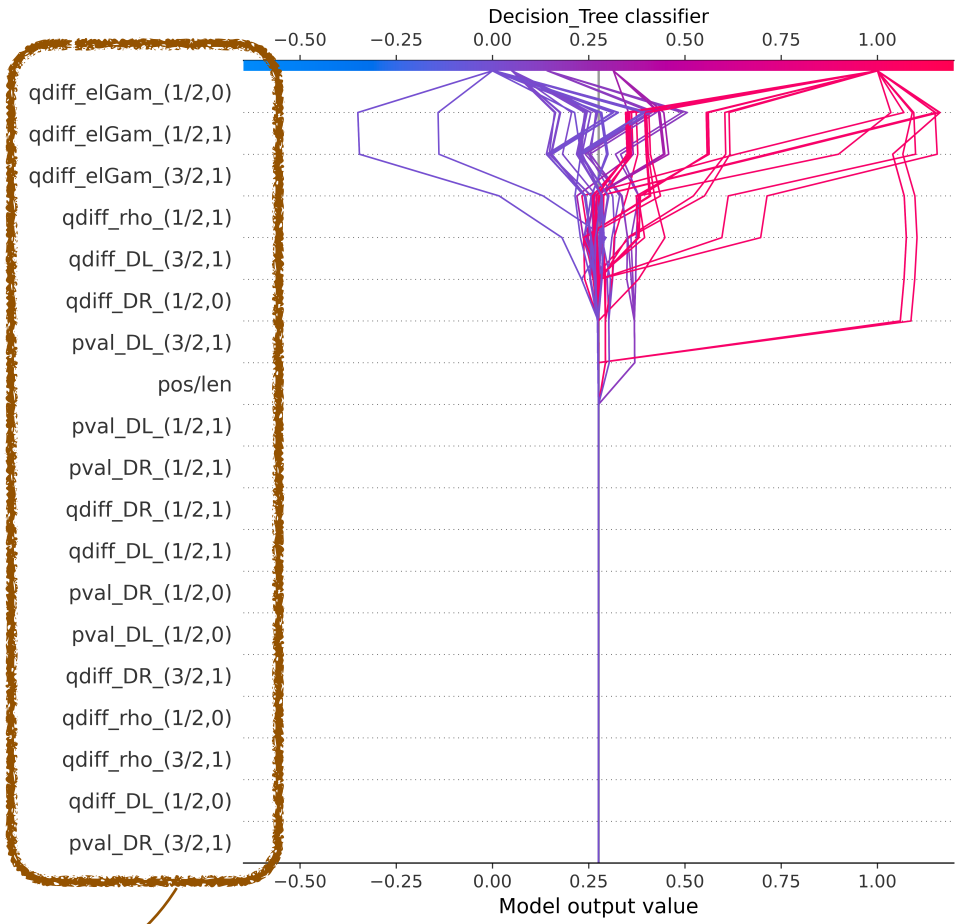

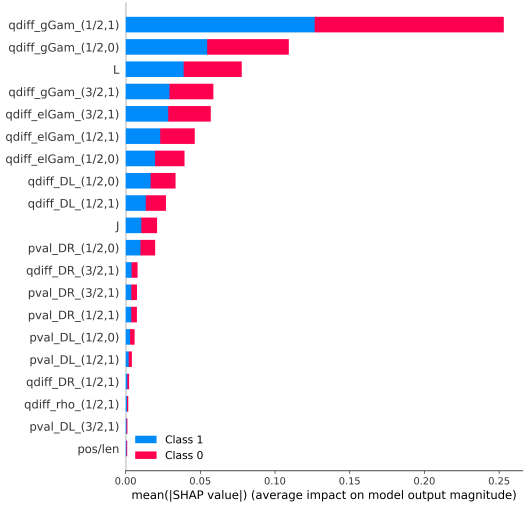

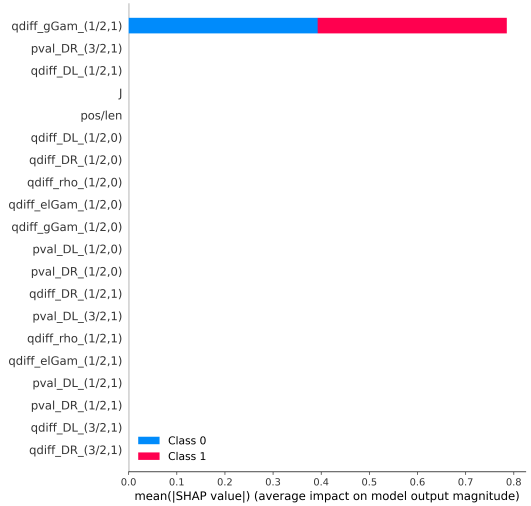

Feature names

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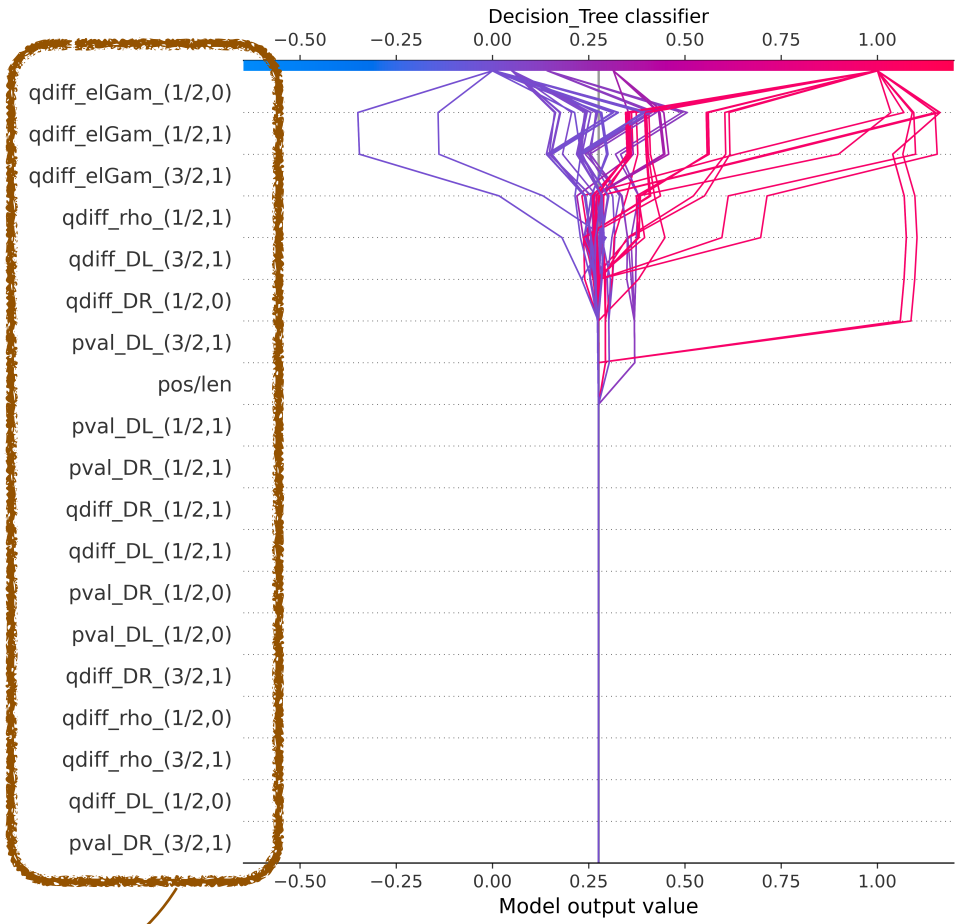

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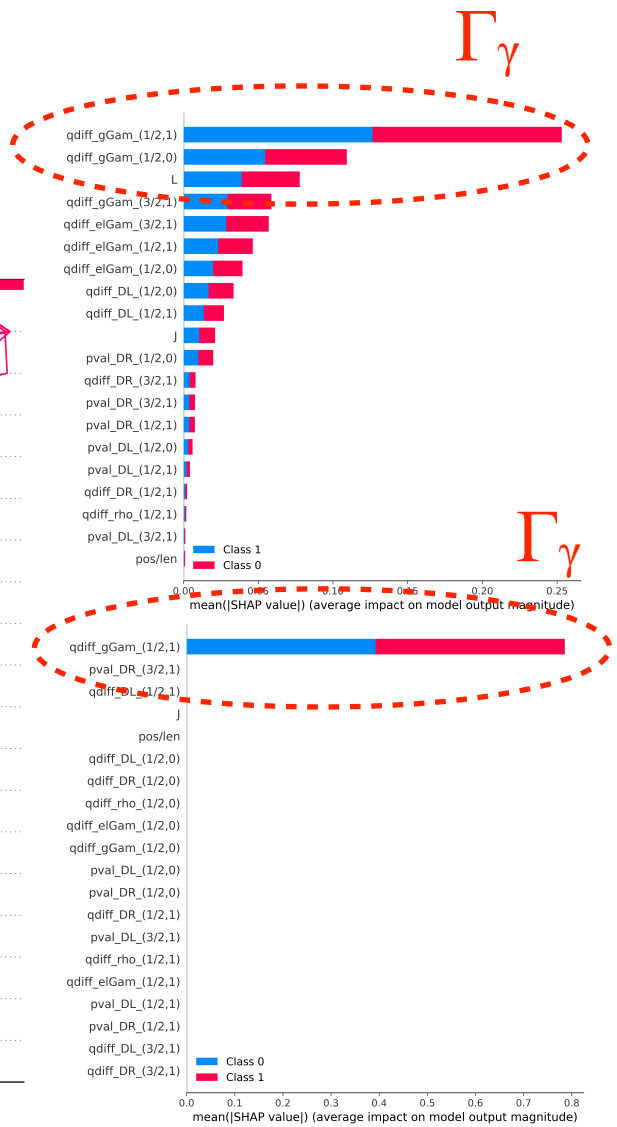
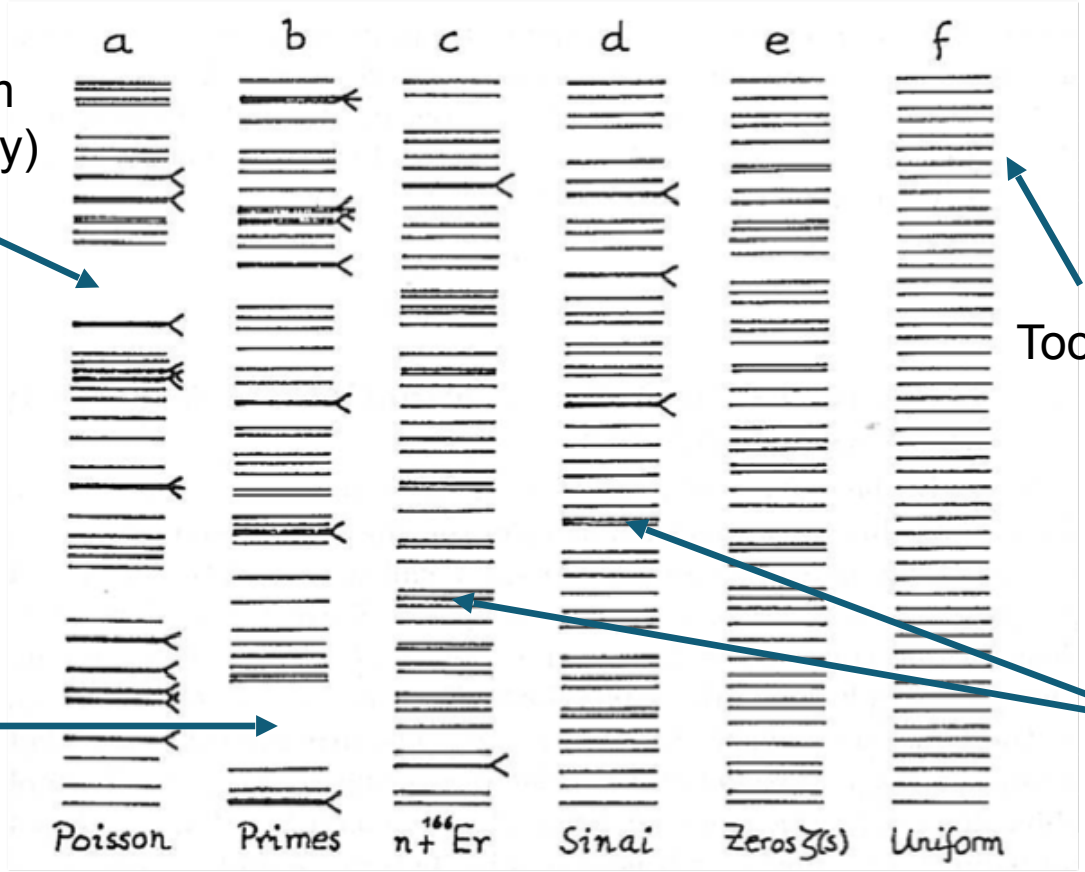


Energies in nuclei are distributed in a distinctive way, best described with Random Matrix Theory

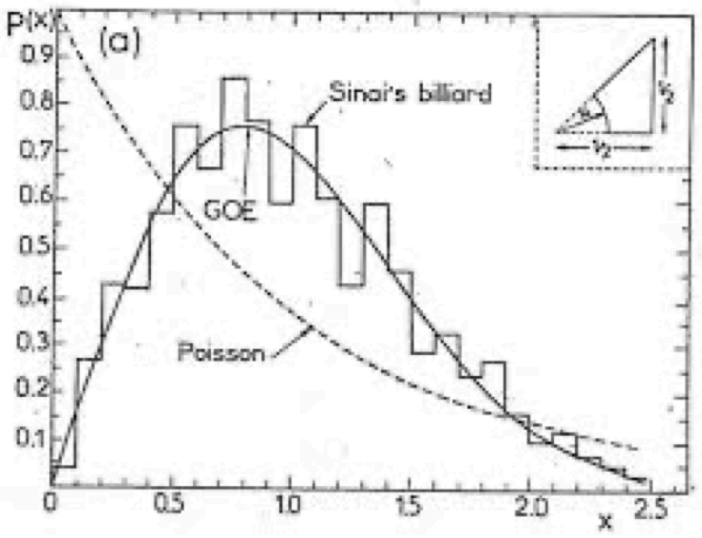
Too random (and clumpy)



Too regular

Too clumpy

Just right



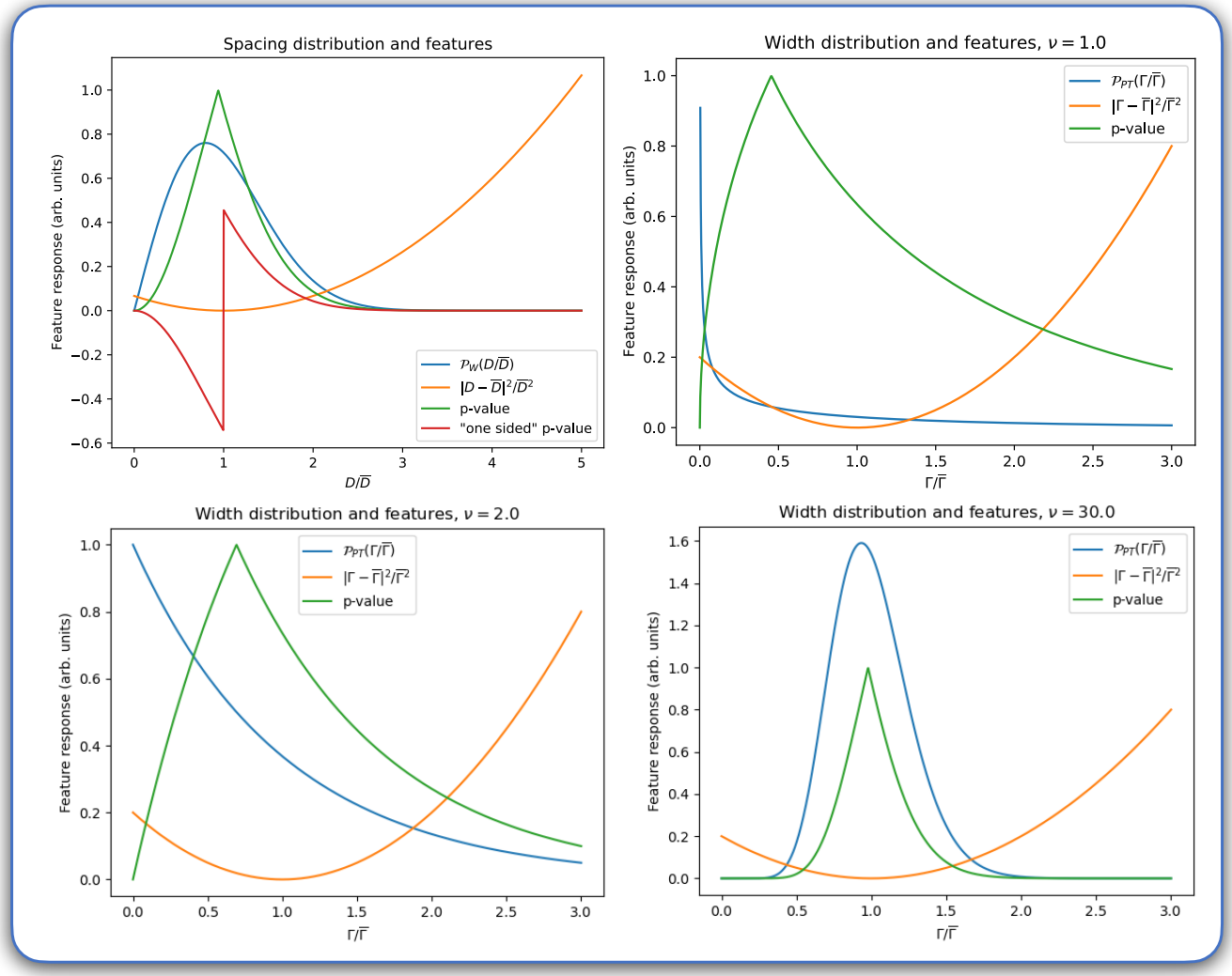
H. A. Weidenmüller and G. E. Mitchell, "Random matrices and chaos in nuclear physics: Nuclear structure", Rev. Mod. Phys. 81, 539 (2009);

RMT suggests some useful qualities:
- Spacings close to average
- Spacings follow expected distribution
- Spacings have L-S-L-S pattern

O. Bohigas and M. J. Giannoni, Lecture Notes in Physics 209 (1984), Springer-Verlag, Heidelberg

Revised feature selection: Spacings & Widths

- **Spacings**:
  - Use “signed p-value” of spacing relative to Wigner dist.
  - If spacing too small, signal with minus sign (indicates resonance in wrong sequence)
  - If spacing too big, indicates missing resonance
- **Test both spacing to left & right**
  - GOE imposes short-long-short-long pattern
  - Experiment with spacing-spacing correlation for same purpose
- **Elastic & Fission widths**
  - Use diff to mean width as using Porter-Thomas leads to lower accuracy for small ν
- **Don’t use capture width by default as prone to exp. bias**
- **All features scaled to remove dependence on nucleus average parameters**
- **Use for all spingroups so can get signal for right/wrong assignments**



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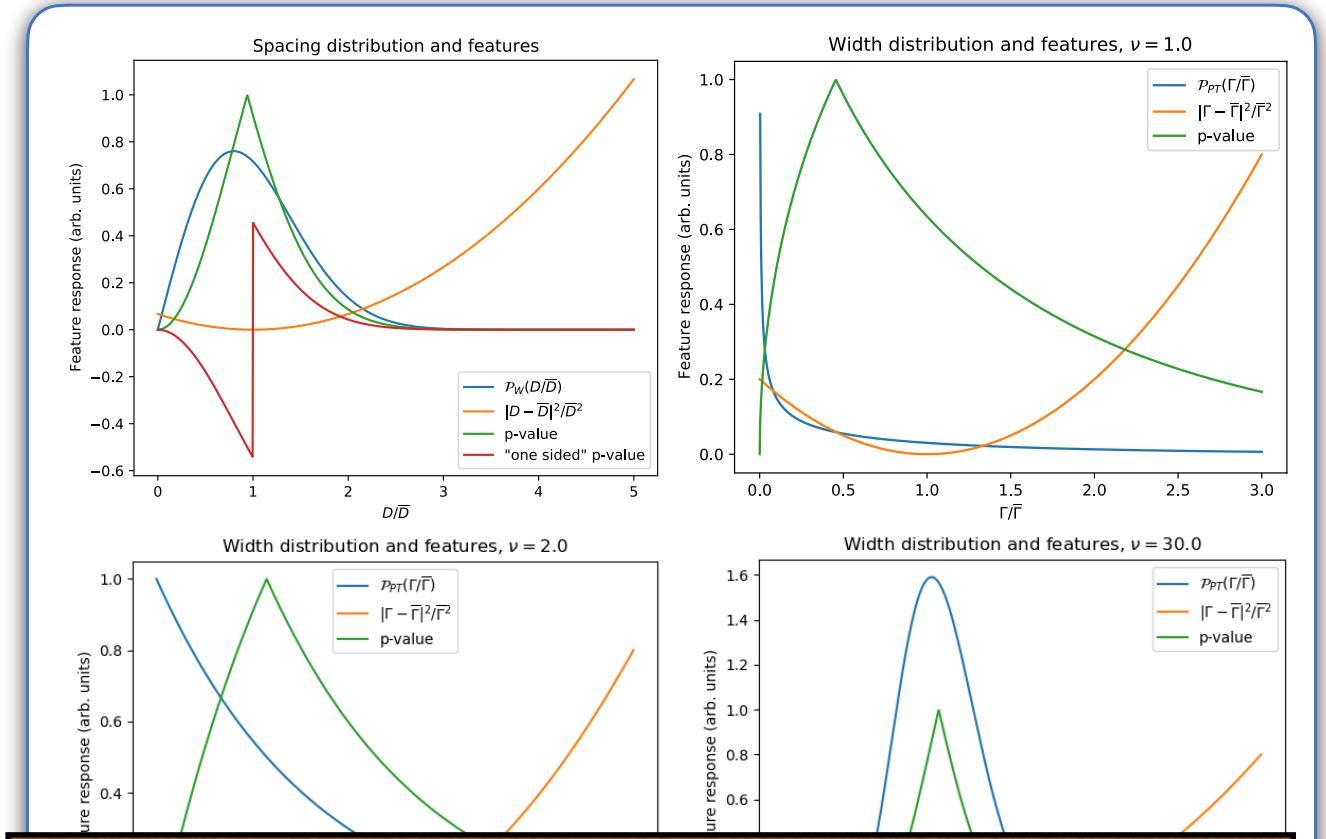

It used to be common for experimentalists to not be able to separate angular momentum and then report resonance widths based on averaged widths: Circular reasoning!

It may be dangerous sometimes to rely heavily on capture widths for spin classification

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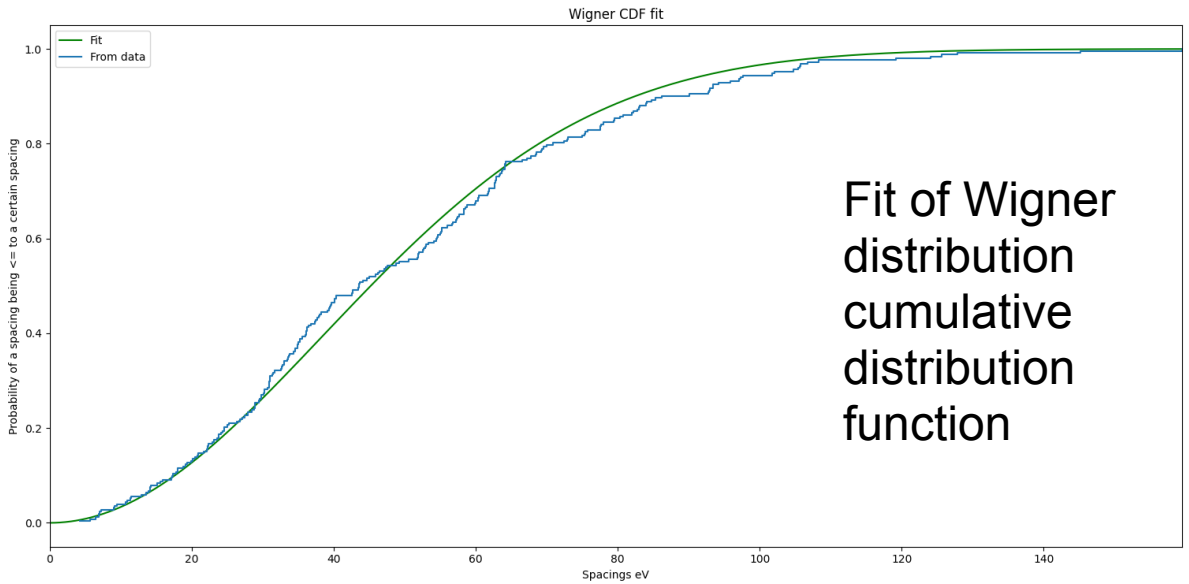
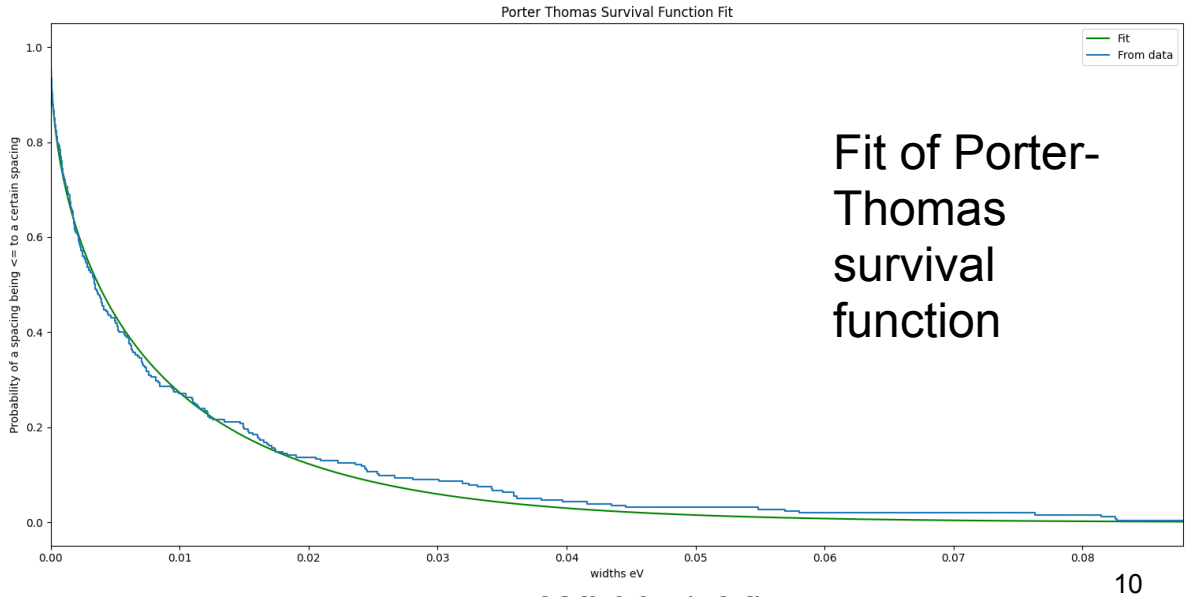
Training data and features need average spacing and channel widths

- Can take from ENDF or *Atlas of Neutron Resonances*
- Can measure directly from sequence prior to reclassification, provided prior L,J assignments exist
- We have not explored iterative updating of parameters, training data and classifier



Fit of Wigner distribution cumulative distribution function

D (eV)



Fit of Porter-Thomas survival function

Width (eV)

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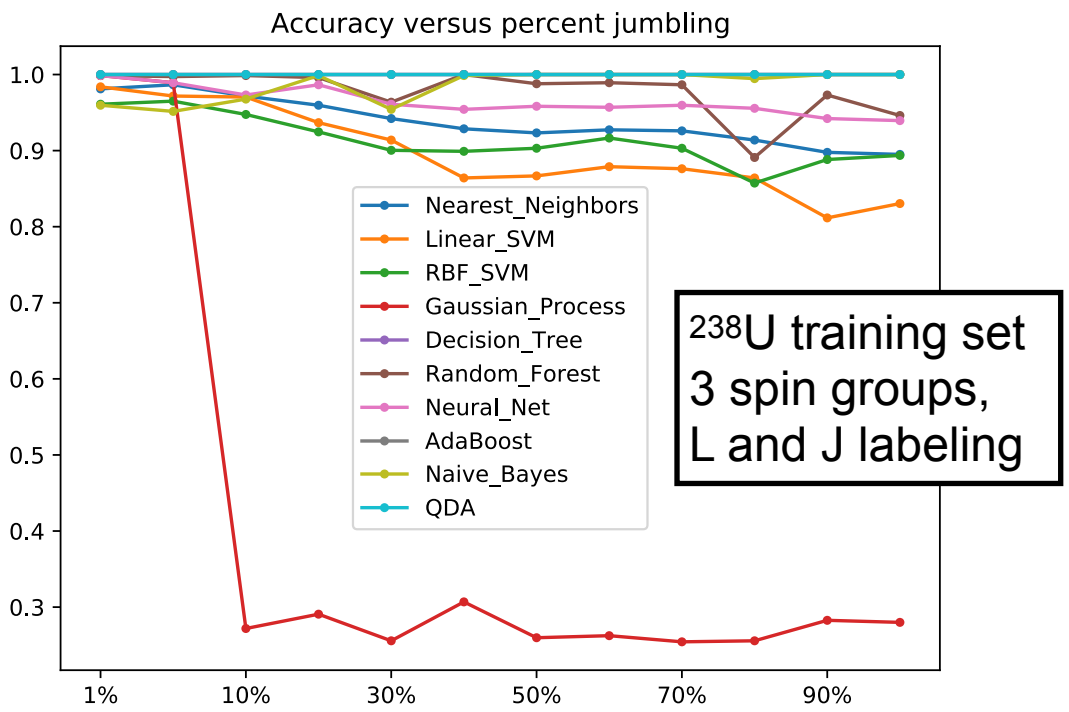
Optimizing the training step



^{238}U training set
3 spin groups,
L and J labeling

Default parametrization straight out of scikit-learn…

…we can do better!

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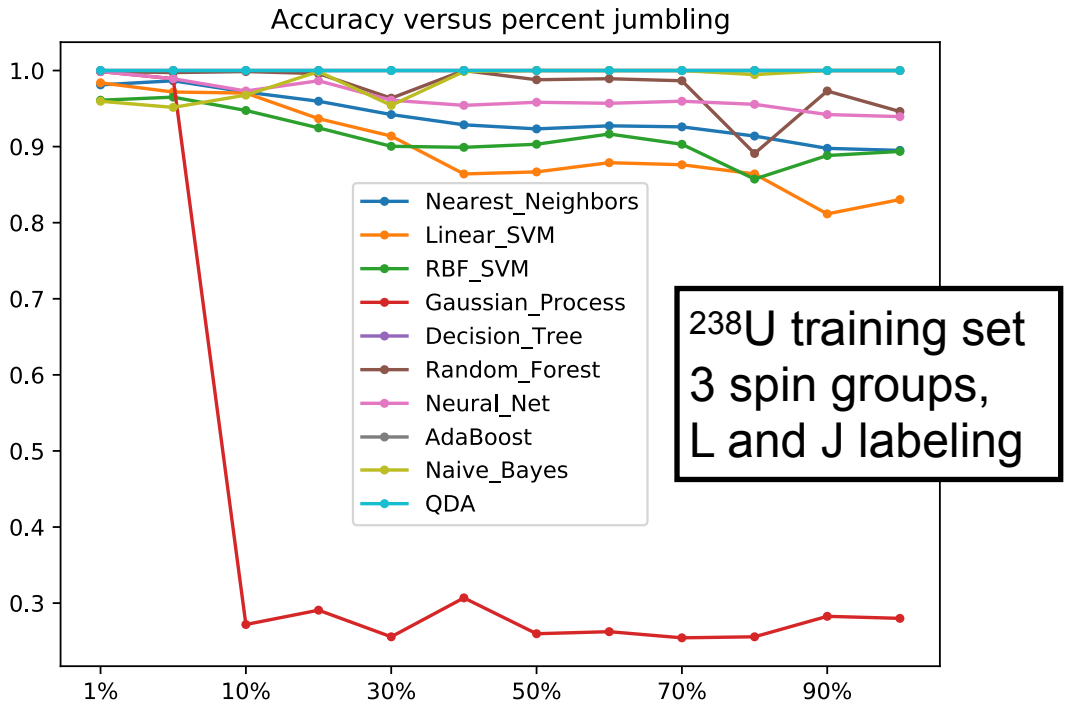

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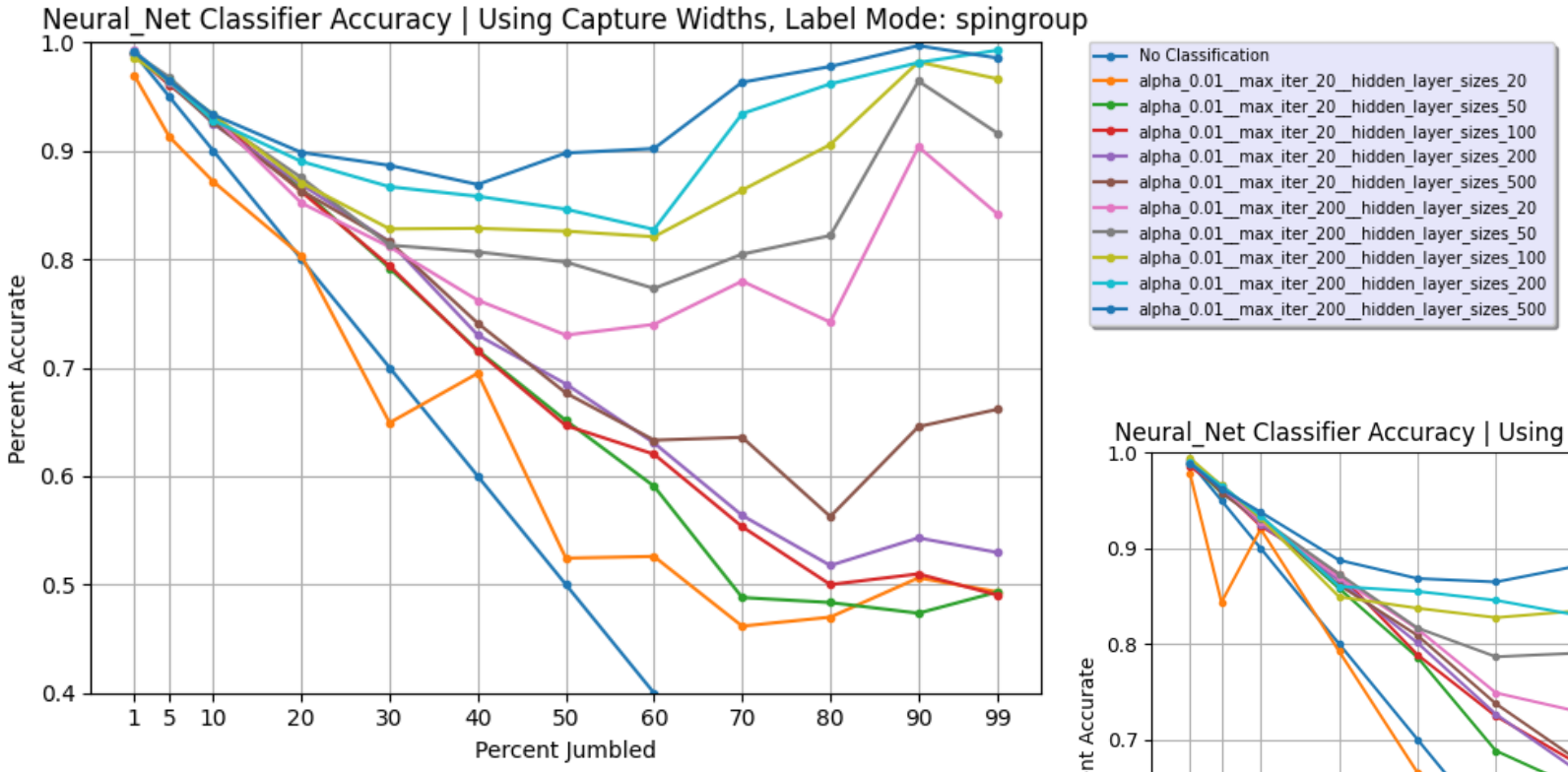
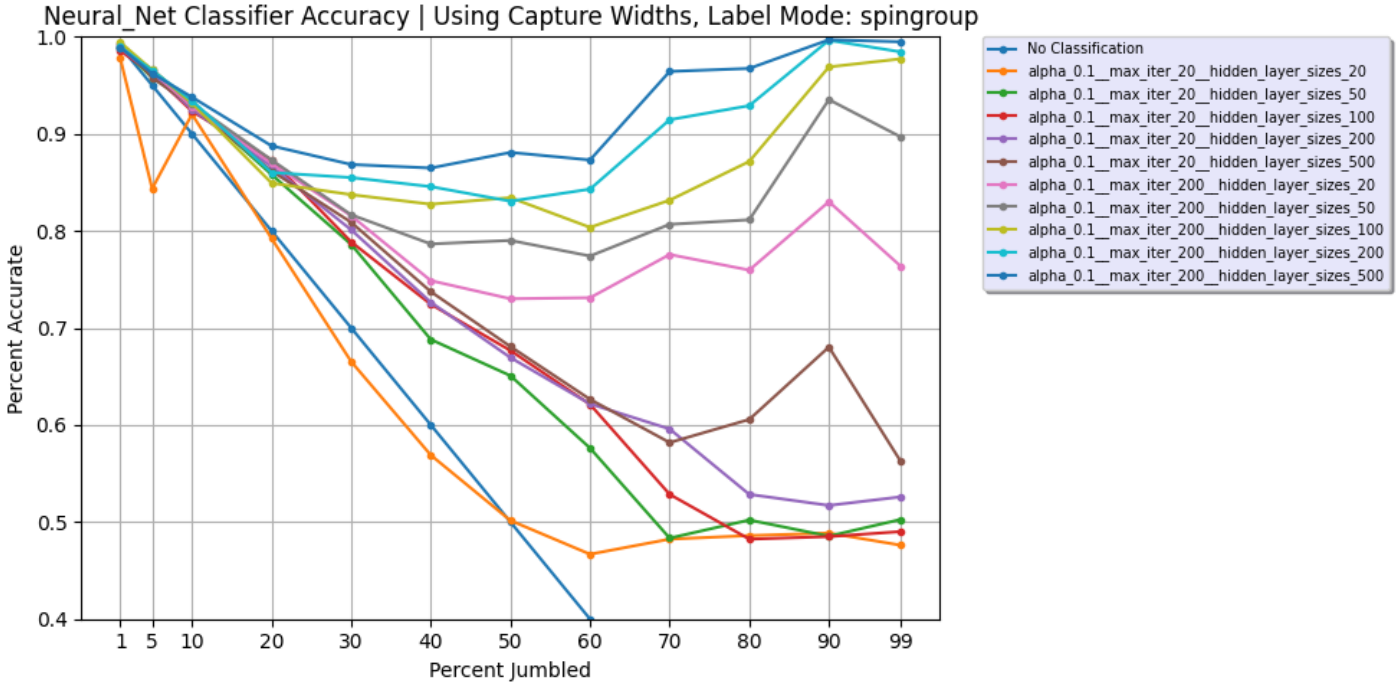
…we can do better!

- Grid search of hyper-parameters
- Began by varying the number of trees in a Random Forest
- Extended to ALL hyper-parameters for ALL classifiers in scikit-learn
- Did many runs so accuracies could be averaged
- Automated batch run to use the 400+ cores (144 dedicated to serial jobs) in the the NNDC computer cluster
- Ran with both Γ_γ feature on and off
- Classification by *L* and spin-group
- **SO MUCH** data that we're still processing them

Examples of the optimization results





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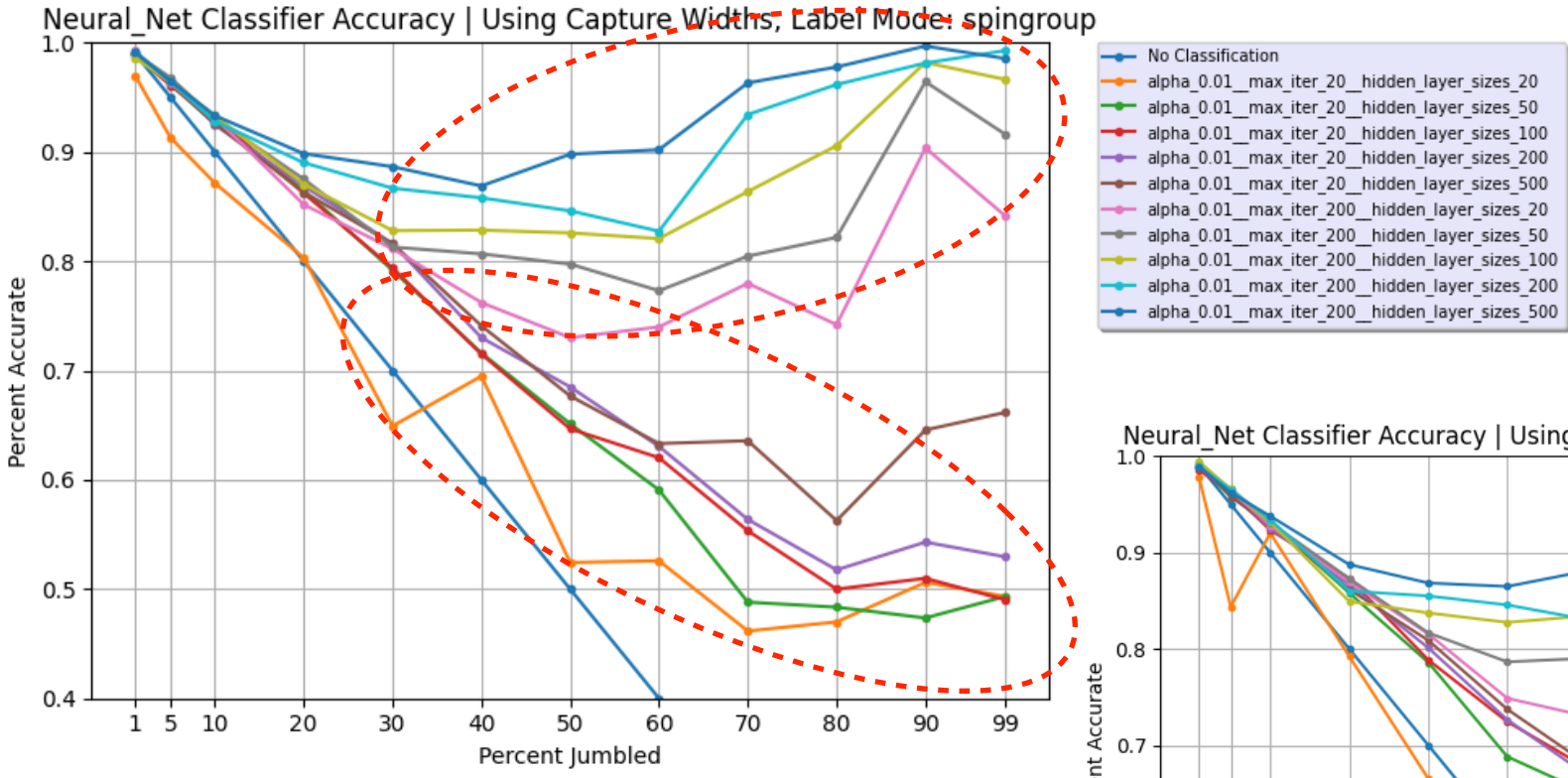

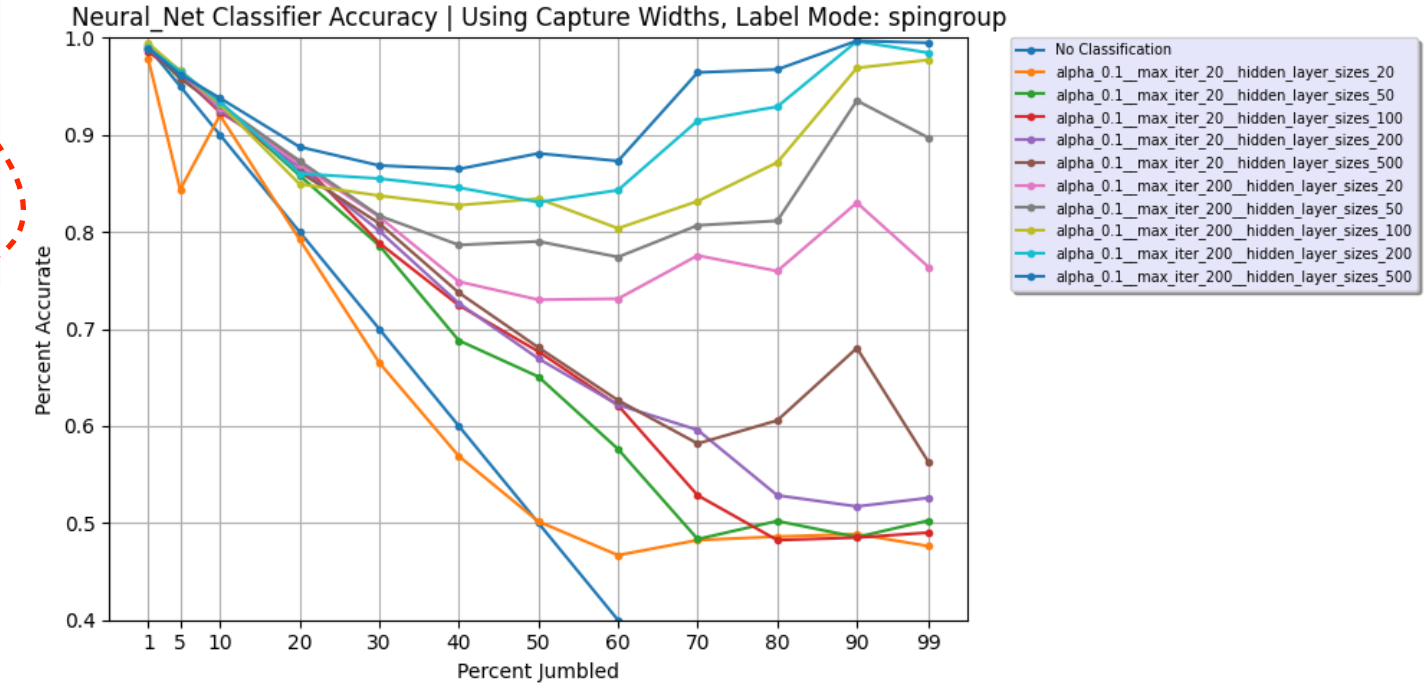

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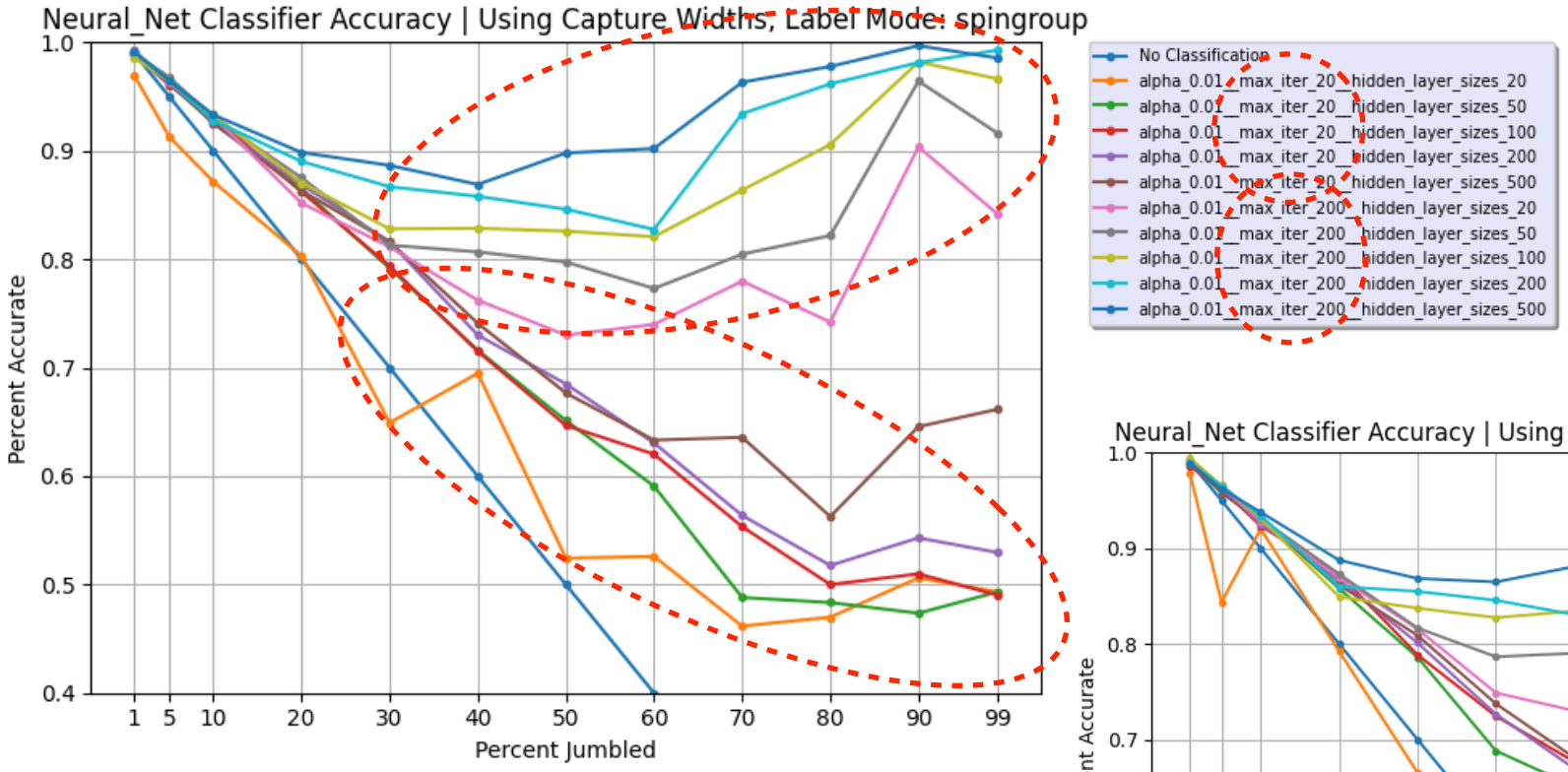

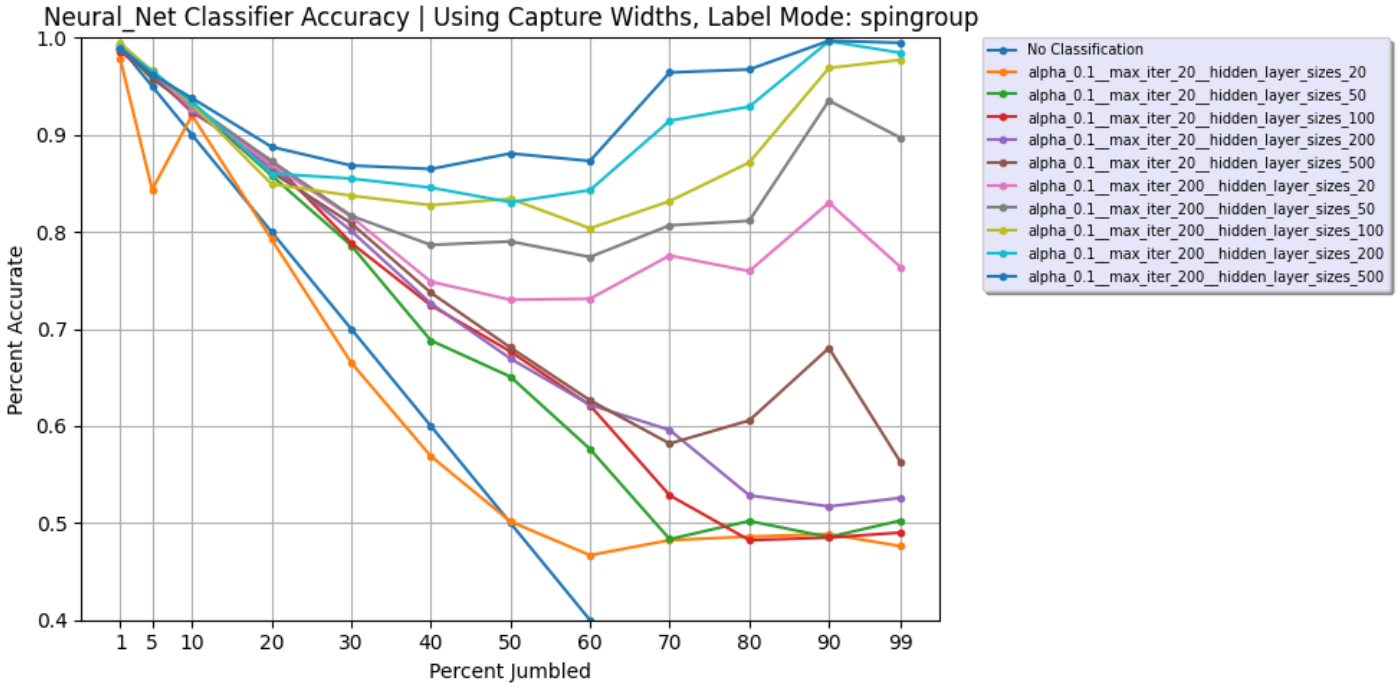

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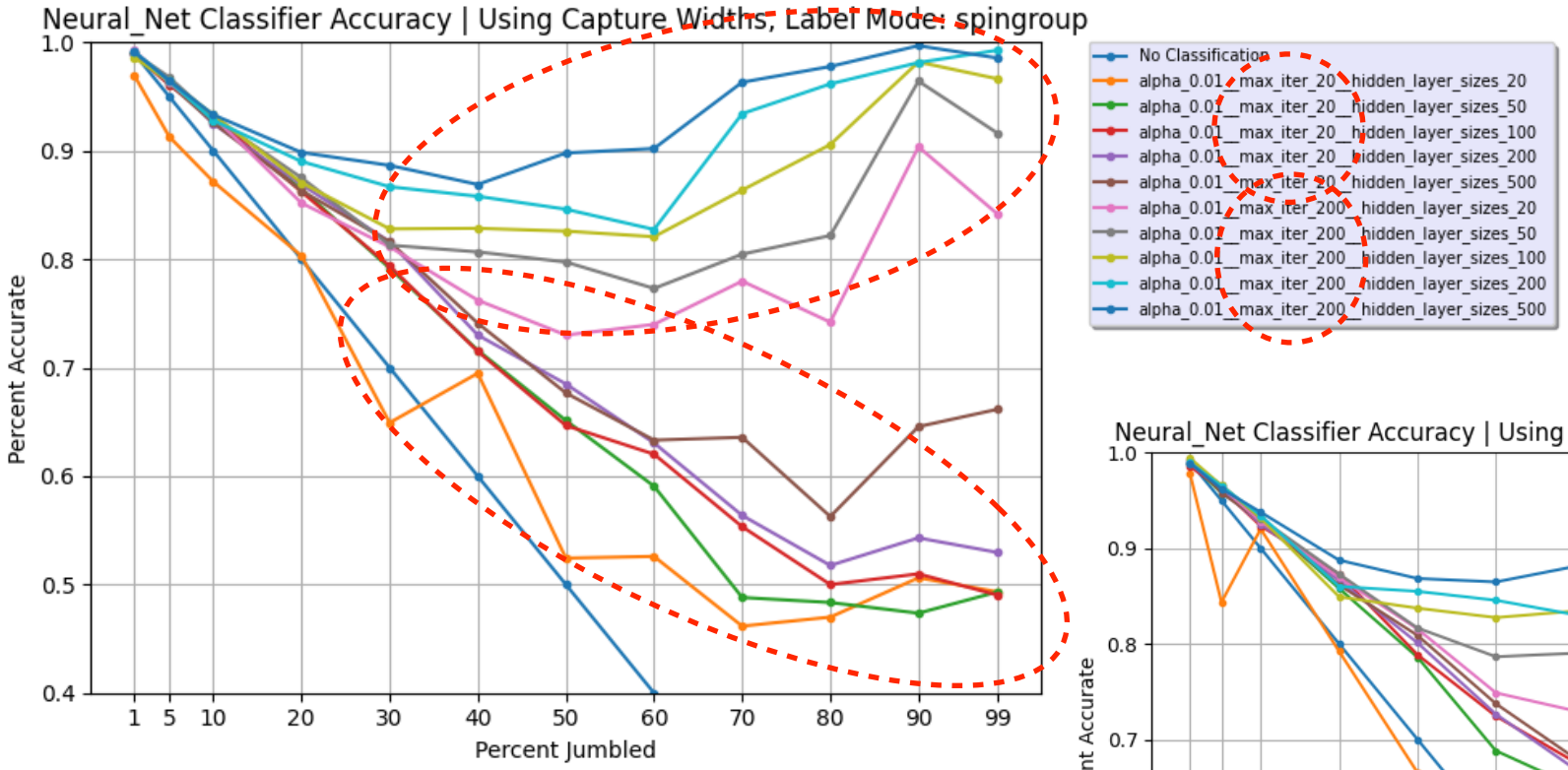
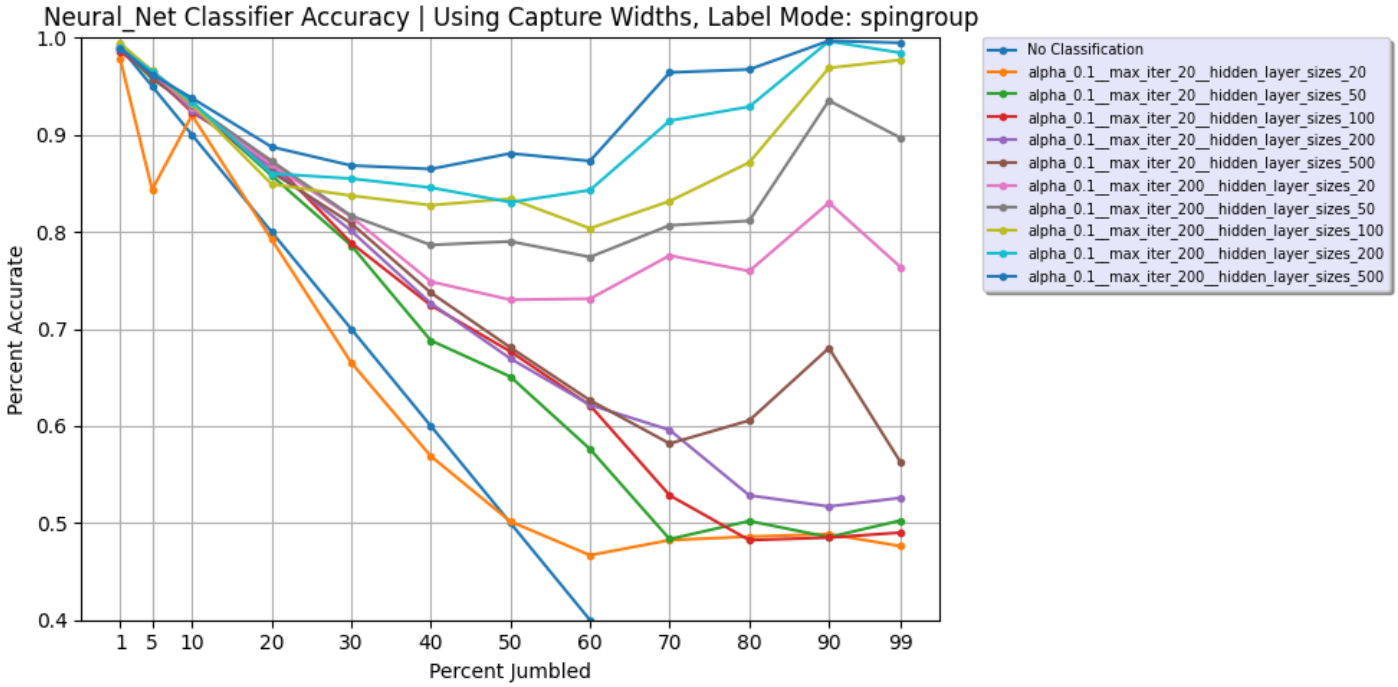


Maximum number of iterations makes significant impact!



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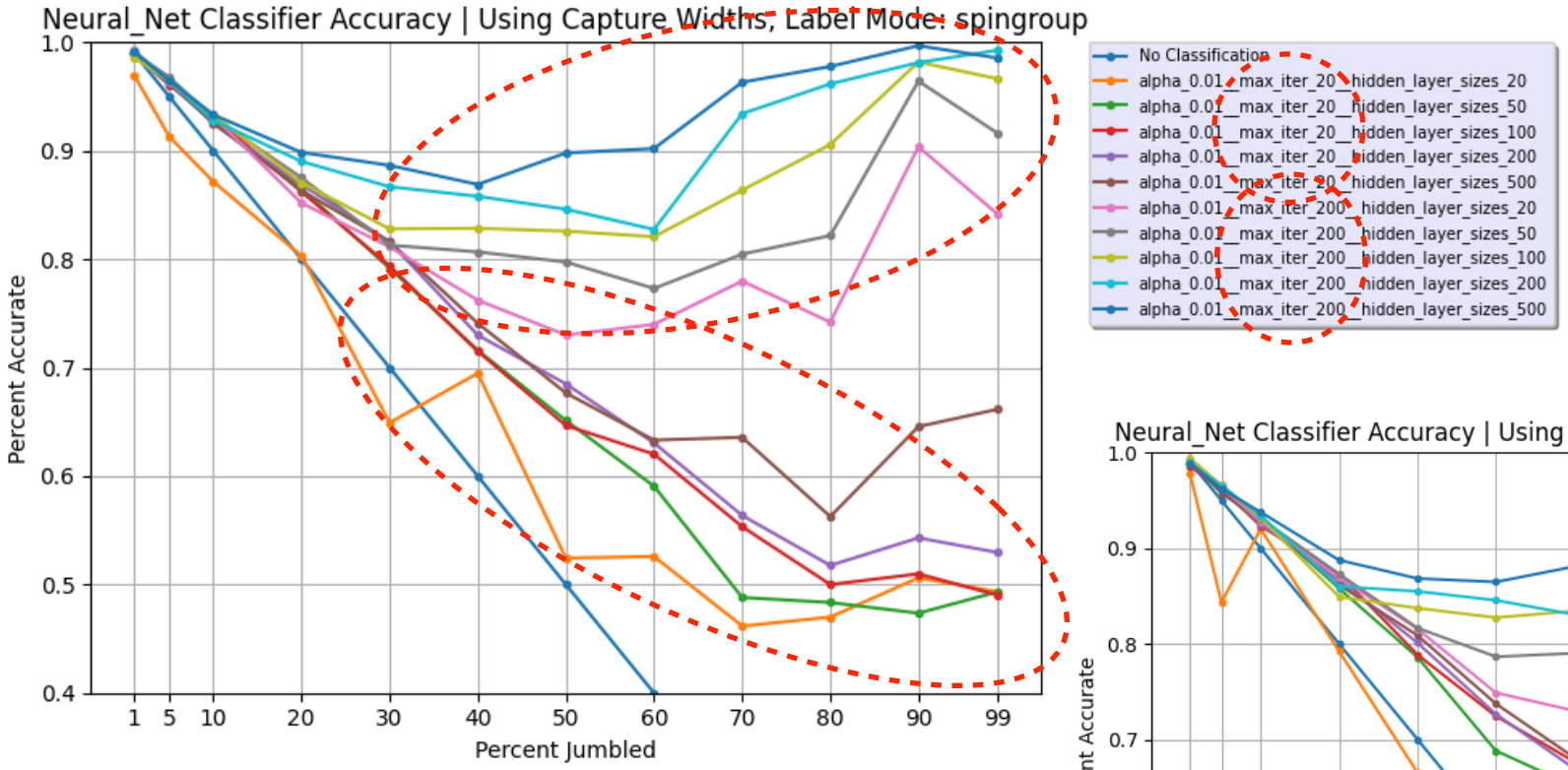

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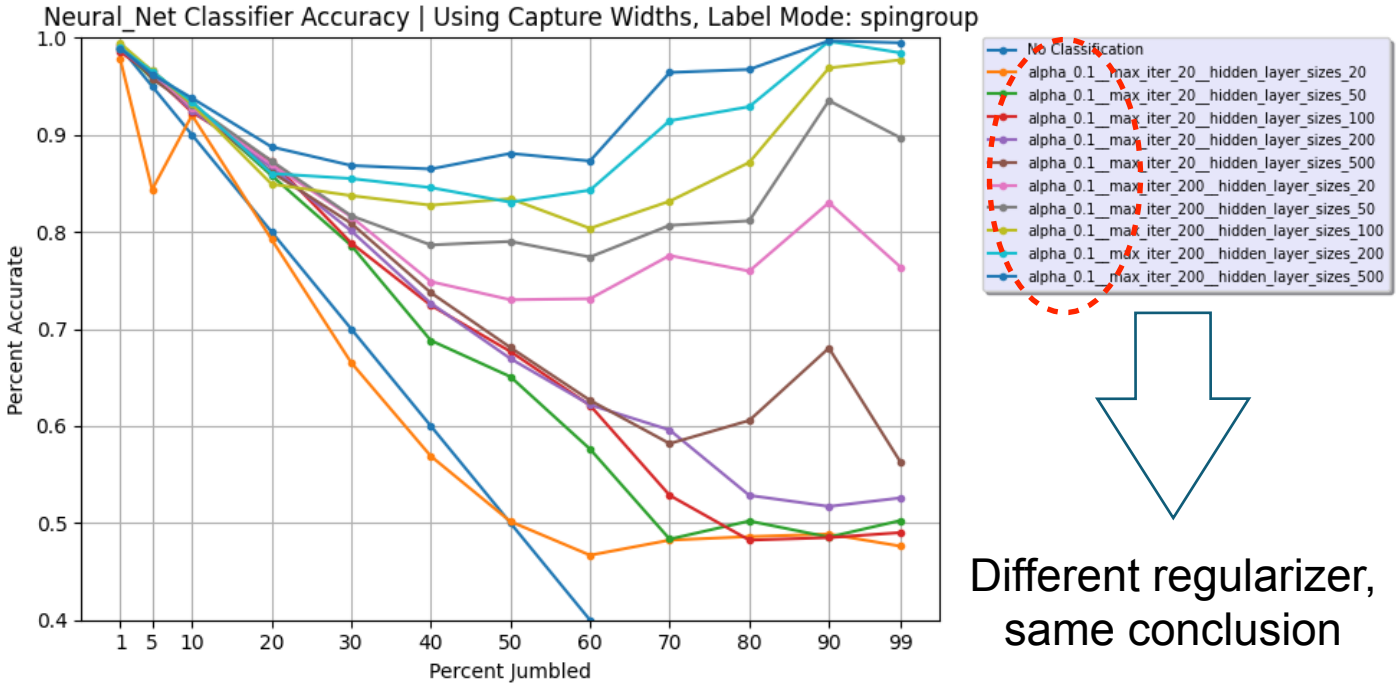

Different regularizer, same conclusion

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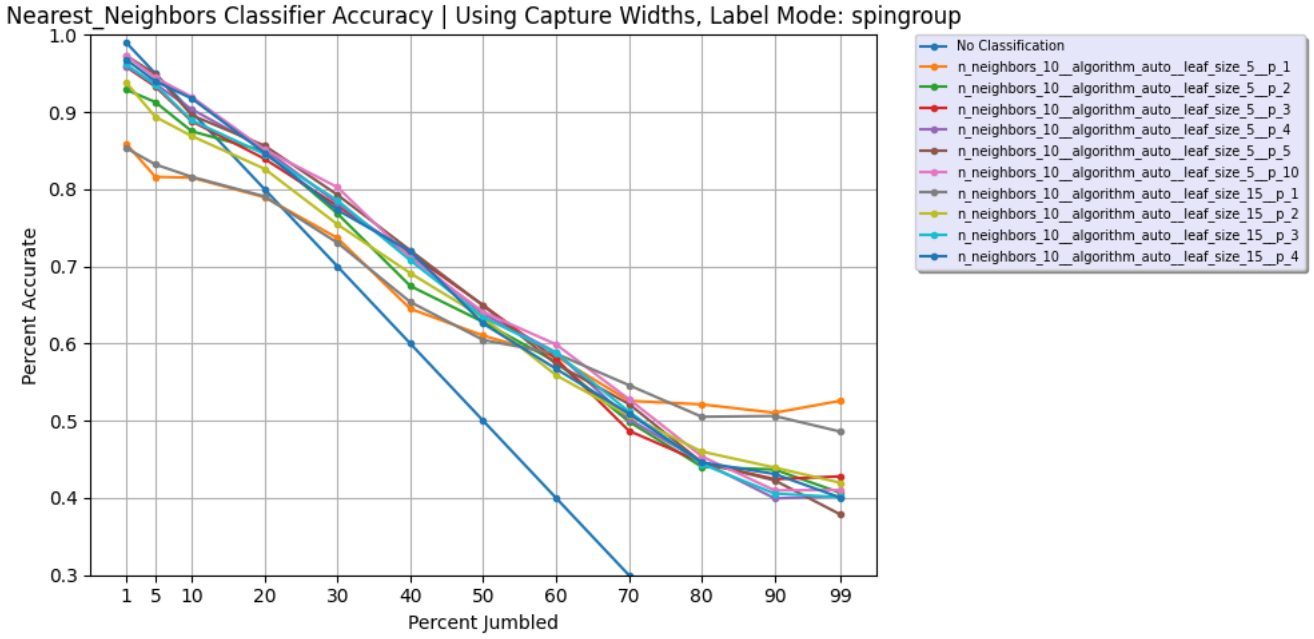

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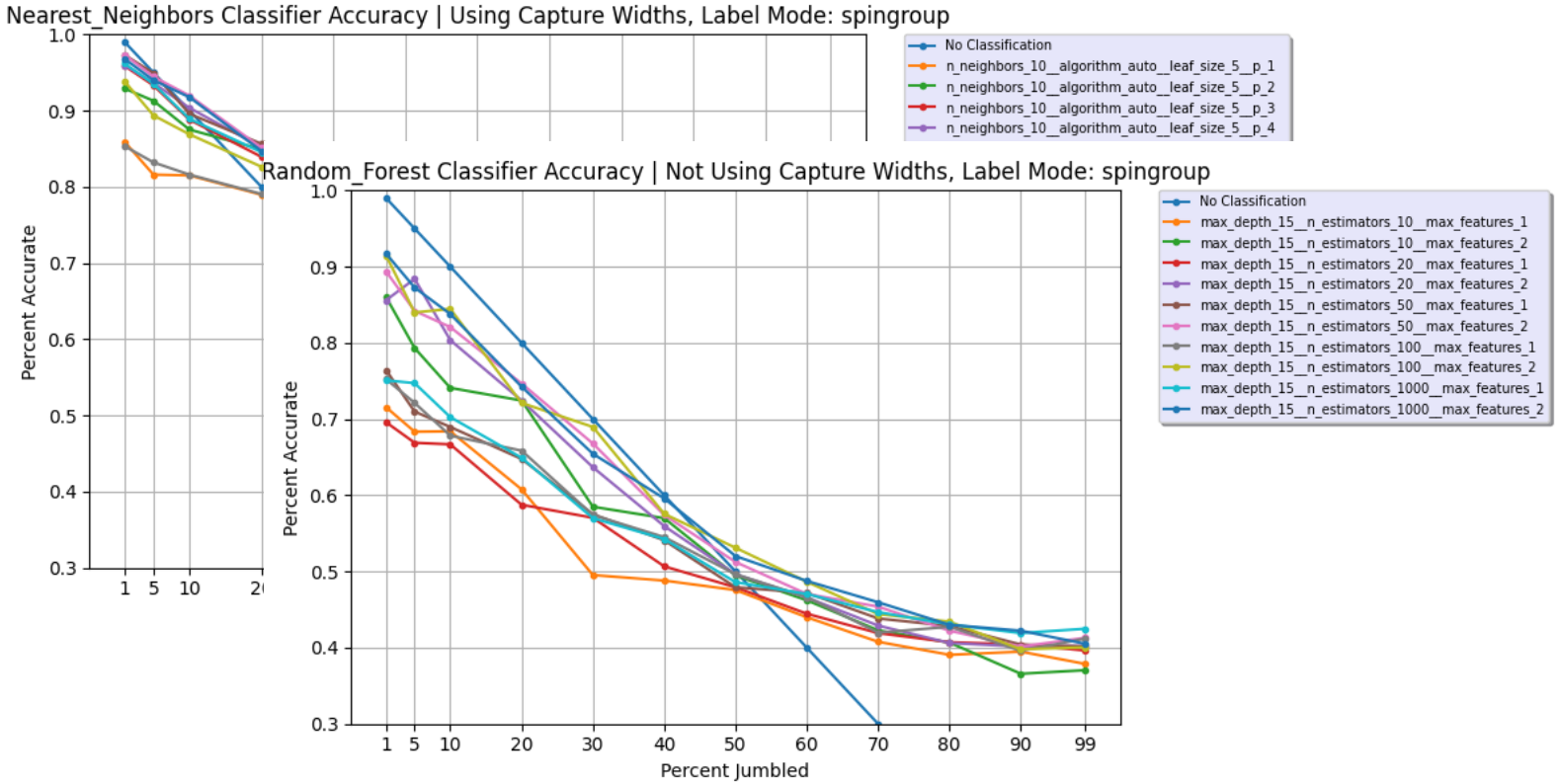

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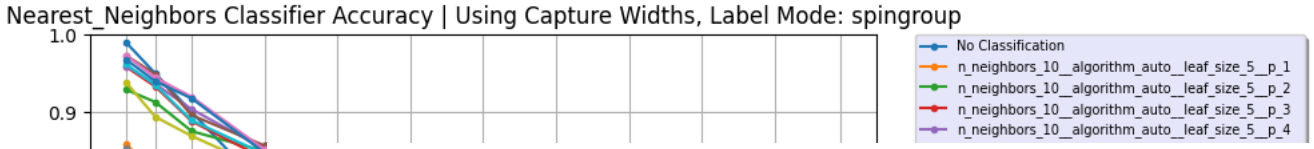

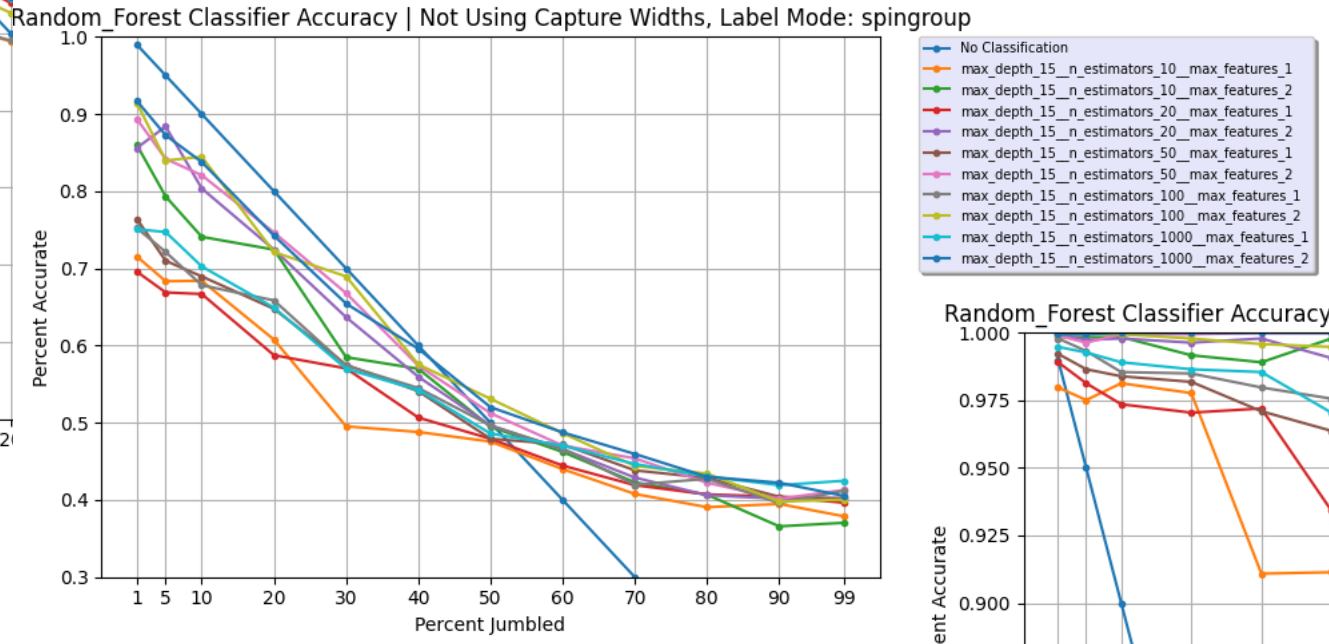

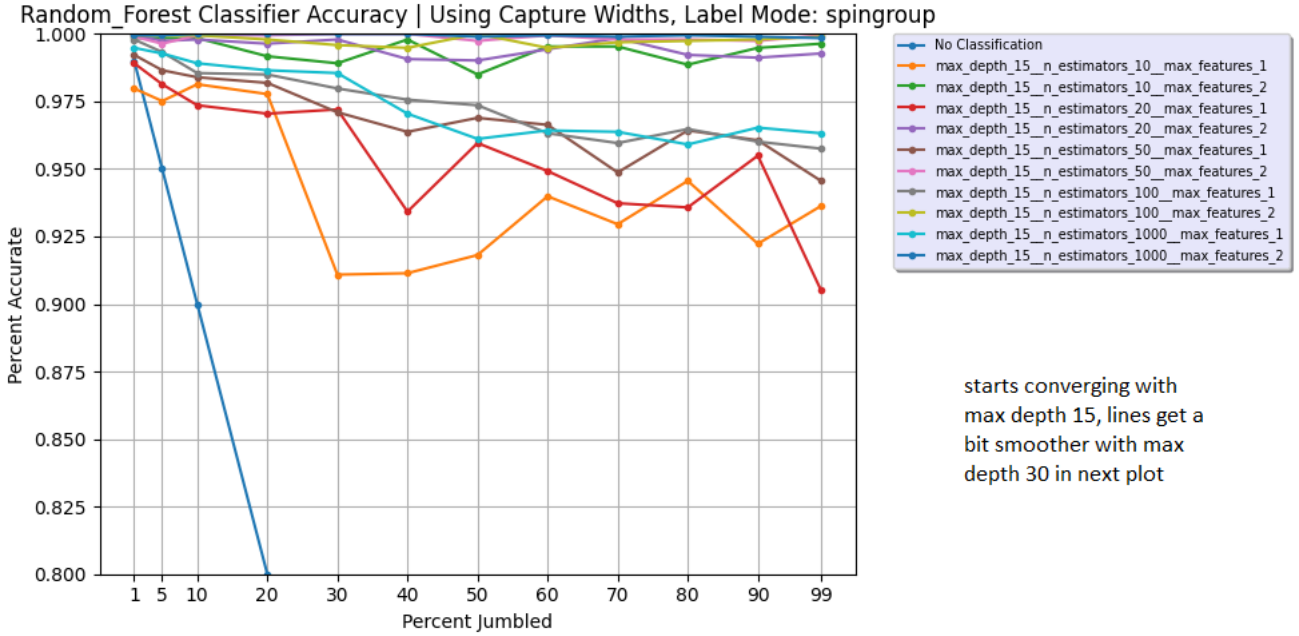

starts converging with max depth 15, lines get a bit smoother with max depth 30 in next plot

Validating with polarized data* - ^{115}In

- Polarized-beam data offers more reliable information about the resonance spin
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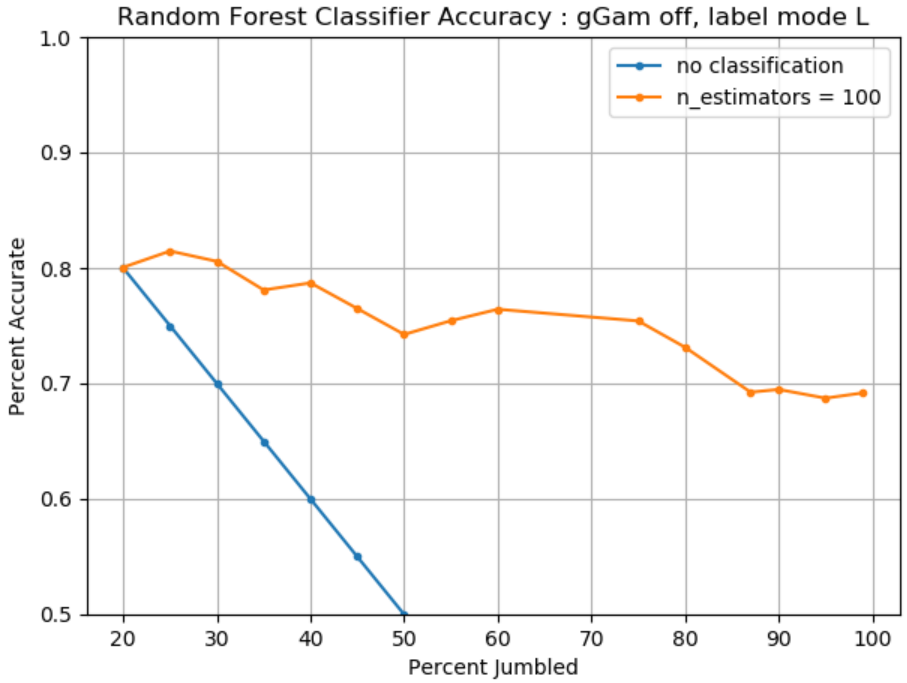

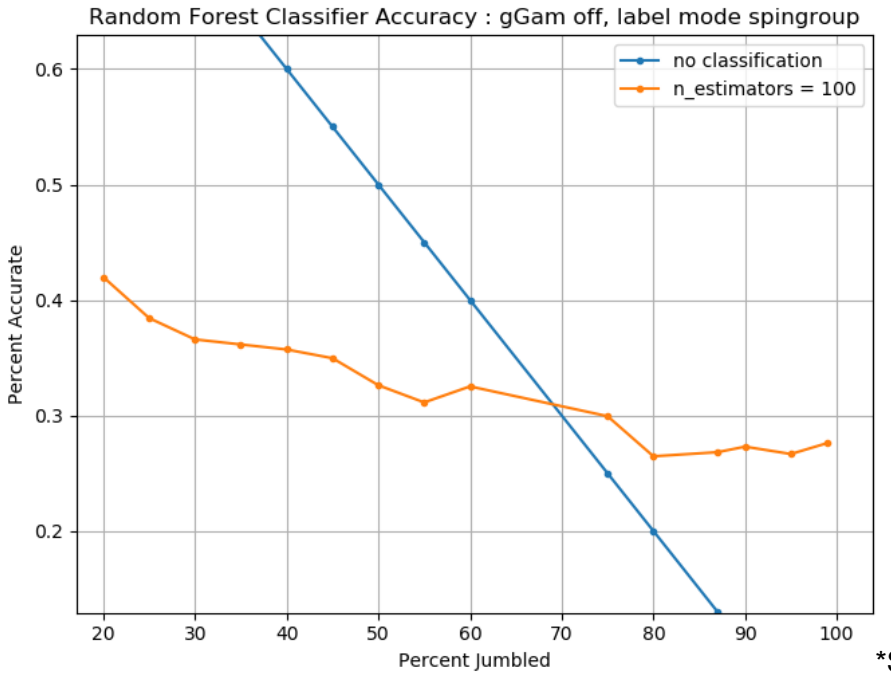

*S. L. Stephenson *et al.*, PRC **61** (2000) 045501

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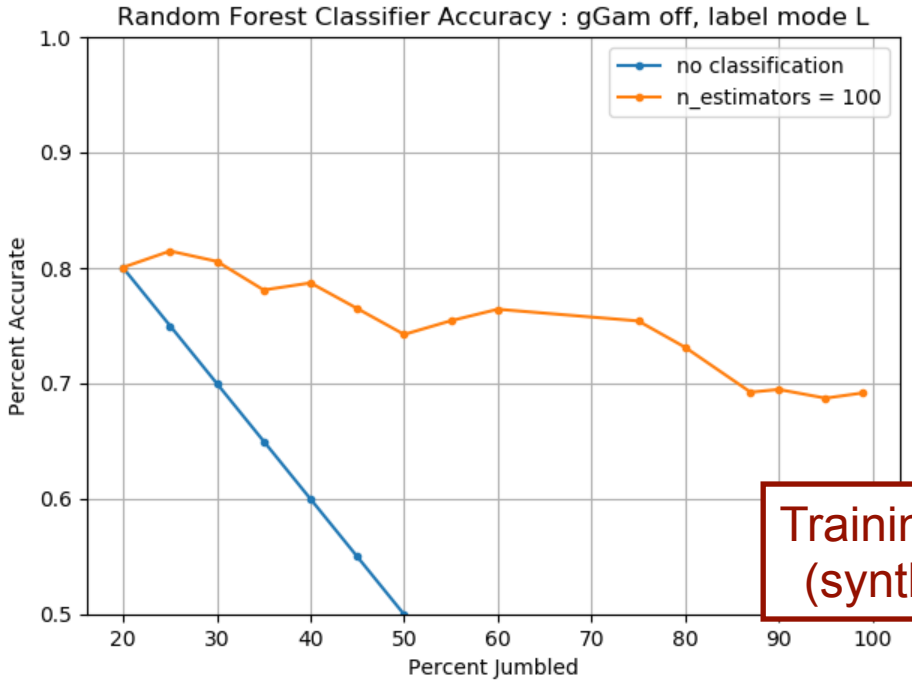

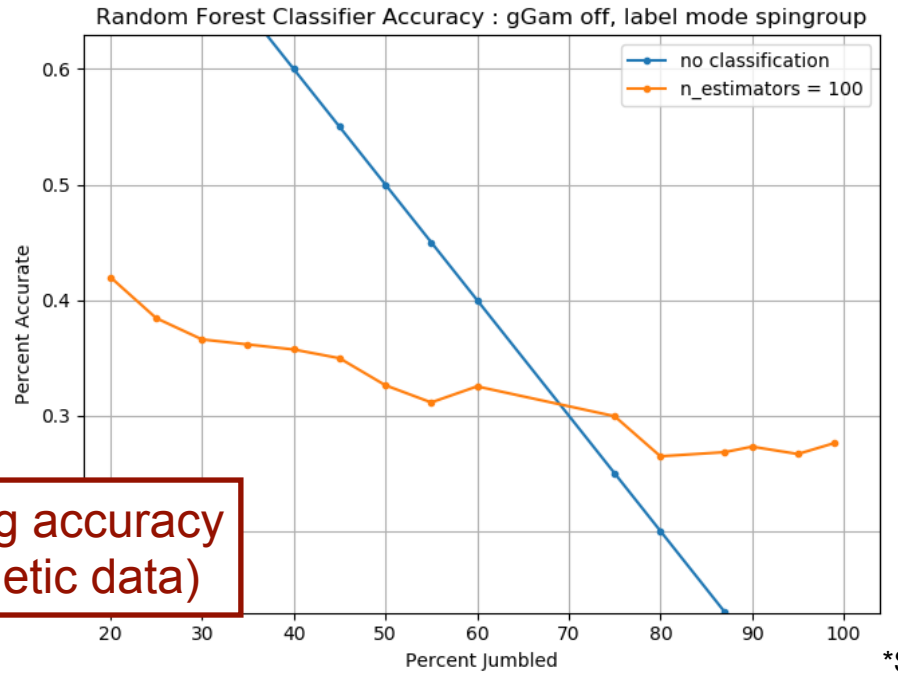

Training accuracy (synthetic data)

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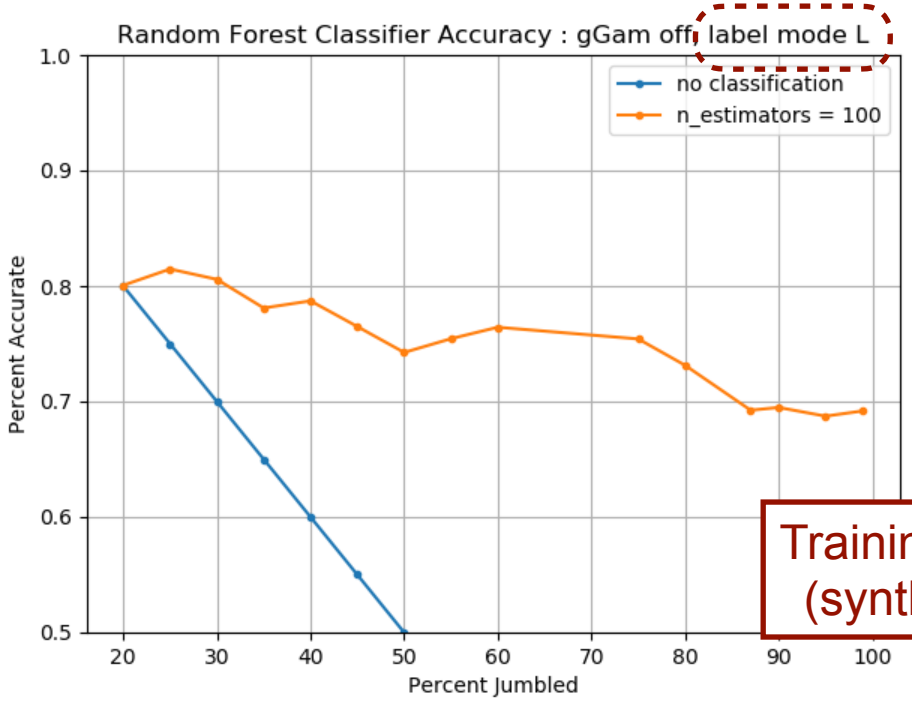

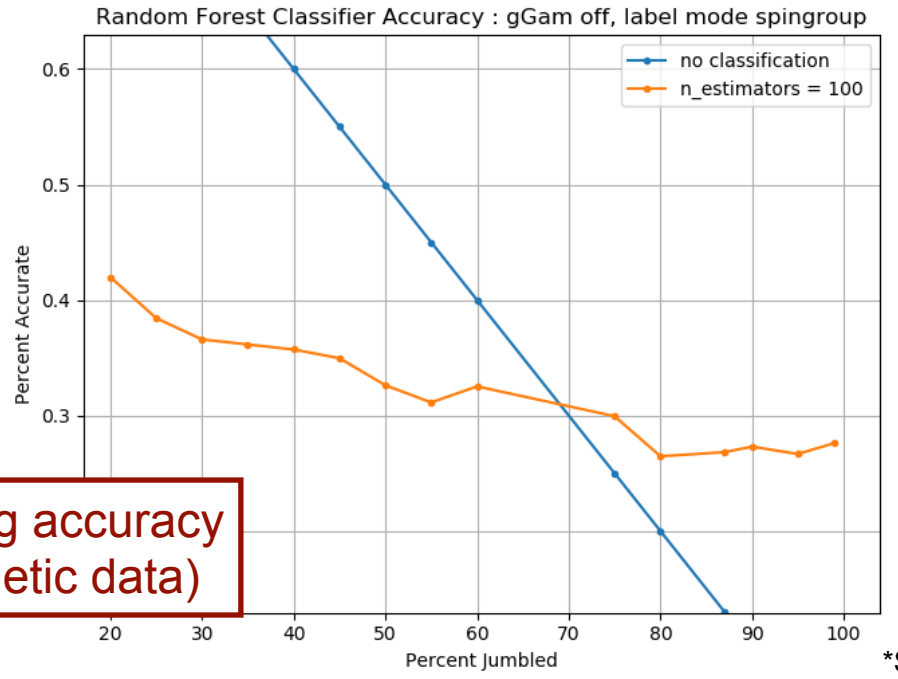

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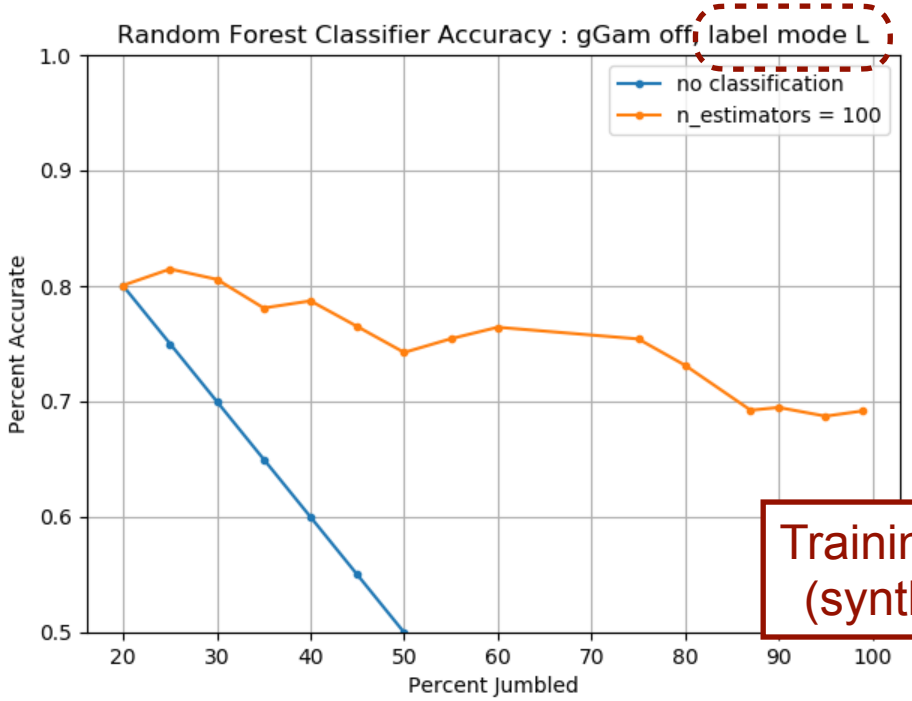

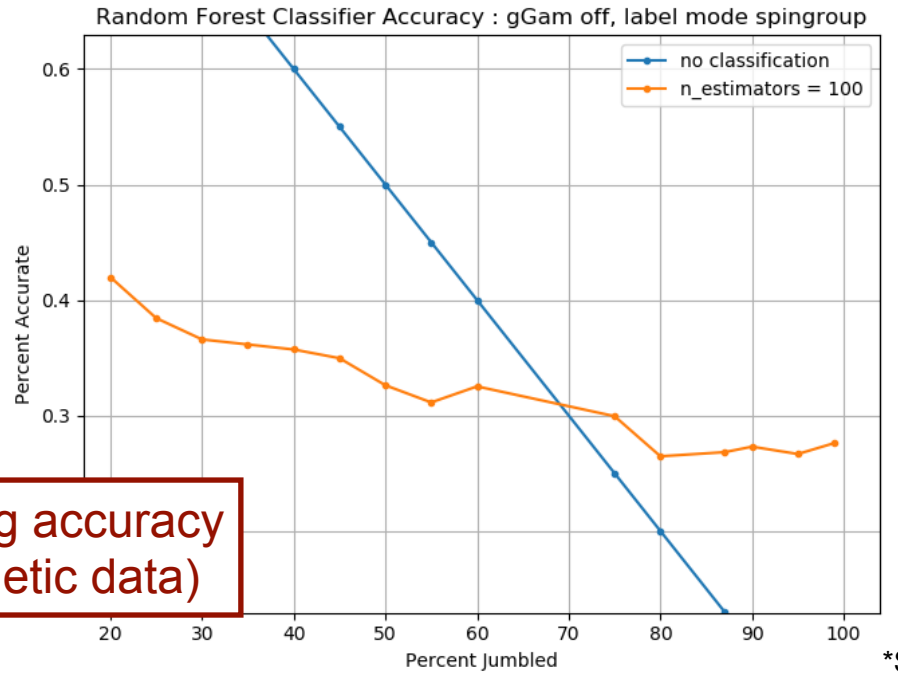

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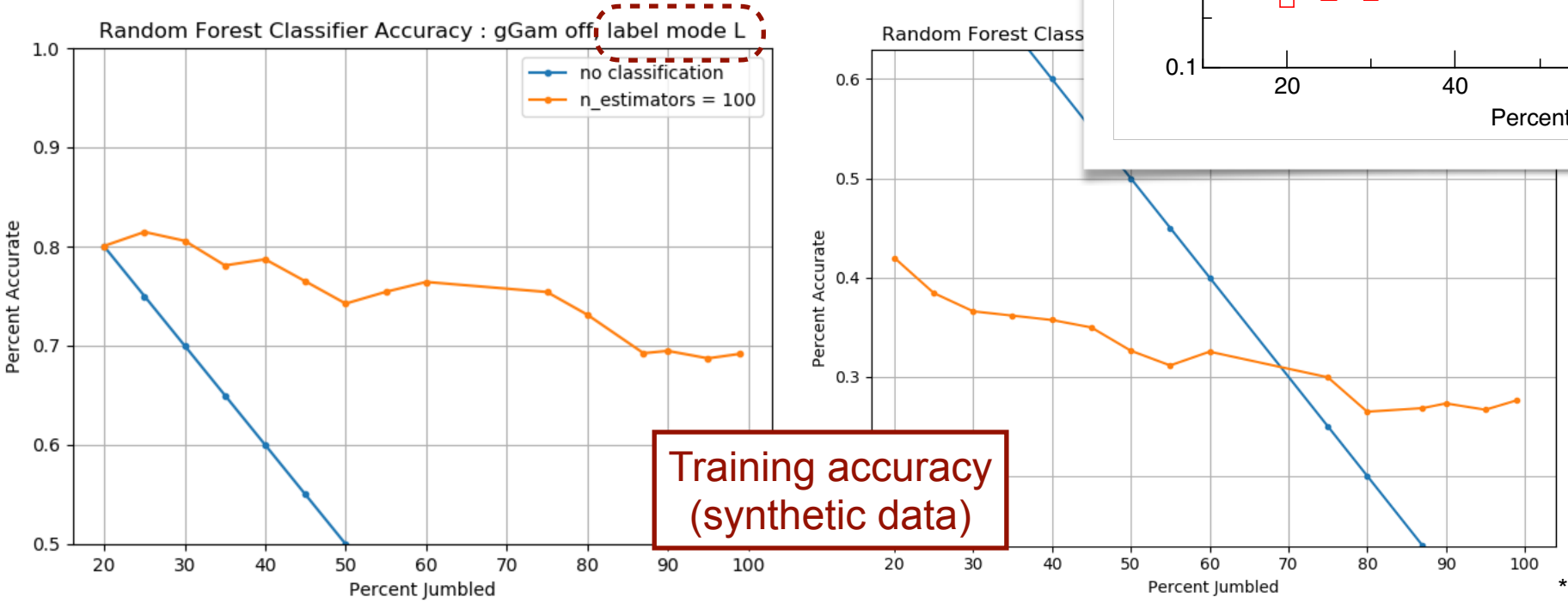

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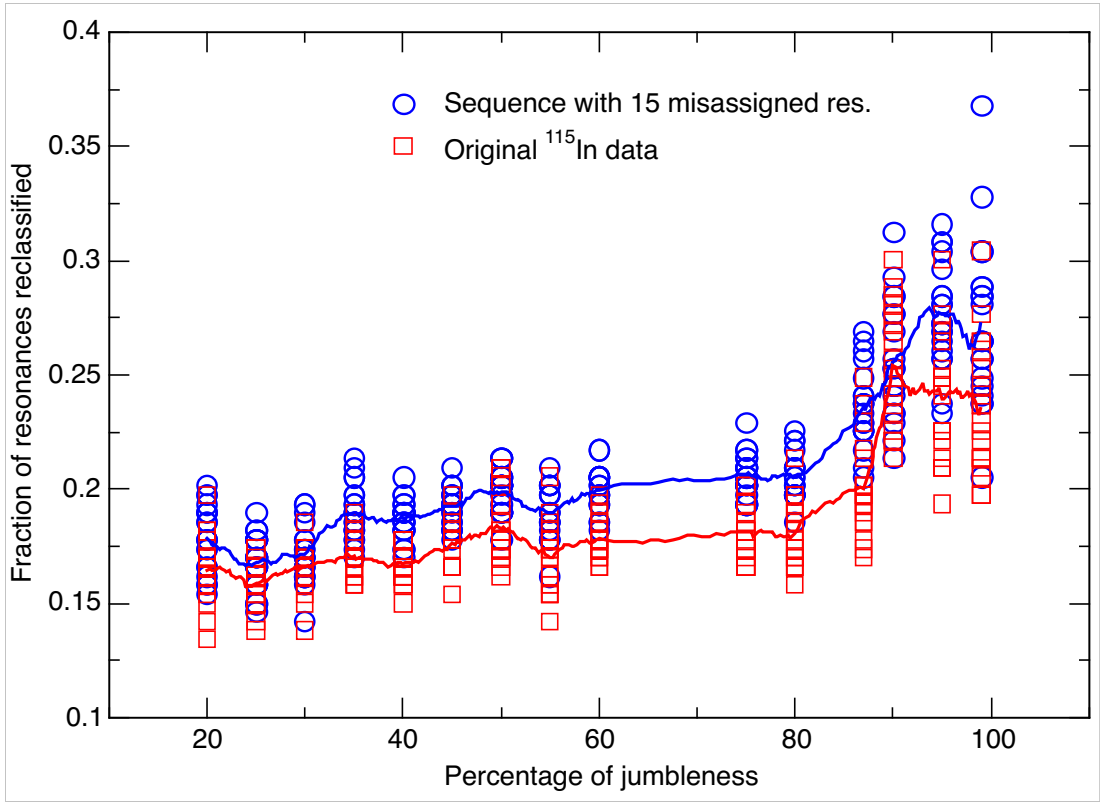

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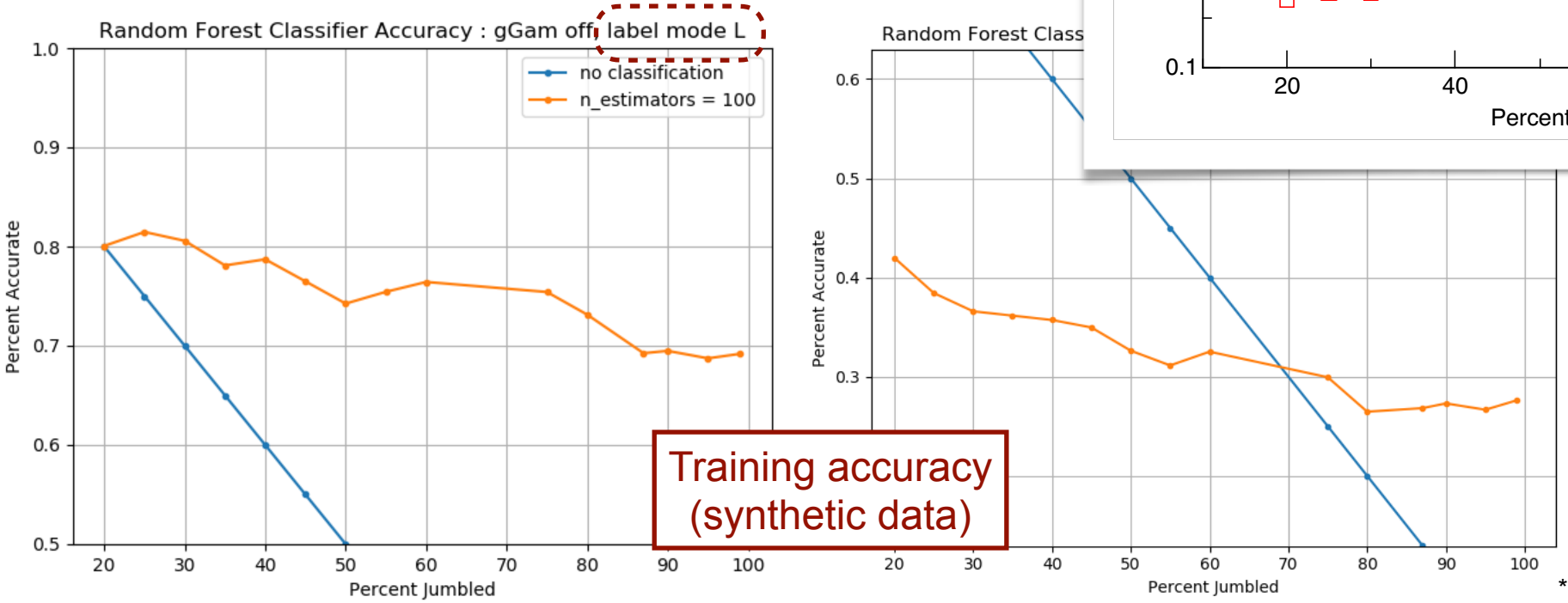

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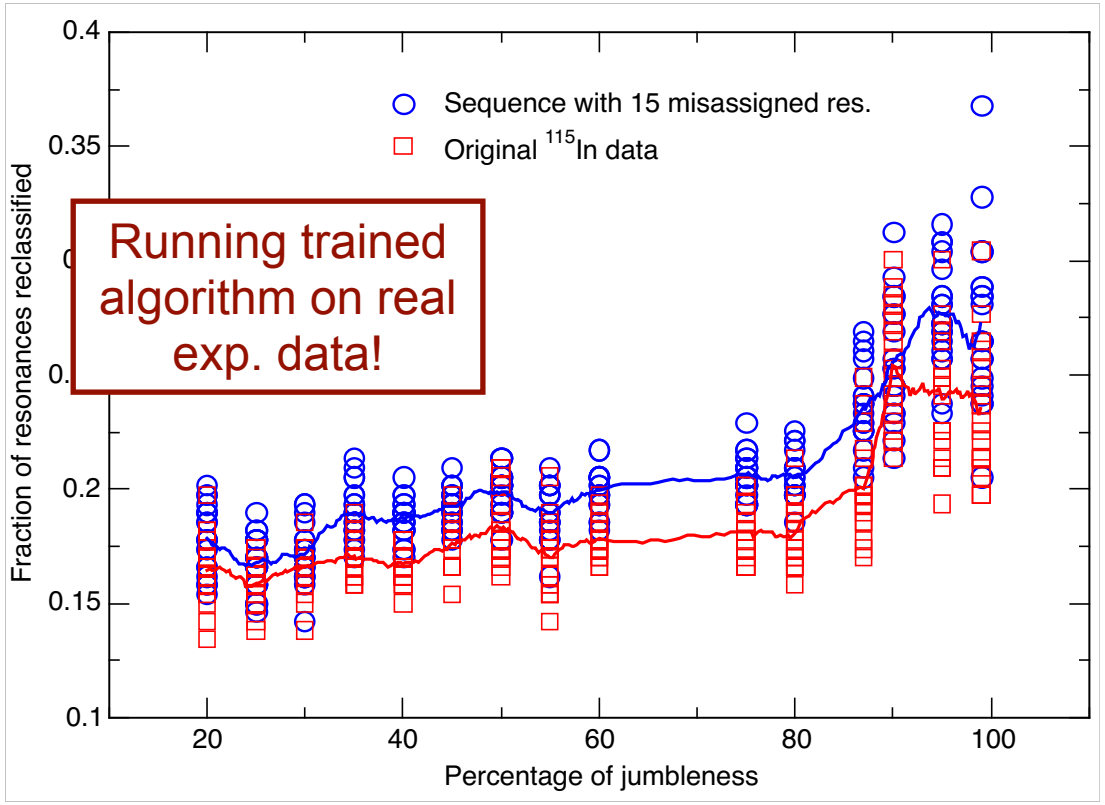

Running trained algorithm on real exp. data!

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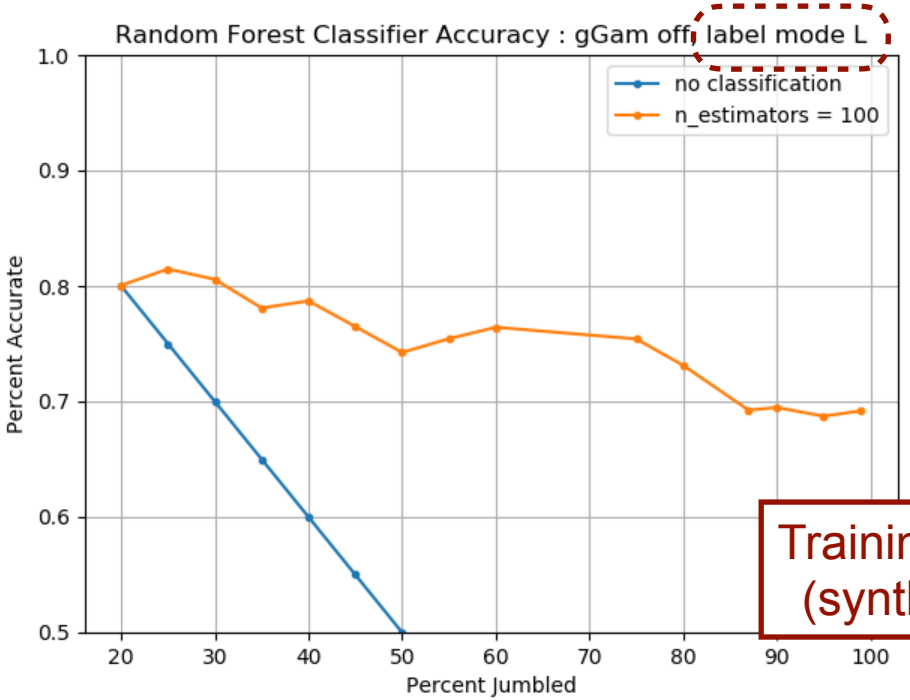

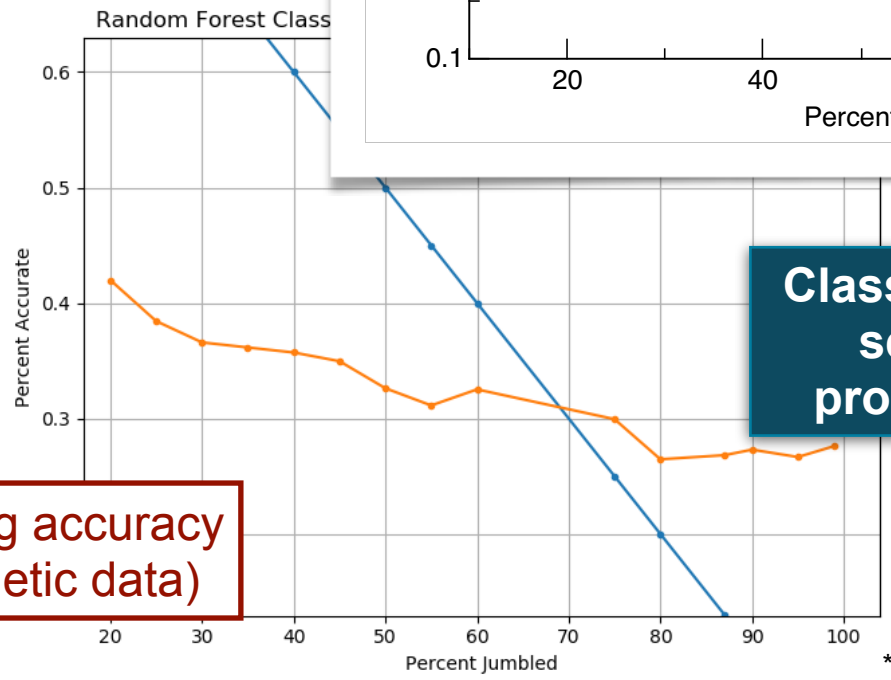

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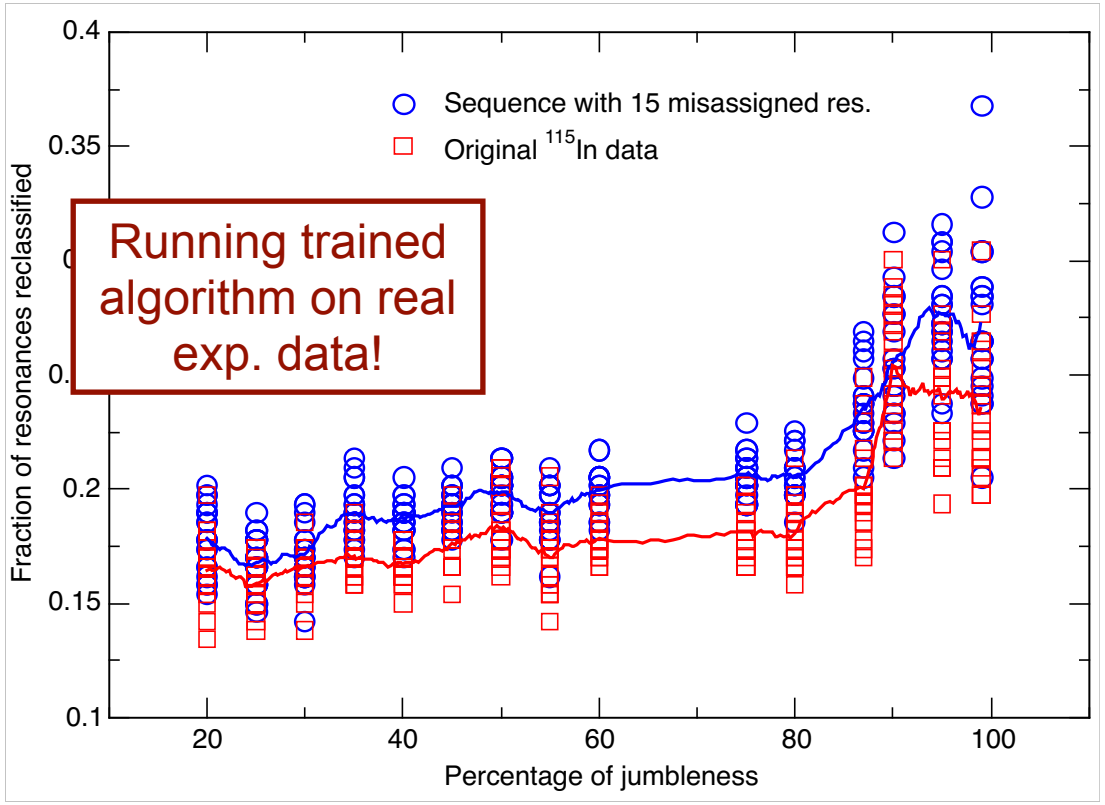

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Classifier correctly detects sequence with more problematic resonances

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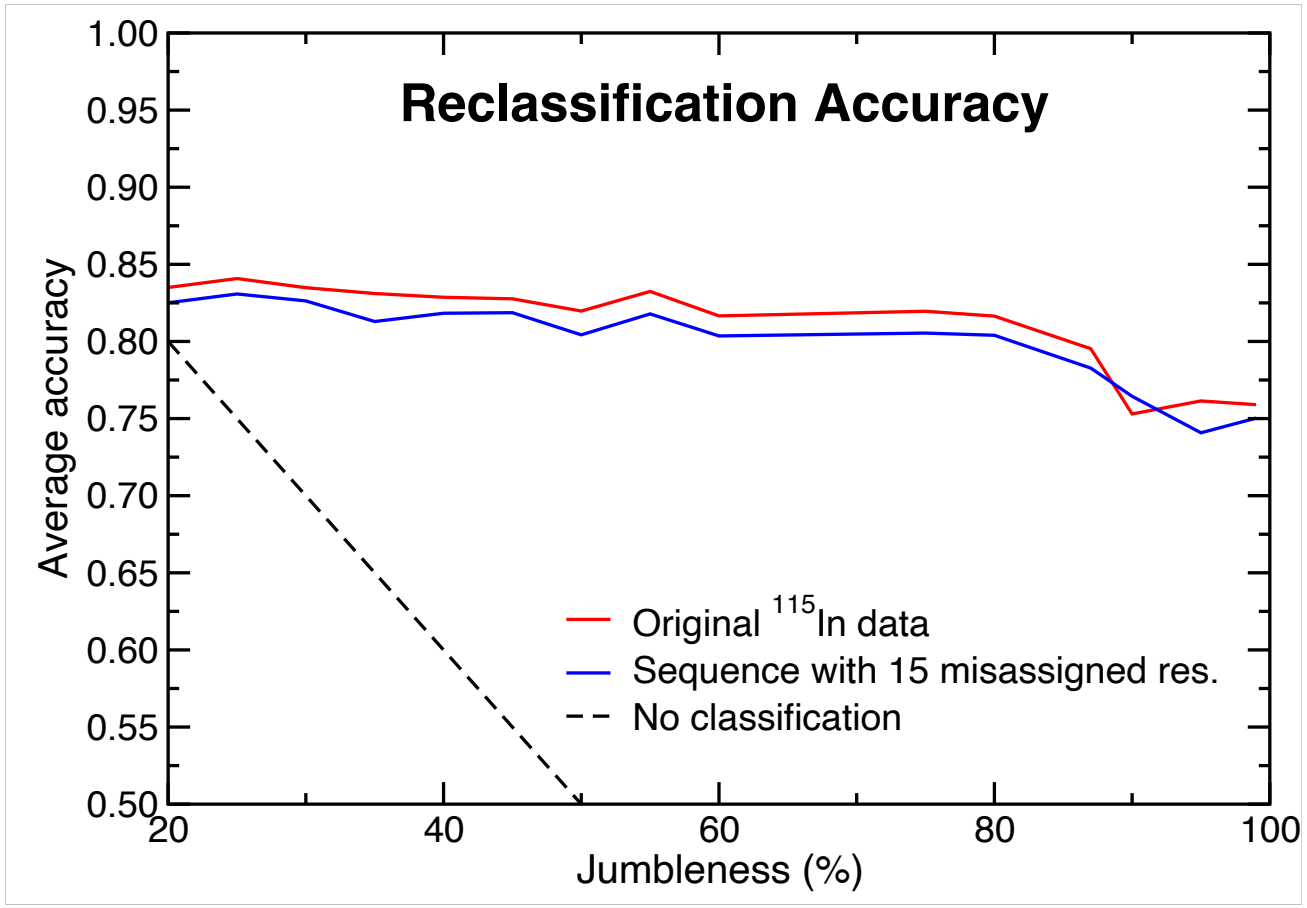

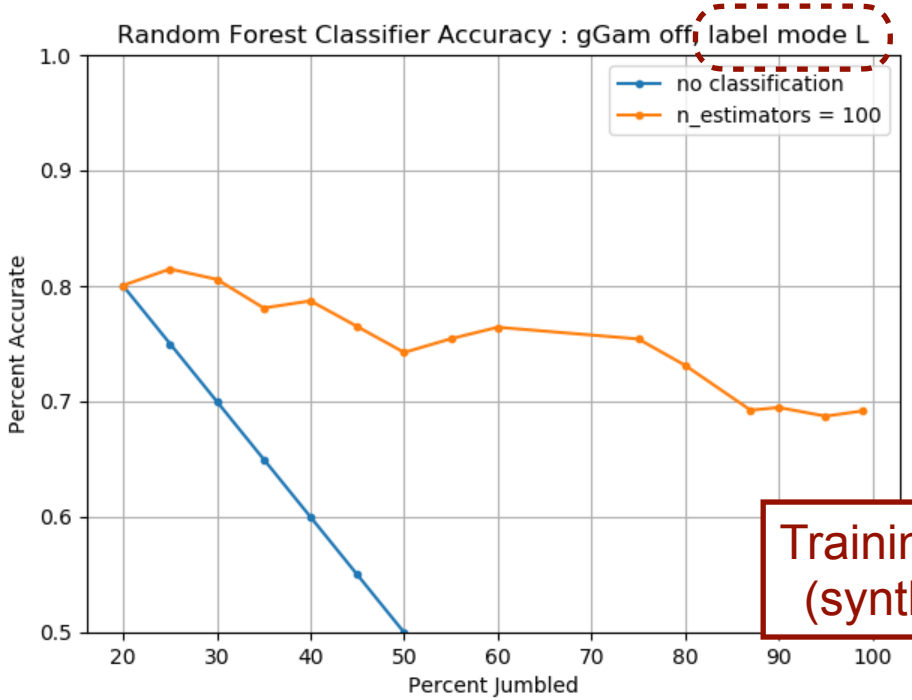

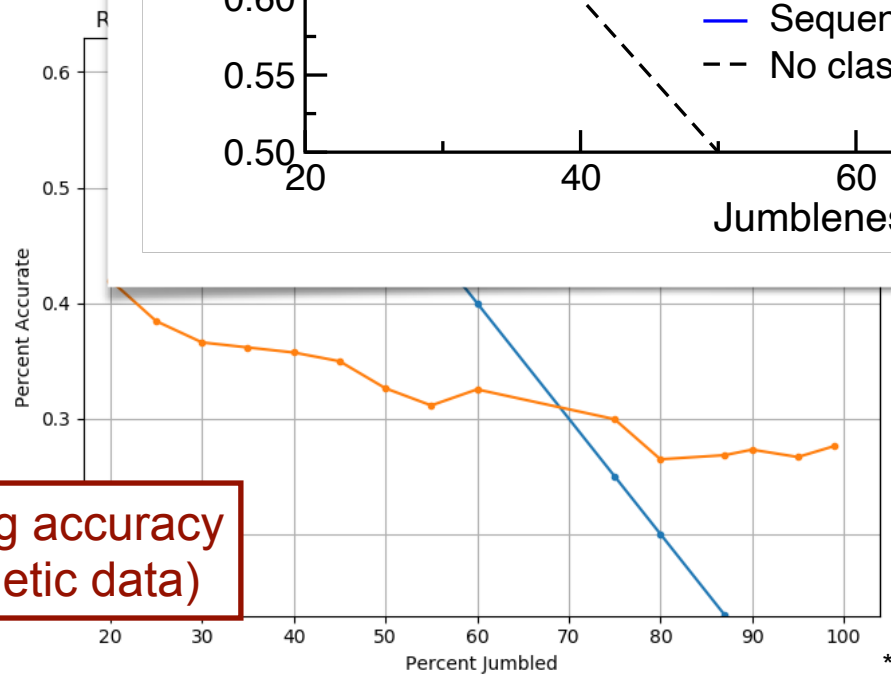

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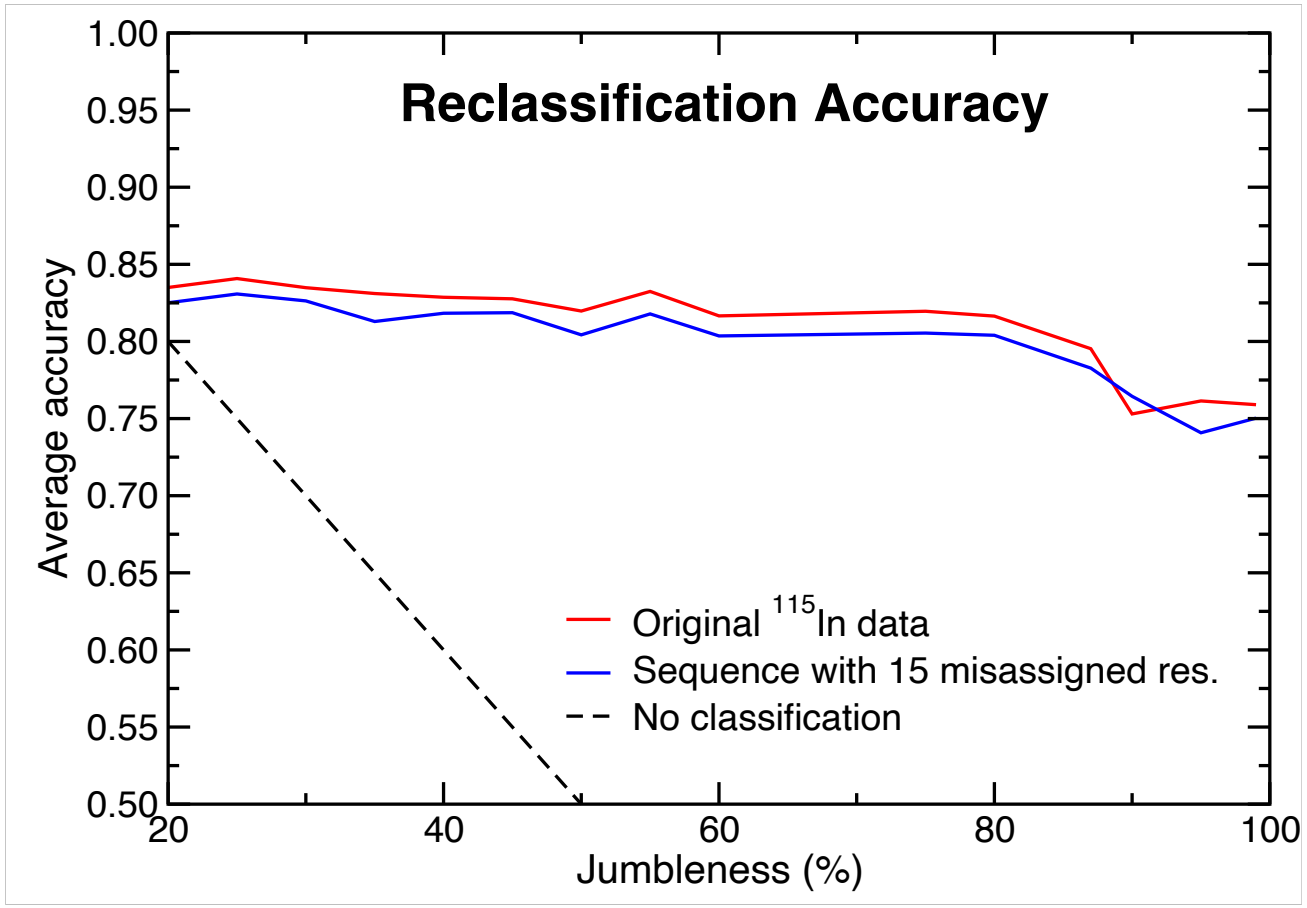

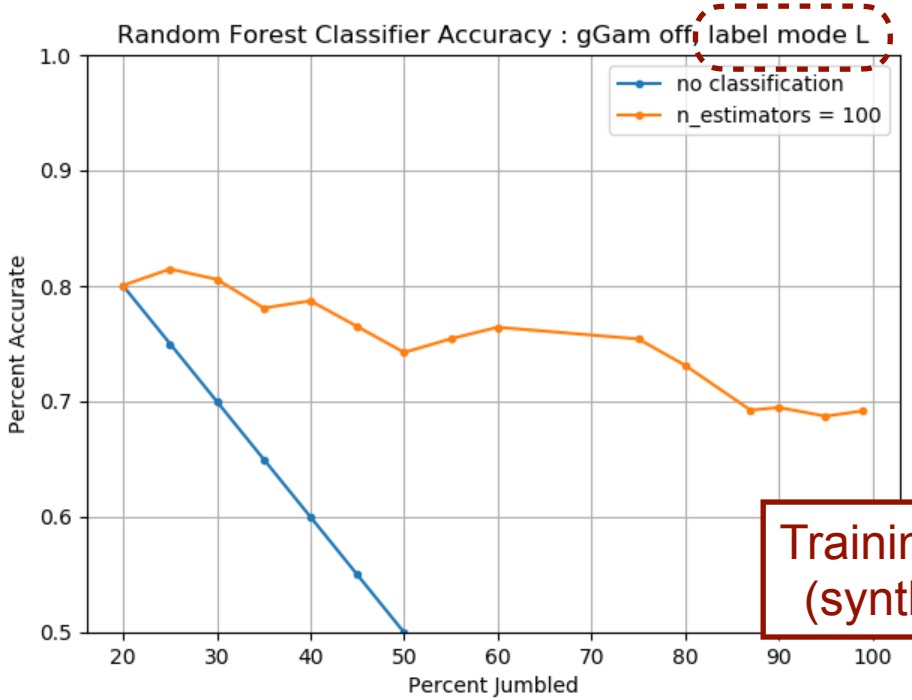

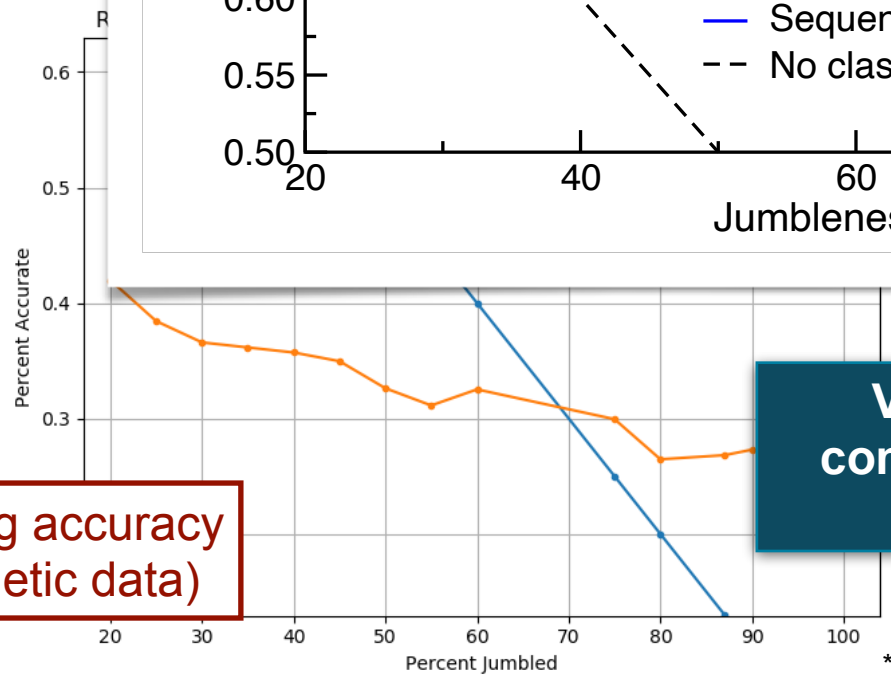

Training accuracy (synthetic data)

Validation accuracy compatible with training accuracy!!

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Conclusion and future perspectives

- We developed a Machine-Learning method to properly assign spins to neutron resonances: automated, general, reproducible
- Fully integrated with evaluated resonances in the Atlas: automation of new editions
- Transfer learning:
    - Train and optimize in synthetic data
    - Validate and deploy to real experimental resonances
- Very encouraging results!
- Will explore other classifiers and hyper-parameter combinations
- Will try to validate further with well-known nucleus (e.g. ^{235}U)
- Publication pipeline planned
- Thanks to all interns who worked and/or are collaborating on this project:


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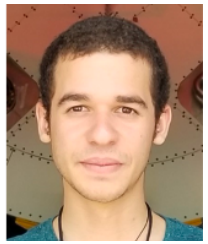
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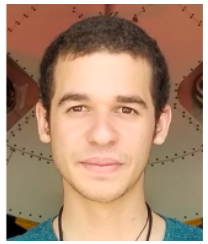
Yale grad student

Sergey Scoville

Graduates in Spring, pursuing grad school



Pedro Rodriguez

PNNL

Mary Fucci

Graduated last Summer, pursuing grad school

Sergio Ruiz

Going into junior undergraduate

Rose-Marie Crawford

Going into junior undergraduate

Brookhaven National Laboratory

Acknowledgements

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