

Example on how to (intelligently) augment the nuclear-data pipeline with machine learning

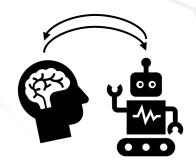
D. Neudecker Feb. 1, 2021 Human pipeline for nuclear data, WANDA 2021

LA-UR-21-20366



The "human pipeline" vs machine learning and automation - a dichotomy??

 Machine learning helps us where human brain is overwhelmed with wealth of data. Conversely, we can integrate expert knowledge in these methods.



 Where can we use automation to free the humans in the nuclear-data pipeline from repetitive work?





 Machine learning is an exciting subject area that draws students/ Postdocs into nuclear data. (Would not say "how to train young students for this new paradigm", but rather how can we learn along with them-with the help of a data scientist.) Students/ Postdocs publications in red









Where in the nuclear-data pipeline can automation and ML help us, a few examples:

Whewell et al., NIMA 978, 164305 (2020). **Schnabel** et al., arxiv:/2009.00521

Tuning Corrections

Arthur et al., ANE **133**, 853 (2019).

Caliva, **De Sousa Ribeiro**, et al., IEEE, 2018.

Differential Experiment

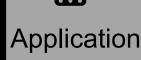
Evaluation

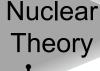
Processing Sensitivity



Generalpurpose Library







Lovell et al., J. Phys. G **47**, 114001 (2020). Grechanuk et al., J. Comput. & Theor. Transport 47, 552 (2019).

 Neudecker et al., NDS 167, 36 (2020).



- Michaud, Kleedtke et al., ANS Transactions 121, 1035 (2019).
- Siefman et al., ANE 151 (2021).





2 examples of LANL work to show how we transfer knowledge to ML and that ML augments the pipeline

Whewell et al., NIMA 978, 164305 (2020). **Schnabel** et al., arxiv:/2009.00521

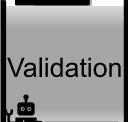
Tuning Corrections

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Differential Experiment

Evaluation

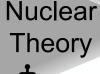
Processing Sensitivity



Generalpurpose Library



Application



Lovell et al., J. Phys. G 47, 114001 (2020).

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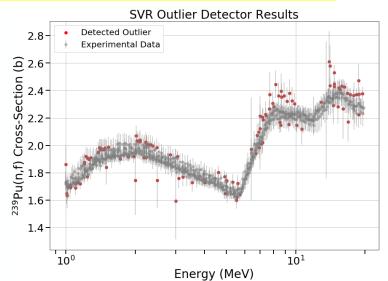




Question: What features of differential exp. lead to systematic discrepancies/ outliers in a database?

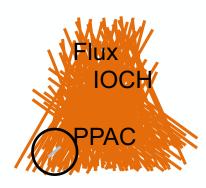
Why traditional techniques fail: the problem has 37 feature categories (100 values) for 24 measurements. ML can help us find trends in data, where

experts are overwhelmed with data.



Needle in the haystack

. . .



Benefit: We are investigating the physics reasons related to discrepancies between experiments or outliers. This can help us:

- Add missing unc/ reject data based on physics reasons → more reliable nuclear data and uncertainties,
- Design experiments with features known to produce reliable exp. data.

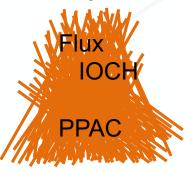


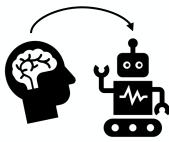




ML find physics expected features and unexpected features related to outliers, brings value to the field.

Needle in the haystack





Expert knowledge fed to ML:

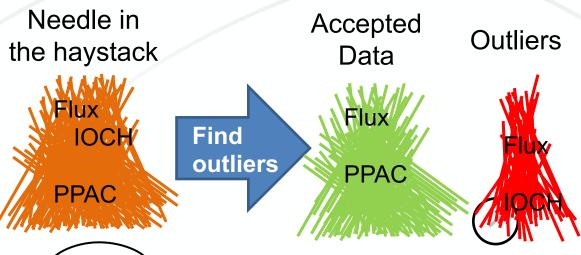
- Exp, data.
- Uncertainties
- Features

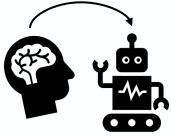






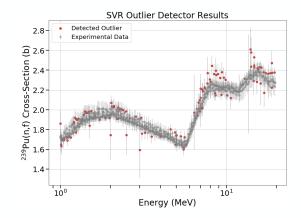
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Expert knowledge fed to ML:

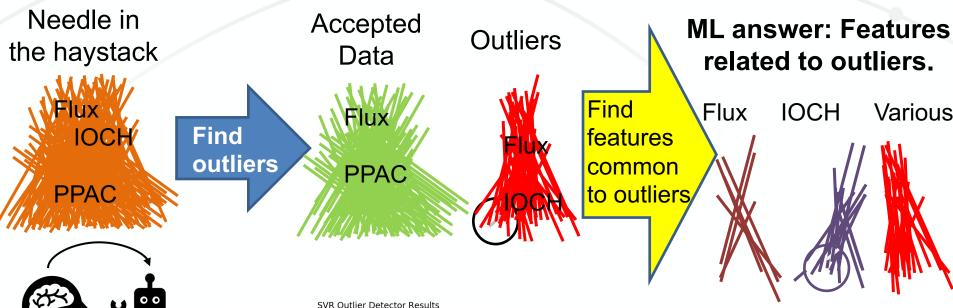
- Exp, data.
- Uncertainties
- Features







ML find physics expected features and unexpected features related to outliers, brings value to the field.

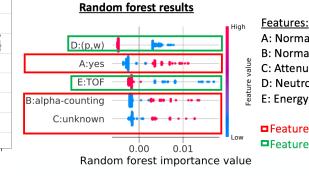


Detected Outlier Experimental Data

<u>a</u> 2.6

Expert knowledge fed to ML:

- Exp, data.
- **Uncertainties**
- **Features**



Legend

- A: Normalization determined
- B: Normalization determination method
- C: Attenuation correction method
- D: Neutron-producing reaction
- E: Energy determination method
- Feature value related to outlying data
- Feature value related to accepted data



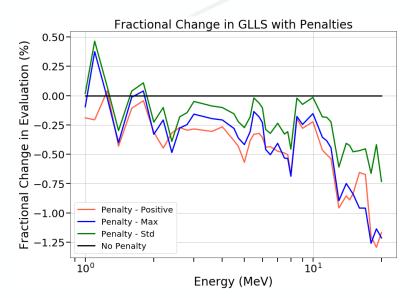


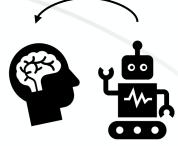
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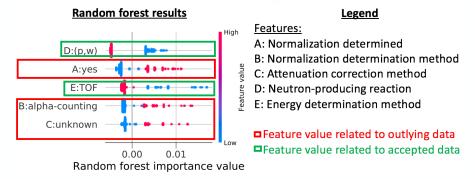
Energy (MeV)



Knowledge gained by ML can influence our evaluated data.







It is always up to the physicist to decide if the results are helpful. ML augments but does not replace expert judgment.

CAVEAT: for this particular problem, we lack the infrastructure to apply ML on a large scale.

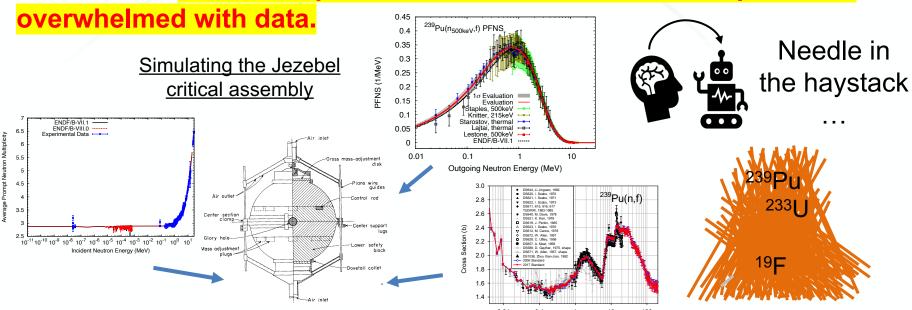
Natural language processing and SG-50 might help.





Question: What nuclear data leads to bias between simulated and experimental criticality?

Why traditional techniques fail: we simulate 1 criticality value with 1000s of nuclear data. ML can help us find trends in data, where experts are



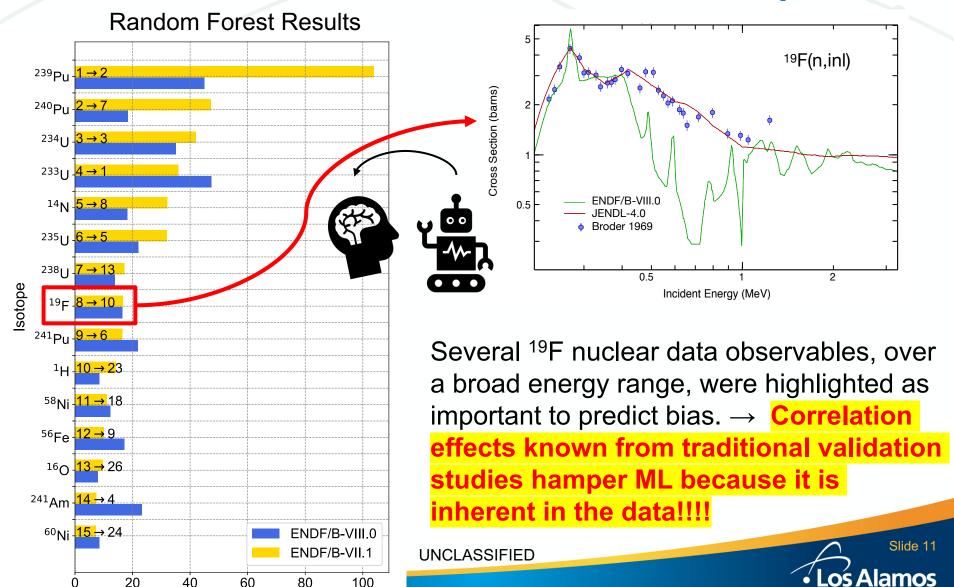
Benefit: This information provides input on what nuclear data might need to be revisited and corrected:

- Resolve timely issues in nuclear data → better data for applications,
- Identify need for integral/ differential experiments or new evaluations.





ML points towards potential issue in ¹⁹F ENDF/B-VIII.0 nuclear data relevant for validation exp.



20

Aggregated SHAP (pcm)

Conclusions:

- Can ML help our nuclear-data pipeline: Absolutely!!!
- ➤ ML's strength: find trends in large amounts of data where human brains are overwhelmed. This information may be crucial to improve our nuclear data.
- ➤ HOWEVER: ML is no silver bullet. It is critical to feed it expert knowledge and use physics intuition to interpret results. We need to:
 - Develop infrastructure and tools to provide data in an easily readable and unambiguously interpretable format (e.g., EXFOR format),
 - Develop experimental data and theory to solve physics questions,
 - Bring statisticians and nuclear-data experts together to correctly interpret the results.

Bottom line: ML is a great tool. We need to use these algorithms along with developing physics data, tools and infrastructure.





Acknowledgements



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