

AI/ML for Nuclear Data

Session Summary

Neural Networks

Gaussian Processes

Supervised Learning Generative Modeling Reinforcement Learning Deep Q Learning

Strong Interest in AI/ML for Nuclear Data

Part I: Prepared Remarks

Opening Plenary	Tim Hallman	Mike Grosskopf	Vladimir Sobes		
Nuclear Data Pipeline		•	•		
Compilations / Experiments	Amanda Lewis	Shinjae Yoo	Michelle Kuchera	Questions / Discussion	
Evaluations / Processing	Leo Neufcourt	Pedro Vicente Valdez	Jutta Escher	Questions / Discussion	
Validation	Denise Neudecker	Jesson Hutchinson		Questions / Discussion	
Applications	Nicholas Schunk	Amy Lovell		Questions / Discussion	
Closing Plenary	Guannan Zhang		•	Questions / Discussion	
	•	Break		•	
Part II: Moderated Discussion					

Part II: Moderated Discussion

Discussion Lead	Kyle Wendt		
Moderated Discussion	All		
Summary	Session Organizers		

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Experiments

Compilations

General Comments

- There is tremendous potential of AI/ML algorithms to address critical ND problems
- To fully and efficiently realize this potential, we should engage AI/ML community
 - to help us train, tune, and use algorithms
 - to explore new uses of existing tools & develop new tools
- ML algorithms currently used in ND should be collected in database with notes on applicability / limitations
- Emphasize that these tools should augment ND expertise, **not replace it**, especially in safety-related projects

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General Comments

- There are many open source tools out there and many other fields have a head start in addressing similar problems
 - Engage them and the AI/ML community
 - Most institutions represented here have strong groups with expertise in this area
- Tools like Tensorflow/Keras/Pytorch/Scikit-learn can be used for rapid exploration of new and innovative ideas
 - Engage the AI/ML community, especially experts in your own lab, to avoid traps in training, over-fitting, mathematically ill-defined applications ...

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Reinforcement Learning

Deep Q Learning

- Long term vision:
 - Faster, more reproducible evaluation of ND using theory/models, differential and integral experiments through AI/ML
 - Assist in generating covariances that can account for potentially discrepant experimental observations
 - Revealing deficiencies in theoretical models.
 - Integration of hard and soft physics constraints with AI/ML tools.
 - AI/ML-guided processing including optimal multigroup.
- Barriers to entry:
 - Bringing uncertainty into the ML predictions.
 - This is not a solved problem in any field.
 - Implementing hard physics constraints in ML methods.
 - Lack of infrastructure, ND formats adapted to ML techniques
- Short term most impactful applications:
 - Acceleration of evaluation through automation, (e.g. feature detection, parameter inference, etc...)
 - Emulation of modern expensive physics models enabling UQ.

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- Long term vision:
 - Automated processing of scientific papers in ND by AI/ML tools for extraction of data, scientifically relevant content, and connection between the different papers for standardized collection and summarization of data and results
 - Emphasize human-in-the-loop methods to augment expert assessment.
 - AI/ML guided design to optimal experiments & use beam time more efficiently.
- Short term most impactful applications.
 - Application of OCR/NLP for extraction of insight from nuclear physics literature adapting recent work law, chemistry, material science, etc.

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• Long term vision:

Experiments

Compilations

- Advancement in validation of ND augmented with AI/ML through optimal experimental design and through new insight
- Validation not just of ND but of the AI/ML tools
 - Building trust through:
 - Stability
 - Robustness
 - Interpretability
- Short term most impactful applications:
 - Use of AI/ML to identify areas of improvement in ND evaluation from benchmark bias
 - Design of optimized integral experiments based on AI/ML

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• Long term vision:

- Integration of emulator/surrogate models into multi-physics codes to facilitate fast, accurate codes across scales and physics
- Utilization of multi-fidelity emulators to leverage information from accurate but slow models to correct fast, lower accuracy models that can be used to explore large parameter spaces for design, optimization, calibration or emulation.
- Identifyings the unexpectedly important reactions to specific applications.

• Barriers to entry:

- Input space, nuclear data libraries, represent an extreme high dimensional space for emulation.
- Short term most impactful applications:
 - Integration of emulators of expensive computer models into optimization/calibration framework outside of current physics models
 - AI/ML to identify features across wide spectrum of integral data (critical and subcritical assemblies, pulsed spheres, radchem, reactor designs, etc)

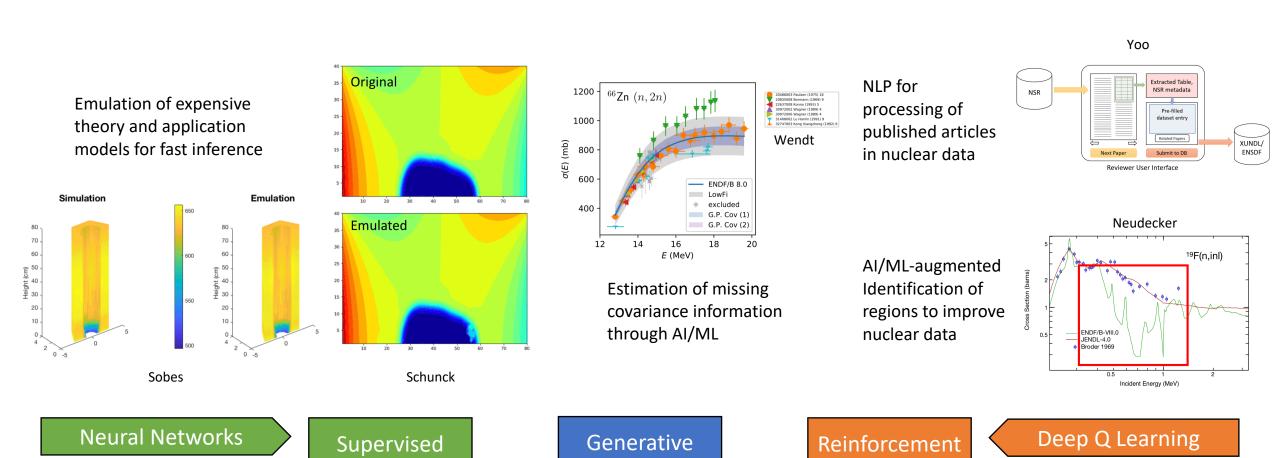
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We strongly encourages entire ND community to embrace the advances that AI/ML tools can have for your work!



Modeling

Learning

Bayesian Optimization

Learning

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