AI IN FUNDAMENTAL NUCLEAR PHYSICS RESEARCH: **CURRENT STATUS* AND THE FUTURE****

* A SOMEWHAT ANECDOTAL PERSPECTIVE

** EXTRAPOLATION COMES WITH LARGE ERROR BARS

MICHELLE KUCHERA DAVIDSON COLLEGE | **AI FOR NUCLEAR PHYSICS** 5 FEBRUARY 2020

CURRENT STATUS*

* A SOMEWHAT ANECDOTAL PERSPECTIVE

CURRENT STATUS: HOW WE ARE "LEARNING"

- Nuclear physics is a broad, distributed "field"
- Large Parallel distributed Effort, less communication / synchronization
- Subfields and groups are developing technology independent of one another

  - very different applications can have similar challenges and neec

  - Vastly different data structures

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Collaboration is what physicists do well

Los Alamos NATIONAL LABORATORY

BERKELEY LAB

Argonne NATIONAL LABORATORY

Jefferson Lab

FRIB

BROOKHAVEN NATIONAL LABORATORY

CURRENT STATUS: TOOLS

- 1990's: first AI-based fundamental physics discovery
  - Single top quark
  - Decision trees, bayesian neural networks (1992)
- Past 5 years: Broader acceptance and adoption: Industry
  - Tensorflow 2015
  - Pytorch 2016

CURRENT STATUS: TOOLS

RECENT TRANSITION TO MODERN ML / AI TOOLS

- RECOGNITION OF ADVANCED, FLEXIBLE TOOLS
- PHYSICISTS TYPICALLY EMBRACE END-TO-END DEVELOPMENT
- LOSE THE NECESSITY TO UNDERSTAND LEARNING PROCESS

PyTorch

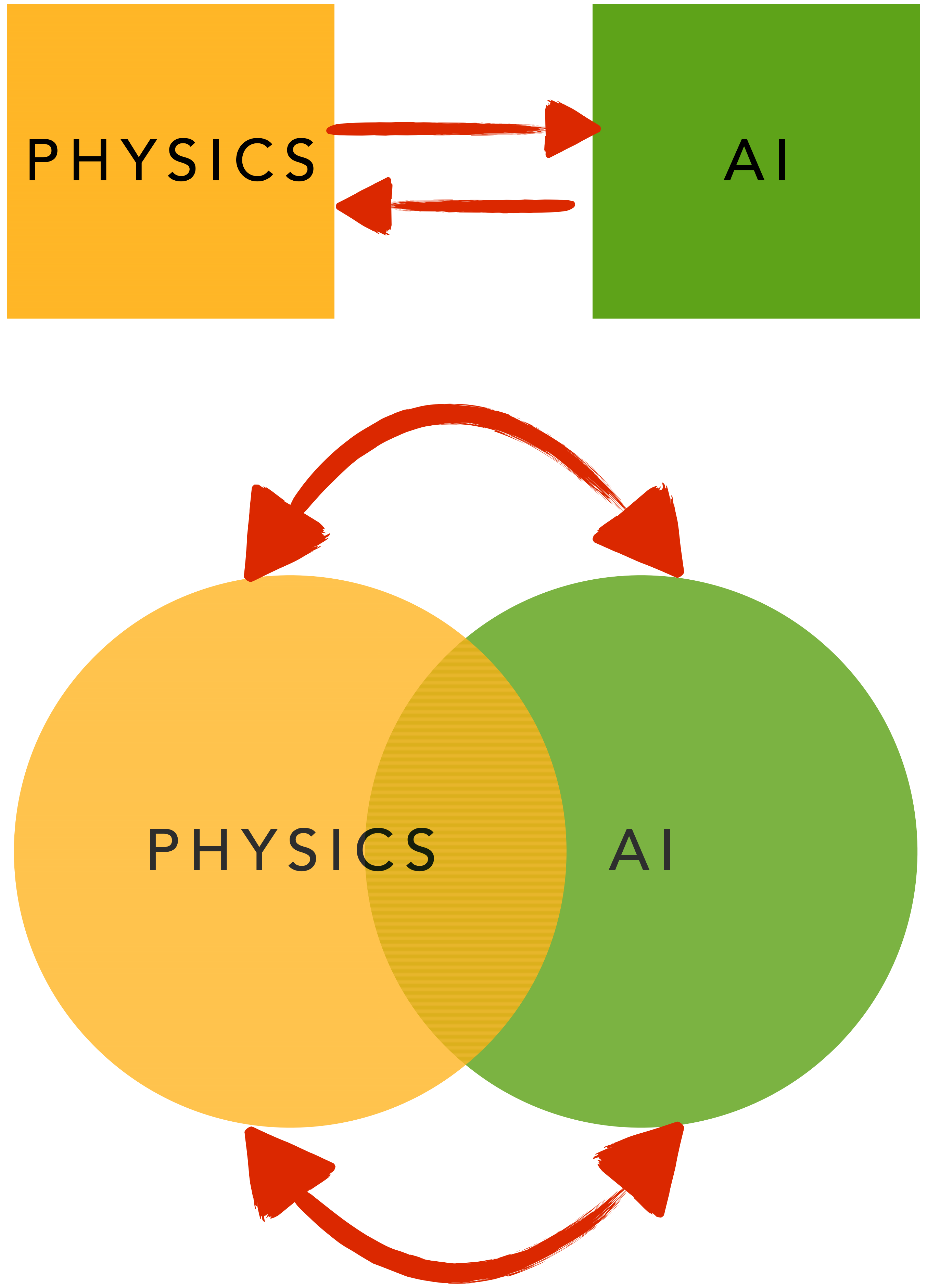
TensorFlow

CURRENT STATUS: COLLABORATIONS

- USERS, NOT INNOVATORS OF NEW AI

- COLLABORATING WITH AI / ML SCIENTISTS AND DATA SCIENTISTS

    - GROUP LEVEL
    - LEARNING CURVE



FUTURE OF AI IN NUCLEAR PHYSICS**

** EXTRAPOLATION COMES WITH LARGE ERROR BARS

FUTURE

FUTURE IS NOW:

Unite across subfields

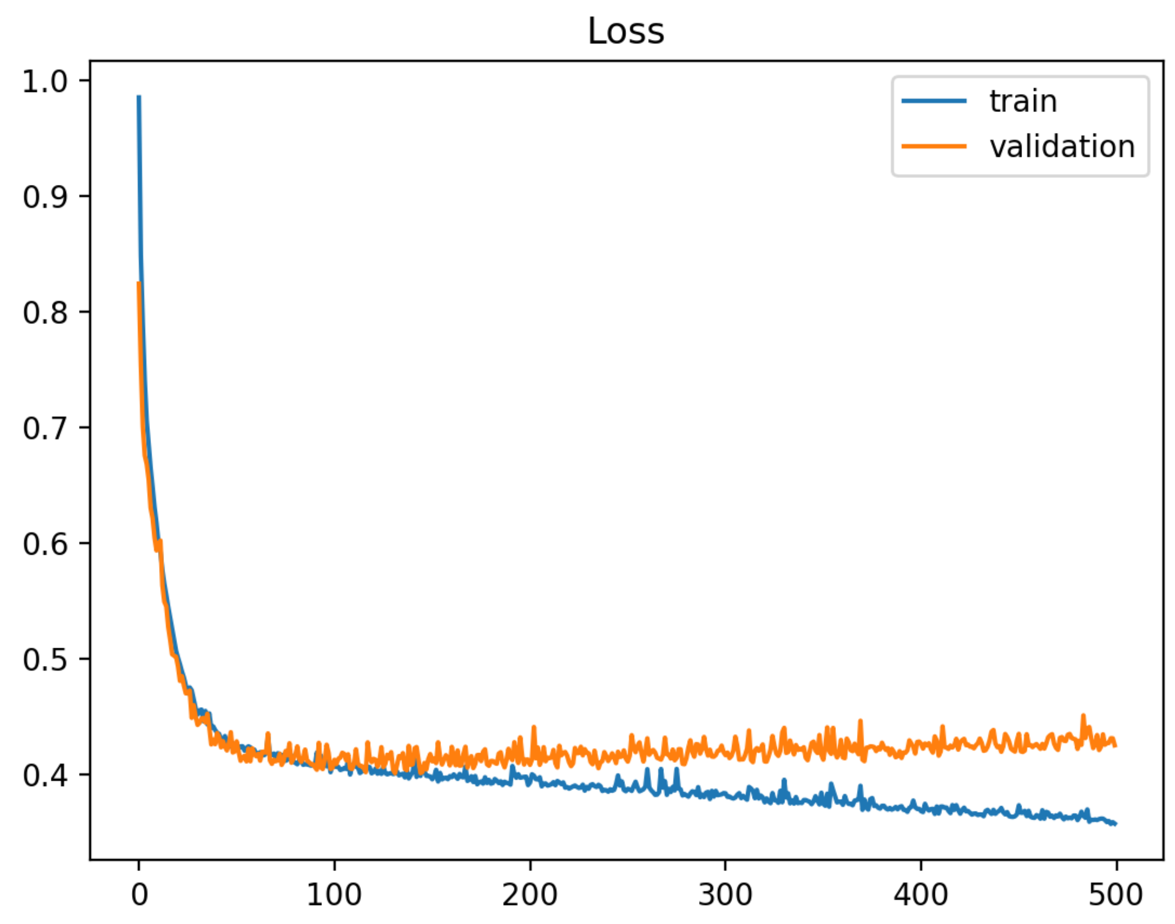
Identify common challenges

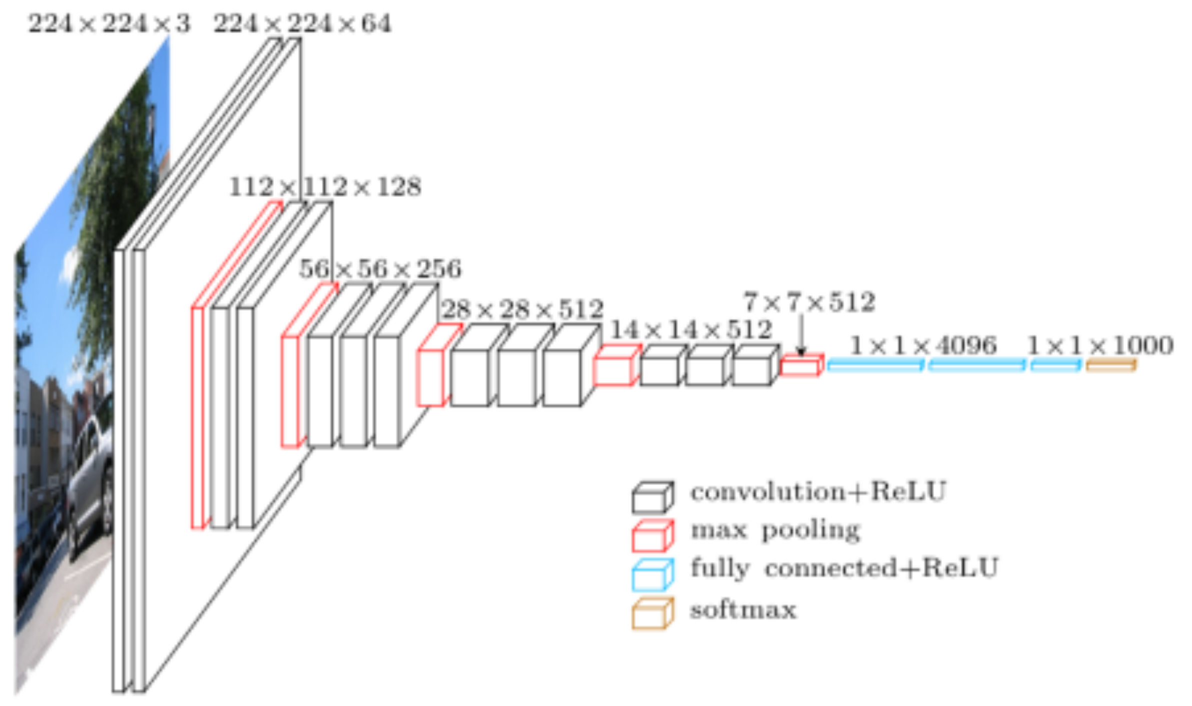
Acknowledge differences

FUTURE: EDUCATION

EDUCATION OF ML / AI METHODS

- We aren't afraid of the mathematics
- standard development and training procedure:
  - how to properly **train**, **monitor**, **tune**, **build** architectures, use pre-existing architectures and **trained models**

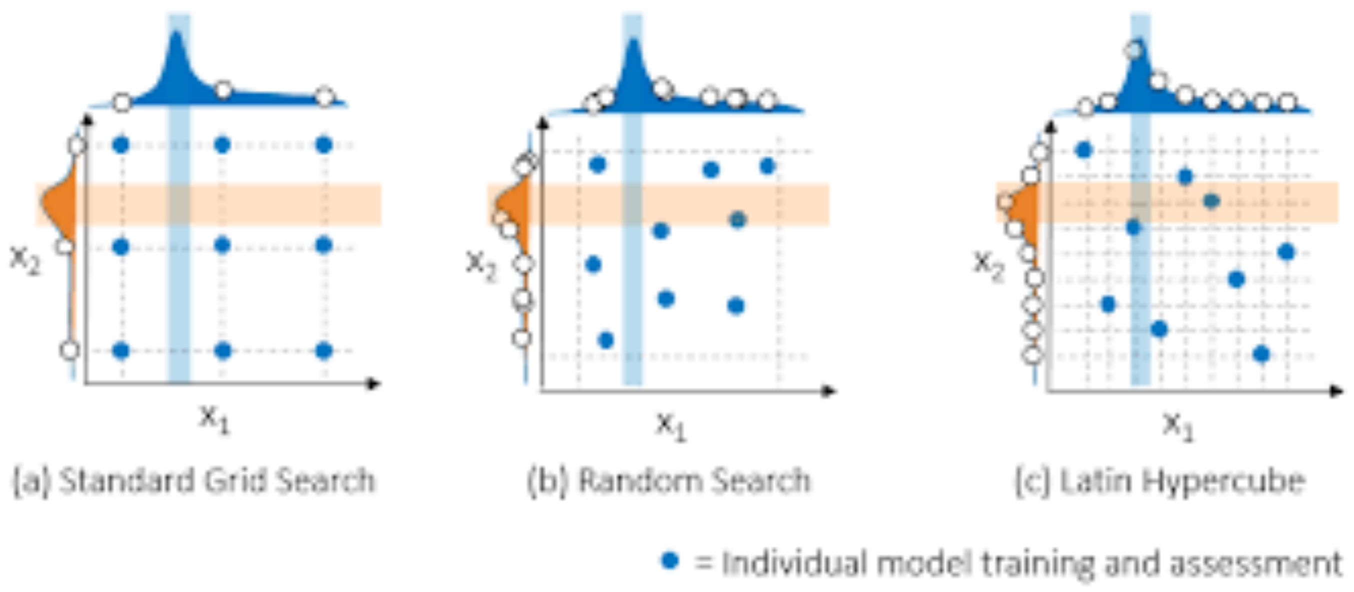


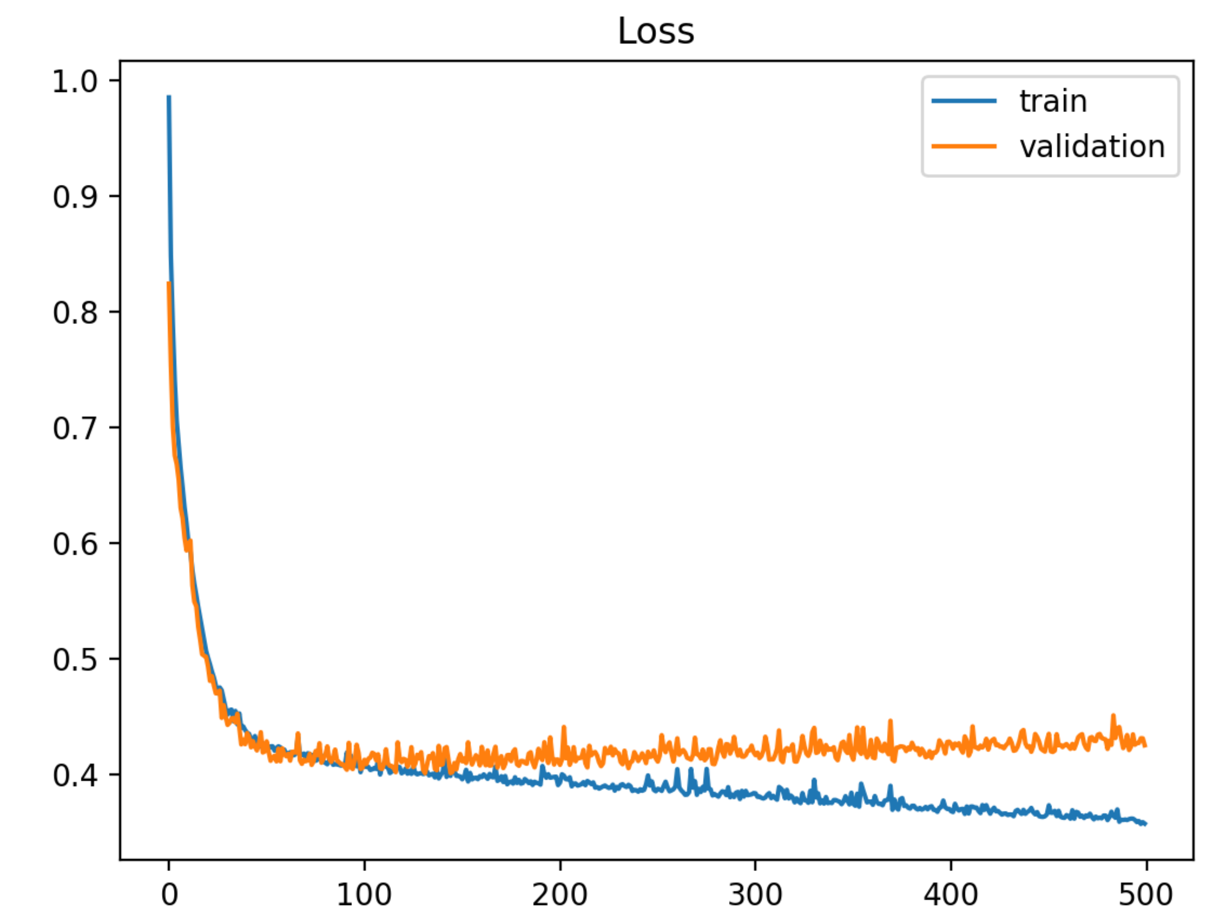


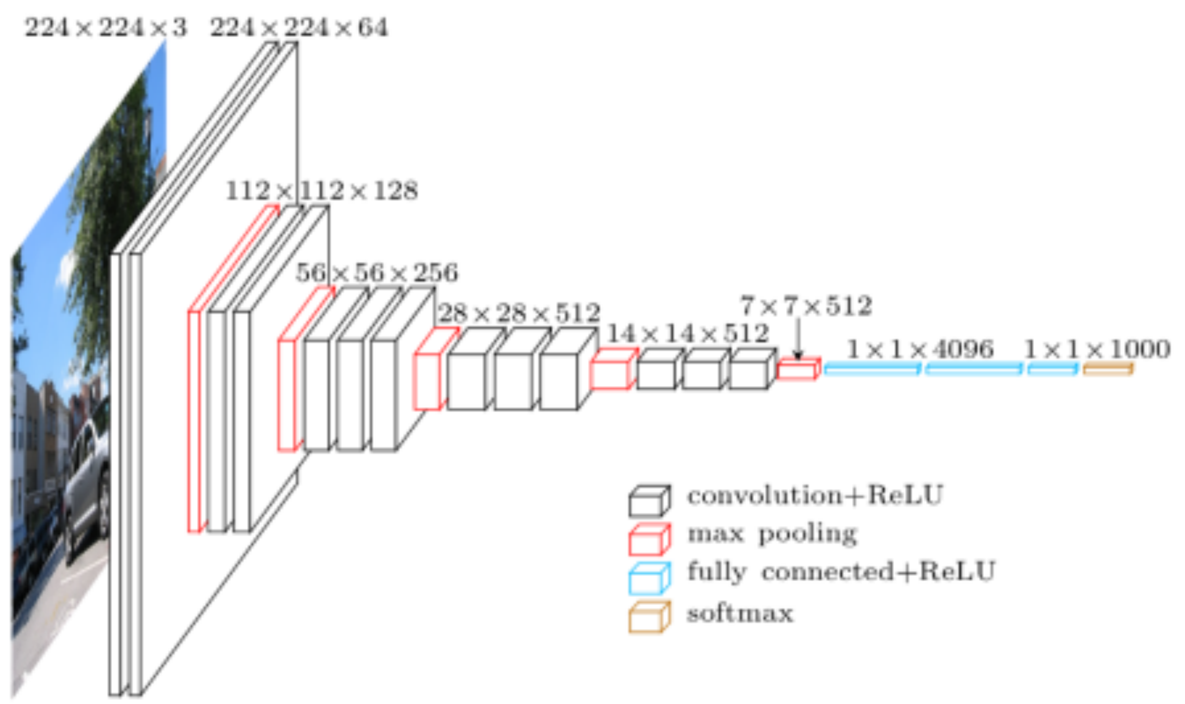
FUTURE: EDUCATION

EDUCATION OF ML / AI METHODS

- We aren't afraid of the mathematics
- standard development and training procedure:
    - **understand limitations:** e.g. loss of AI benefits when:
        - building domain knowledge into models
        - interpretable learning methods







FUTURE: DATA

DATA

- Provide data structures that can be easily presented to models (unite?)
- Accessible public datasets:
  - Non-NP students and AI researchers: Kaggle grab and play format and problem description

FUTURE: COLLABORATION

- **Stronger collaboration:**
  - AI scientists
  - Industry
- **How:**
  - NP presents challenges that are not addressed in current technologies
  - NP presents datasets that expose limitations of cutting edge methods
  - Work together, with both parties privy to the others' motivations

PERSPECTIVES: GUANNON ZHANG

- Heuristics used in ML/AI training significantly prohibits reproducibility, such that a lot of “new” ML/AI models and methods can not be verified.

applied mathematician
uncertainty quantification, AI, ML

Oak Ridge National Laboratory

PERSPECTIVES: GUANNON ZHANG

- Training ML/AI with physical constraints

- Most existing ML/AI training algorithms are non-constraint optimization, but ML/AI problems related to nuclear data may require either hard or soft constraints.

- Soft constraints could be handled by adding regularization terms to the loss function, but hard constraints are generally difficult to handle.

applied mathematician

uncertainty quantification, AI, ML

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PERSPECTIVES: GUANNON ZHANG

- Generalization gap

  - Since the loss function only involves training data, the global optimum of the loss function may not be a good choice for your ML/AI model.

  - If the training data can fully represent the entire population, global optimum is the best. Otherwise, a local minimum with small curvature is preferred.

applied mathematician

uncertainty quantification, AI, ML

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PERSPECTIVES: GUANNON ZHANG

Stability and Robustness of AI/ML prediction

• Stability means the sensitivity of ML model output with respect to small perturbations of inputs

- Deep NNs may have stability issues when viewing them as dynamical systems, i.e. ODEs

- Possible strategies include implicit neural networks, reversible networks

• Robustness means the ML can alleviate the influence of adversarial attacks

- Intentionally or non-intentionally generated or crafted data to hurt the predictability of deep neural networks, e.g., mis-classification.

applied mathematician
uncertainty quantification, AI, ML

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THANK YOU!!

DAVIDSON