



Pacific Northwest
NATIONAL LABORATORY

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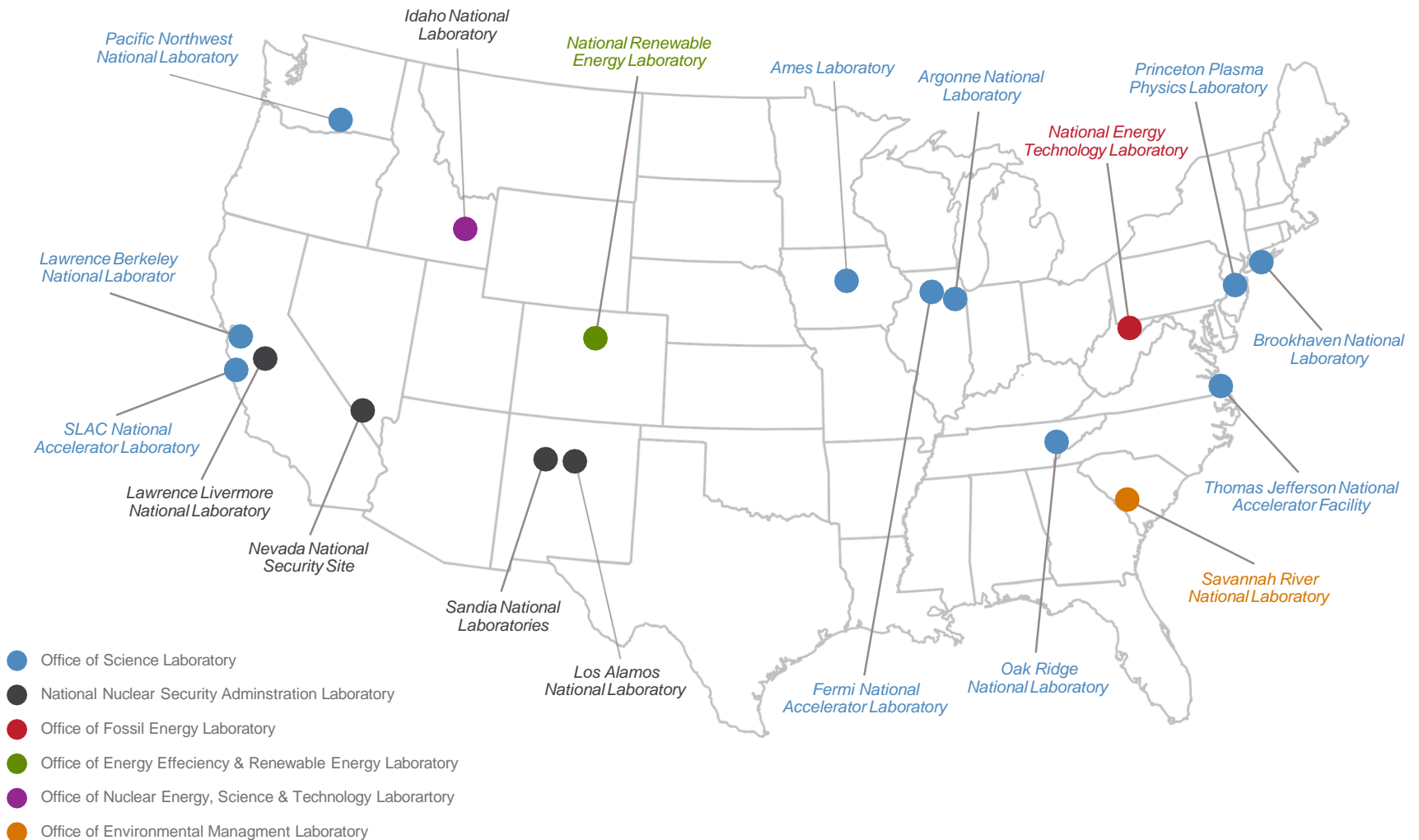
Deep Learning for Scientific Discovery



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.

PNNL is Mission Driven



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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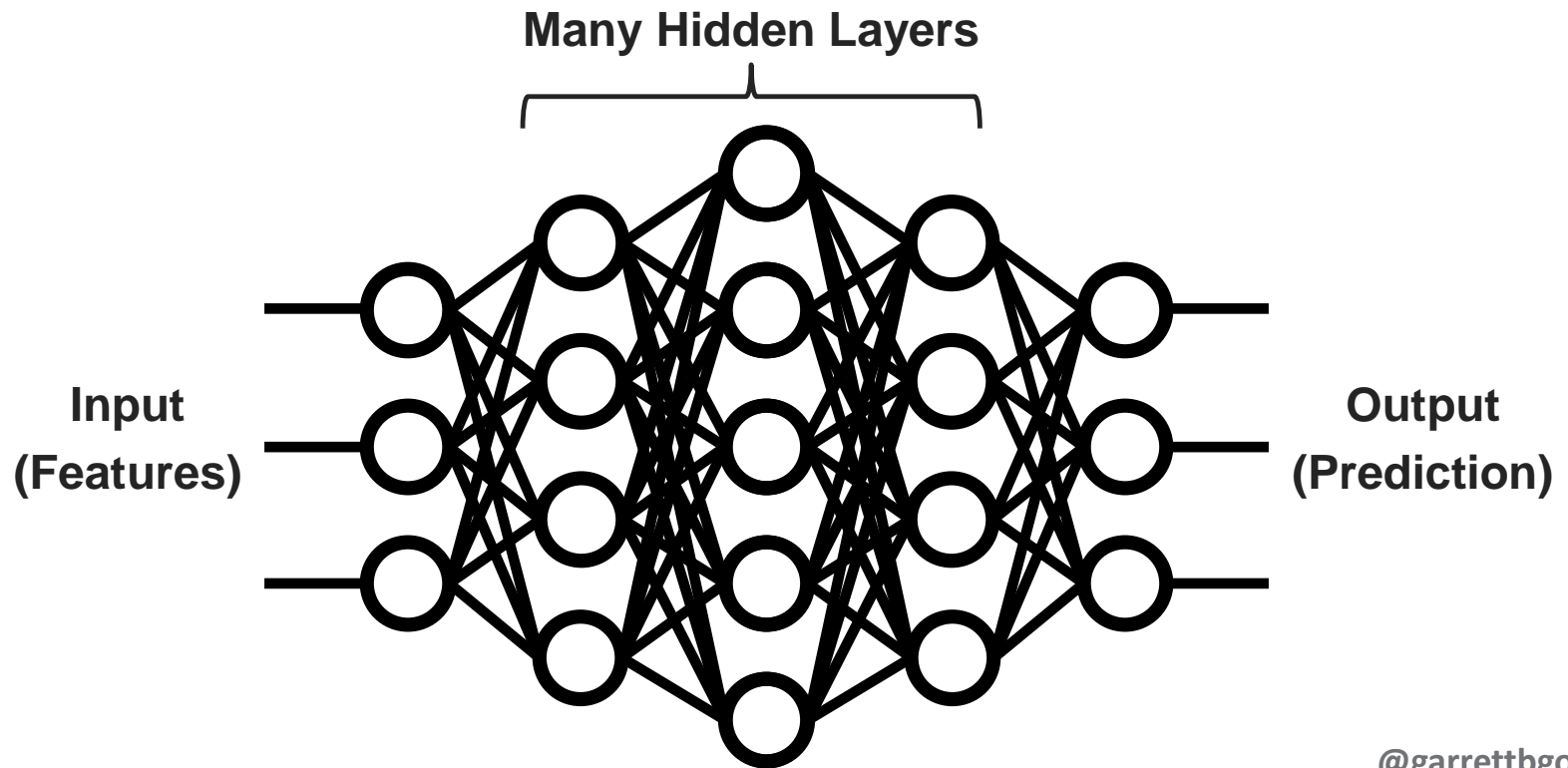
What is Machine Learning?

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



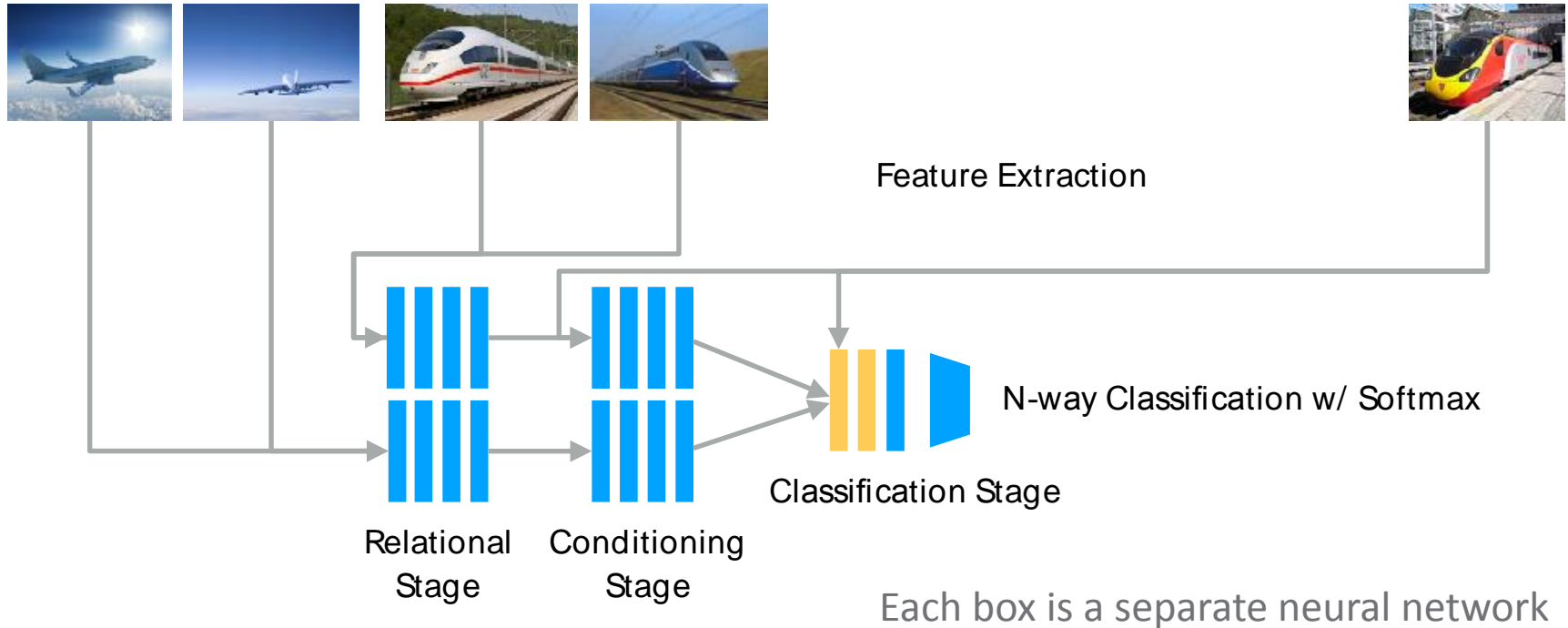
@garrettbgoth

Then



What is Deep Learning?

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



NOW

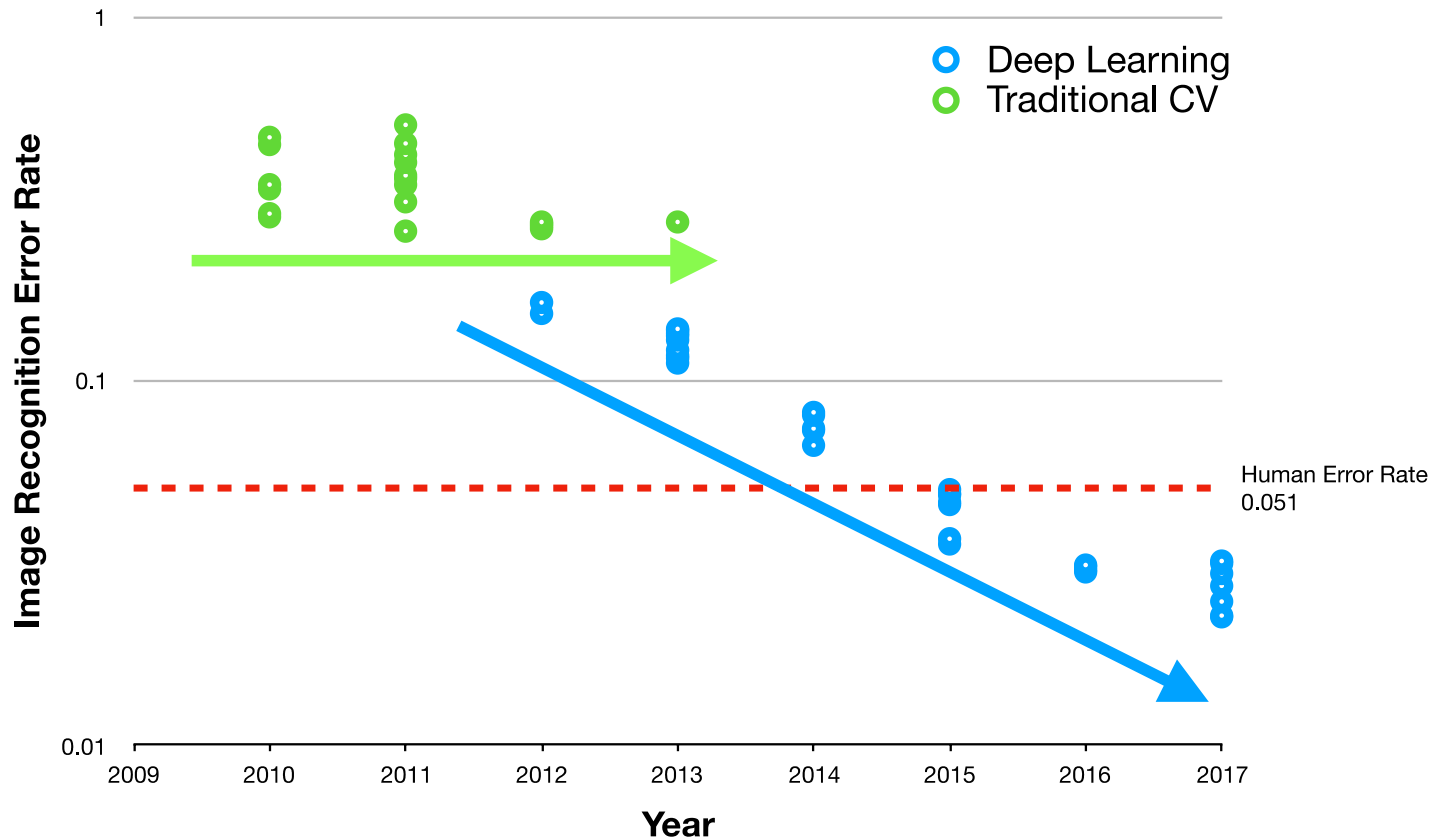


What Changed?

- ▶ **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?

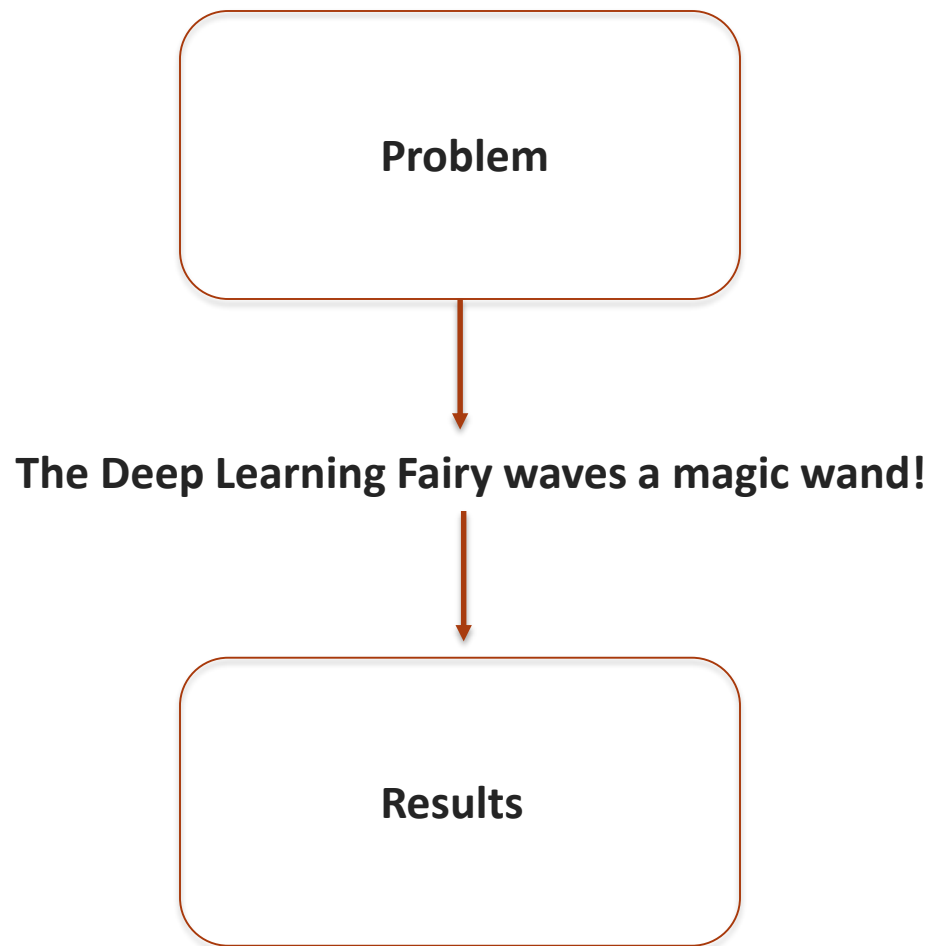
Top-10 ImageNet Classification Error Rate



Deep learning can help to break the "soft barriers"

Now

Protected Information | Proprietary Information



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

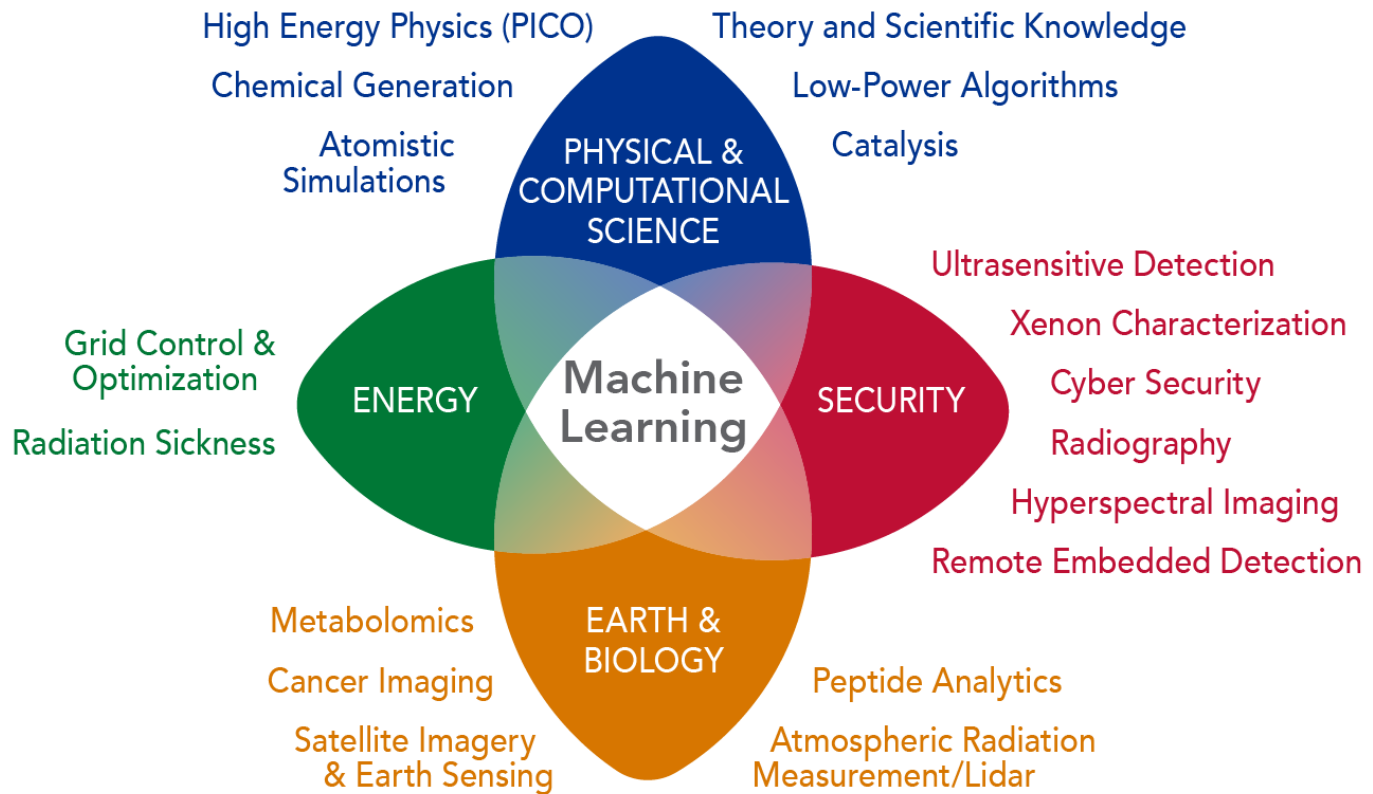
Requirements for Success

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



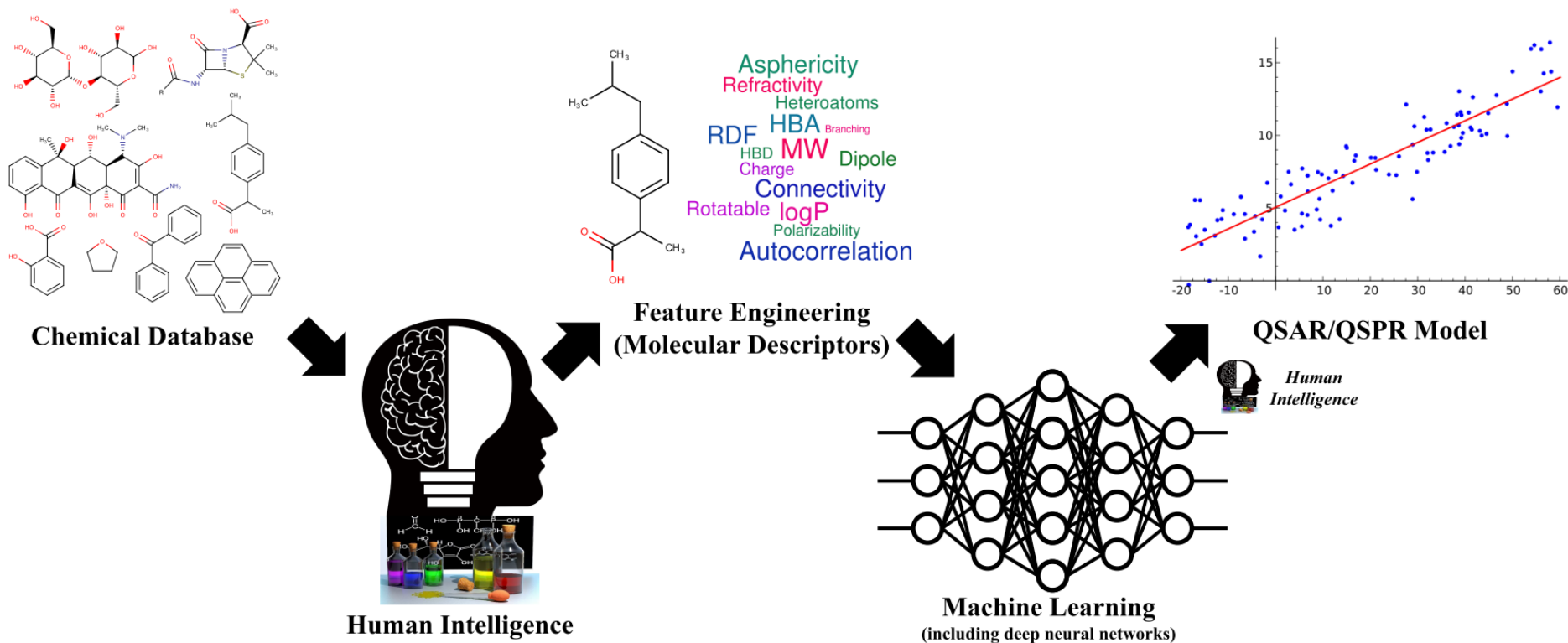


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Machine Learning in Chemistry

Machine Learning Tool Approach

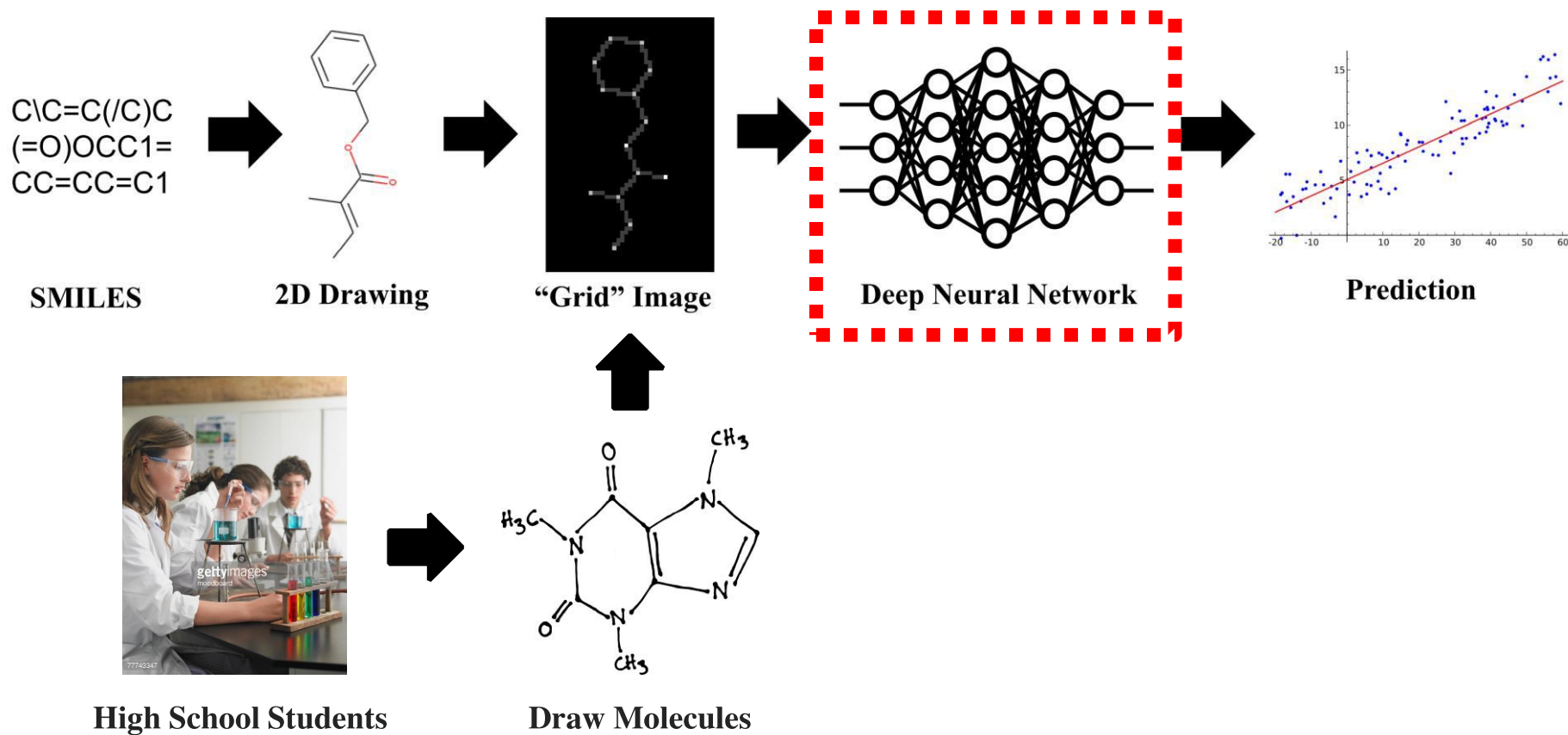




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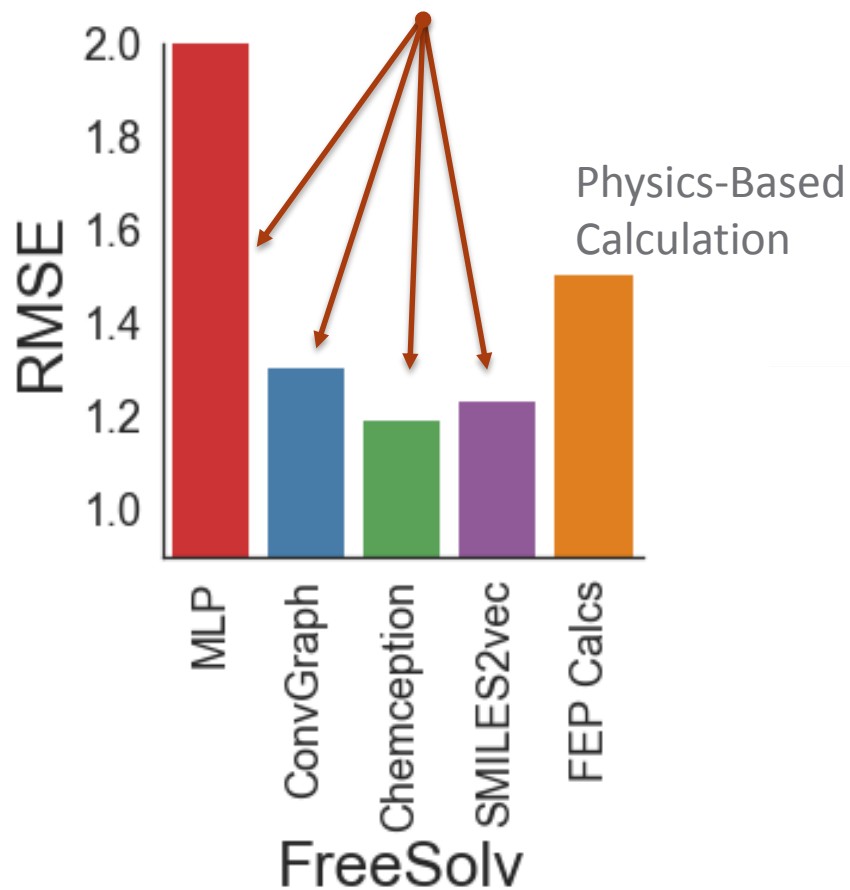
Can we remove the scientist?



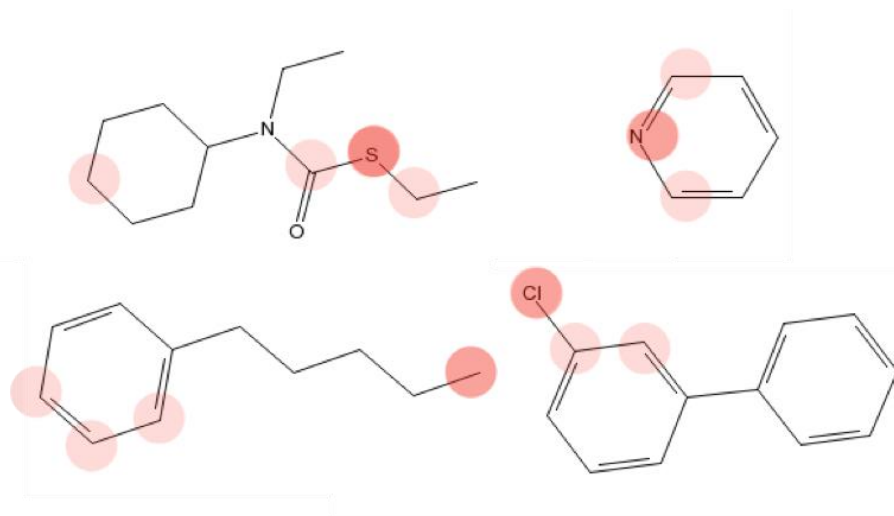


Does it work?

Deep Learning
Can Reach “Chemical Accuracy”

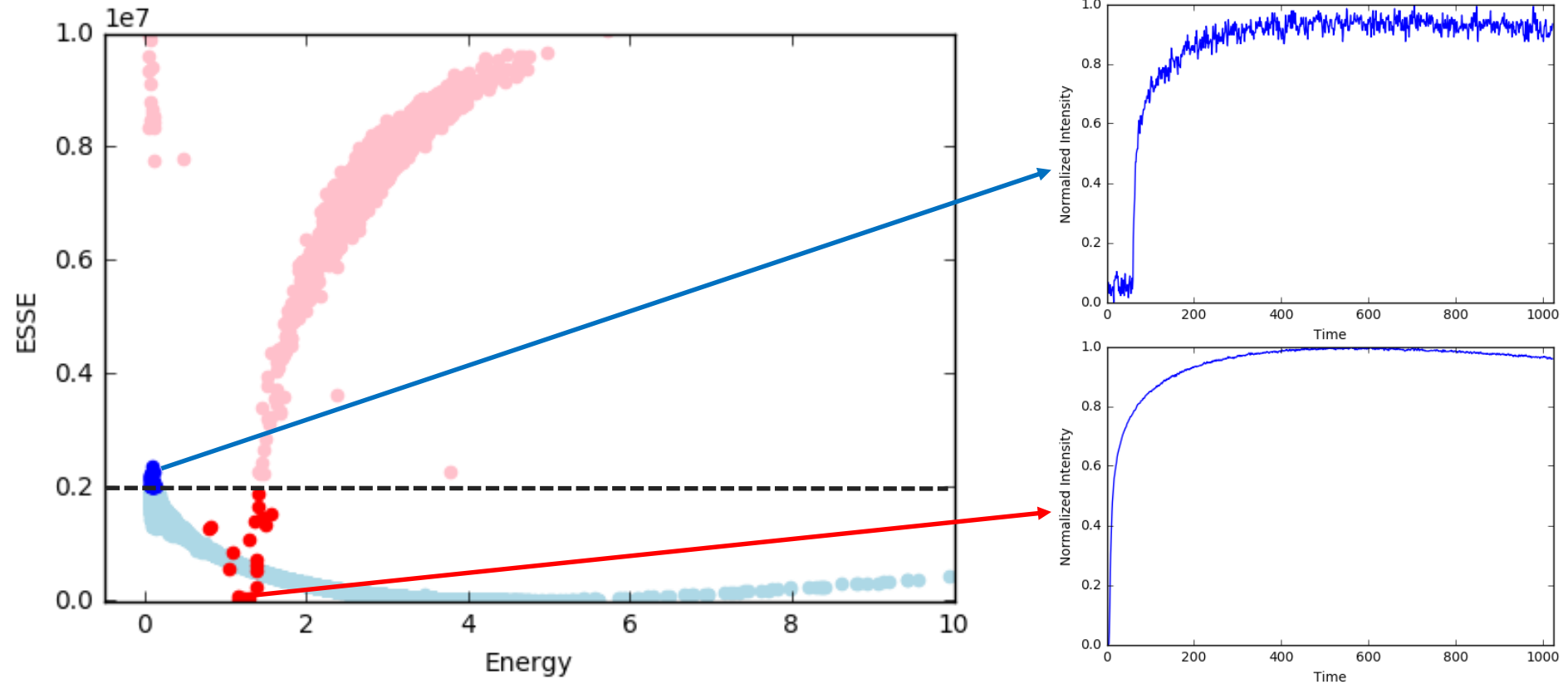


Neural network “explanations”



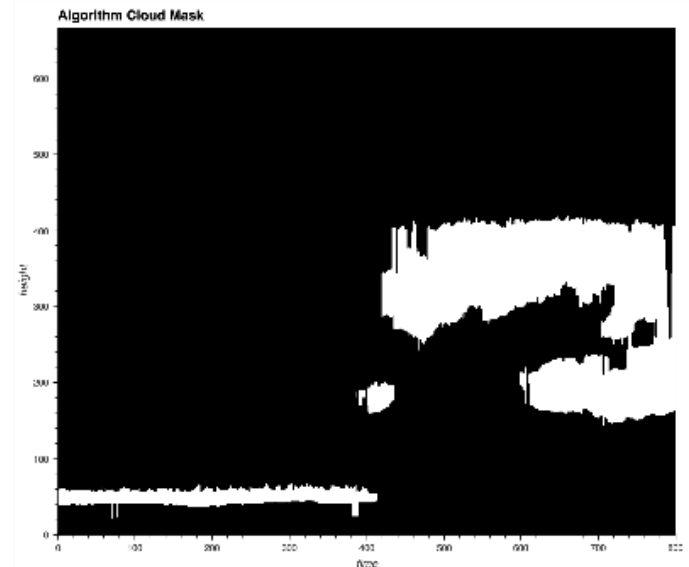
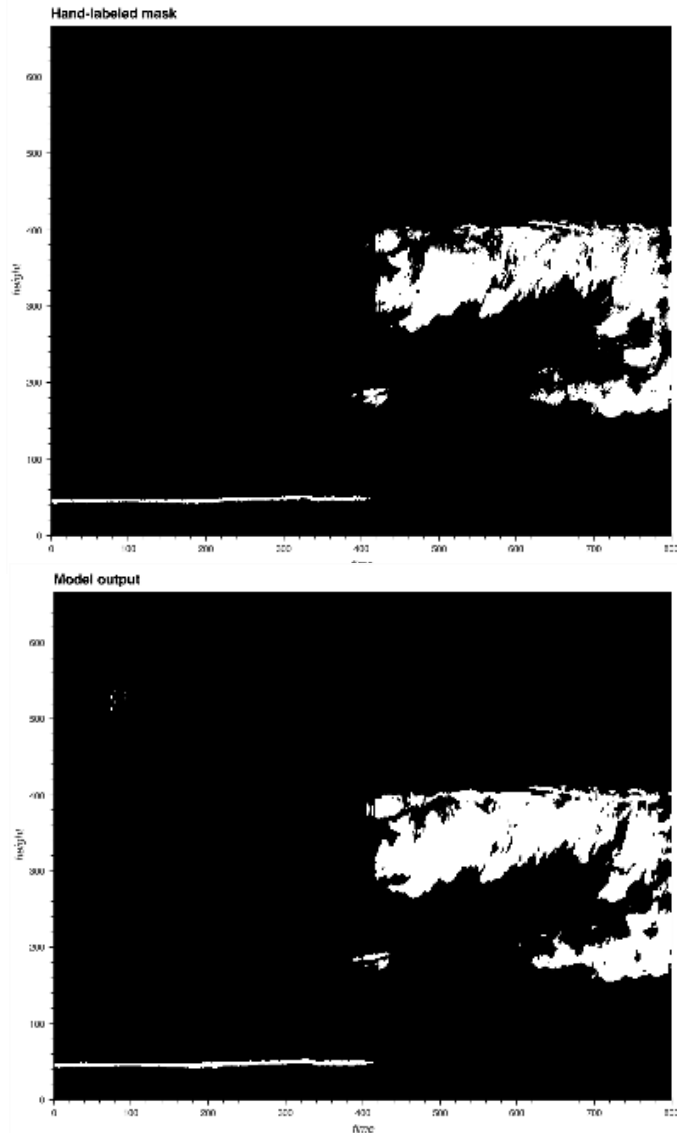


Ultrasensitive Measurements



Deep Learning can help improve signal processing

Lidar Cloud Detection with Deep Neural Networks



Contact



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