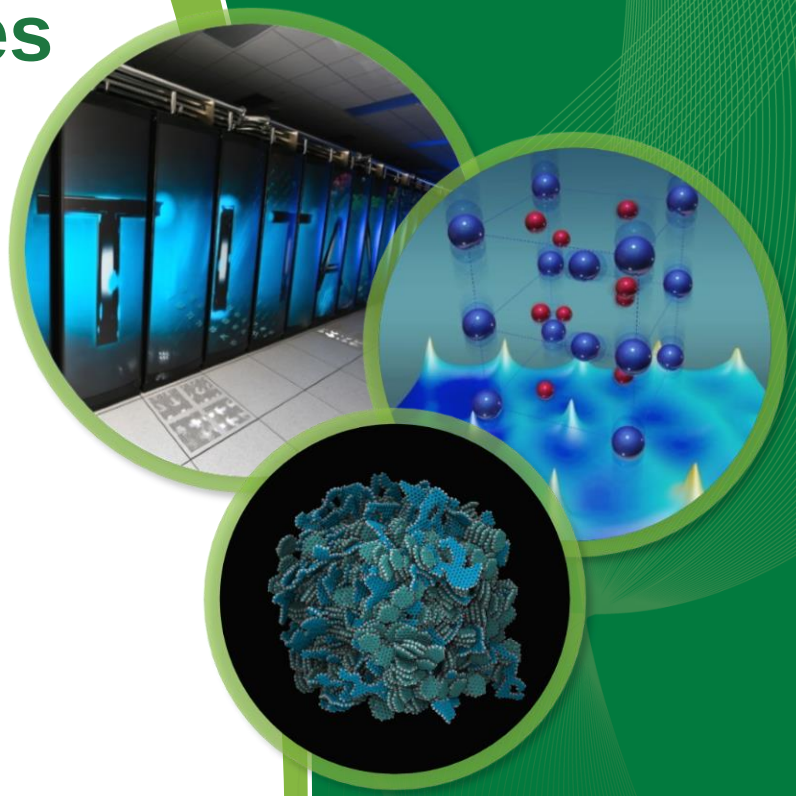
ORNL Publication ID: 112595

Machine Learning: Issues and Opportunities



ARPA-E Machine Learning-Enhanced Energy-Product Development Workshop

June 21-22, 2018

Falls Church, VA

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Oak Ridge National Laboratories

With thanks to

Celia Merzbacher

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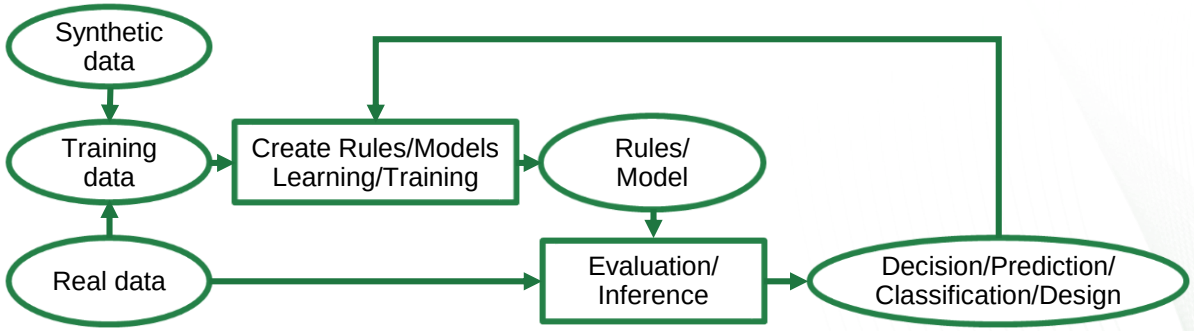
Rich Archibald

What are Artificial Intelligence (AI) and Machine Learning (ML)

- A class of data analytics algorithms in which the rules and/or models are not known a priori and are learned as part of the process
  - Process data to identify correlations
  - Complexity of the model is a potential problem

- Computers trained to perform tasks that if performed by a human would be said to require intelligence
  - Knowledge-based tasks
  - Computers are good at working with data, not “meaning”



Hope/Hype/Hard Truth

- Hope
  - The convergence of big data, HPC, and AI will enable the accumulation and automation of functional knowledge across many application spaces.
- Hype
  - AI solutions are superior to collective intelligence of the experts for multi-modal data challenges
  - Effective translation of AI tools is straightforward
- Hard truths
  - AI solutions, thus far, are effective at executing narrowly defined tasks, identifying correlations in complex data
  - Need for sustainable heterogeneous data and compute infrastructure to advance AI innovation
  - Access to and availability of ”good” and “labelled” data is one of the biggest challenges for AI
  - Vulnerability threats for AI (hacking, intentional manipulation) are a huge concern for deployment

Taxonomy of AI Uses

- Classification and regression
- Surrogates

dimension reduction

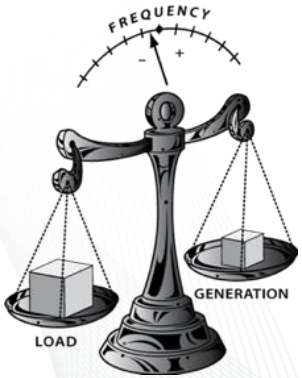
- Control
- Inverse problems, design and optimization

Near Infrared (single band) WorldView-3 image

CODA cloud detection saliency map for image above

Use Case: Smart Grid

Application challenges	• Integrating variable distributed energy resources (DERs) with intelligent interfaces • Integrating storage at multiple layers • Integrating electric vehicles (EV) • Managing demand – Residential, Commercial, Industrial – Enabling energy coordination and trading between buildings and trading between buildings and grid
Technology challenges	• Connectivity across DERs • Scalable control and diagnostics algorithms that are driven by data • Actionable, real-time situational awareness • Data and physical system security, including privacy



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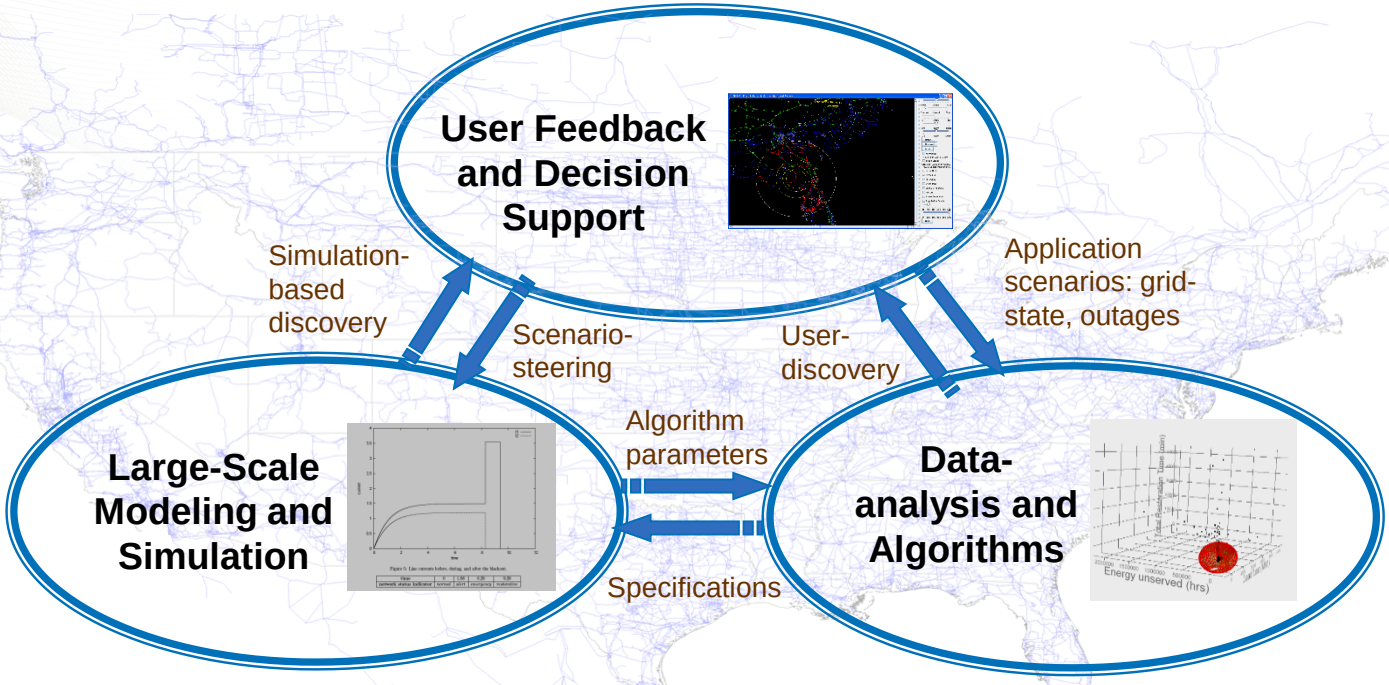
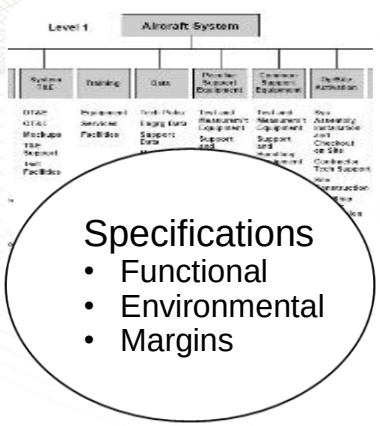
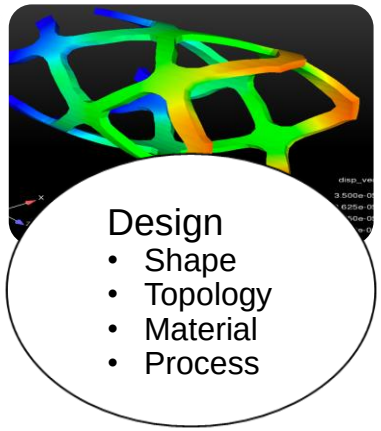
Smart Grid: Leveraging A Data-rich Environment

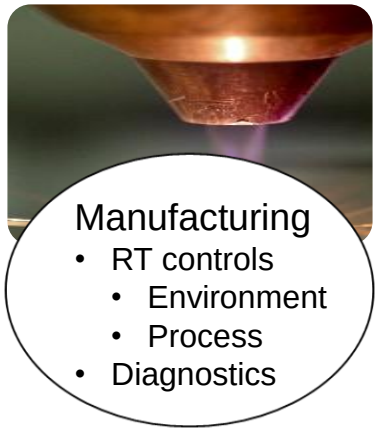


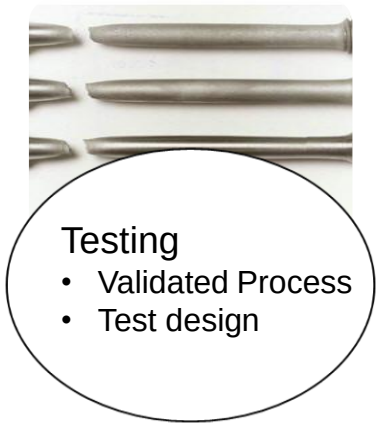
- Learning algorithms for wide-area, hierarchical information sources
  - Distribution: Intelligent loads, SCADA devices, DERs
  - Transmission: Protection systems, power flow control
  - Generation: Planning and coordination
  - Control: Situational awareness, fine-grained control of DERs, enhanced reliability and resilience

Use Case: Additive Manufacturing

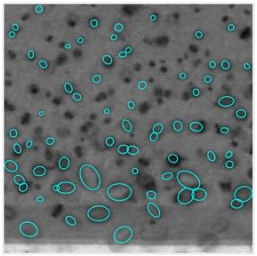








- Impact of machine learning
  - Surrogate models
  - Steering high-fidelity simulation
  - Design, particularly materials and processes
  - Real time diagnostics and control during manufacturing
    - Defect detection and mitigation
    - Control of local structures
  - Predicted performance based on manufacturing data
  - Test design and control



Ensemble methods

- Statistical methods to improve the performance of machine learning algorithms
  - E.g., decision trees, k-NN
  - Most common application is perhaps the random forest
  - Not effective for stable learners
  - Most effective for weak learners
- Bootstrap aggregation (bagging)
  - Random selection of training data to improve stability and reduce variance
- Boosting
  - Ensembles of weak learners to create a stronger learner
  - Can be sequential or parallel
- Stacking
  - A trained meta-learner

Random Forest/Decision Trees
Feature Selection and Dimension Reduction

- Problem: Do an approximate combinatorial search to establish a feature-to-function relationship
  - A full search requires 2^n computations
- Idea: Mine decision trees for patterns
- Decision trees -
  - More naturally explainable
  - Weak learners
  - Prone to overfitting

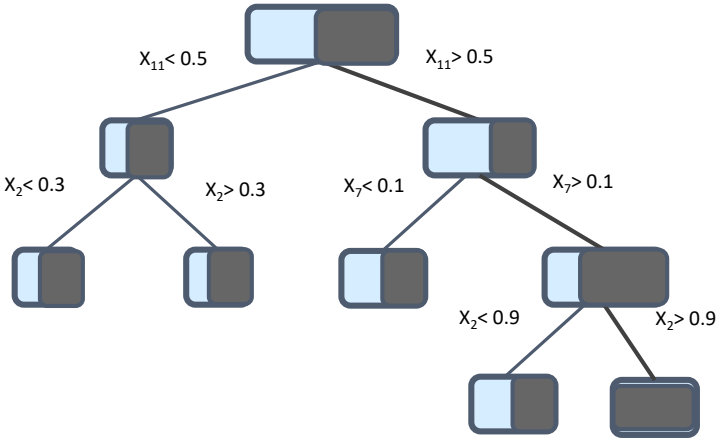
Random Forest/Decision Trees

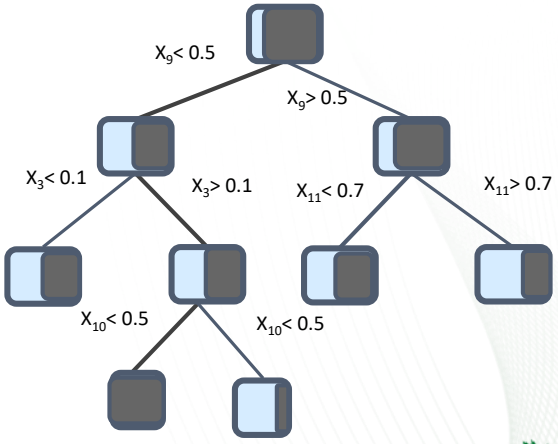
- Step 1 – determine branching criterion
- Step 2 – limit depth to prevent over-fitting

Decision tree

- Step 3 – apply bootstrap aggregation (bagging)
  - Select α "large" and $n' = \alpha n$
- Step 4 – apply feature bagging
  - Select $p' = \sqrt{p}$
- Step 5 – boost (combine trees)

Random Forest





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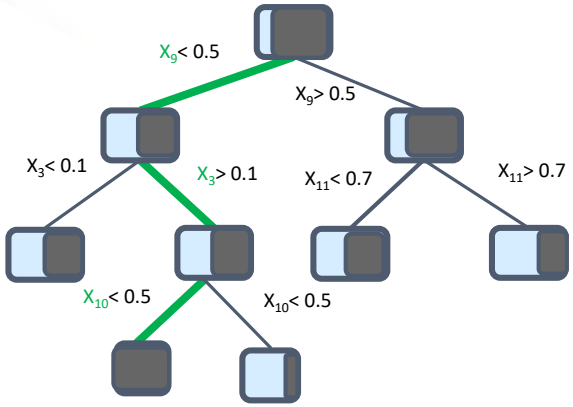
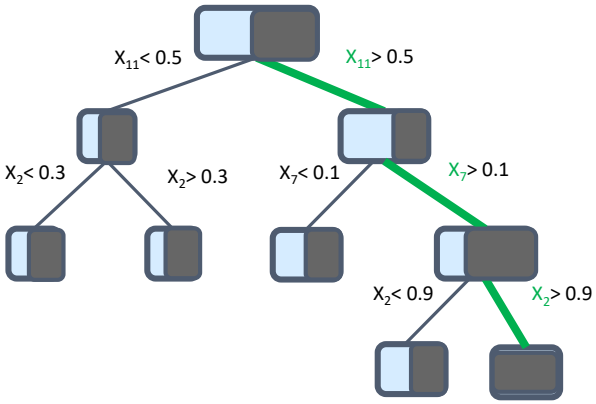
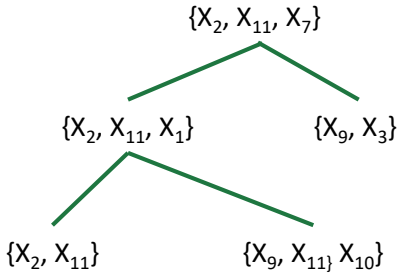
Random Forest/Decision Trees

- Step 6 – Identify branching patterns and select feature sets



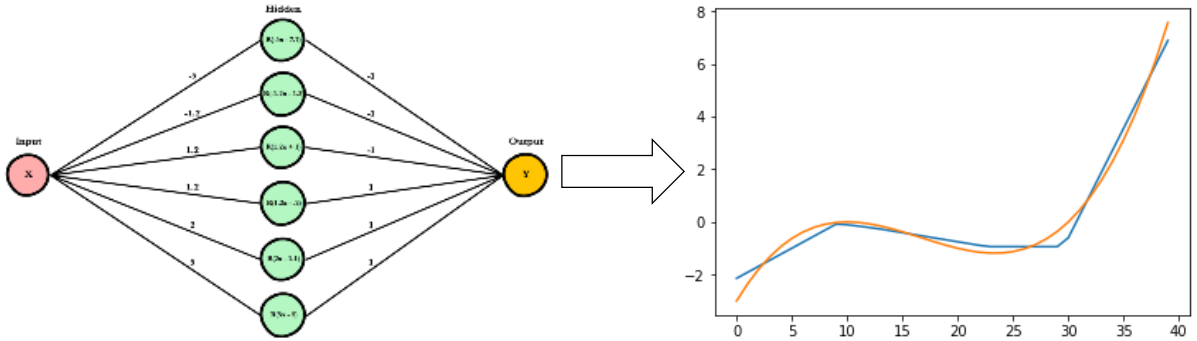


- Step 7 – create new RF branching on selected sets



Neural Networks

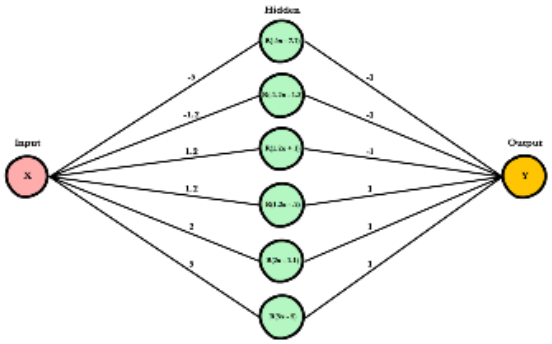
- A NN is simply a function approximation, and a NN with a single hidden layer can approximate any function

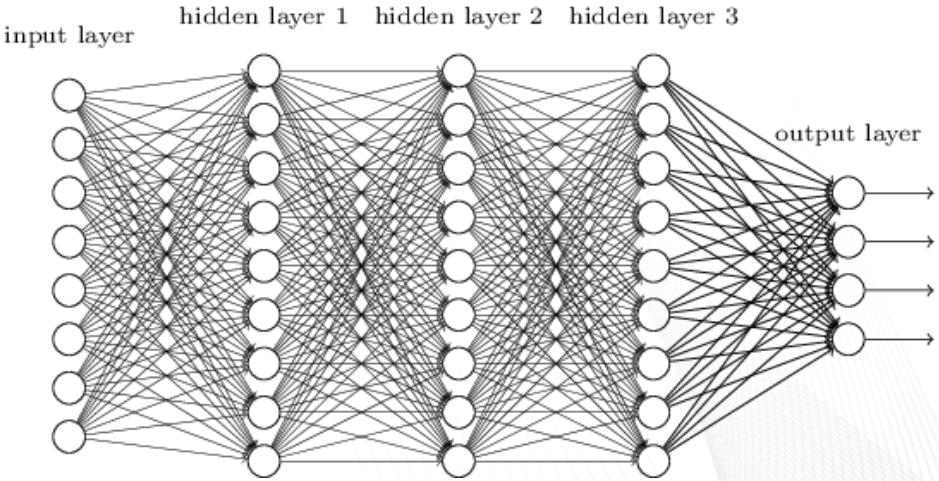


- Great for models when a specific model form is not known, but not much capability beyond basic statistical methods.
- NNs languished for decades

Neural Networks – Significant Advances
Deep Neural Networks

- Deep neural networks (DNNs) were introduced
  - Width increases the ability to approximate a function
  - Depth increases the abstractions,
    reduces the number of parameters but
    increases the computational requirements for training
  - Still susceptible to overfitting
  - Still an art



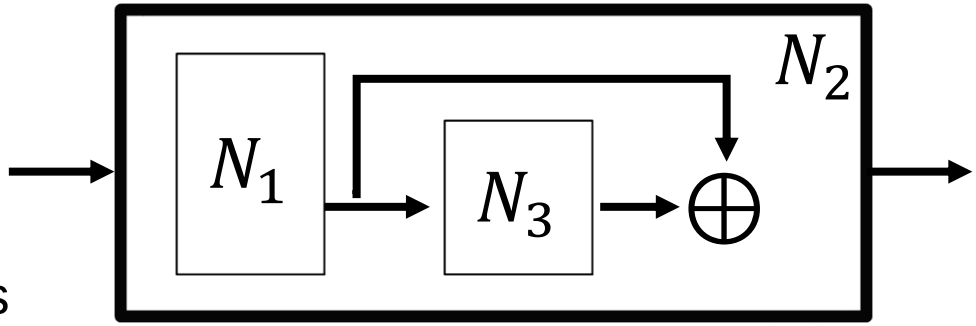


Neural Networks – Accelerated Training

- Key idea for many improvements

$$\text{If } N_1 \subseteq N_2, \text{ then } L(N_1) \geq L(N_2)$$

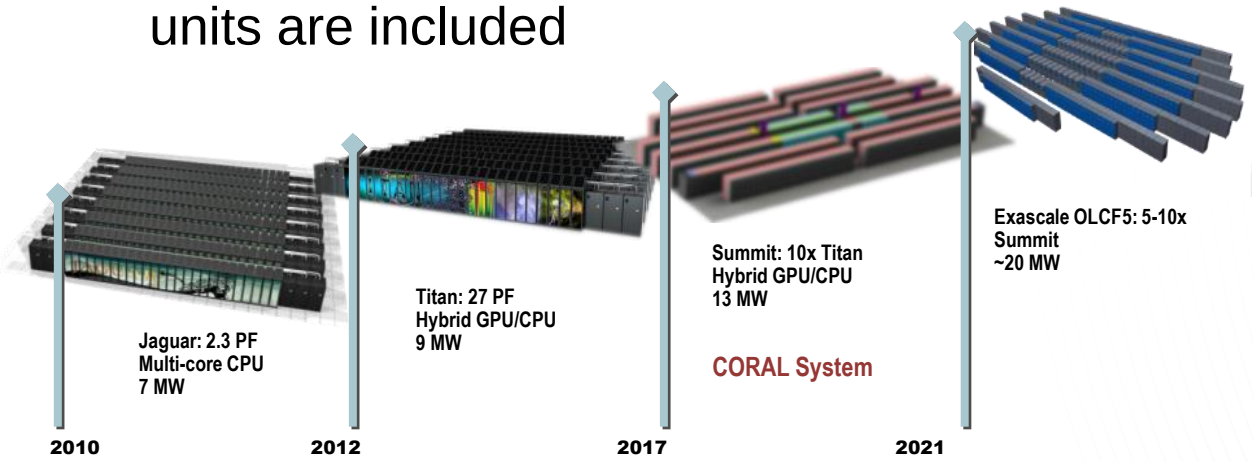
- Leads to
  - Residual networks
  - Inception networks
  - Feature reuse
  - Convolutional networks



- Training DNNs became algorithmically tractable
  - Stochastic gradient descent

Neural Networks – HPC

- We have the ability to collect and store large amounts of data
- Computational power continued to increase, with architectural improvements that are amenable to neural networks
  - For example, GPU became practical for accelerated computations.
  - Reduced-precision tensor core units are included



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Issue: “Syntactic” Space vs. “Semantic” Space

- Humans tend to think in semantic space, i.e., in terms of the meaning.

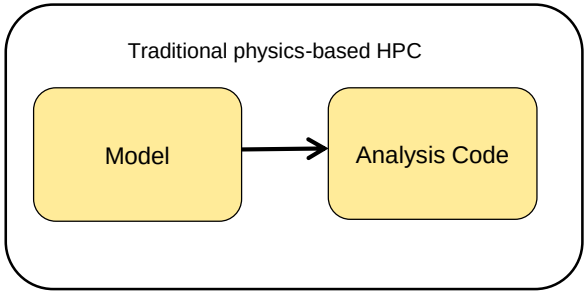
And metrics in semantic space are fundamentally different from those in syntactic space

- Implications
  - Easy to spoof classification systems
  - Transfer learning doesn’t map well.

    (Humans tend to transfer learning in semantic space, e.g., transfer what I learned about human behavior in kindergarten to how I drive. Most AI approaches transfer in syntactic space or transfer parts of the model (a sort of “gene transfer”).

Issue: Verification, Validation, Explainability and Interpretability

- Verification
  - Is the model implemented correctly?
- Validation
  - Is the model (including training data) appropriate for the decisions being made?
  - Must be evidence based
  - Requires some form of UQ, robustness guarantees and bounds on “distortion”



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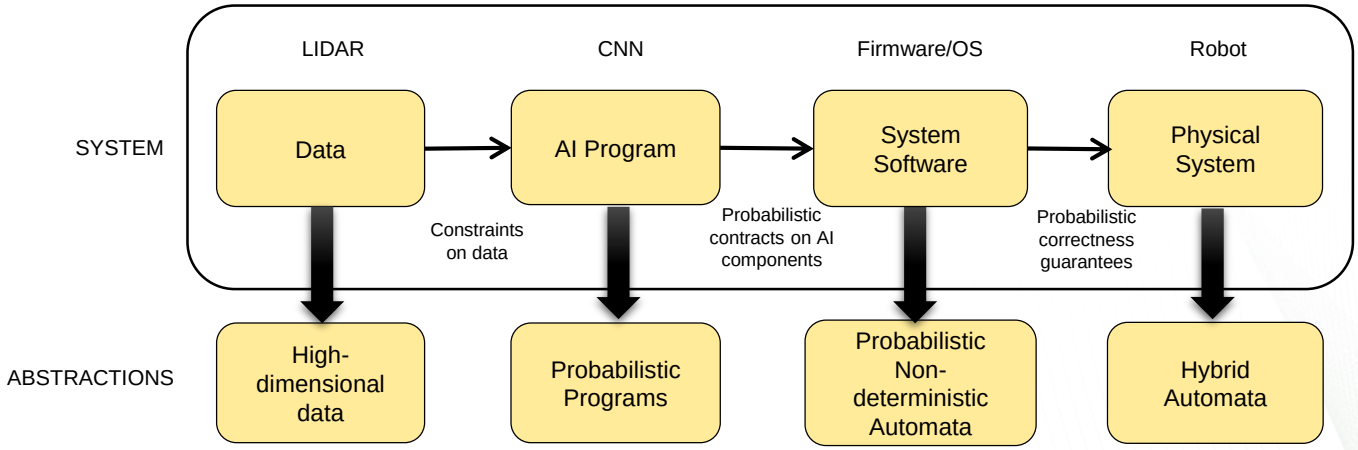
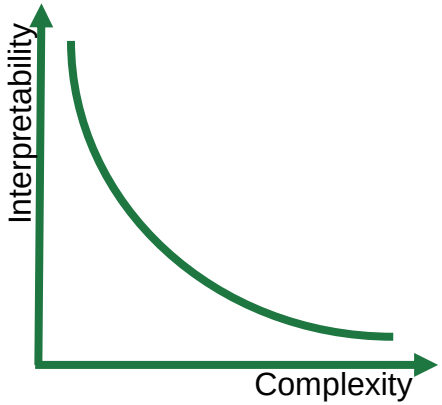
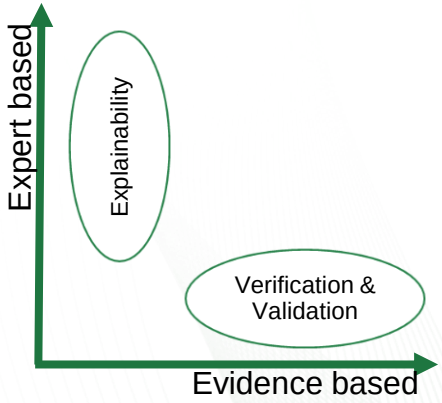


Issue: Verification, Validation, Explainability and Interpretability

- Interpretibility
  - Can a human understand the model? For example, do the basis vectors in a dimension reduction algorithm have a physical meaning?
- Explainability
  - Can the model present a sequence of steps that can justify the answer to an expert?
  - Expert based
- Reproducibility
  - Does the same experiment lead to the same conclusion?
  - Can we run different experiment and not contradict our conclusion?
  - If we create a new model with the same data, do we get the same conclusions?
  - Required for good science
-





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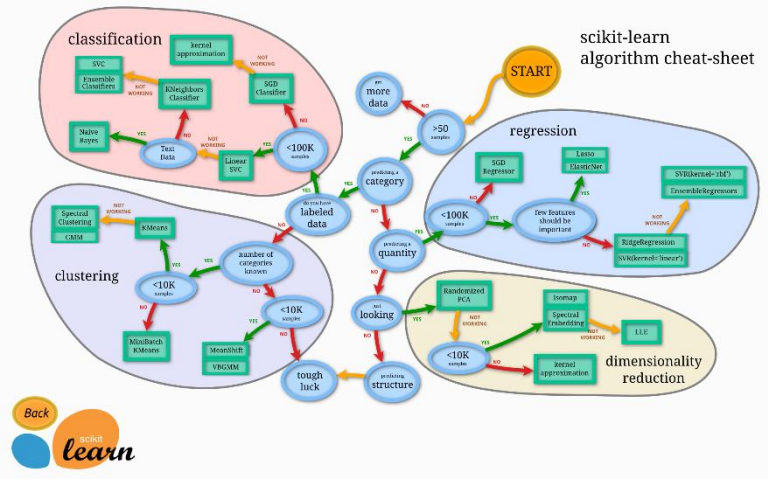
Issue: Data Is A Major Problem

- Need more data than was imagined just a few years ago
  - We are looking for complex correlations
  - Using primarily statistical methods
- Labelled data is a problem
  - Generating labels is expensive and labor intensive (e.g., Mechanical Turk)
  - Need to move toward reinforcement learning
- Synthetic data and simulated environments are partial solutions
  - But an AI can learn the flaws in these systems

Issue: AI Is An Art

- Choosing the model form and hyper parameters is often ad-hoc and requires experience and insight
- AI models must be tuned
- Neural networks design is difficult and often requires tuning
- Interpreting the results requires expertise



> "Machine learning methods are often described in papers at an abstract level, for maximum generality. However, a good choice of hyperparameters is usually necessary to make them work well on real-world problems, and tricks are often used to make most efficient use of these methods and extend their capabilities."
>
> G. Montrevan, et.al., "Methods for Interpreting and Understanding Deep Neural Networks."

Six Research Areas To Be Addressed

- Data quality and statistics
  - Even if we have enough data, it is not necessarily good data
  - Dealing with bias
- Machine learning
  - Needs to accelerate
  - Very model dependent
- Merging physics and AI
  - We can't violate the laws of physics
- Verification, validation and explainability
  - Is the answer right, is the model appropriate, and can we understand it
  - What is the human-computer interface
- Computing
  - How do we use "big" computers
  - How do we use accelerated nodes
- Deployment
  - Computing at the edge
  - privacy, ethics and regulations