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Deep Learning for Scientific Discovery



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Does deep learning work?

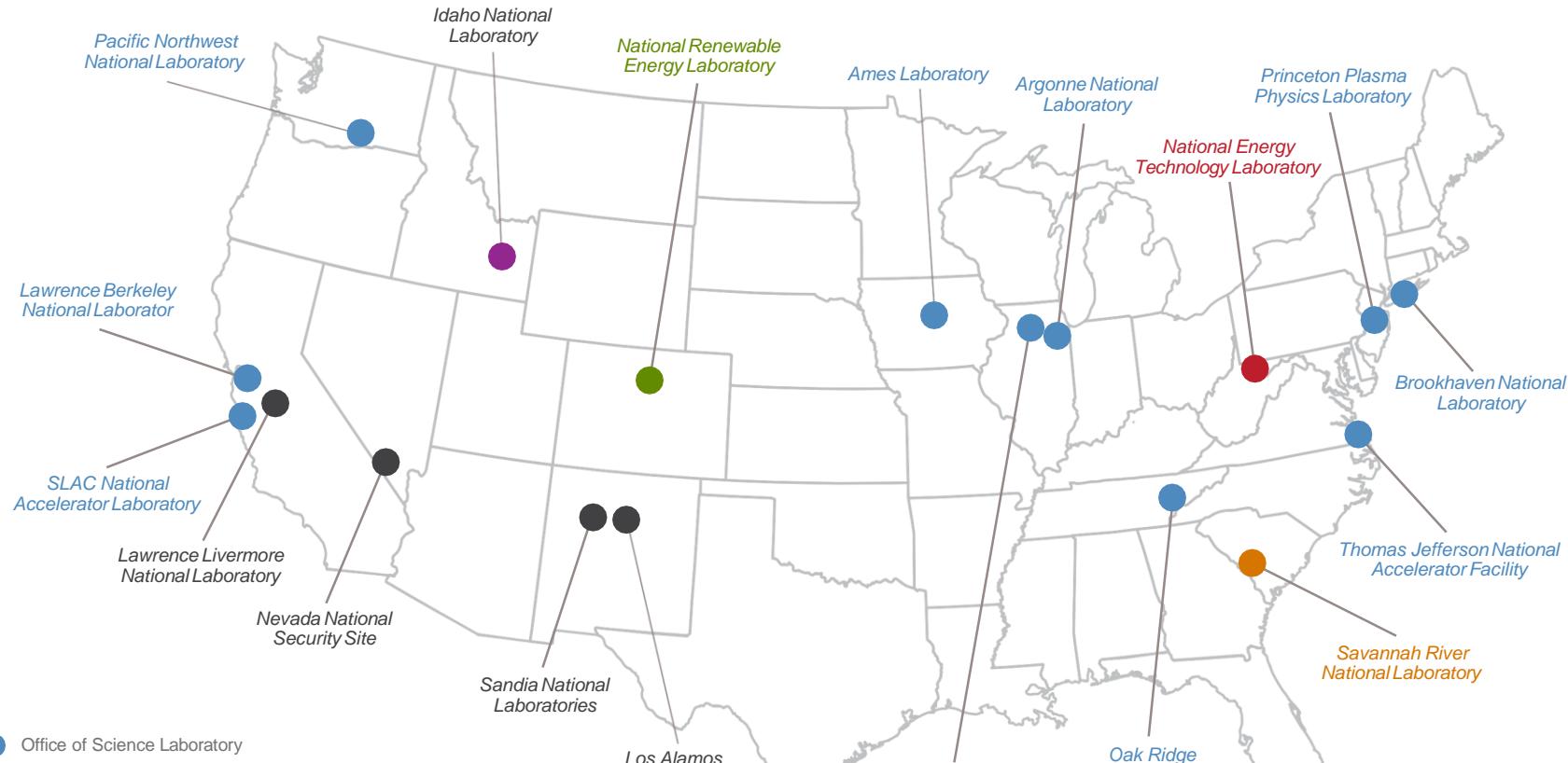
- ▶ Yes, if you have **data** and a **metric for success**.
- ▶ But! how **well** it works can't be known until you try.



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PNNL is Mission Driven



- Office of Science Laboratory
- National Nuclear Security Administration Laboratory
- Office of Fossil Energy Laboratory
- Office of Energy Efficiency & Renewable Energy Laboratory
- Office of Nuclear Energy, Science & Technology Laboratory
- Office of Environmental Management Laboratory



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PNNL's Science Vision



Earth

- Clouds and Aerosols
- Water Cycle
- Microbial Communities



Energy

- Energy Storage
- Energy Conversions
- Control and Security



Security

- Ultra-Trace Detection
- Novel Signatures
- Data-Driven Discovery





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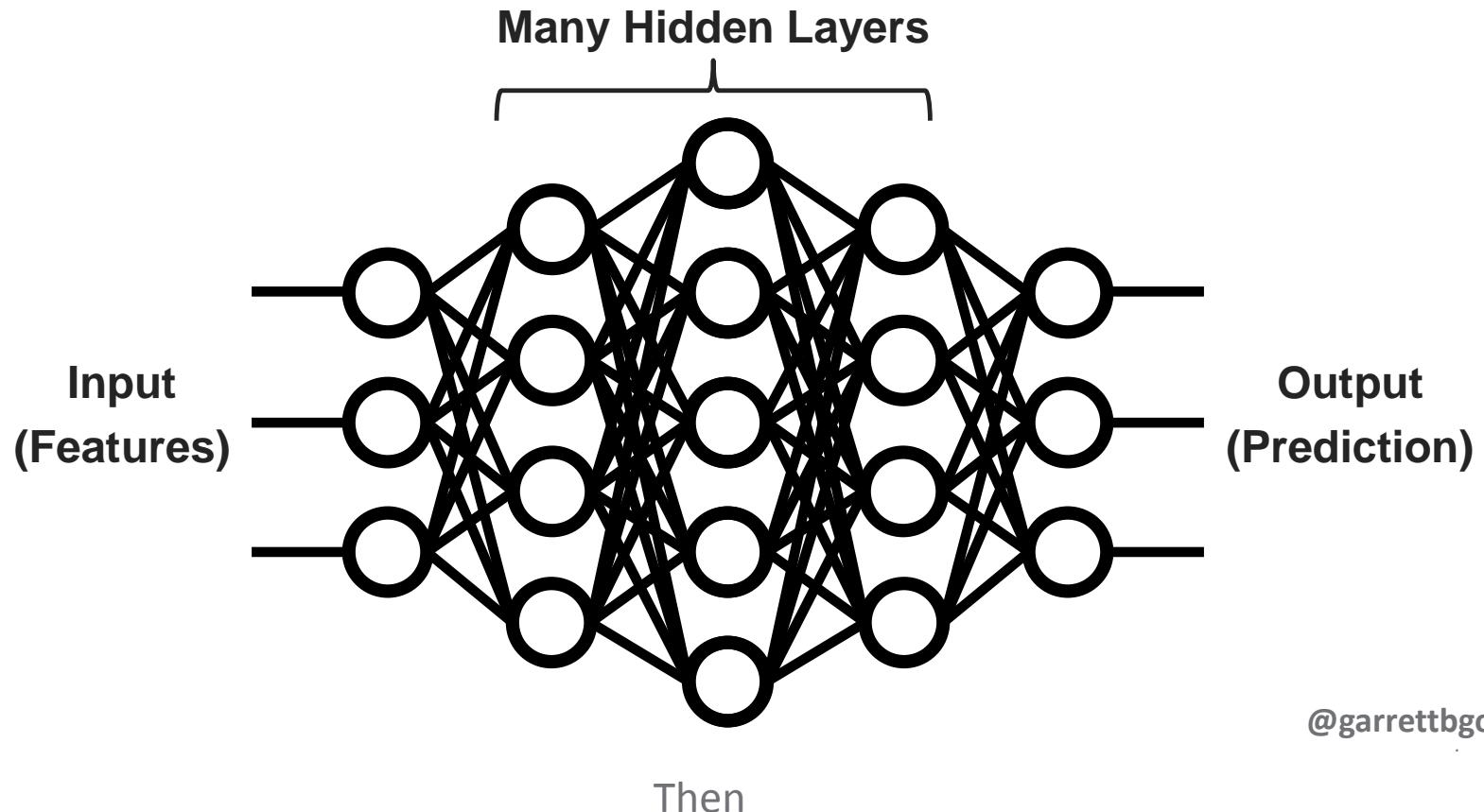
What is Machine Learning?

Machine learning is a subfield of computer science and artificial intelligence that enables machines to learn without being explicitly programmed



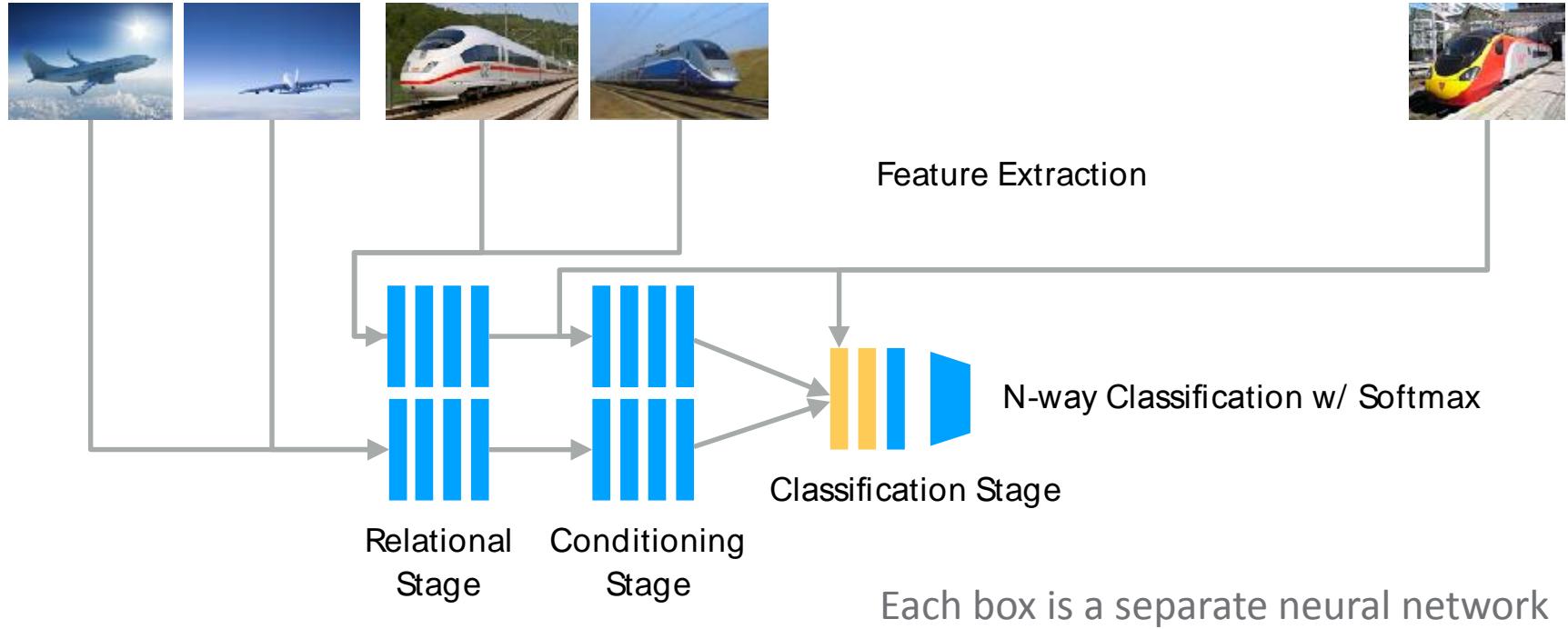
What is Deep Learning?

- ▶ Deep Learning is neural networks from the 1970's and 1980's -- fully realized



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- Deep Learning is neural networks from the 1970's and 1980's -- fully realized



NOW



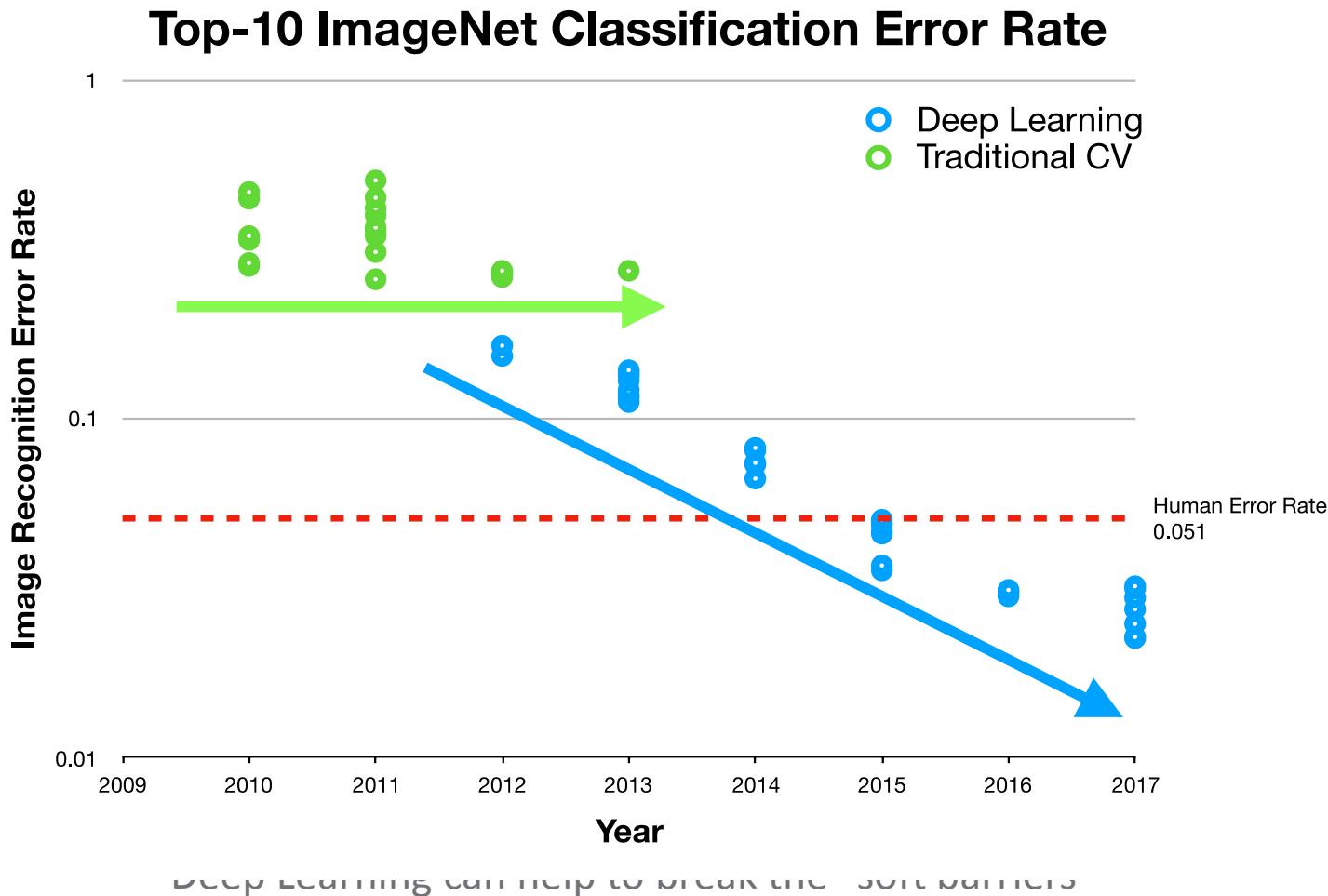
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What Changed?

- ▶ **More Data**
- ▶ **Better Computing (Graphics Processing Units)**
- ▶ Better optimizers (ADAM, RMSProp,...)
- ▶ Better numerics (Rectified Linear Units, BatchNorm,...)
- ▶ Better architectures (Residuals, LSTM...)
- ▶ Better software (Keras, Tensorflow, PyTorch...)

Why Deep Learning?

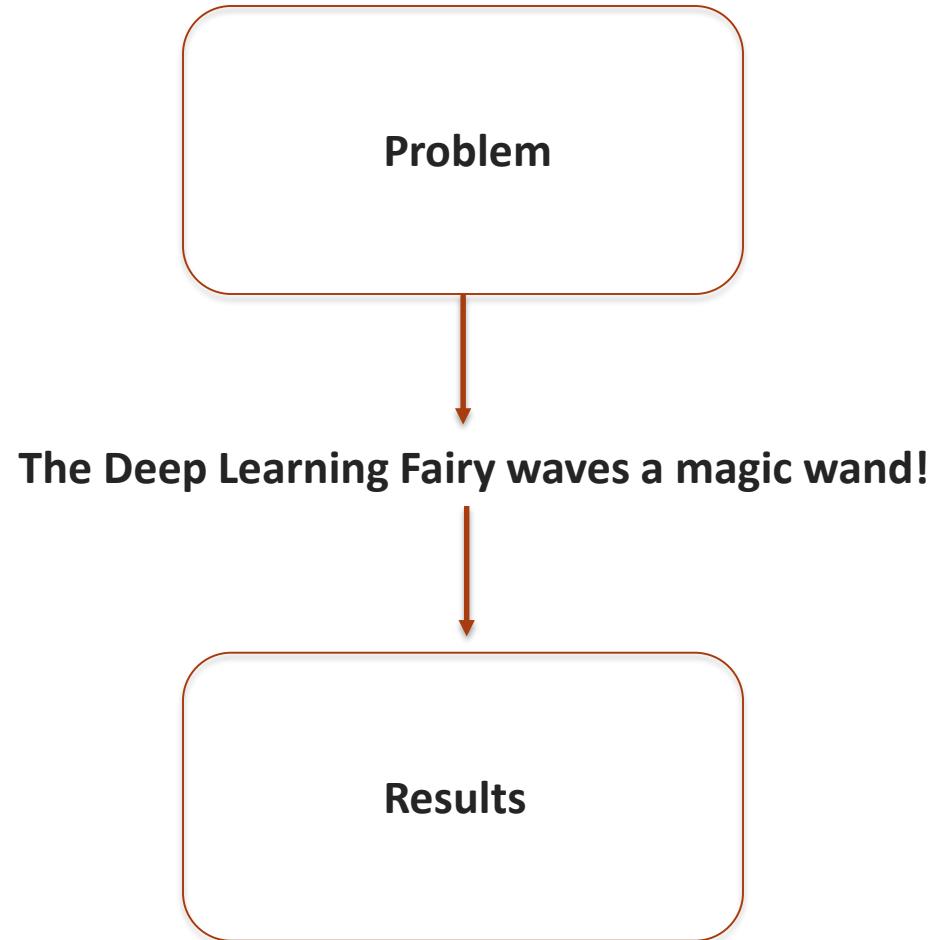


Now

Protected Information | Proprietary Information



Myths



Equivalently: “Can we use deep learning to understand X?”



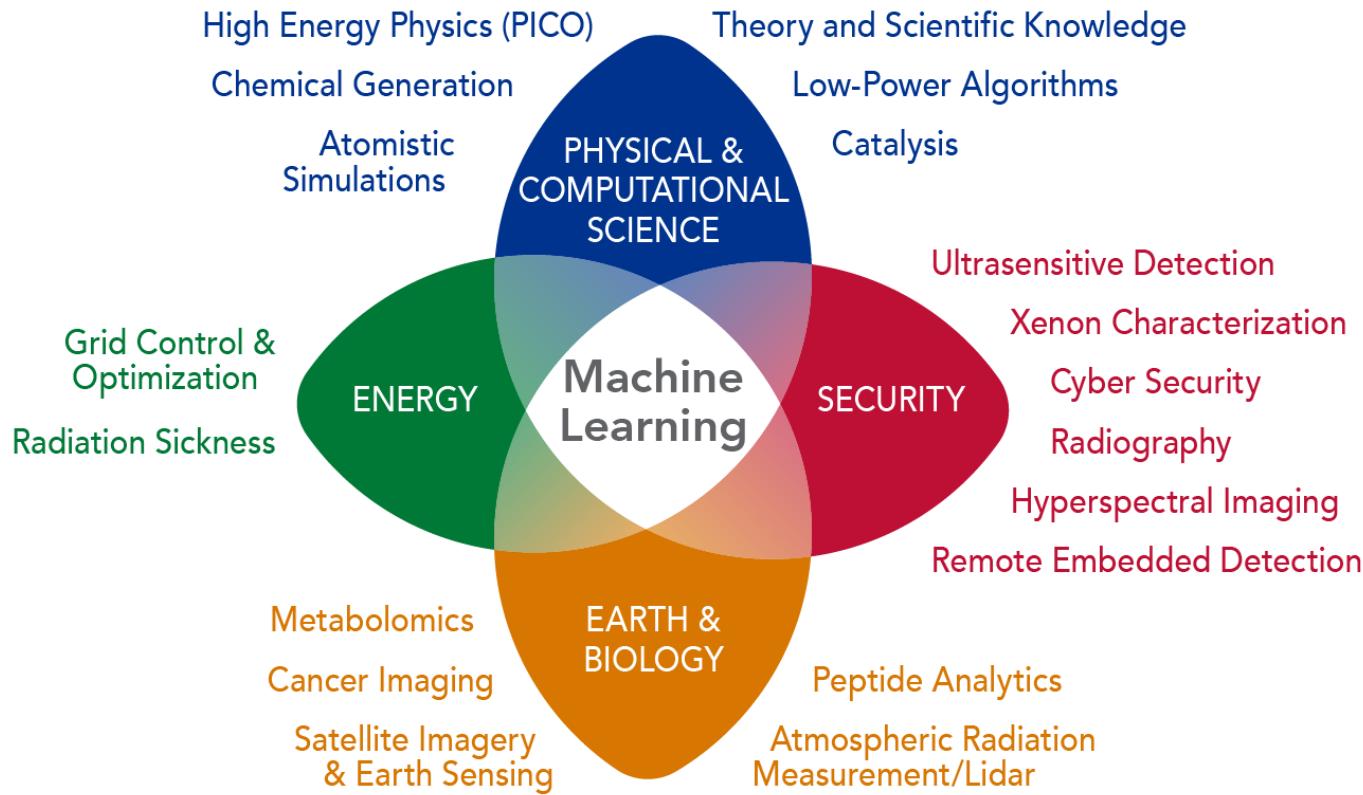
Requirements for Success

1) Scientific Goal

2) Data – You need data to learn the patterns

3) A quantitative metric – You need to know if you are getting closer to success.

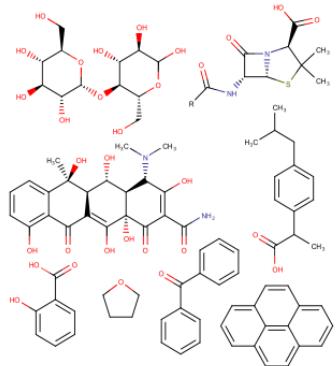
Deep Learning for Scientific Discovery at PNNL



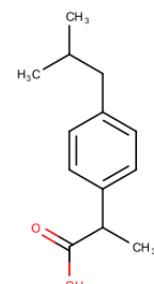


Machine Learning in Chemistry

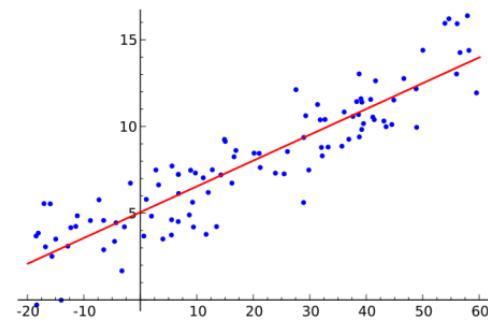
Machine Learning Tool Approach



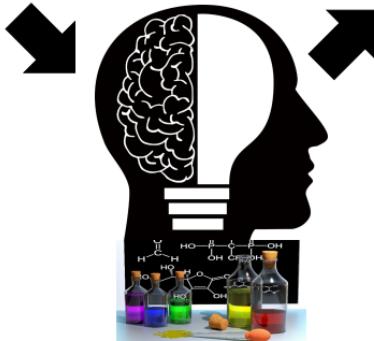
Chemical Database



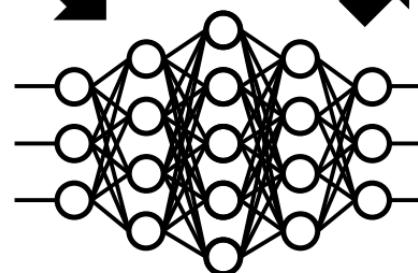
Asphericity
Refractivity
Heteroatoms
RDF
HBA
HBD
MW
Dipole
Branching
Charge
Connectivity
Rotatable
logP
Polarizability
Autocorrelation



Feature Engineering
(Molecular Descriptors)



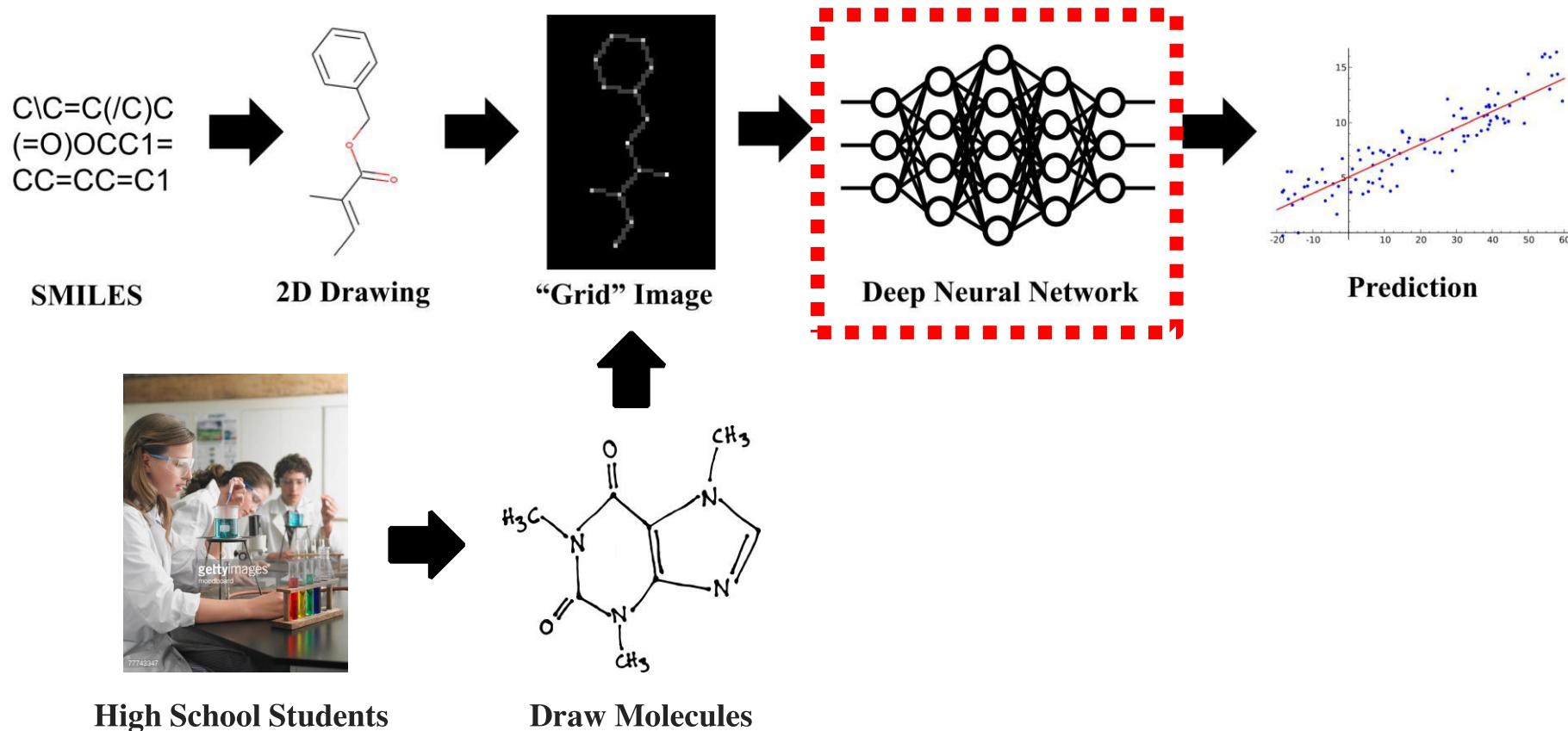
Human Intelligence



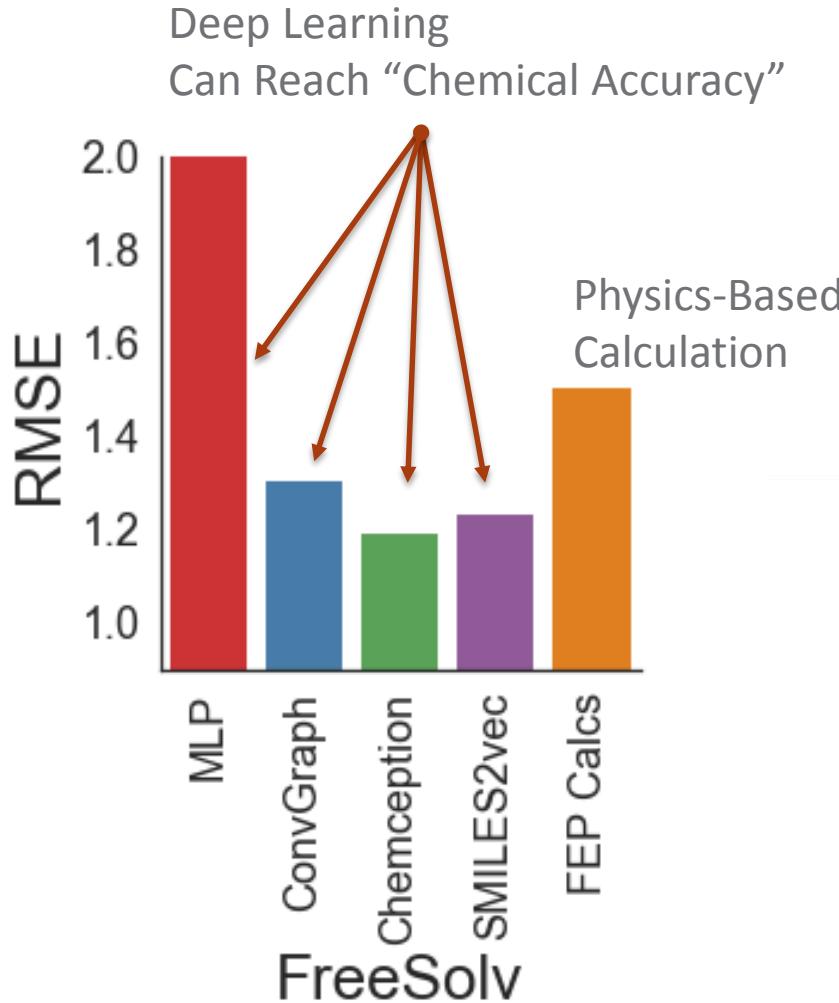
Machine Learning
(including deep neural networks)

QSAR/QSPR Model
Human
Intelligence

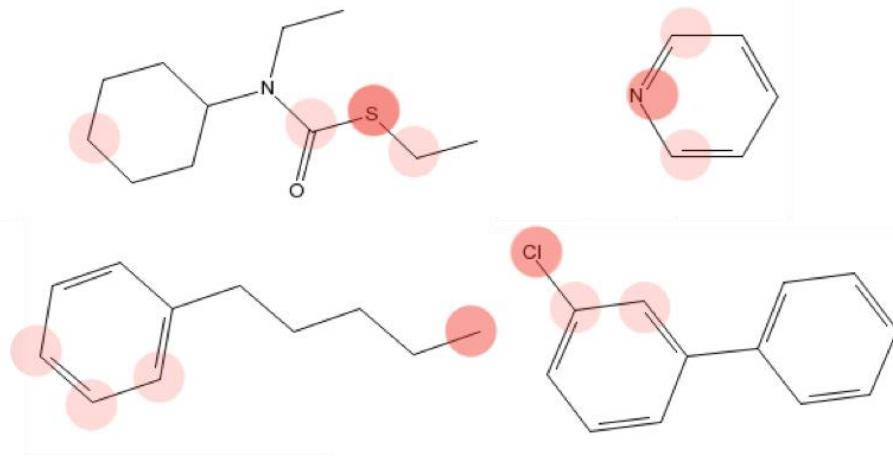
Can we remove the scientist?



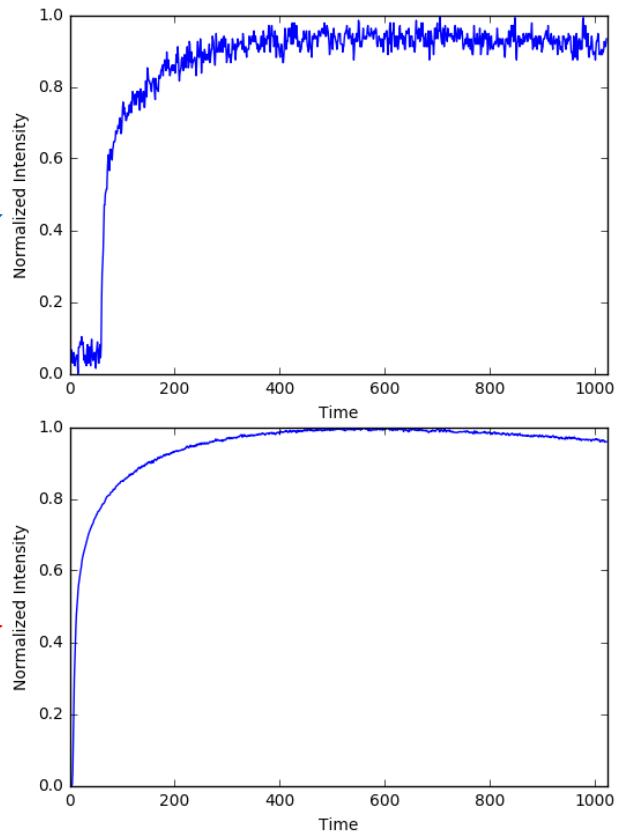
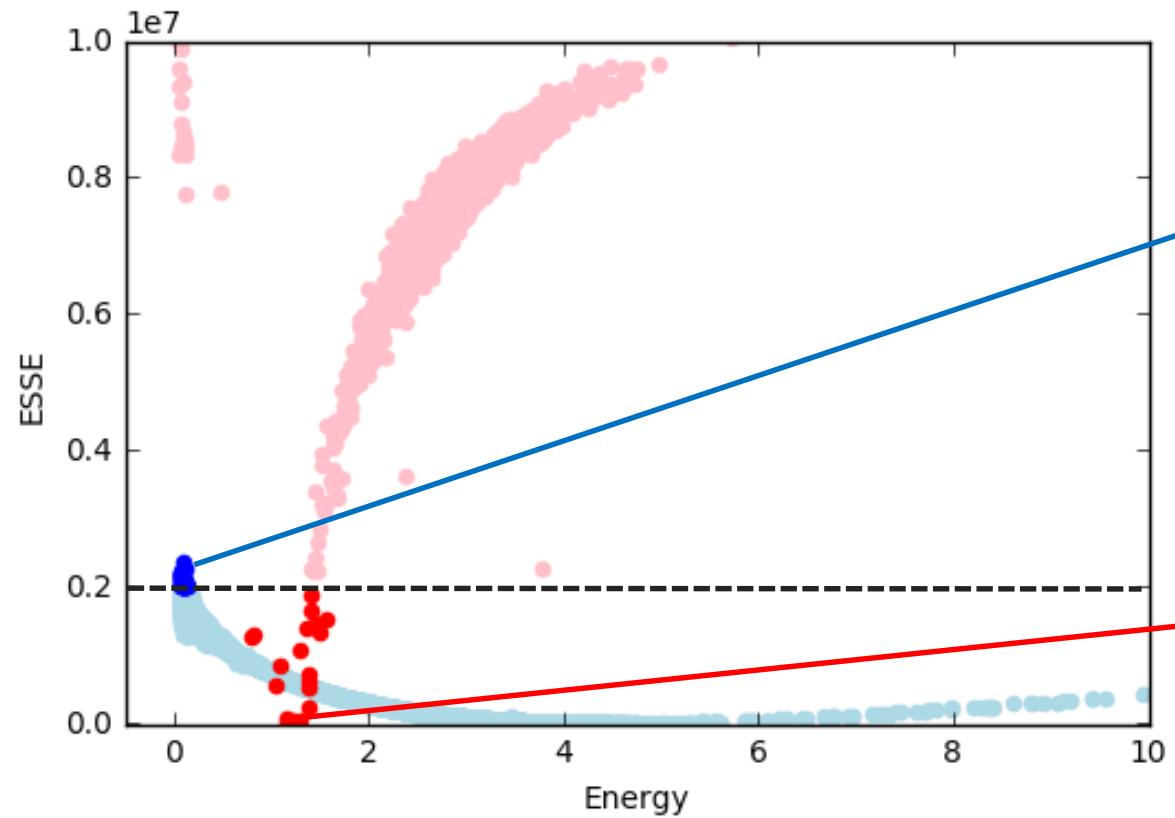
Does it work?



Neural network “explanations”



Ultrasensitive Measurements



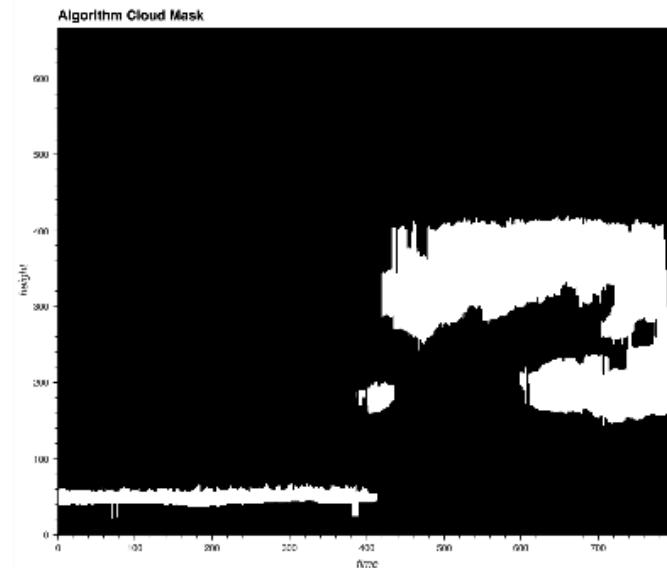
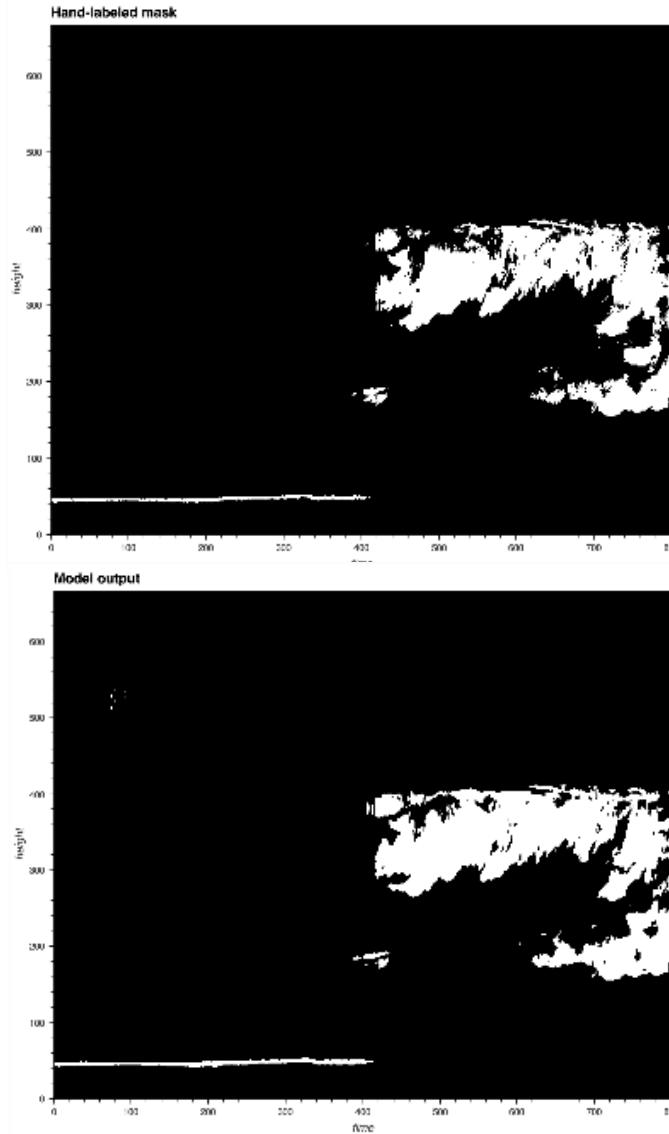
Deep Learning can help improve signal processing

Lidar Cloud Detection with Deep Neural Networks



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