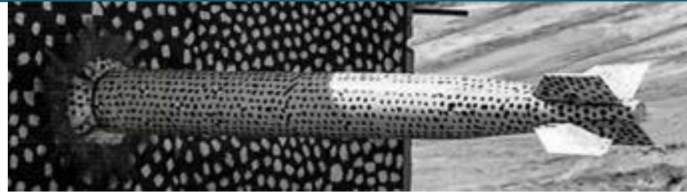




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SAND2019-12441PE

Artificial Intelligence and Machine Learning: Overview and Applications for Power Systems



Raymond Byrne, David Stracuzzi, Warren Davis,
Jean-Paul Watson, Matthew Reno, Logan Blakely



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1. Introduction to Artificial Intelligence and Machine Learning (Ray Byrne)
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7. Future Research Directions and Conclusions



Introduction to Artificial Intelligence and Machine Learning

Raymond H. Byrne (rhbyrne@sandia.gov)

September 9, 2019

Why is Artificial Intelligence a Hot Topic?



Examples of Successful Artificial Intelligence (AI) Applications:



Self-driving cars, lane departure detection, etc.



Credit card fraud detection



amazon alexa

Personal assistants



Conversation optimization



Customer interaction optimization (travel, etc.)



Music recommendations



Existing client interactions - luxury travel concierge



Product recommendations



Product recommendations



Thermostat control

What is AI? – Federal Perspective



“The term ‘artificial intelligence’ means the full extent of Federal investments in AI, to include: R&D of core AI techniques and technologies; AI prototype systems; application and adaptation of AI techniques; architectural and systems support for AI; and cyberinfrastructure, data sets, and standards for AI”

– Presidential Executive Order

“The research priorities outlined in this AI R&D Strategic Plan focus on areas that industry is unlikely to address on their own, and thus, areas that are most likely to benefit from Federal investment. These priorities cut across all of AI to include needs common to the AI sub-fields of perception, automated reasoning/planning, cognitive systems, machine learning, natural language processing, robotics, and related fields. Because of the breadth of AI, these priorities span the entire field, rather than only focusing on individual research challenges specific to each sub-domain. To implement the plan, detailed roadmaps should be developed that address the capability gaps consistent with the plan.”

- National AI Research and Development Strategic Plan (pg5)



<https://www.whitehouse.gov/presidential-actions/executive-order-maintaining-american-leadership-artificial-intelligence/>

<https://www.whitehouse.gov/wp-content/uploads/2019/06/National-AI-Research-and-Development-Strategic-Plan-2019-Update-June-2019.pdf>

What is AI? – DOE Perspective from the Artificial Intelligence & Technology Office



“Artificial Intelligence has the power to literally change the world we live in by tackling some of the biggest problems facing humanity – from improving our environment, to advancing our understanding of the cosmos; from increasing cyber security to improving crop production, . . .”

–Rick Perry

“Artificial Intelligence or AI is a new way of thinking, of discovering, of dreaming. AI reimagines computer programming to mirror human reasoning. It gives us the power to search through vast datasets to discover new patterns and hidden correlations to solve deeper mysteries to see future horizons.”

– Mindy Overbaugh (DOE)

“It’s the process of trying to make computer act intelligent, make them act like humans.”

-Kathy Yelick (Berkeley Lab)

“Artificial intelligence is a way to take our ability to reason and put it into a more automated format in a computing system.

– Conrad James (SNL)





The diagram illustrates the architecture of an Expert System. A **Non-expert user** (represented by a stick figure) interacts with the system via a **User Interface**. The user sends a **Query** to the User Interface, and the system provides **Advice** back to the user. The User Interface is connected to the **Inference Engine**, which in turn interacts with the **Knowledge Base**. The Knowledge Base is linked to **Knowledge from an expert** (represented by a cartoon expert figure). The entire system is enclosed in a dashed box labeled **Expert System**.

```
graph LR; User[Non-expert user] -- Query --> UI[User Interface]; UI -- Advice --> User; subgraph Expert_System [Expert System]; UI <--> IE((Inference Engine)); IE <--> KB[Knowledge Base]; end; KB -.->|Knowledge from an expert| Expert[Expert];
```

The diagram illustrates a neural network with three layers: Input, Hidden, and Output. The Input layer consists of three red circles, the Hidden layer consists of three blue circles, and the Output layer consists of two green circles. Every circle in the Input layer is connected to every circle in the Hidden layer, and every circle in the Hidden layer is connected to every circle in the Output layer, representing a fully connected architecture.

The diagram illustrates Agent Based Modeling. The top part shows a network of agents (represented by yellow and blue figures) interacting within a red environment. A speech bubble indicates a specific agent's internal state or action. Below, a graph shows three fuzzy membership functions (cold, warm, hot) plotted against temperature, illustrating how agents might perceive or act based on temperature.

Huang Ling-fang, "Artificial Intelligence," *2010 The 2nd International Conference on Computer and Automation Engineering (ICCAE)*, Singapore, 2010, pp. 575-578.

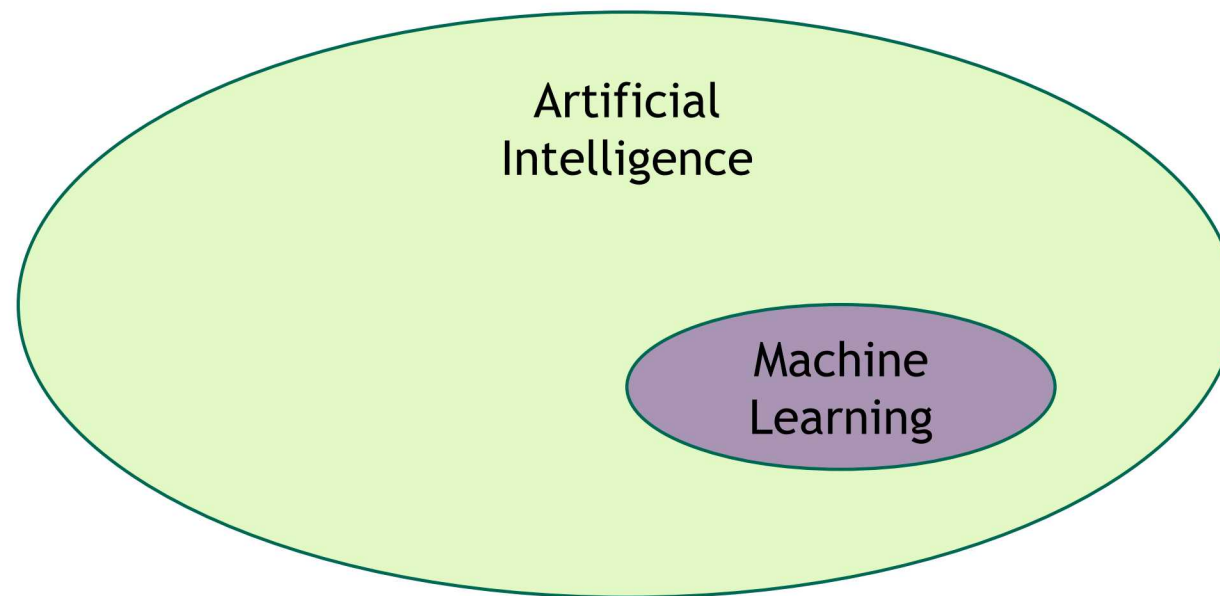
AI versus Machine Learning



Machine learning is considered a subset of artificial intelligence

Artificial Intelligence: a branch of computer science which studies building machines capable of intelligent behavior

Machine Learning: a computer learns to perform a task, often without explicit instructions, by studying a training set of examples



K. Bakshi and K. Bakshi, "Considerations for artificial intelligence and machine learning: Approaches and use cases," *2018 IEEE Aerospace Conference*, Big Sky, MT, 2018, pp. 1-9.

P. Louridas and C. Ebert, "Machine Learning," in *IEEE Software*, vol. 33, no. 5, pp. 110-115, Sept.-Oct. 2016.

Machine Learning is a Subset of AI



Tables making comparisons are often incorrect ... since machine learning is a subset of AI, every machine learning approach has some application to AI

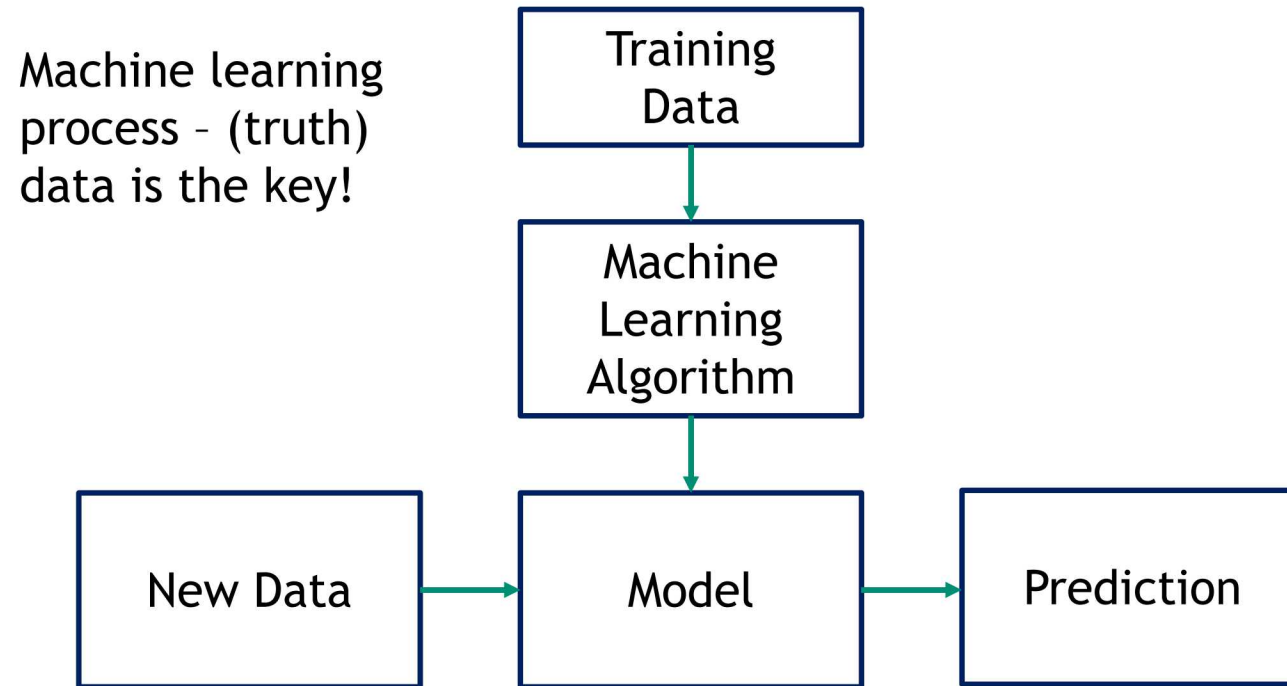
Machine Learning Example	AI application
Image segmentation and classification to visually identify manufacturing flaws	Image segmentation and classification is a key component in AI applications (e.g., humanoid robots, etc.)
Linear regression to predict future samples of a time series (e.g., GDP growth)	Numerous AI applications related to prediction (e.g., motion of images in a scene for autonomous navigation and obstacle avoidance)
Natural language (text and voice) processing for translation (e.g., Google translate) of business documents	Natural language processing is required for any AI application that involves language
Pattern recognition applied to credit card fraud detection	Pattern recognition applied to autonomous grasping (e.g., pick up the ball not like the others)
Product recommendations to improve customer experience and boost online sales	Product recommendations provided by an AI assistant

In addition, there are many fields of AI that are not application specific and are not related to machine learning ... examples include research on planning and cognitive architectures

Machine Learning

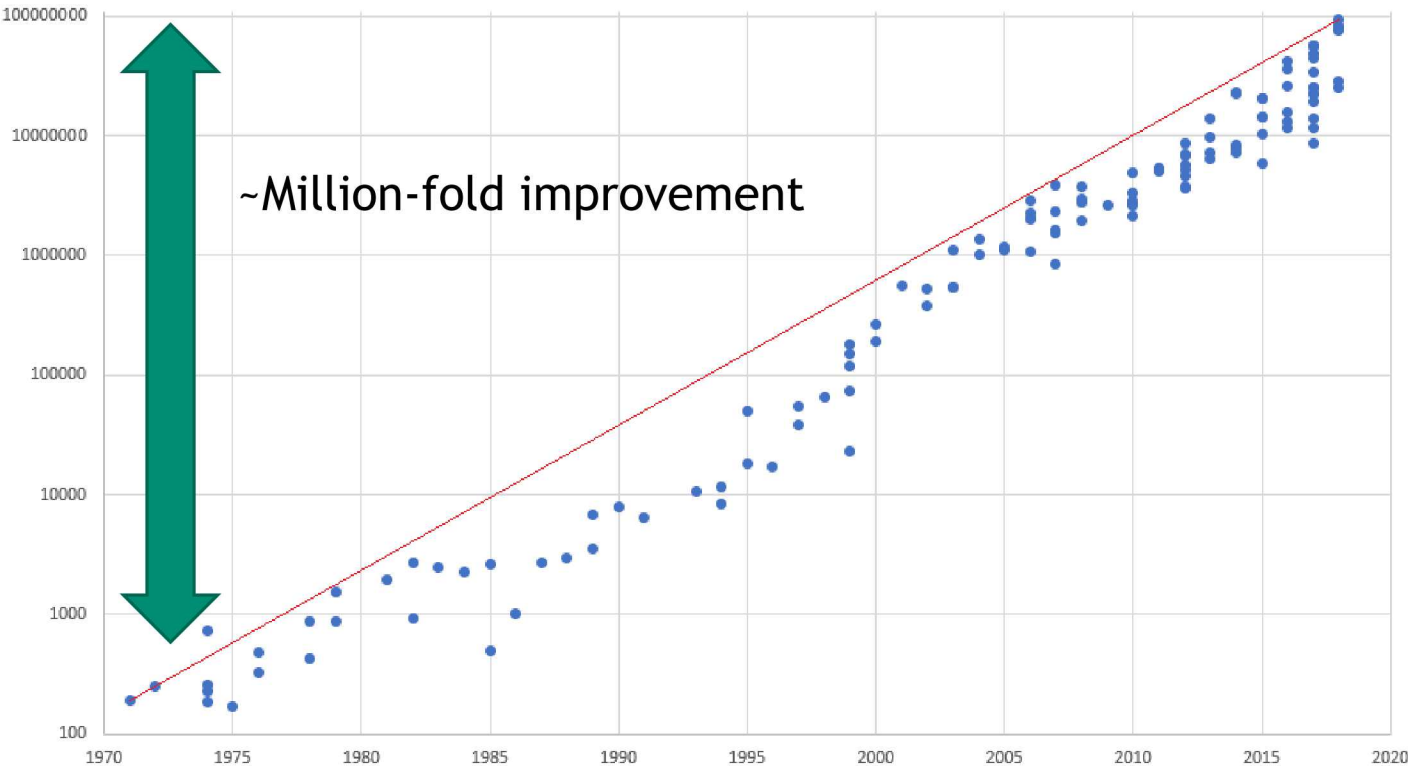


While there are many machine learning techniques, the basic process flow is the same for all approaches

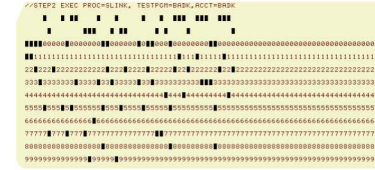




Moore's Law is Alive and Well!
Transistors per Square Millimeter by Year



Moore's Law: the number of transistors on an IC would double every few years.



~80 bytes/punch card
133 bytes/sec



1951 - 7200 bytes/sec



1980 - 5MB, 0.625MB/sec
1990 - 400MB, 0.7MB/sec
2008 - 750GB, 64MB/sec

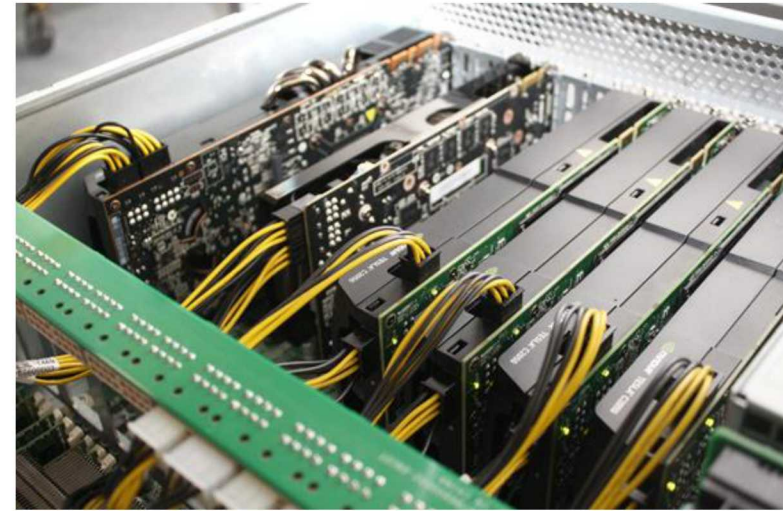
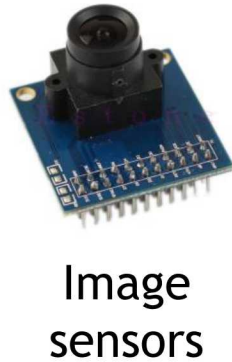
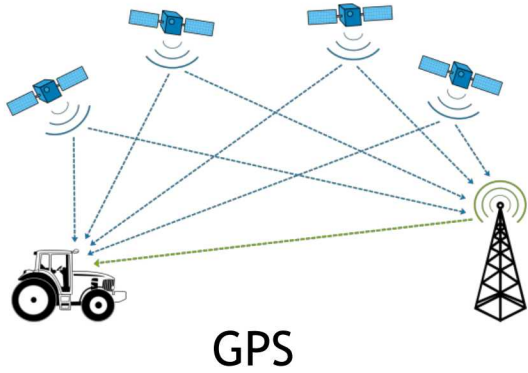


today - solid state drive
4TB, 500MB/sec

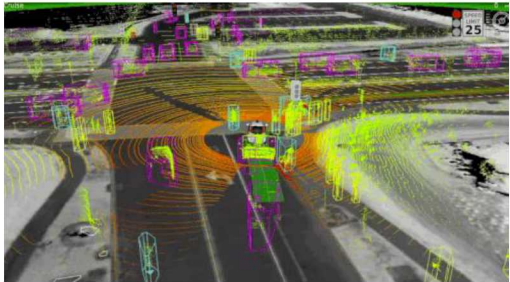
Enabling Technological Advances (continued)



Low cost, high performance sensors, platforms



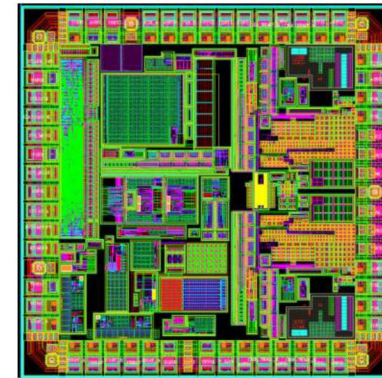
Graphical Processing Units (GPUs)



LIDAR (Light Detection and Ranging)



UAVs

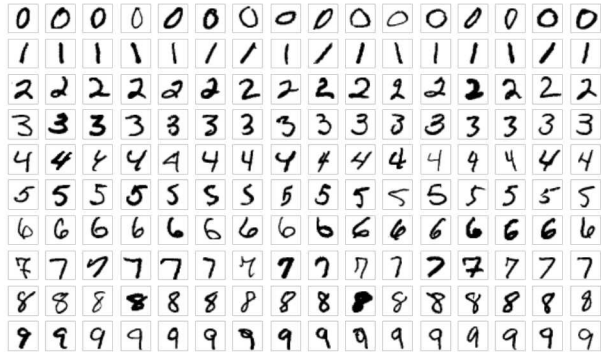


Application Specific Integrated Circuits (ASICs)

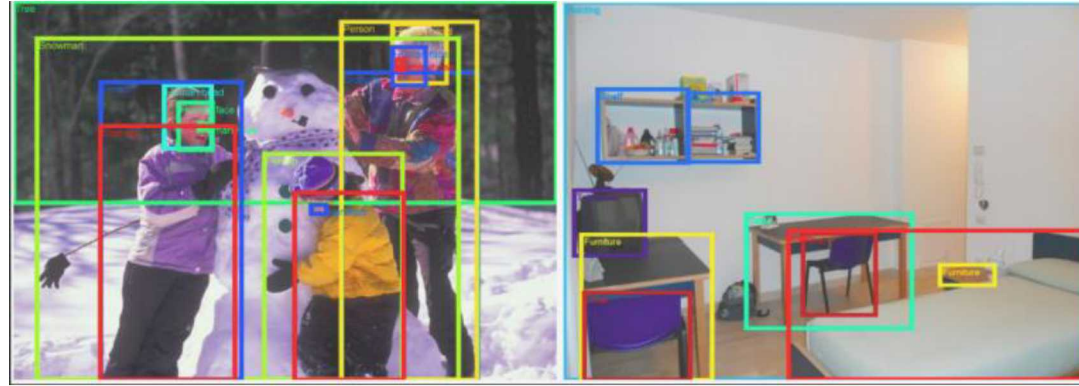
Enabling Technological Advances (continued)



Truth data for training/validation – there are a large number of datasets available for image processing, natural language processing, and audio/speech processing



MNIST - 70,000 handwritten digits

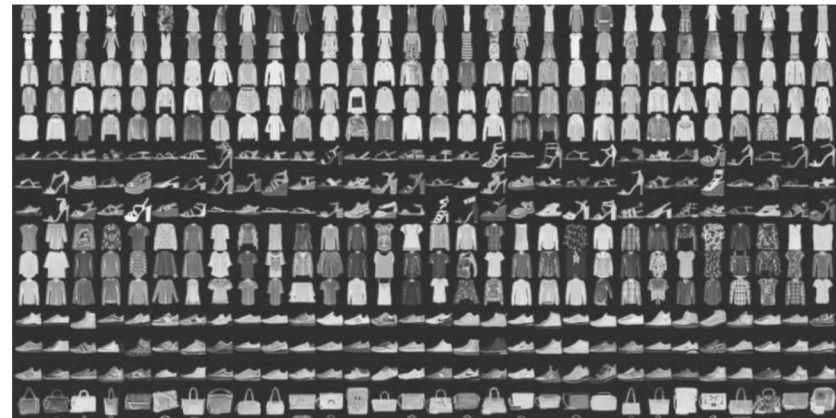


Open Images Dataset - 9 Million annotated images



The Street View House Numbers (SVHN), 600,000 images

Fashion-MNIST, 70,000 images



A Brief History of AI – The Turing Test



Proposed by Alan Turing in 1950

Three players

- A – computing machine
- B – human being
- C – interrogator

All communication is through a textual device (e.g., keyboard)

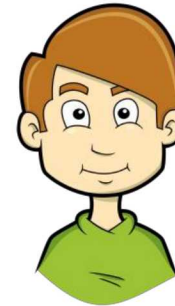
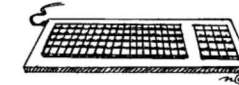
Can the interrogator identify the human and computer?

Turing predicted that a computer could convince ~33% of the judges after 5 minutes of questioning by the year 2000

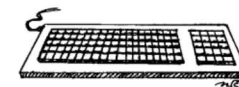
June 2014, A chatbot called Eugene Goostman, which simulates a 13-year-old Ukrainian boy, convinced 30% of the judges



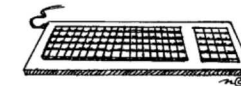
A - computer



B - human



C - interrogator



A Brief History of AI – the Dartmouth Workshop



The term “artificial intelligence” was first coined by John McCarthy, Marvin Minsky, Nathaniel Rochester, and Claude Shannon in 1956

They proposed a summer workshop on artificial intelligence at Dartmouth College



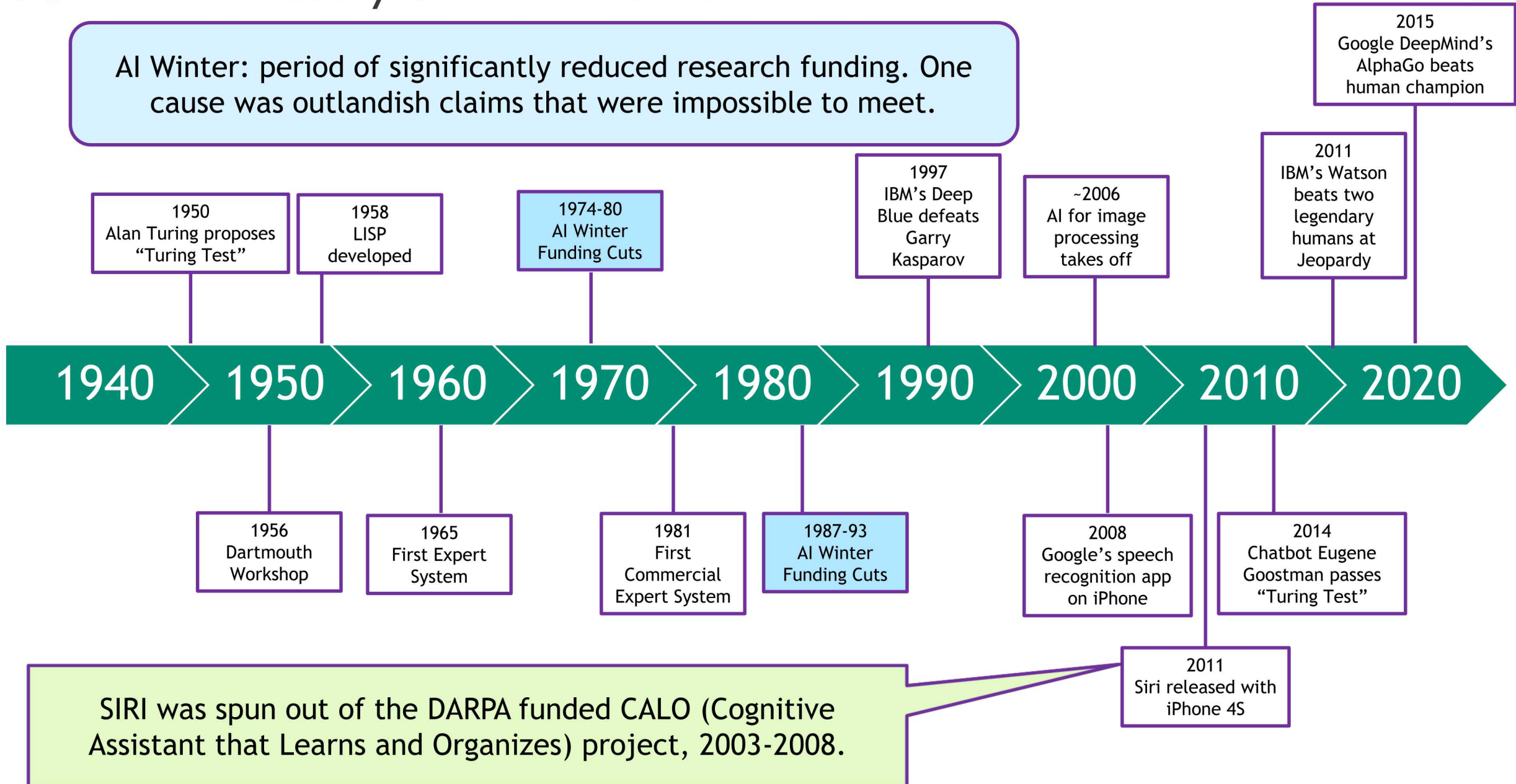
Topics included:

- ***Automatic Computers*** – “If a machine can do a job, then an automatic calculator can be programmed to simulate the machine. The speeds and memory capacities of present computers may be sufficient to simulate many of the higher functions of the human brain, but the major obstacle is not the lack of machine capacity, but our inability to write programs taking full advantage of what we have.”
- ***How Can a Computer be Programmed to Use a Language*** – “It may be speculated that a large part of human thought consists of manipulating words according to rules of reasoning and rules of conjecture. From this point of view, forming a generalization consists of admitting a new word and some rules whereby sentences containing it imply and are implied by others. This idea has never been very precisely formulated nor have examples been worked out.”
- ***Neuron Nets*** – “How can a set of (hypothetical) neurons be arranged so as to form concepts. Considerable theoretical and experimental work has been done on this problem ...”
- **Theory of the Size of Calculation** – you have to understand the size of the calculation to measure the efficiency of an algorithm
- **Self Improvement** – a truly intelligent machine will carry out self-improvement
- **Abstractions** – machine methods of forming abstractions from sensory and other data
- **Randomness and Creativity** – conjectured that creative thinking involves some randomness

A Brief History of AI - Timeline



AI Winter: period of significantly reduced research funding. One cause was outlandish claims that were impossible to meet.



Research in Machine Learning Applied to Energy Systems

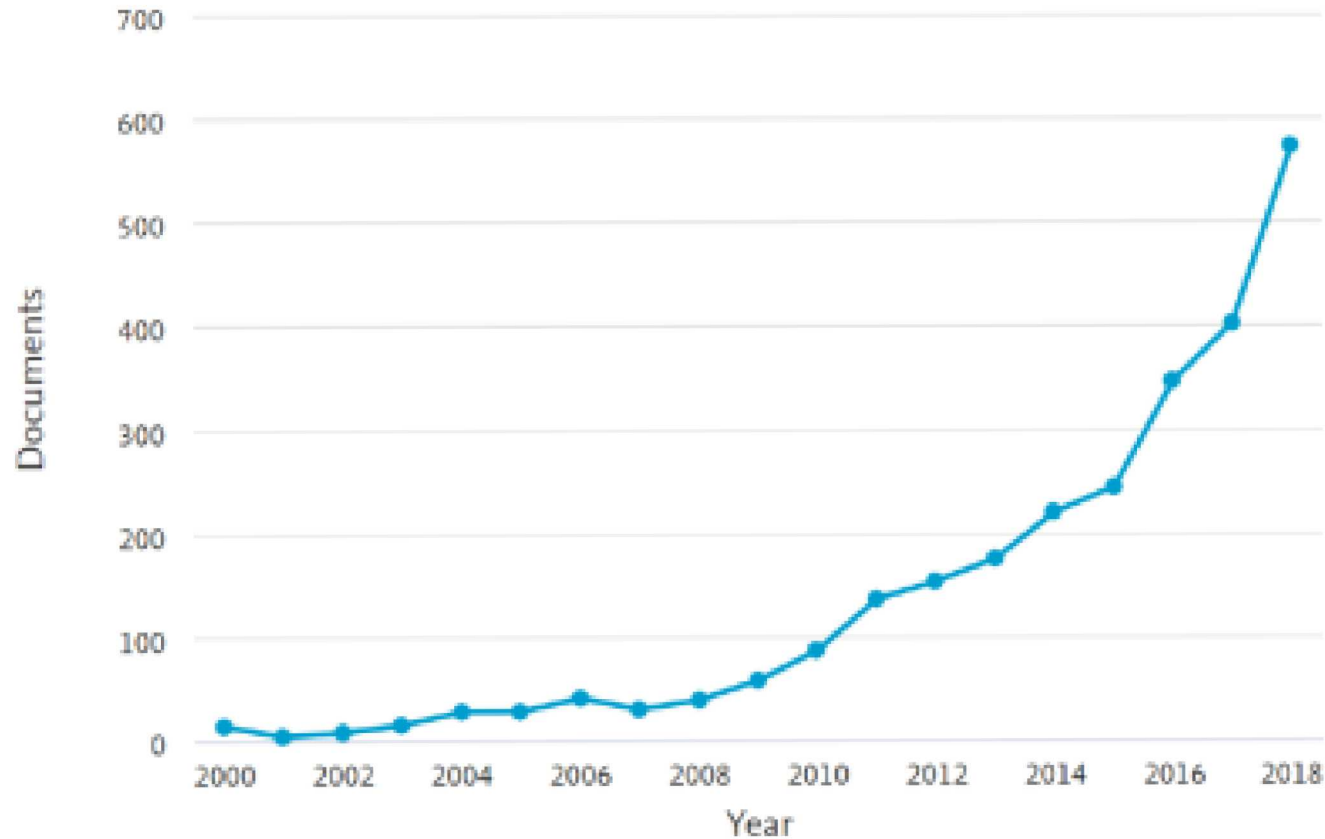


Figure 2. The growth in the number of articles during the past two decades.

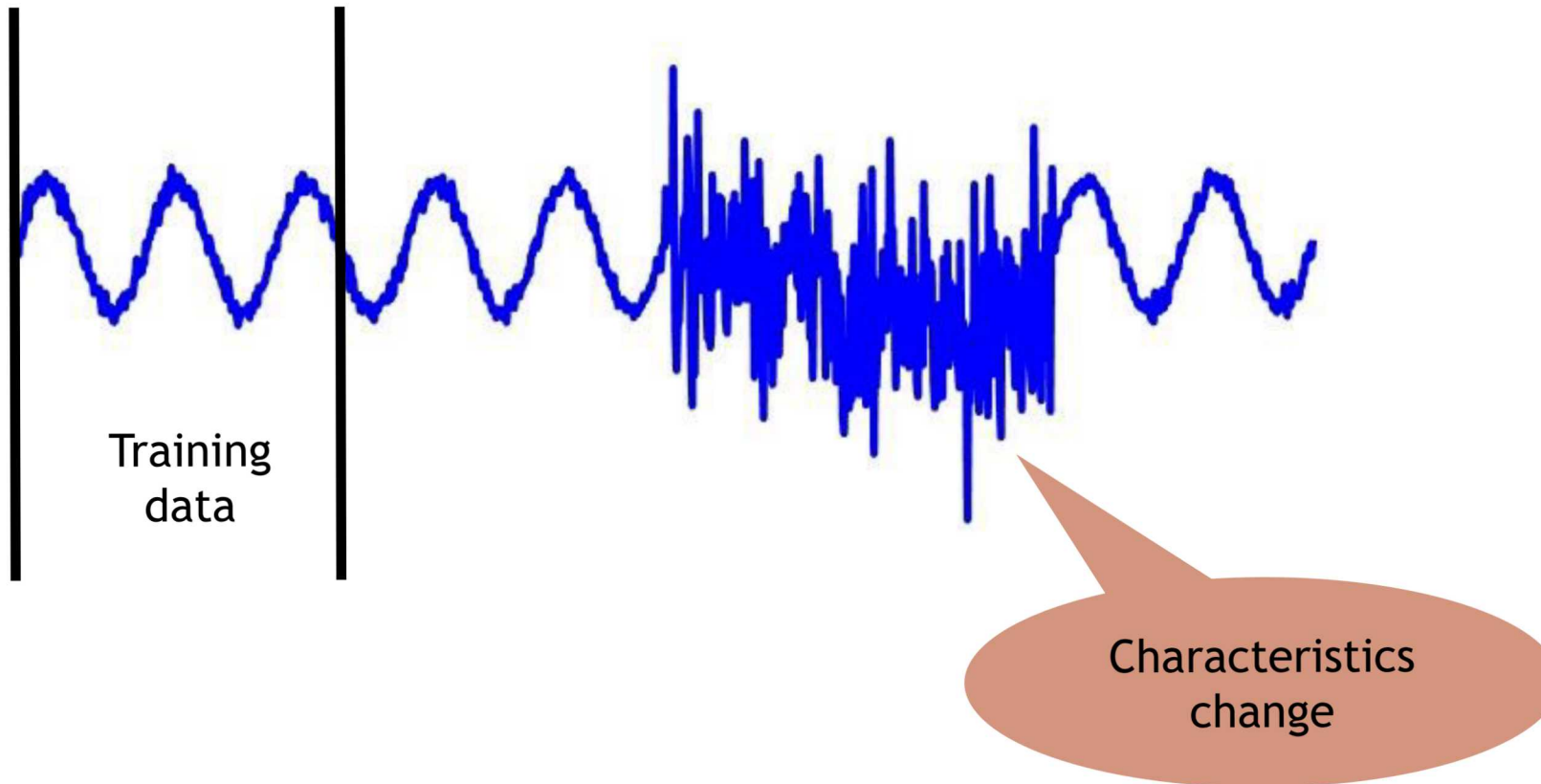
A. Mosavi, M. Salimi, S. F. Ardabili, T. Rabczuk, S. Shamshirband, and A. R. Varkonyi-Koczy, "State of the Art of Machine Learning Models in Energy Systems, a Systematic Review," *Energies*, vol. 12, no. 7, Apr. 2019.

Limitations of Machine Learning



Performance of a ML algorithm can be very good if the characteristics of the training data match the observed data

If the characteristics of the data change over time, and this is not captured in the training data, the performance of the ML algorithm can vary widely

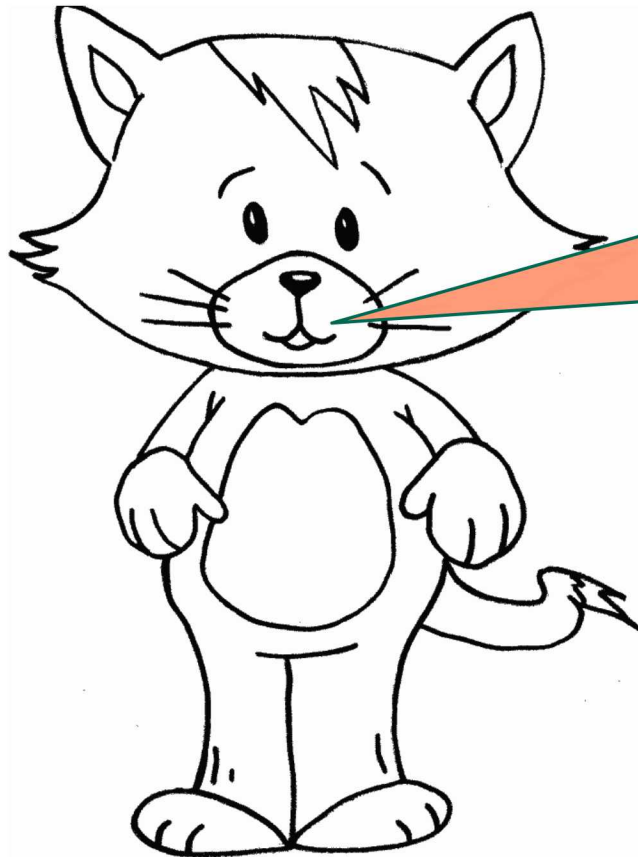


Limitations of Machine Learning



For some problems, there is a known non-machine learning solution that is efficient, elegant, and robust

Is machine learning the best fit for my problem?



**Wow, I applied
machine learning
to solve my
problem!**

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Machine Learning Overview

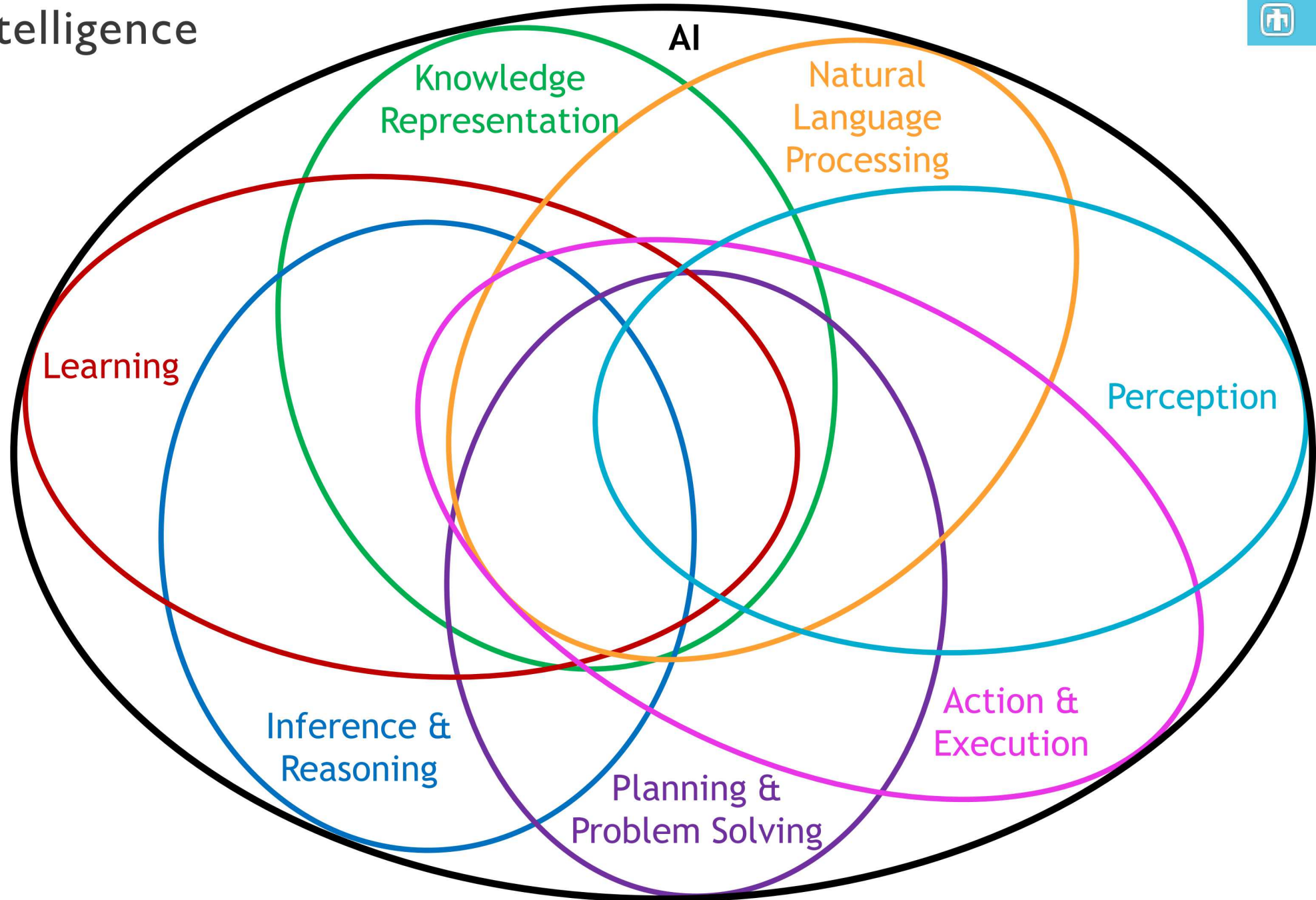
David J. Straczuzi (djstrac@sandia.gov)

September 9, 2019

“The automation of activities that we associate with human thinking ...”
(Bellman, 1978)

“The art of creating machines that perform functions that require intelligence when performed by people.”
(Kurzweil, 1990)

“The study of the computations that make it possible to perceive, reason, and act.”
(Winston, 1992)



What is Machine Learning?



Machine Learning coined in 1959 by Arthur Samuel while trying to use data to improve performance of a checkers playing program.

Samuel, A.L. (1959). Some studies in machine learning using the game of checkers. *IBM Journal of Research and Development*.



IBM, 1956



*A computer program is said to **learn** from **experience** E with respect to some class of **tasks** T and **performance measure** P if its performance at tasks in T , as measured by P , improves with experience E .*

– Tom Mitchell, *Machine Learning*, 1997

Many Types of Tasks and Methods



Tasks:

- Supervised vs Unsupervised
- Classification
- Clustering
- Regression
- Anomaly Detection
- Time Series Analysis
- Policy Learning
- Transfer Learning

Methods:

- Decision Trees
- Rule-Based Methods
- Neural Networks
- Inductive Logic
- Support Vector Machines
- Bayesian Methods
- Genetic Algorithms
- Statistical Algorithms
- Ensembles

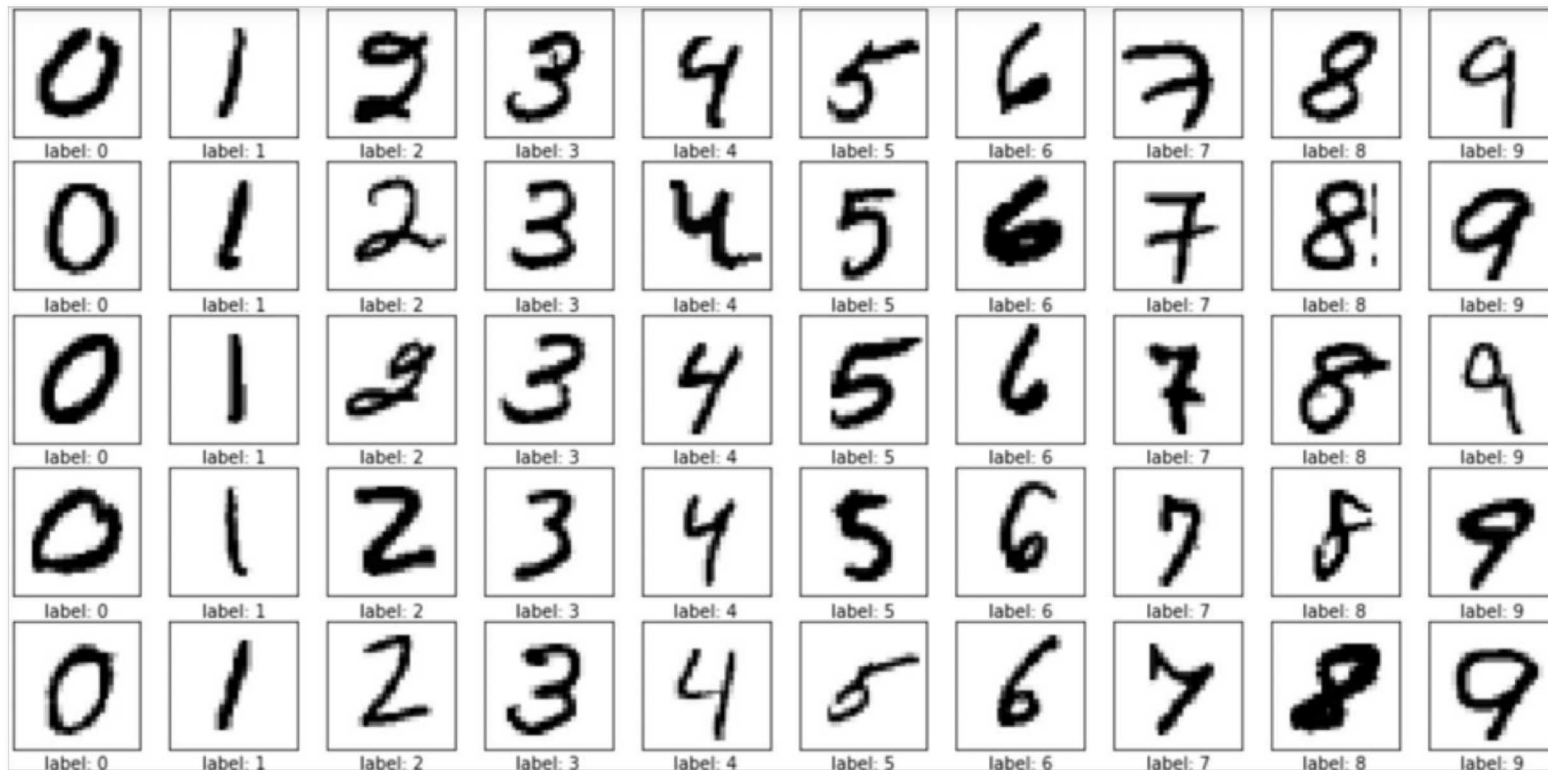
Example Problem: Handwriting Recognition



Task (T): Recognizing and classifying handwritten numbers within images

Performance measure (P): Percent of numbers correctly classified

Experience (E): Database of handwritten numbers with given classifications



How Does Machine Learning Work?



Data / Experience

$X = \{x_1, x_2, \dots, x_n\}$		Y

Model

$$Y=f(x)$$

Loss Function

$$\epsilon = \frac{1}{N} \sum_{i=0}^n g(f(x_i) - Y_i)$$

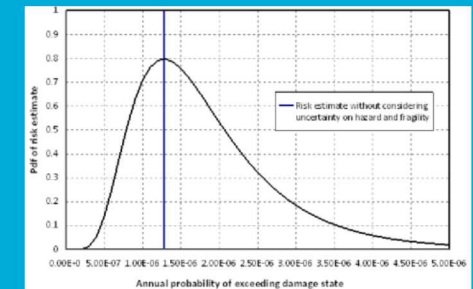
Learning Algorithm

```
if (settings[0].compareTo("s")==0) {  
  if (name.compareTo("") !=0) {  
    name += "_";  
  }  
  name += etr.getString(settings[1]);  
} else if (setting [0].compareTo("d") == 0){  
  if (name.compareTo("") !=0) {  
    name += "_";  
  }  
  name += DateUtils.format(etr.getDate(settings[1]))  
} else if (setting [0].compareTo("d") == 0){  
  if (name.compareTo("") !=0) {  
    name += "_";  
  }  
}
```

Parameterized Model

$$f(x) = \theta_1 x_1 + \theta_2 x_2 + \dots$$

Predictions & Evaluation



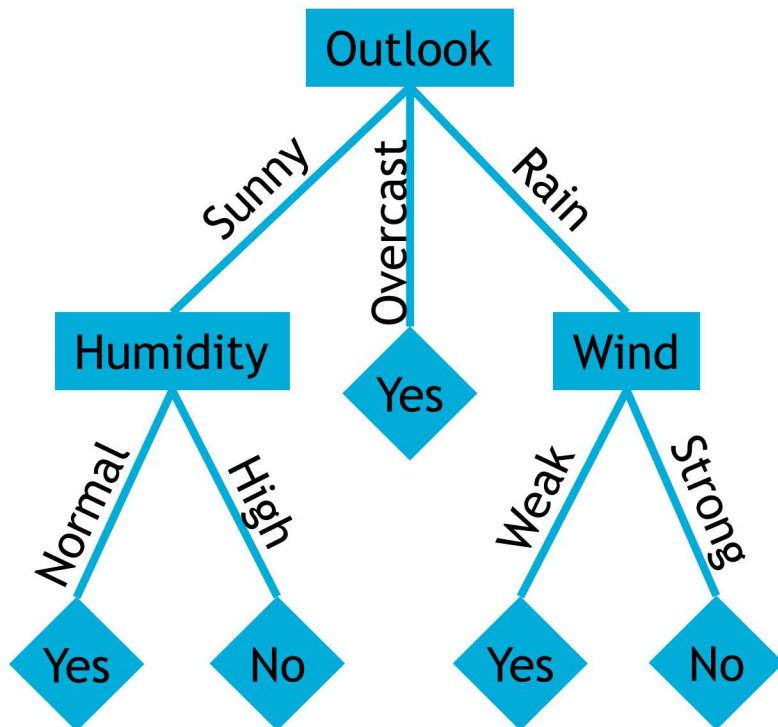
Learning Example : Decision Trees



Task: Determine if Bill will play tennis given weather observations

Performance Metric: Prediction accuracy

Experience: Past observations



Day	Outlook	Temperature	Humidity	Wind	Play Tennis?
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Learning Example: Data Preprocessing and Feature Engineering



- Many learning algorithms take a set or sequence of **vectors** as input
 - Raw data needs to be encoded in this format
 - For many data types, there are existing encoding conventions
- **Feature engineering** uses domain knowledge to create these encodings
 - Highly manual and time consuming
 - Quality of learned model often dependent on feature encodings

Example: Play Tennis?

Outlook: {sunny, overcast, rain} or
 {sunny, partly cloudy, mostly cloudy, cloudy, drizzle, rain, downpour} or
 RGB image from TennisCam

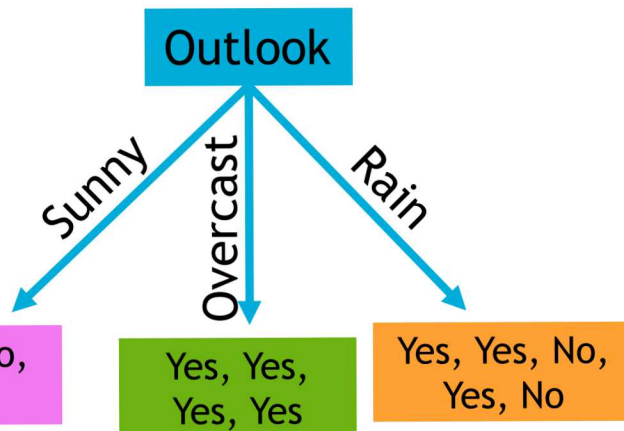
Temperature: {hot, mild, cool} or
 {hot, warm, mild, cool, cold} or
 {-20F, -19F, ... , 114F, 115F} or
 continuous

Learning Example: Decision Trees

General Approach:

- Split the data based on information theory (entropy)
- Entropy measures the distribution of positive and negative examples in each block
- Greedy search through attribute (feature) space

$$\text{Gain} = \text{Entropy}_{\text{all data}} - \text{Sum of Entropies}_{\text{after split}}$$



Day	Outlook	Temperature	Humidity	Wind	Play Tennis?
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

G=0.247

G=0.029

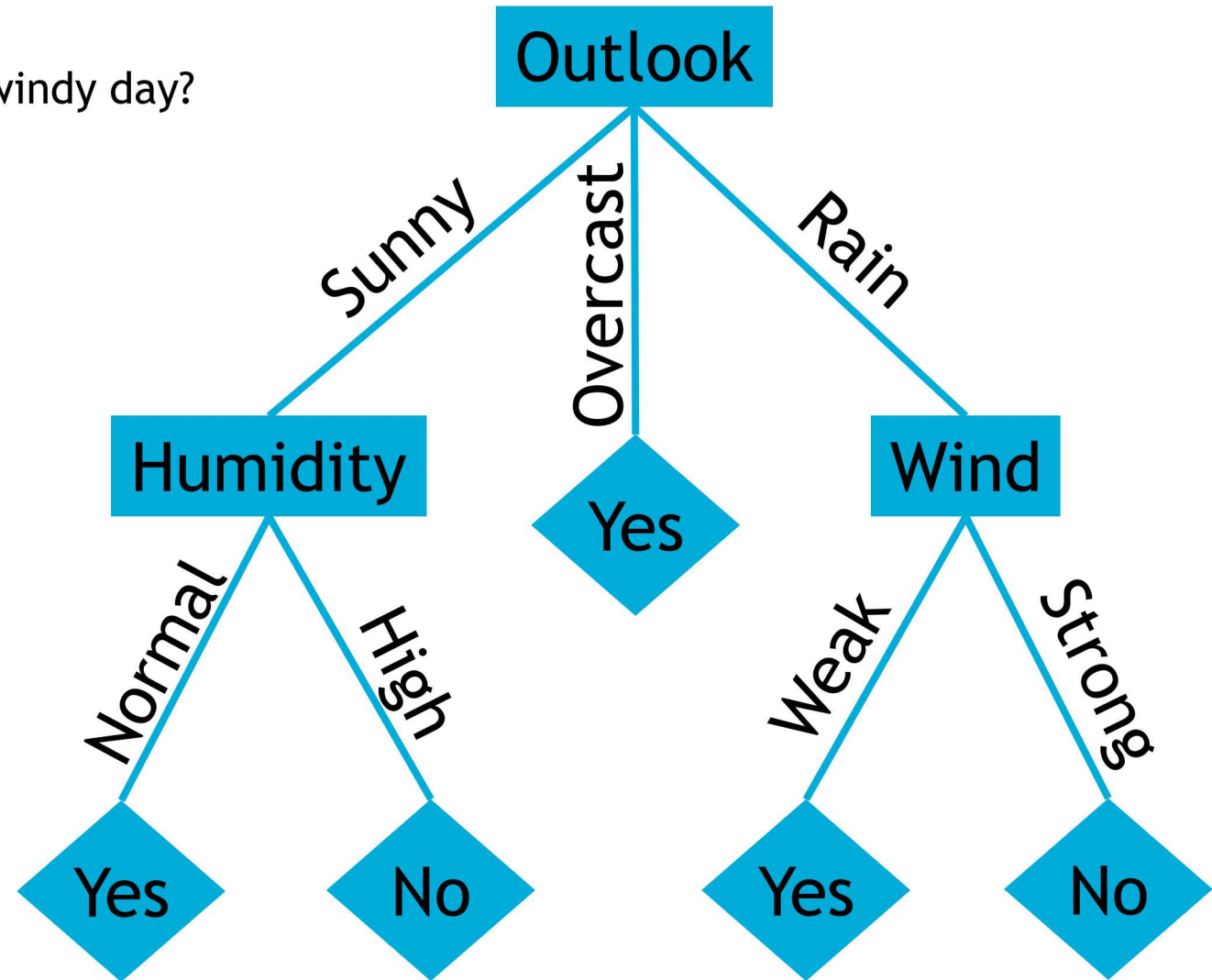
G=0.152

G=0.048

(Day 15) What will happen on a sunny, cool, humid, windy day?

Many design decisions affect performance:

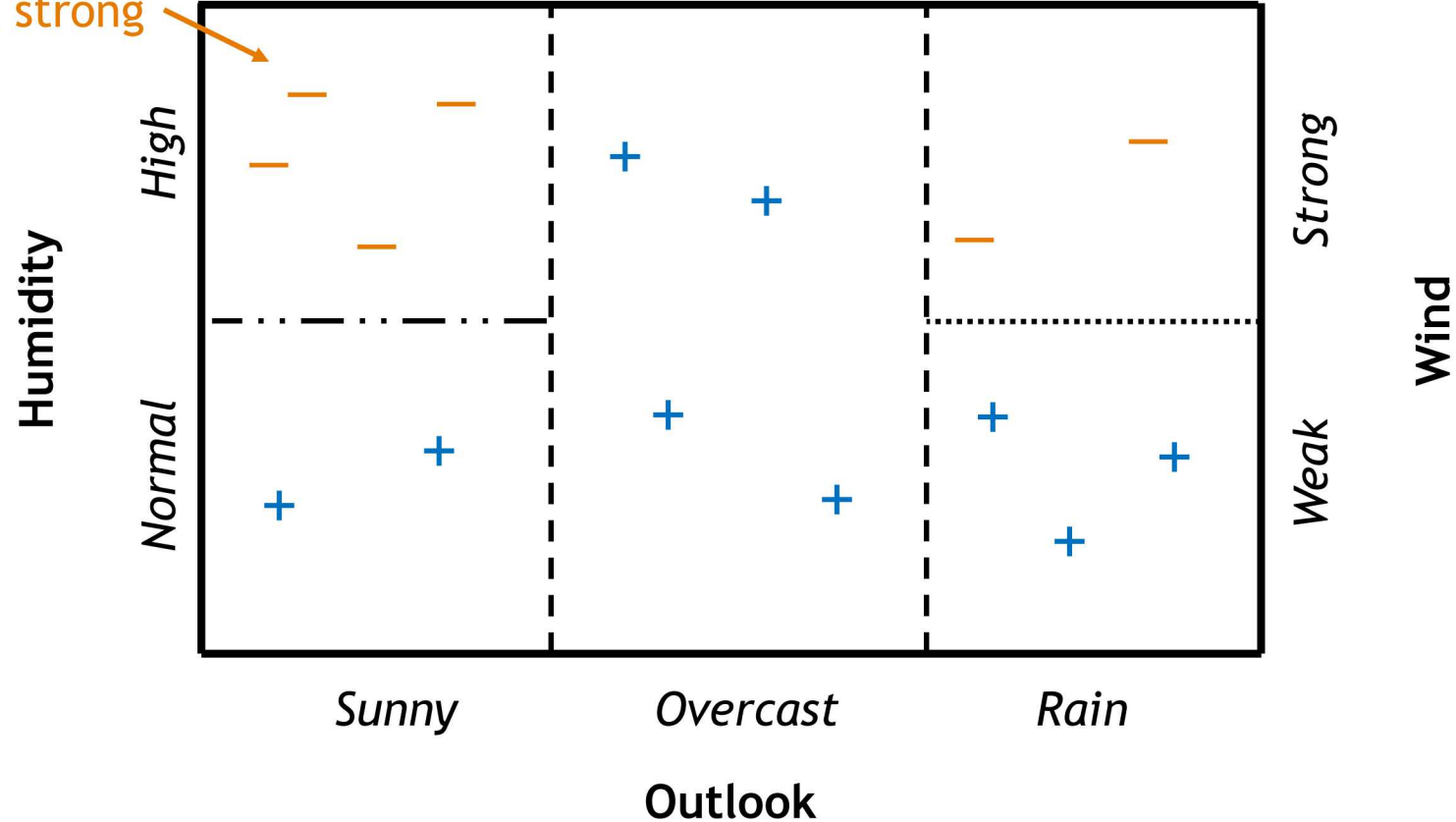
- Training data
(number and quality of examples)
- Which variables describe the data
- Splitting criterion
- Binary versus multivariate splits
- What to do with numeric variables
- Stopping criterion



Decision Tree Hypothesis Space



sunny, cool, high, strong



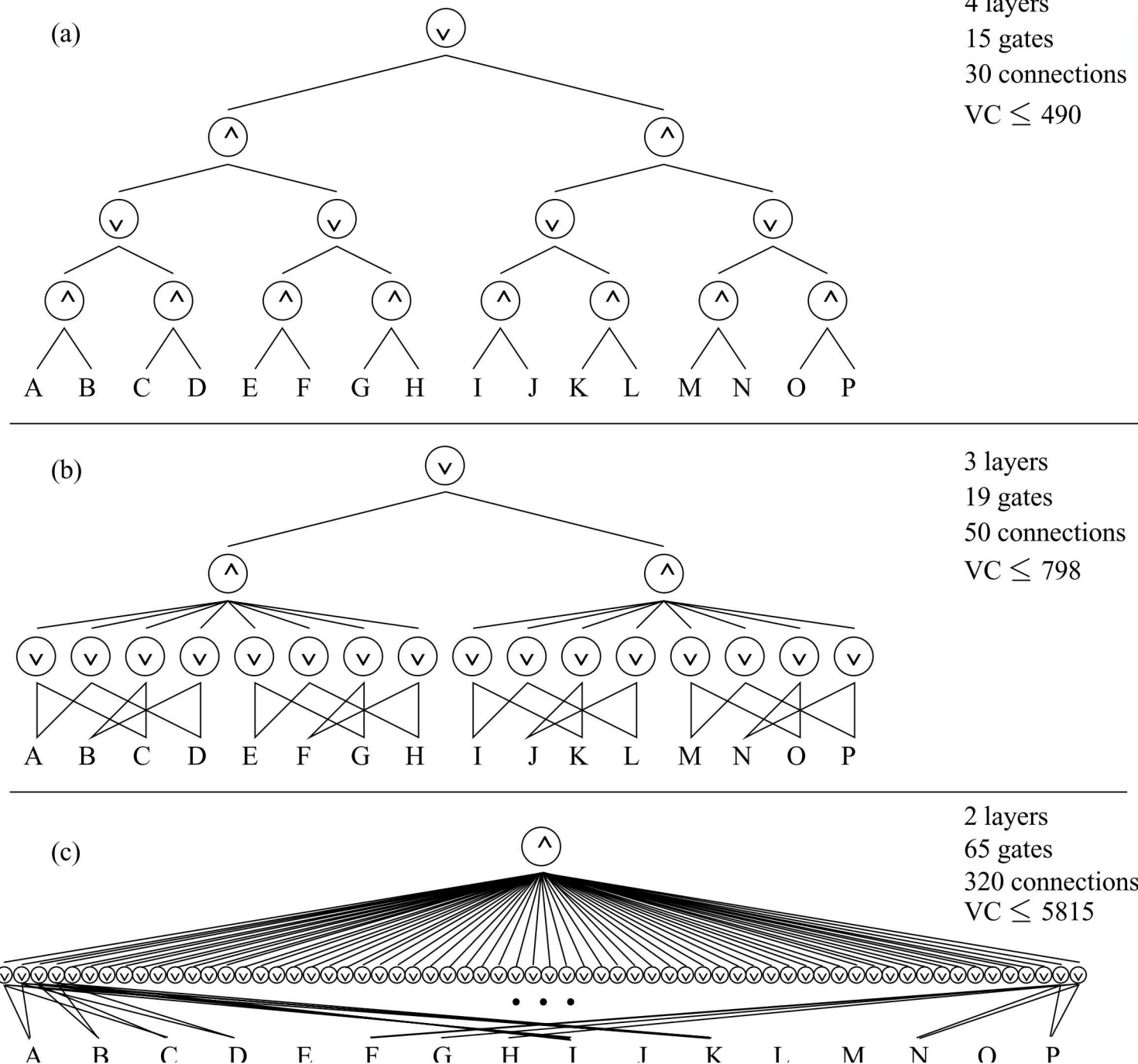
Note: Original data was in 5 dimensions. Only showing 3 here compressed into 2.

Bias-Variance Trade-Off

Always choose the simplest model that can fit the data.

- Circuits (a), (b), (c) represent same logical function
- Can view gates and connections as learnable parameters
- All things equal, (a) is a much easier learning problem and most likely to generalize well.

Many theoretical constructs attempt to explicitly manipulate this trade, yet it remains a vexing problem.



Learning Example: Image Analysis



Task: Classify pixels as tree, grass, roof, water, concrete, or boat

Performance Metric: Accuracy

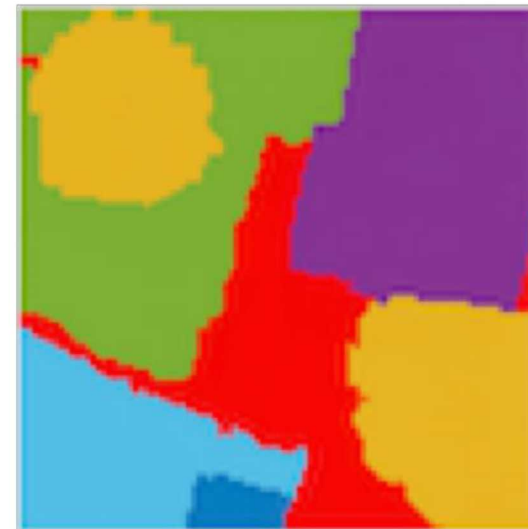
Experience: Labeled pixels



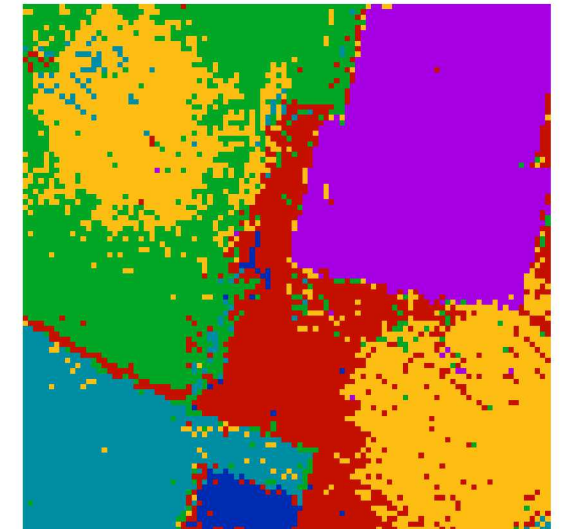
RGB Color



Height



Labels



Predictions

Learning Example: Image Analysis

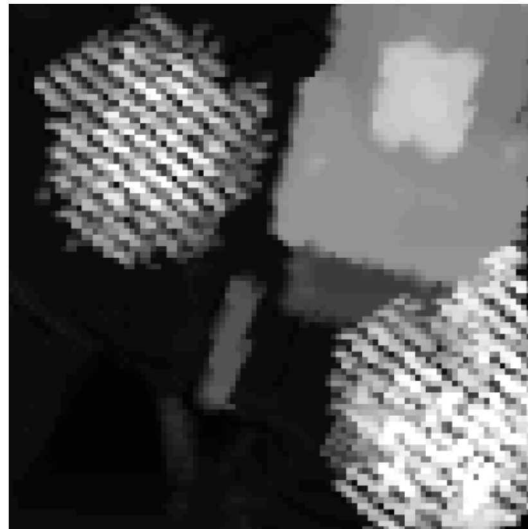


As we develop an application, we need to ask:

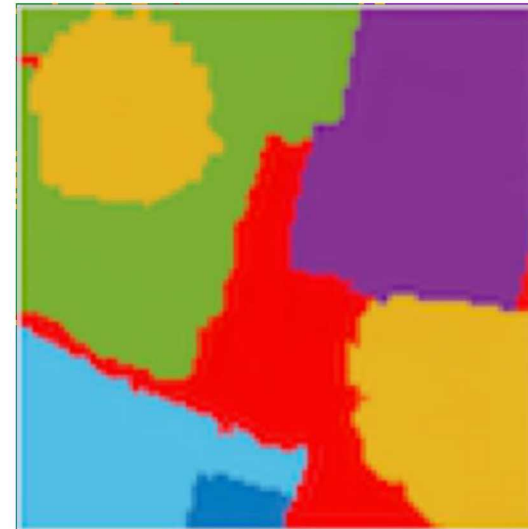
- How else might we formulate the problem?
- What input variables might provide the most information?
- How good are my labels?
- What is the most appropriate knowledge representation?
- What is the most appropriate performance metric?
- Given the task and the data, what learning algorithms are likely to perform well?



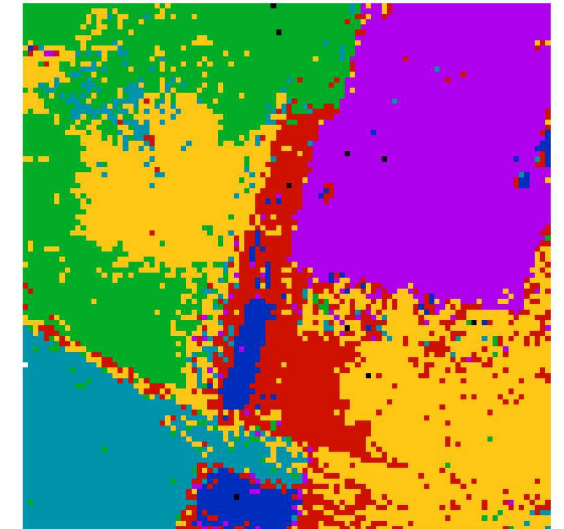
RGB Color



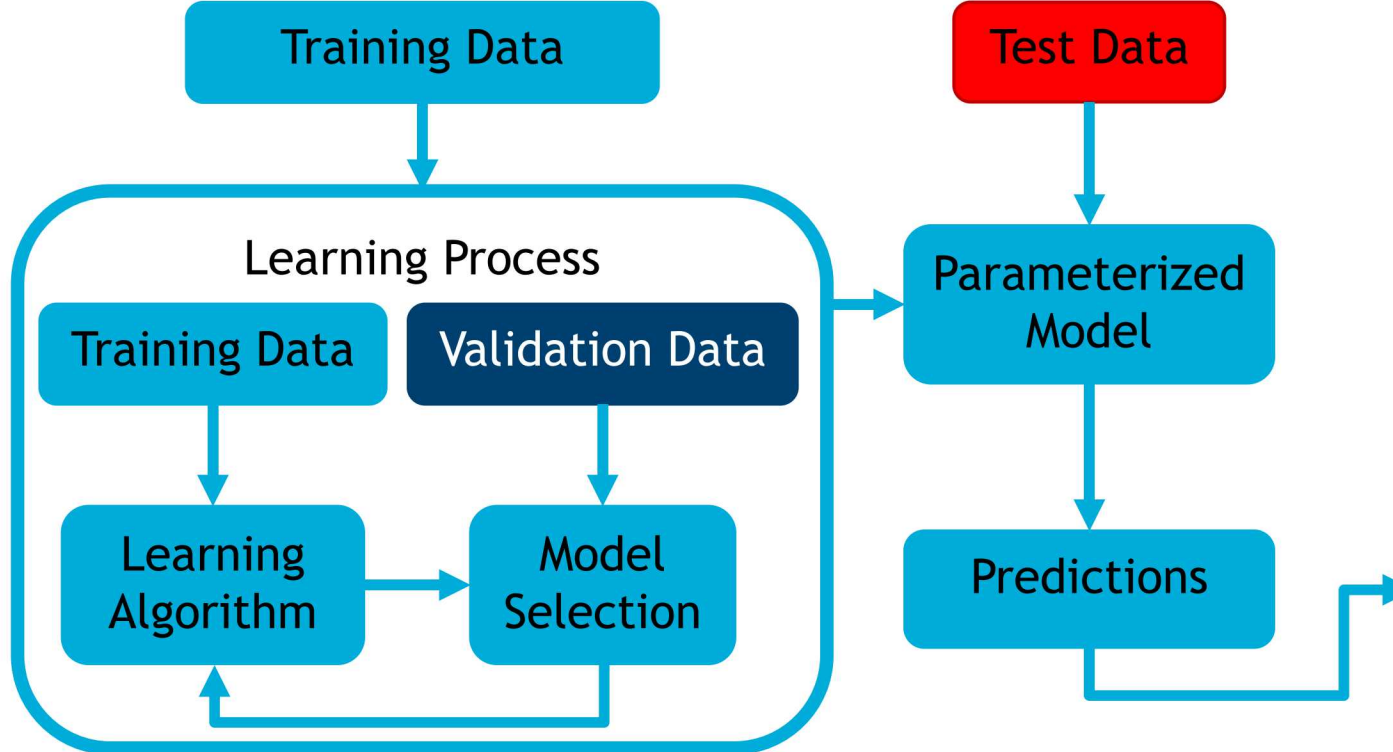
Height



Labels



Predictions with
Color Only (78%)



- Many ways to formulate error and performance metrics
- Highly dependent on the data, task, and goals
- Extrapolation ability is difficult to evaluate
- Hard to determine if/when we are extrapolating

- Accuracy = $(TP + TN) / n$
- Precision = $TP / (TP + FP)$
- Recall (Sensitivity) = $TP / (TP + FN)$
- F-score = $(P * R) / (P + R)$
- Confusion Matrices
- Log Loss = $\frac{-1}{N} \sum_{i=1}^N \sum_{j=1}^M y_{ij} \times \log(p_{ij})$
- ROC Curves: calibrate classification thresholds
- P-R Curves: similar to ROC; lots of negatives
- Regression metrics:
 - Root Mean Squared Error
 - Mean Absolute Error
 - R^2 – variance explanation

All of these can be applied with cross validation, random resampling, and stratification

Learning Example: Time Series Application



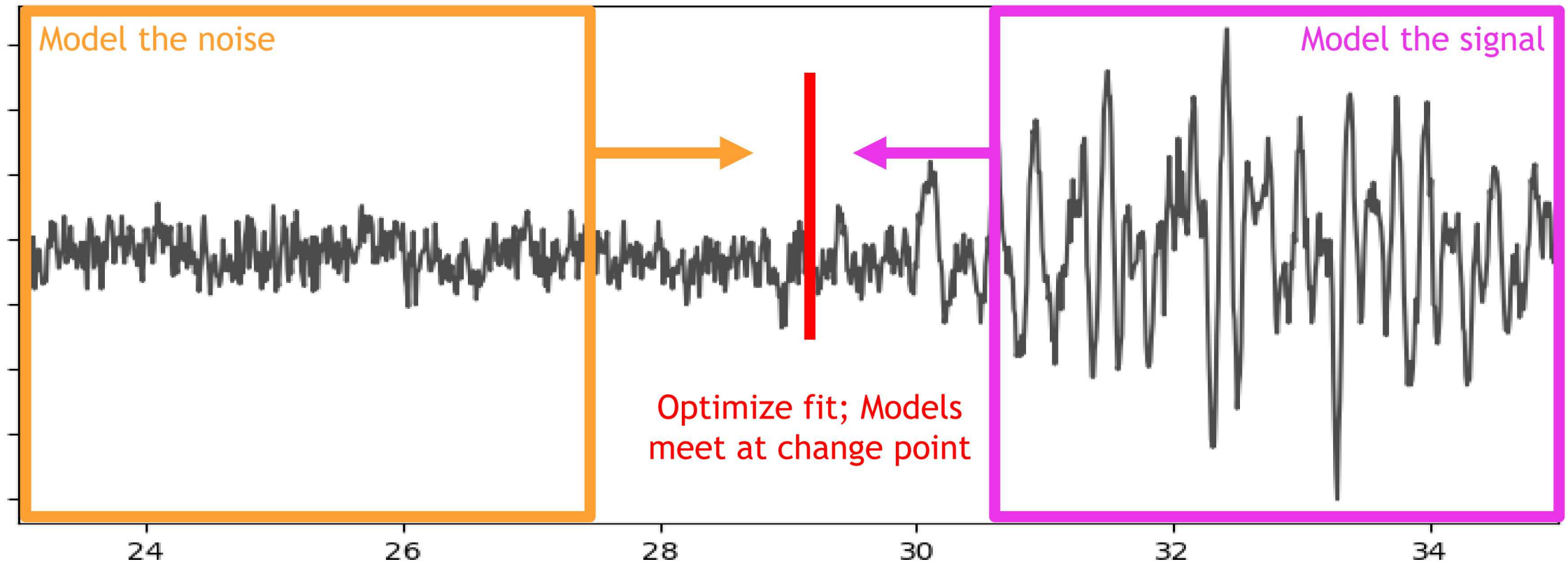
Task: Change detection

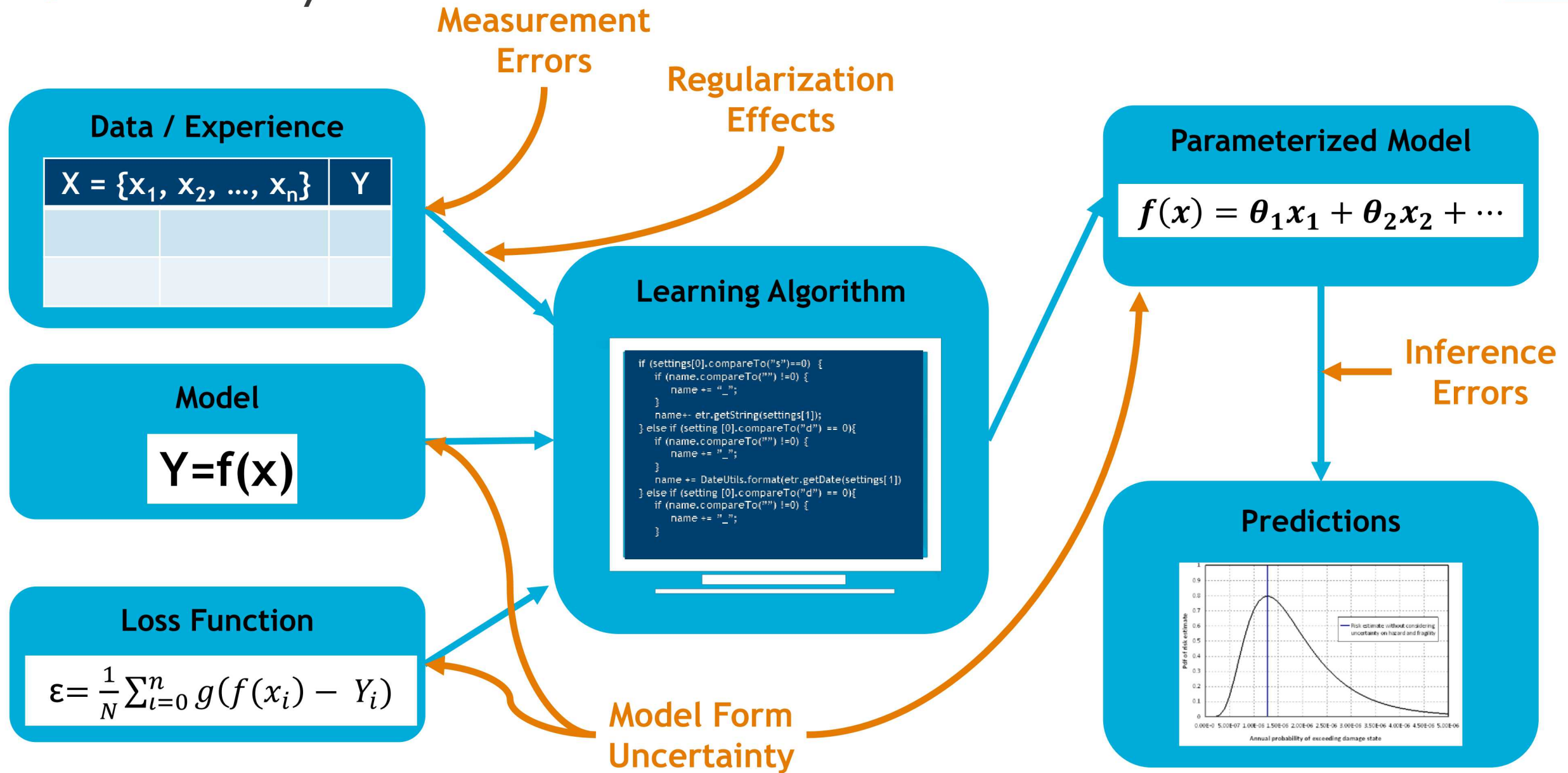
Want to know, as precisely as possible,
when the signal first arrived

Performance Metric: *No Ground Truth!!*

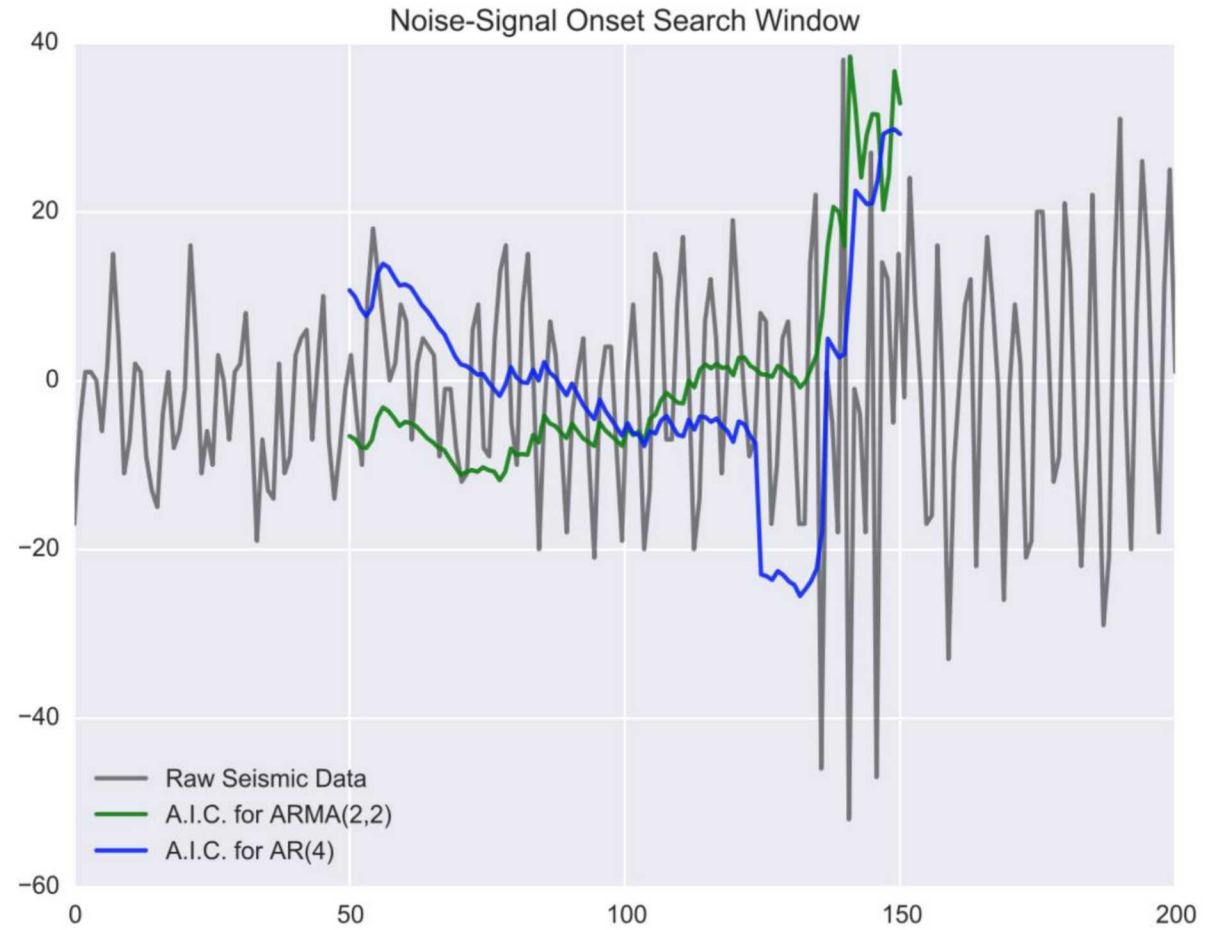
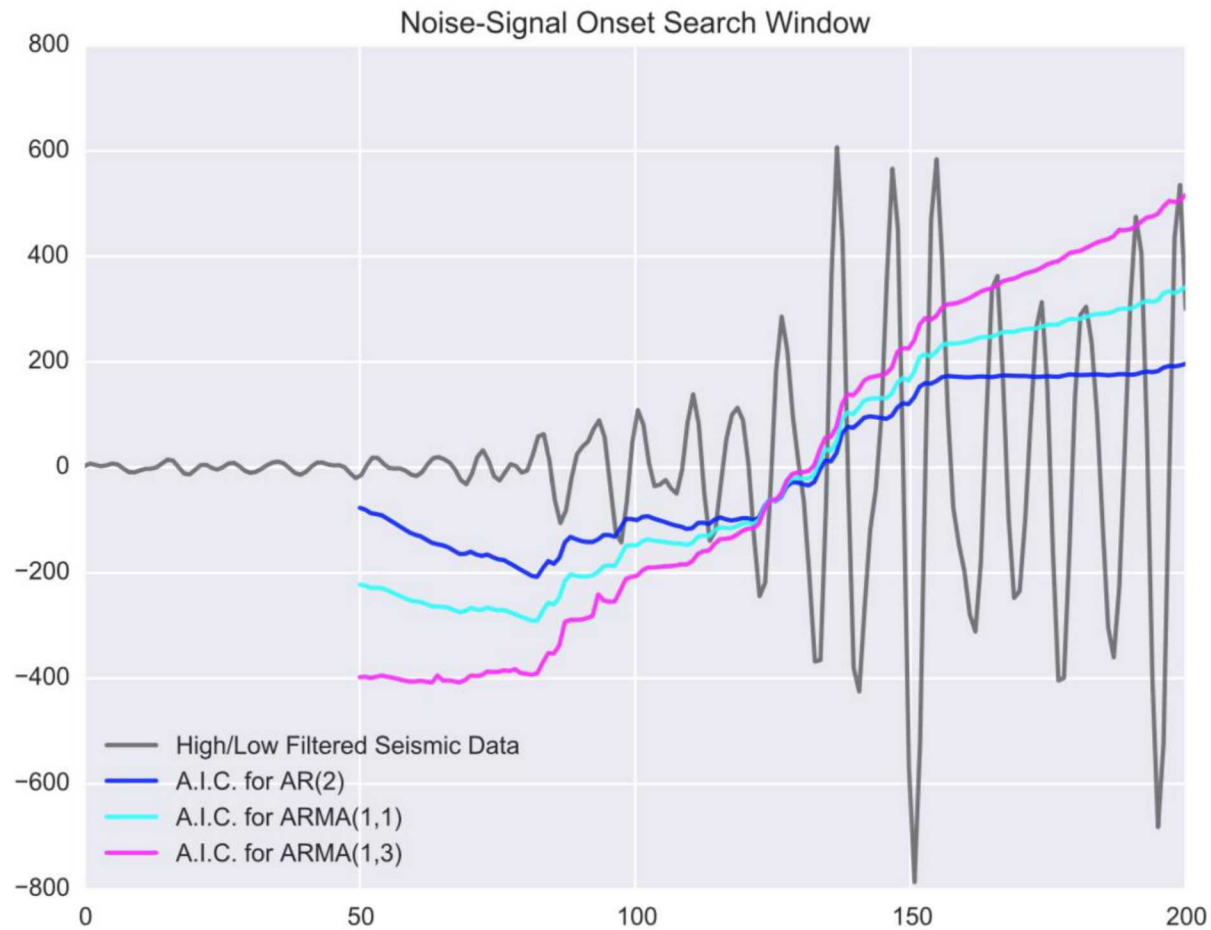
Internal distance metrics only

Experience: Waveform data,
containing both signal and noise

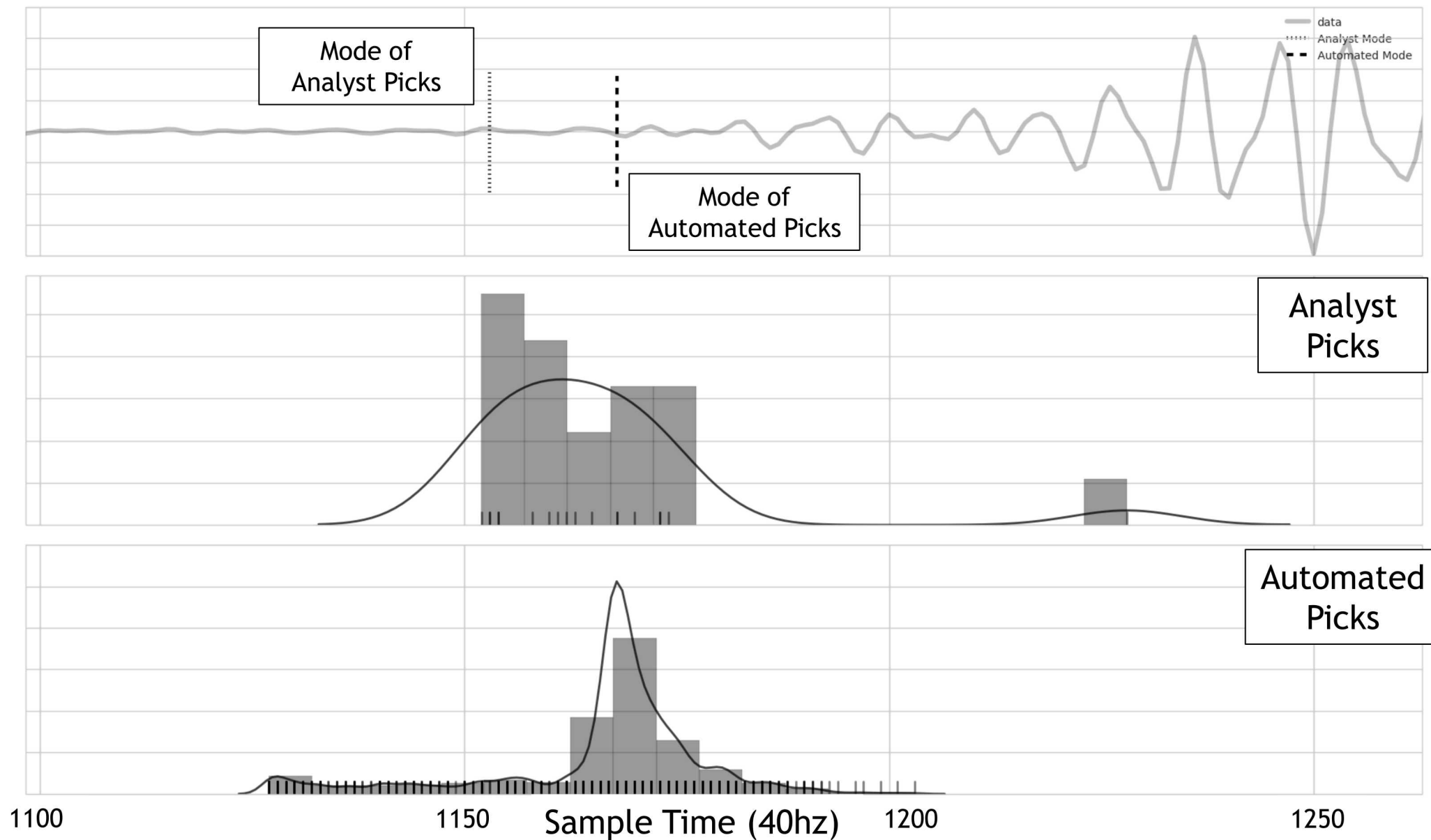




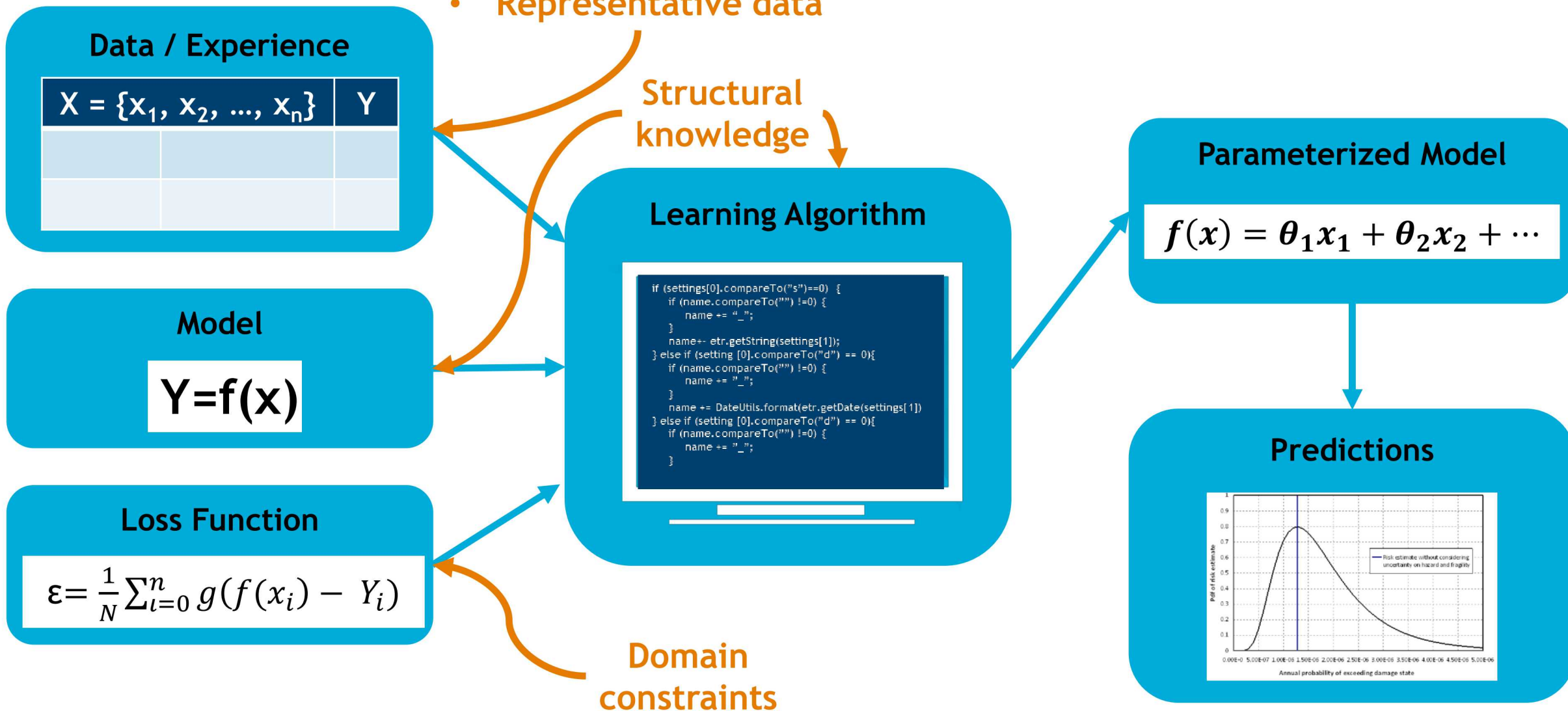
Uncertainty Example: Seismic Onset Detection



Uncertainty Example: Seismic Onset Detection



- Variable selection
- Representative data



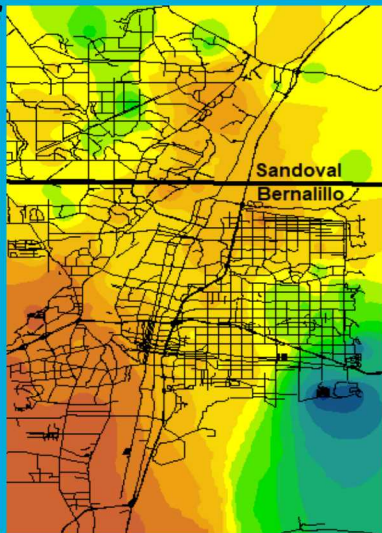
Domain
constraints



Sparse measurements

Example: Given sparse network of rainfall sensors and doppler radar, compute rainfall distribution map for entire region.

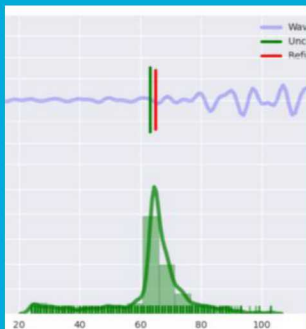
Becomes input to hydrology simulations.



Event detection

Example: Given seismograph network, identify all onset times and estimate relative detection quality.

Becomes input to slowness inversion.



Predictive Model Induction

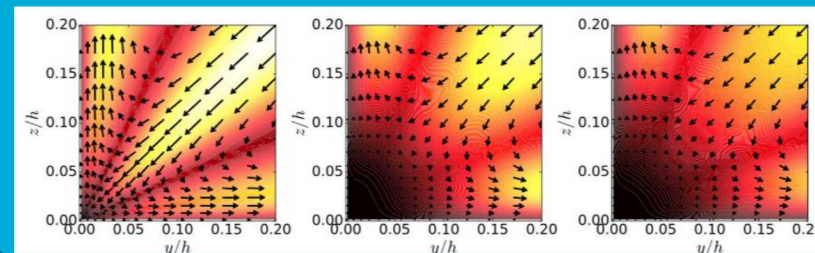
Example: Given URL format rules and known examples of benign and malicious links, learn to distinguish between the two.

<https://www.facebook.com/help/cookies/?ref=sitefooter>

HostName Path Parameters

Error correction

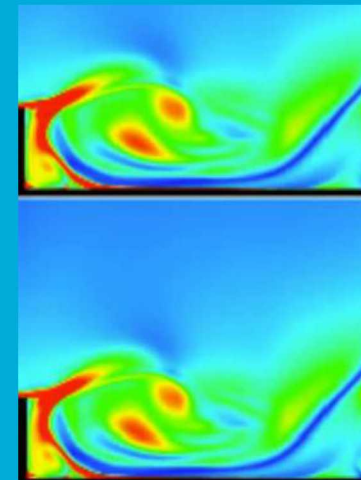
Example: Compare mod/sim results to observations, learn an error term for the simulation model. Error term may use observables not included in the model.



Surrogate models

Example: Given high-fidelity model and simulations, predict physical model outputs for given conditions.

Use learned model as inexpensive proxy for the high-fidelity model.





Textbooks on AI & ML

- Hastie, T., Tibshirani, R. and Friedman, J. (2009). *The Elements of Statistical Learning*. Springer
- Mitchell, T.M. (1997). *Machine Learning*. McGraw-Hill
- Russell, S. and Norvig, P. (2009). *Artificial Intelligence: A Modern Approach (3rd Ed)*. Pearson
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- Kearns, M.J. and Vazirani, U. (1994). *An Introduction to Computational Learning Theory*. MIT Press
- Rissanen, J. (2007). *Information and Complexity in Statistical Modeling*. Springer
- Vapnik, V.N. (1999). *The Nature of Statistical Learning Theory (2nd Ed)*. Springer

Bayesian Methods

- Gelman, A., Carlin, J.B., Stern, H.S., Dunson, D.B., Vehtari, A. and Rubin, D.B. (2013). *Bayesian Data Analysis (3rd Ed)*. CRC Press
- Kruschke, J.K. (2015). *Doing Bayesian Data Analysis (2nd Ed)*. Academic Press.

Evaluation

Cohen, P.R. (1995). *Empirical Methods for Artificial Intelligence*. MIT Press

Zheng, A. (2015). *Evaluating Machine Learning Models*. O'Reilly

Uncertainty

Stracuzzi, D.J., Darling, M.C., Peterson, M.G., Chen, M.G. (2018). *Quantifying Uncertainty to Improve Decision Making in Machine Learning*. Sandia National Laboratories, SAND2018-11166.

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Bauer, T. (in preparation). *Human Constrained Machine Learning: A Brief Survey and Ideas for Capability Development*. Sandia National Laboratories (SAND Report)

Karpatne, A., et al. (2017). Theory-Guided Data Science: A New Paradigm for Scientific Discovery from Data. *IEEE Transactions on Knowledge and Data Engineering*, 29 (10).



Machine Learning Approaches and Data Considerations

Warren L. Davis IV (wldavis@sandia.gov)

September 9, 2019



- Factors in deciding upon a machine learning approach
- Classes of Machine Learning
 - Supervised Learning
 - Unsupervised Learning
 - Semi-Supervised Learning
 - Reinforcement Learning
- Information Representation

Deciding Upon a Machine Learning Approach



What problem are you trying to solve?

- Predict a category
- Predict a value
- Group data
- Find anomalies
- Find correlations
- Optimize parameters

What data is available?

- Numerical
- Categorical
- Images/Audio/Video
- Text
- ...



Tasks

- Regression (continuous response)
- Classification (discrete response)
 - Binary (2 classes)
 - Multiclass (>2 classes)

Experience (data)

- Regression: input-output pairs
- Classification: feature-label pairs

Performance measures

- Many different methods

Iris Data (subset)

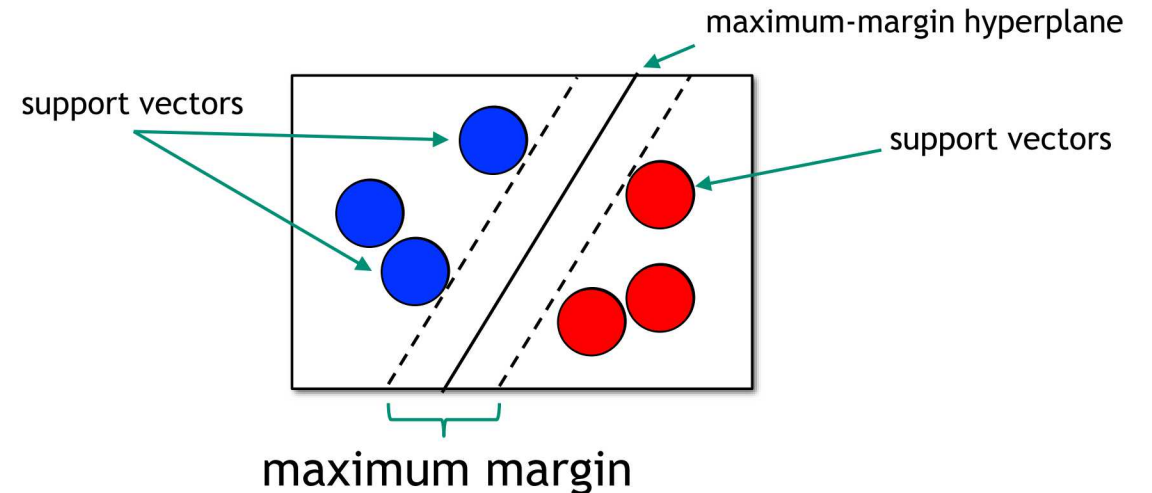
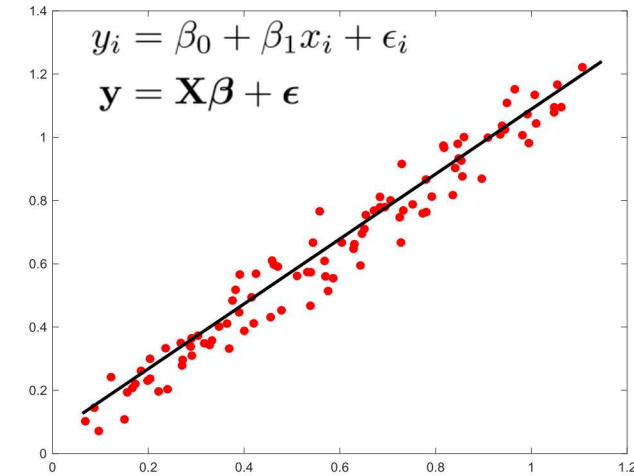
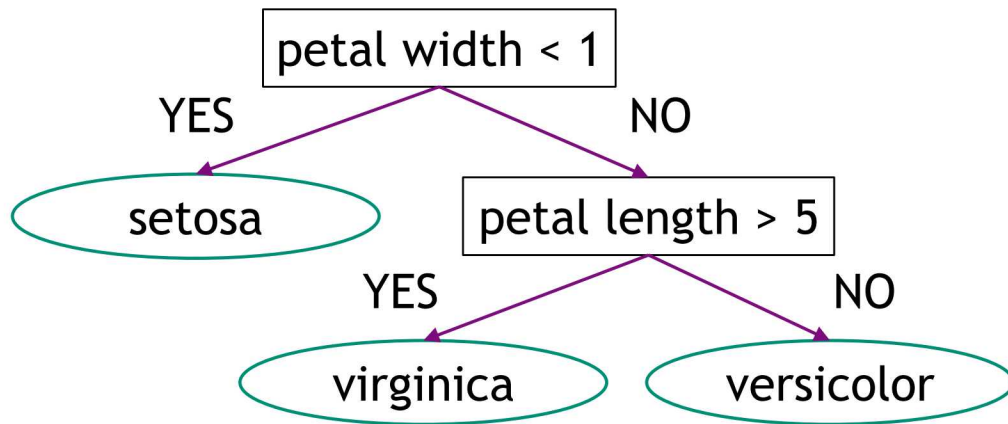
Sepal length	Sepal width	Petal length	Petal width	Species
5.1	3.5	1.4	0.2	setosa
4.9	3	1.4	0.2	setosa
4.7	3.2	1.3	0.2	setosa
4.6	3.1	1.5	0.2	setosa
5	3.6	1.4	0.2	setosa
7	3.2	4.7	1.4	versicolor
6.4	3.2	4.5	1.5	versicolor
6.9	3.1	4.9	1.5	versicolor
5.5	2.3	4	1.3	versicolor
6.5	2.8	4.6	1.5	versicolor
6.3	3.3	6	2.5	virginica
5.8	2.7	5.1	1.9	virginica
7.1	3	5.9	2.1	virginica
6.3	2.9	5.6	1.8	virginica
6.5	3	5.8	2.2	virginica

Features
Label

Examples of Supervised Learning



- Linear Regression
- Support Vector Machines
- Naïve Bayes
- Decision Trees / Random Forests
- Neural Networks
- k-Nearest Neighbor



Neural Networks

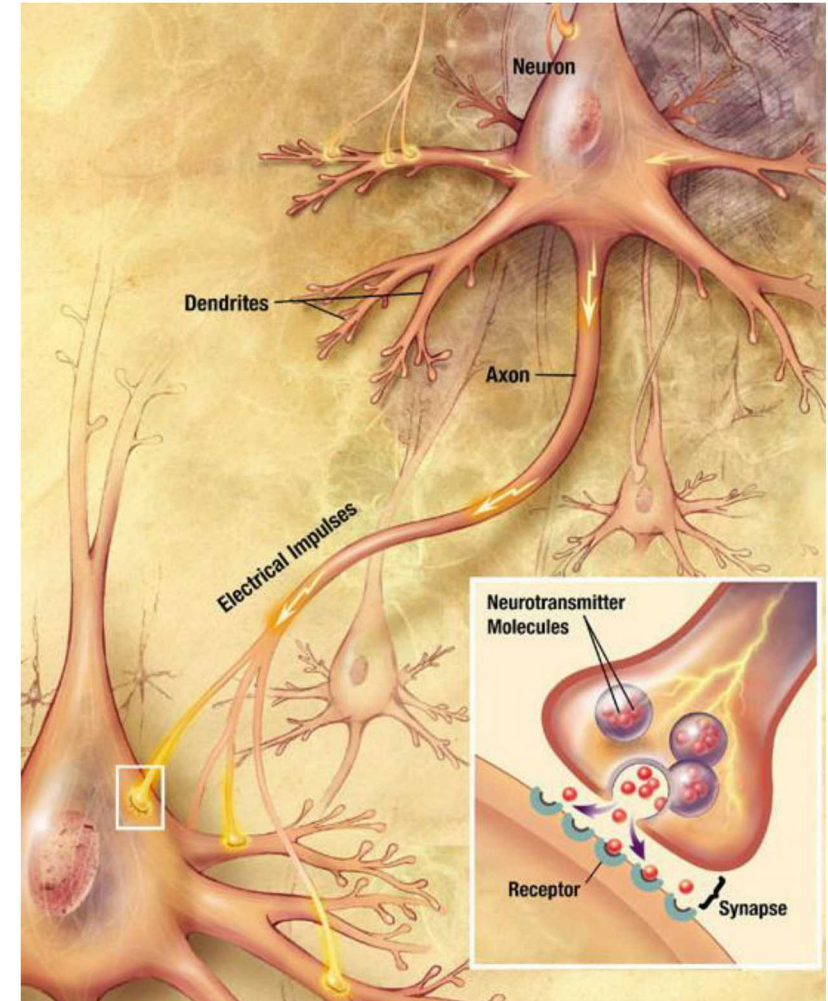


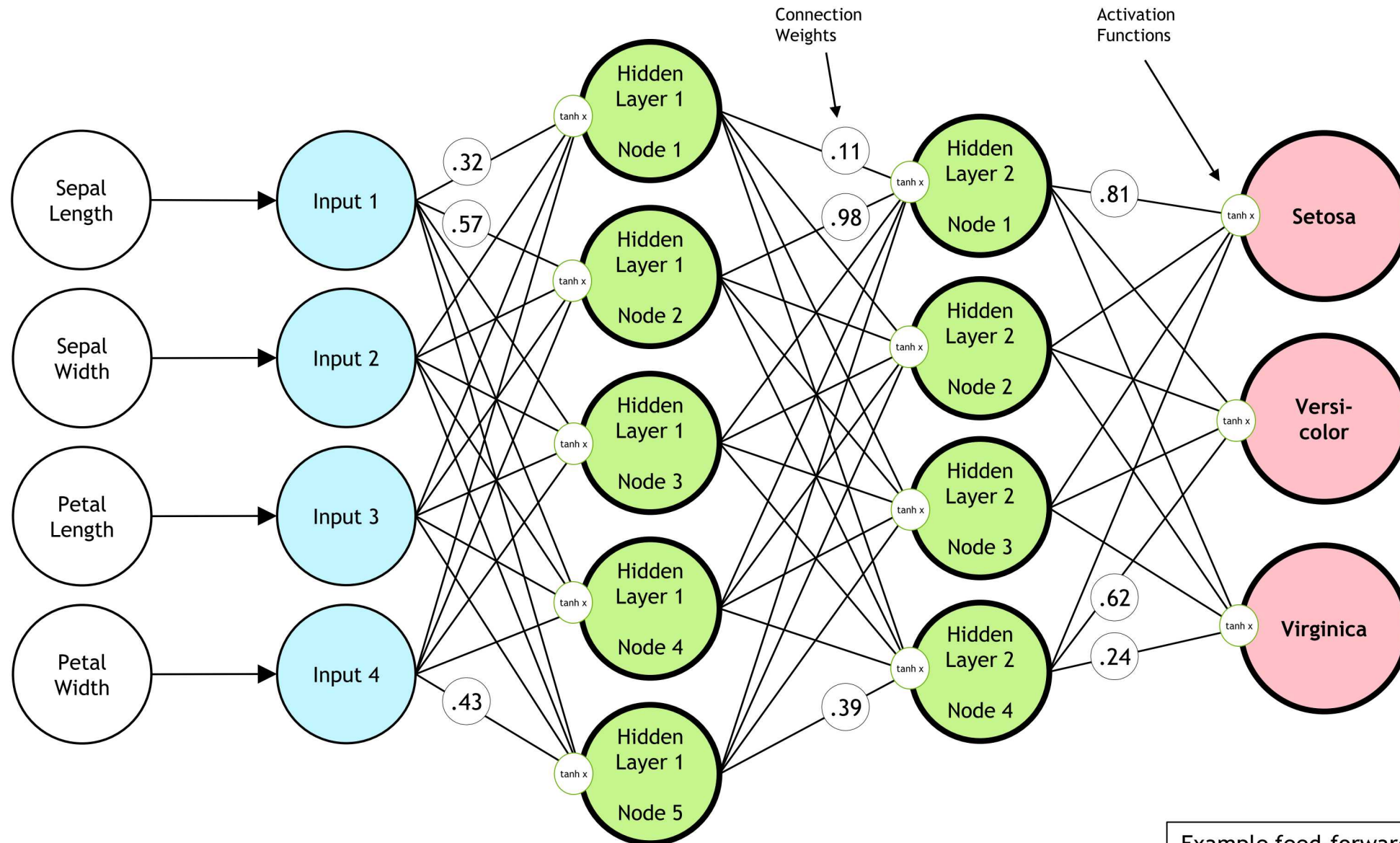
Brain has neurons that communicate with other neurons through electrical impulses.

- Approximately 100 billion in human brain

Connections strengthen with experience

Neural networks are mathematical models inspired by the connectionist model of the brain





Example feed-forward neural network



Convolutional/Deep Networks

- Convolutional networks take advantage of local dependencies
- Deep networks capitalize on the power of deeper networks to encode/represent higher level, latent features
- Deep convolutional networks revolutionized the processing of images, sounds, and video
- Applicable to other modalities

Recurrent Neural Networks

- Takes data of varying length
- Useful for temporal and sequential data (e.g., text, signal processing)

Autoencoders/Generative Adversarial Networks

- Autoencoders create compressed representations of the original data
 - Useful in anomaly detection, compression, domain feedback
- Variational autoencoders can generate new data
- Generative Adversarial Networks pit two models (usually neural networks) against each other
 - Generator creates new samples
 - Discriminator learns to tell original samples from generated samples
 - Generator and Discriminator co-evolve
 - "Battle-tested" generator produces high quality new samples

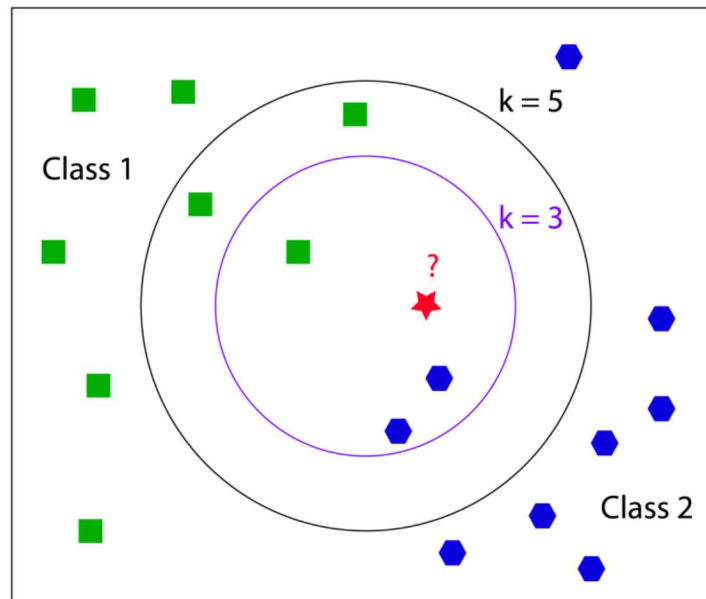
k-Nearest Neighbor



Input: k closest instances (nearest neighbors) in feature space

Output

- Regression: average values of k nearest neighbors
- Classification: majority class of k nearest neighbors



kNN: example of **instance-based learning**

- Function only approximated locally
- Computation deferred until prediction



Tasks

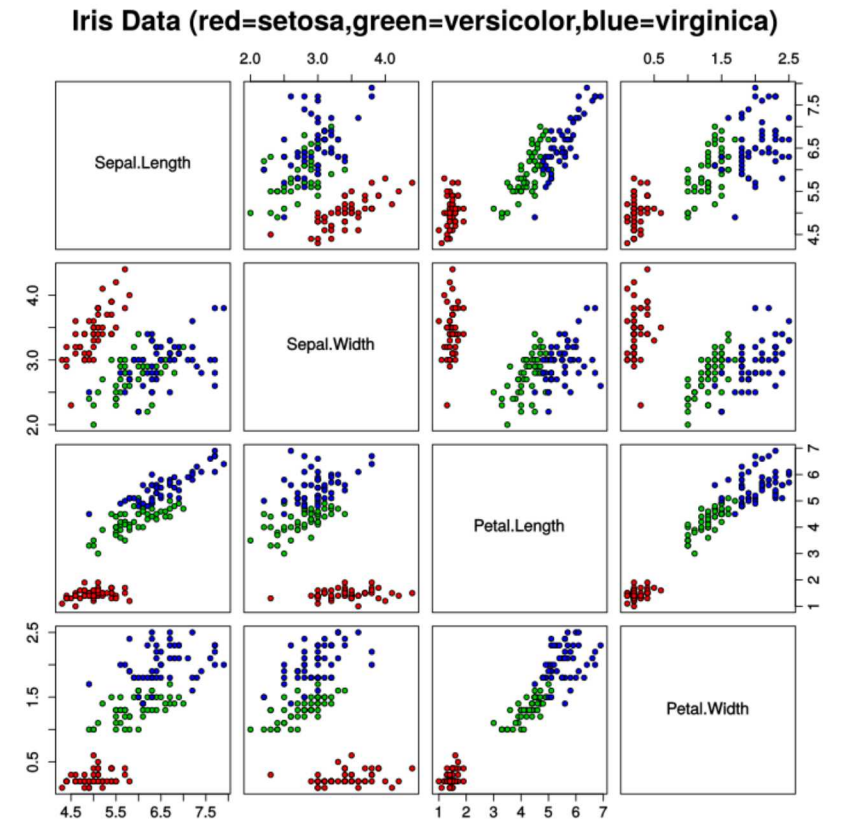
- Clustering (grouping)
- Dimensionality reduction
- Anomaly detection
- Association
- Generative modeling

Experience (data)

- Instances are unlabeled

Performance measures

- Challenging due to lack of labels/known solutions
- Validation often leverages labeled data sets (labels only used in testing)



K-means Clustering



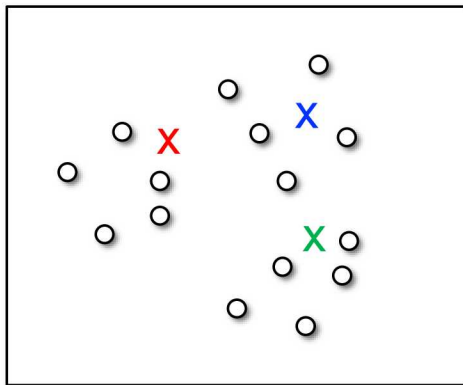
Task

- Group data instances by distance into K groups
- Data instances are points in a multidimensional feature vector space

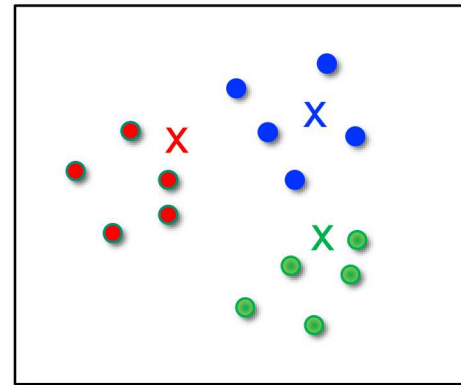
Standard Algorithm

1. Initialize cluster centroids randomly
2. Iterate until convergence
 - a) **Assign** each instance to the cluster whose centroid is “closest”
 - b) **Update** the centroids given the current cluster assignments

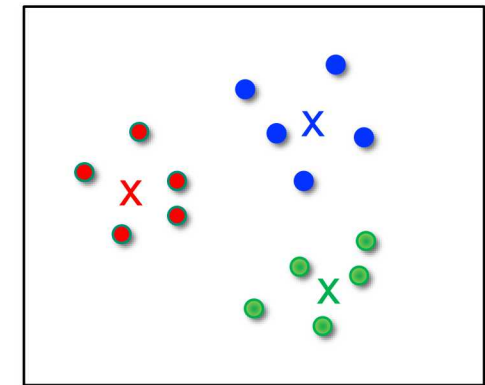
cluster centroid =
arithmetic mean of
the points in the
cluster



Centroids (x) and cluster assignments (color) at **start of iteration**



Assignment of instances to cluster with closest centroid



Update centroids based on new cluster assignments

Task

- Group data instances by distance into K groups
- Data instances are points in a multidimensional feature vector space

Challenges

- What value to use for K ?
 - Most often chosen by the user/analyst/subject matter expert
- How to initialize the centroids?
 - Random instances as centroids vs. random cluster assignments
- How to compute distances?
 - Euclidean distance often used
 - Often data- and problem-dependent
- When to stop iterating?
 - Assignment stagnation often used
 - K -means clustering is equivalent to local minimization

Other Partitional Clustering Methods



***K*-medoids**

- *K*-means like algorithm using medoids (median values of cluster points) instead of means for assignments

Fuzzy *K*-means

- Fuzzy set membership for observations

DBSCAN

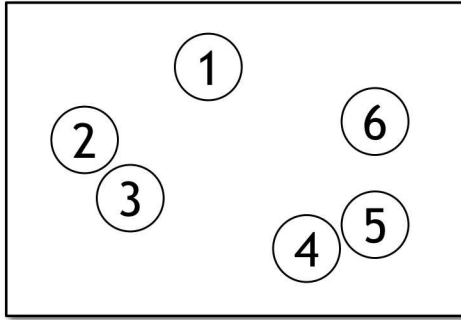
- density-based clustering with outlier detection and no predetermined number of clusters

Gaussian Mixture Models

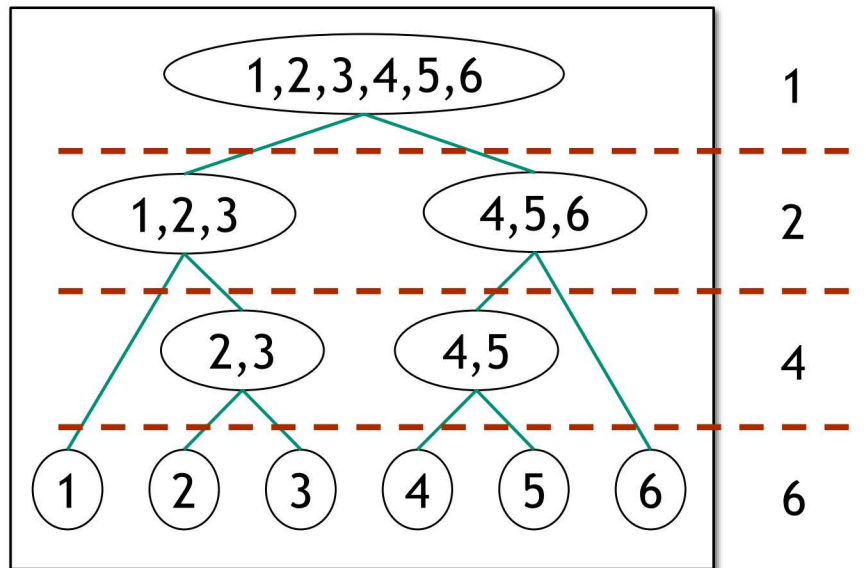
- *K*-means like algorithm with Gaussian distribution assumptions & probabilistic assignment

Spectral Clustering

- Useful for exploiting affinities (e.g., connections, similarities), in data points, regardless of Cartesian proximity



Data in 2D Feature Space



Dendrogram

Clusters

Clustering Approaches

- Agglomerative
 - Merging from bottom to top
- Divisive
 - Splitting from top to bottom

Metric

- Distance between data points

Linkage Criteria

- Distance between sets
 - Single: minimum
 - Complete: maximum
 - Average

Number of clusters

- Choose a level to cut dendrogram

Tasks

- Supervised Learning Tasks

Experience (data)

- Small amount of labeled data
- Mostly unlabeled data

Performance measures

- Supervised Learning measures

Training model

- Train a model using labeled data
- Use model to predict labels for unlabeled data
- Add (some) unlabeled data and predicted labels to labeled data
- Repeat

Co-training

- Multiple classifiers working in tandem
- Requires independence between classifiers

Tasks

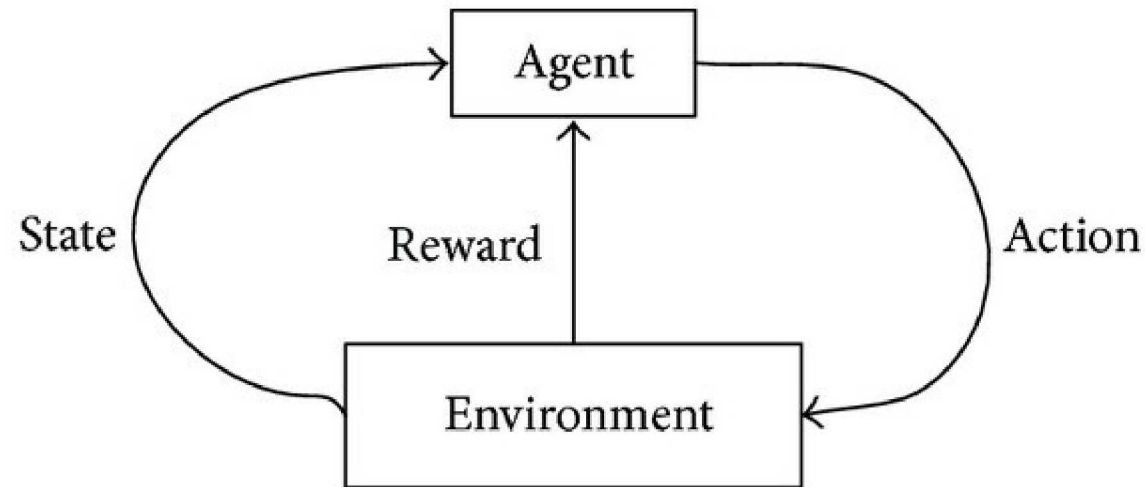
- Take the best action based on current state (i.e., information available)

Experience (data)

- Interactions with the environment/system
- State of environment/system

Performance measures

- Maximize reward
- Minimize risk



Information Representation is Key to Machine Learning Success



Aforementioned examples assume that the data is already in the correct form to solve the problem

Knowledge Elicitation

- Gaining knowledge from Subject Matter Experts

Feature engineering / Data wrangling

- Getting the data in a form useful for answering the pertinent questions
- Often an iterative process

Feature selection

- Some features may be irrelevant
- Many algorithms are robust to this, but irrelevant features can degrade performance or cause machine learning methods to take longer than desired

Data properties

- Are the relevant features included?
- Is there enough of the data?
- Is the data drawn from the correct distribution?



Tools

- **Scikit-learn**
 - <https://scikit-learn.org/>
- **PyTorch**
 - <https://pytorch.org>
- **Tensorflow**
 - <https://www.tensorflow.org>

Data

- **UCI Machine Learning Repository:**
 - <https://archive.ics.uci.edu/ml/index.php>
- **Kaggle:**
 - <https://www.kaggle.com/datasets>



Optimization with Application to Machine Learning and Power Systems

Jean-Paul Watson (jwatson@sandia.gov)

September 9, 2019

What Do We Mean By “Optimization”?



Linear programming (LP)

$$\begin{aligned} \arg \min_x \quad & c^T x \\ \text{s.t.} \quad & Ax \leq b \\ & x \in Q^n \end{aligned}$$

“Standard” form:

$$\begin{aligned} \arg \min_x \quad & c^T x \\ \text{s.t.} \quad & Ax = b \\ & x \geq 0 \\ & x \in Q^n \end{aligned}$$

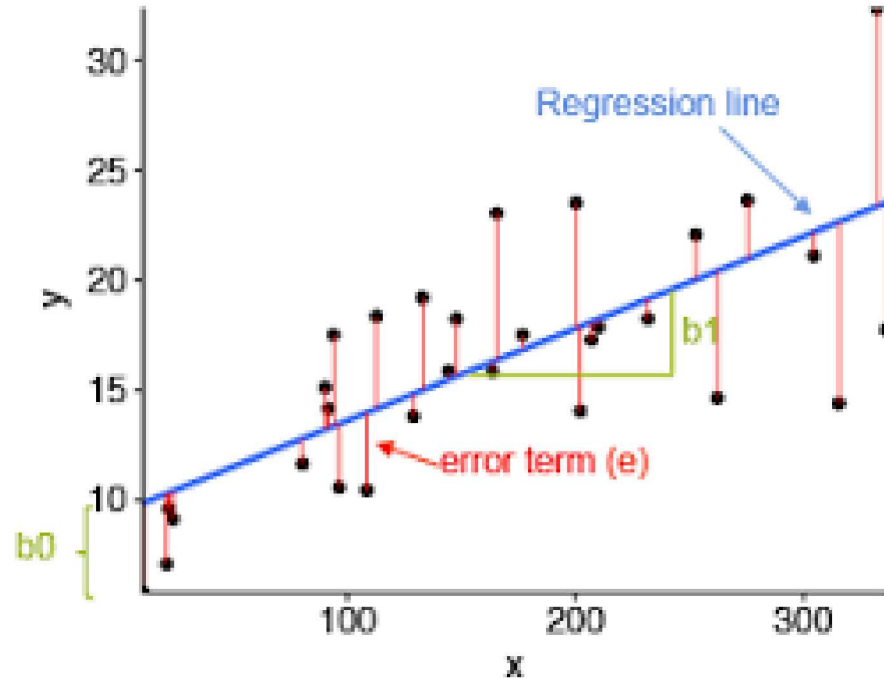
Classic example: Linear Assignment Problem (LAP)

$$\begin{aligned} \arg \min_x \quad & \sum_{j \in N} \sum_{i \in N} c_{ij} x_{ij} \\ \text{s.t.} \quad & \sum_{i \in N} x_{ij} = 1 \quad \forall j \in N \\ & \sum_{j \in N} x_{ij} = 1 \quad \forall i \in N \\ & x_{ij} \geq 0 \quad \forall i \in N, j \in N \end{aligned}$$

We generally assume that an algebraic description of the underlying problem is available

Popular extensions:

- Mixed-integer programming
- Non-linear programming
- Stochastic programming
- Robust optimization

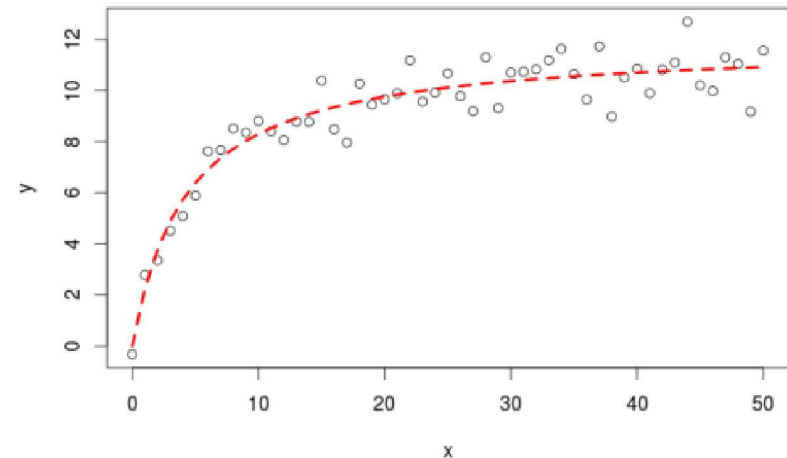
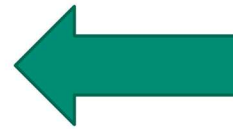


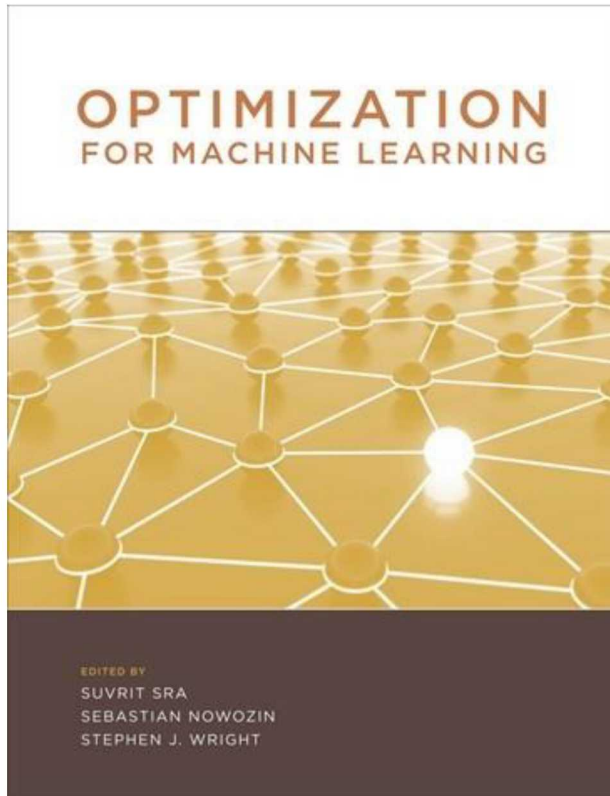
Linear regression is an optimization problem

$$\text{Find } \min_{\alpha, \beta} Q(\alpha, \beta), \quad \text{for } Q(\alpha, \beta) = \sum_{i=1}^n \hat{\varepsilon}_i^2 = \sum_{i=1}^n (y_i - \alpha - \beta x_i)^2$$

↑
Slope-intercept
parameters of a line

Non-linear regression is still an optimization problem - you just shift from linear programming to non-linear programming models and methods



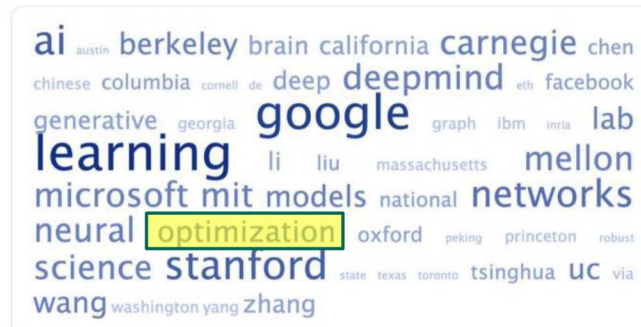


MIT Press



“The interplay between optimization and machine learning is one of the most important developments in modern computational science. Optimization formulations and methods are proving to be vital in designing algorithms to extract essential knowledge from huge volumes of data.”

A word doodle of accepted papers at @NeurIPSConf -- Learning is more than deep.



ICML | 2019

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Wed Jun 12th 04:00 -- 04:20 PM @ Room 103	Accelerated Linear Convergence of Stochastic Momentum Methods in Wasserstein Distances			Oral
Bugra Can · Mert Gurbuzbalaban · Lingjiong Zhu				In Convex Optimization
Video ▾				
Wed Jun 12th 04:20 -- 04:25 PM @ Room 103	SGD without Replacement: Sharper Rates for General Smooth Convex Functions			Oral
Dheeraj Nagaraj · Prateek Jain · Praneeth Netrapalli				In Convex Optimization
Slides ▾ Video ▾				
Wed Jun 12th 04:25 -- 04:30 PM @ Room 103	On the Complexity of Approximating Wasserstein Barycenters			Oral
Alexey Kroshchinskii · Nazari Tupitsa · Darina Dvinskikh · Pavel Dvurechenski · Alexander Gasnikov · Cesar Uribe				In Convex Optimization
Slides ▾ Video ▾				
Wed Jun 12th 04:30 -- 04:35 PM @ Room 103	Estimate Sequences for Variance-Reduced Stochastic Composite Optimization			Oral
Andrei Kulunchakov · Julien Mairal				In Convex Optimization
Slides ▾ Video ▾				
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Jeff HaoChen · Suvrit Sra				In Convex Optimization
Slides ▾ Video ▾				
Wed Jun 12th 05:00 -- 05:05 PM @ Room 103	First-Order Algorithms Converge Faster than $O(1/k)$ on Convex Problems			Oral
Ching-pai Lee · Stephen Wright				In Convex Optimization
Slides ▾ Video ▾				



Many talk sessions at major machine learning conferences would be at home at optimization conferences



Journal of Machine Learning Research 7 (2006) 1265–1281

Submitted 7/06; Published 7/06



This is even before the deep learning revolution...

The Interplay of Optimization and Machine Learning Research

Kristin P. Bennett

*Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, NY 12018, USA*

BENNEK@RPI.EDU

Emilio Parrado-Hernández

*Department of Signal Processing and Communications
University Carlos III de Madrid
Leganés (Madrid), 28911, Spain*

EMIPAR@TSC.UC3M.ES

Editors: Kristin P. Bennett and Emilio Parrado-Hernández

Abstract

The fields of machine learning and mathematical programming are increasingly intertwined. Optimization problems lie at the heart of most machine learning approaches. The Special Topic on

Machine Learning and Large Scale Optimization examines this interplay. Machine learning researchers have embraced the advances in mathematical programming allowing new types of models to be pursued. The special topic includes models using quadratic, linear, second-order cone, semi-definite, and semi-infinite programs. We observe that the qualities of good optimization algorithms from the machine learning and optimization perspectives can be quite different. Mathematical programming puts a premium on accuracy, speed, and robustness. Since generalization is the bottom line in machine learning and training is normally done off-line, accuracy and small speed improvements are of little concern in machine learning. Machine learning prefers simpler algorithms that work in reasonable computational time for specific classes of problems. Reducing machine learning problems to well-explored mathematical programming classes with robust general purpose optimization codes allows machine learning researchers to rapidly develop new techniques. In turn, machine learning presents new challenges to mathematical programming. The special issue include papers from two primary themes: novel machine learning models and novel optimization approaches for existing models. Many papers blend both themes, making small changes in the underlying core mathematical program that enable the develop of effective new algorithms.

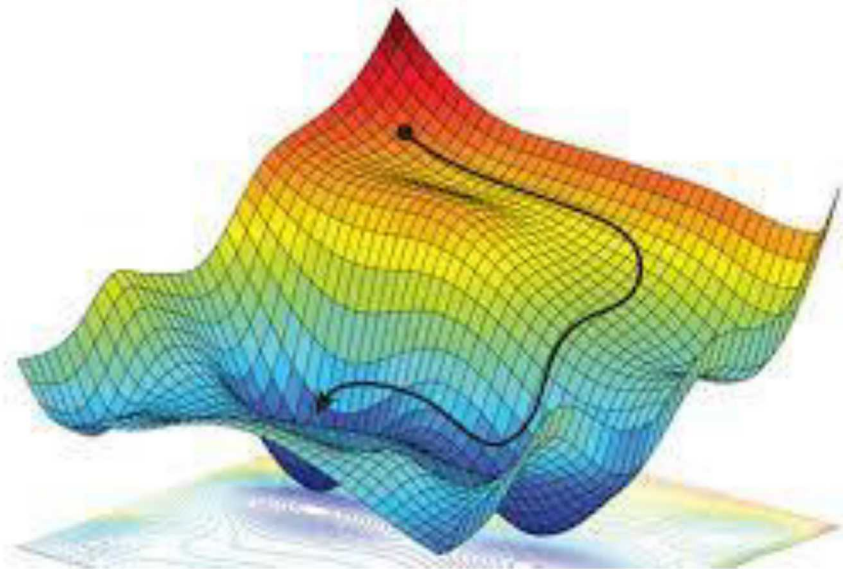


”Optimization problems lie at the heart of most machine learning problems”

Machine Learning and Optimization (4)



Stochastic gradient descent (SGD) - a now standard optimization method - is at the center of the deep learning revolution



Training of deep (autoencoder) neural networks is a non-linear optimization problem to minimize reconstruction errors

There is still much more that optimization can do for machine learning, e.g.,

- Rigorous proofs of global optimality
- Basis for adversarial machine learning
- From neural net training to architecture design

But: SGD is a *local* method for solving a non-linear optimization model

- A heuristic - not a rigorous, complete solution method
- Absolutely no guarantee of optimality
- Nor any indication of how far you are from a global optimum

Most of Power Systems Operations and Planning is Optimization...



Decision making in power systems looks at processes ranging from very large time constants to near real-time:

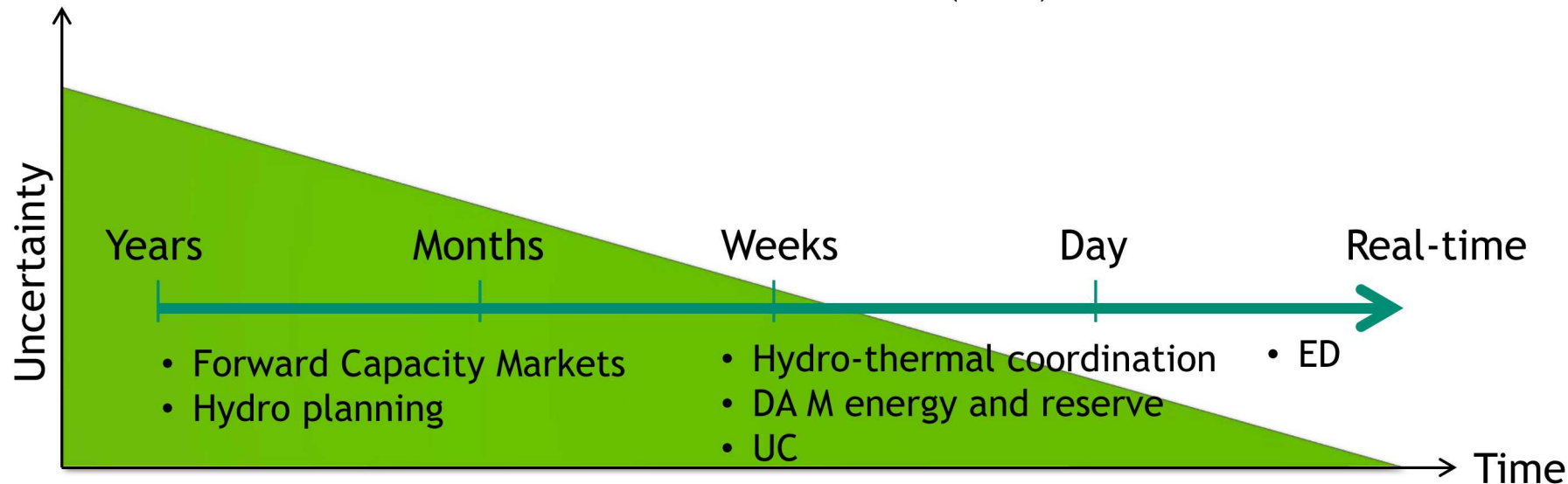
Years, Seasons, Months, Weeks: Resource adequacy, transmission and hydro resource planning

Days: Hydro-thermal coordination, day-ahead UC of energy and reserves, intra-day UC

Hours: intra-day look-ahead processes, dynamic economic dispatch

Minutes: Economic Dispatch (ED)

Seconds: Automatic Generation Control (AGC)



Every problem at the five minute and larger time scales is formulated and solved as an optimization problem

ML for Power Systems Optimization: Warm Starting



The time required to solve operations problems such as commitment and dispatch can be significantly lowered by up to 80% via “warm starting” - use historical data to fit a ML model that predicts what are likely to be high-quality solutions for a given



Learning to Solve Large-Scale Security-Constrained Unit Commitment Problems

Álison S. Xavier¹, Feng Qiu¹, and Shabbir Ahmed²

¹ Energy Systems Division, Argonne National Laboratory, Argonne, IL, USA. {axavier,fqiu}@anl.gov

² School of Industrial and Systems Engineering, Georgia Institute of Technology, Atlanta, GA, USA.
sahmed@isye.gatech.edu

Abstract. Security-Constrained Unit Commitment (SCUC) is a fundamental problem in power systems and electricity markets. In practical settings, SCUC is repeatedly solved via Mixed-Integer Linear Programming, sometimes multiple times per day, with only minor changes in input data. In this work, we propose a number of machine learning (ML) techniques to effectively extract information from previously solved instances in order to significantly improve the computational performance of MIP solvers when solving similar instances in the future. Based on statistical data, we predict redundant constraints in the formulation, good initial feasible solutions and affine subspaces where the optimal solution is likely to lie, leading to significant reduction in problem size. Computational results on a diverse set of realistic and large-scale instances show that, using the proposed techniques, SCUC can



A Distributed Framework for Solving and Benchmarking Security Constrained Unit Commitment with Warm Start

Publisher: IEEE

4 Author(s) Yonghong Chen ; Fengyu Wang ; Yaming Ma ; Yiyun Yao [View All Authors](#)

26
Full
Text Views



Abstract

Authors

Keywords

Metrics

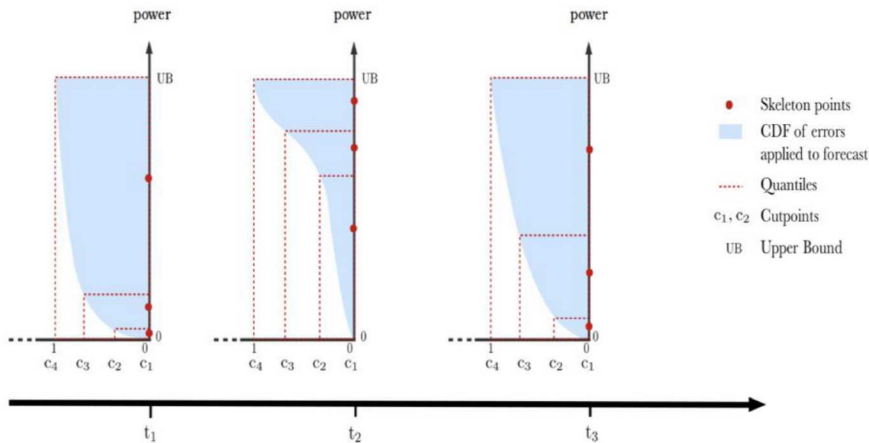
Abstract:

This paper discusses several methods to improve commercial optimization solver performance on day ahead security constrained unit commitment through warm start and lazy constraint settings. Data analytics is performed to greatly improve the quality of the initial commitment solution and lazy constraint setting. A distributed optimization framework is proposed to take advantage of the diversity from prevalent solvers (GUROBI and CPLEX) and different warm start strategies. A systematic distribution profile based benchmarking method is also proposed.

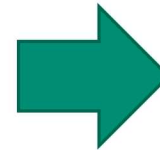
Published in: [IEEE Transactions on Power Systems](#) (Early Access)

Related techniques hold even more promise in the context of stochastic power systems operations problems, which are significantly more difficult in practice

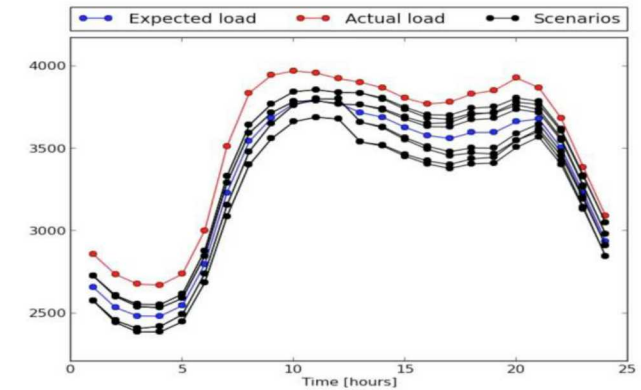
Historical forecasts and corresponding actuals are fed into ML algorithms to characterize error distributions...



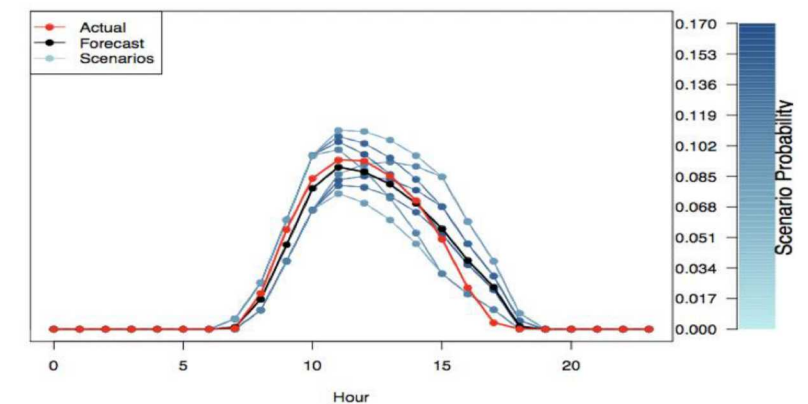
.. which are then used to construct probabilistic scenarios for operations



Day-Ahead Scenarios for Bulk Load



Day-Ahead Scenarios for Bulk Solar



Probabilistic scenarios form the basis for stochastic power systems operations and planning problems - and they are provided by ML



(Examples of) Machine Learning for the North American Energy Resilience Model (NAERM)

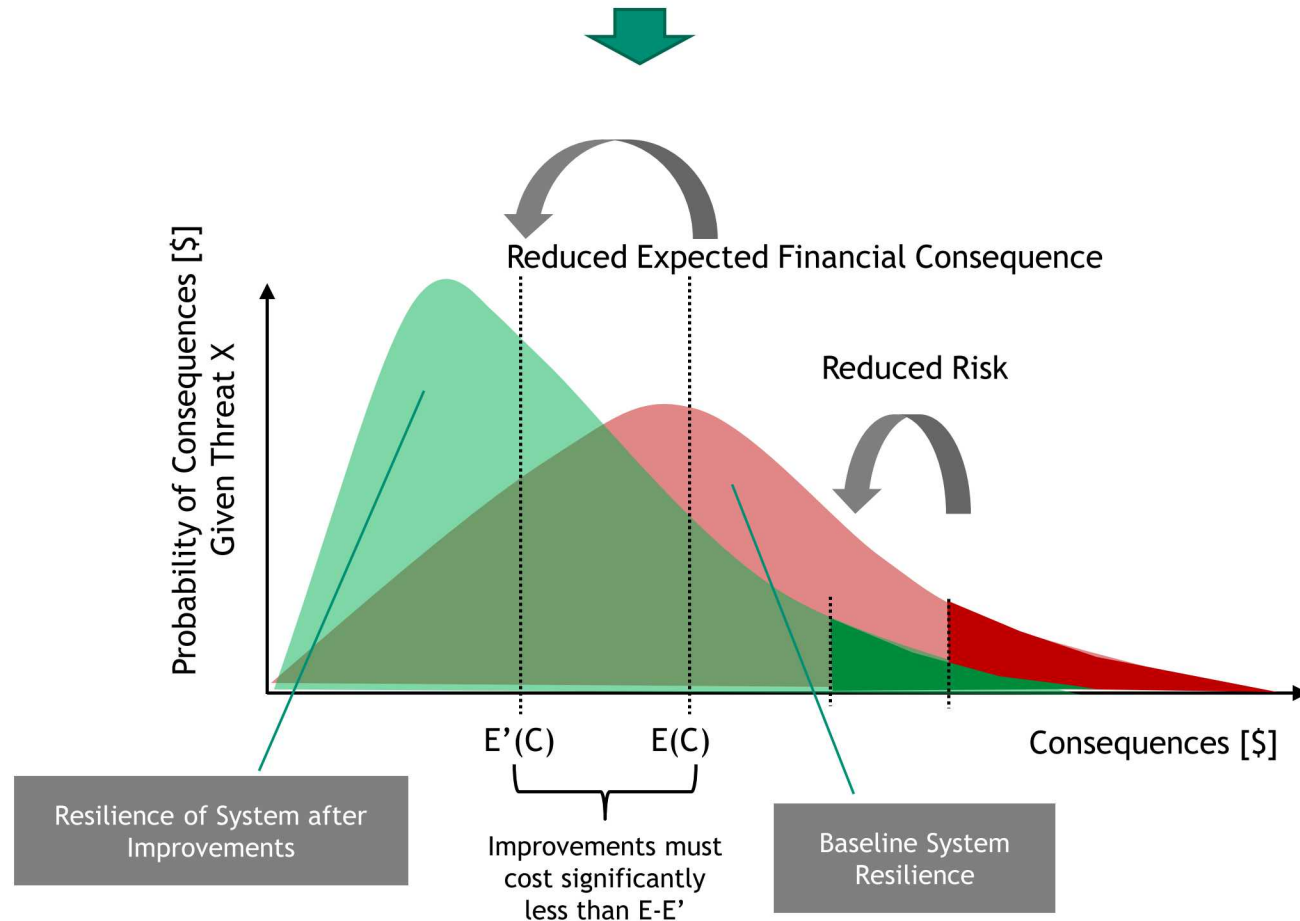
Jean-Paul Watson (jwatson@sandia.gov)

September 9, 2019

Resilience Quantification: Stochastic Models are Critical



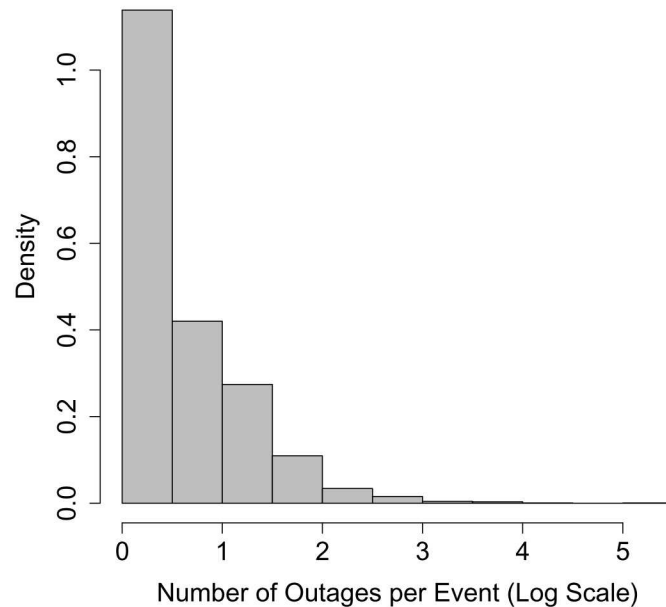
ML is central to developing probabilistic models of threats - which are critical inputs to resilience analysis



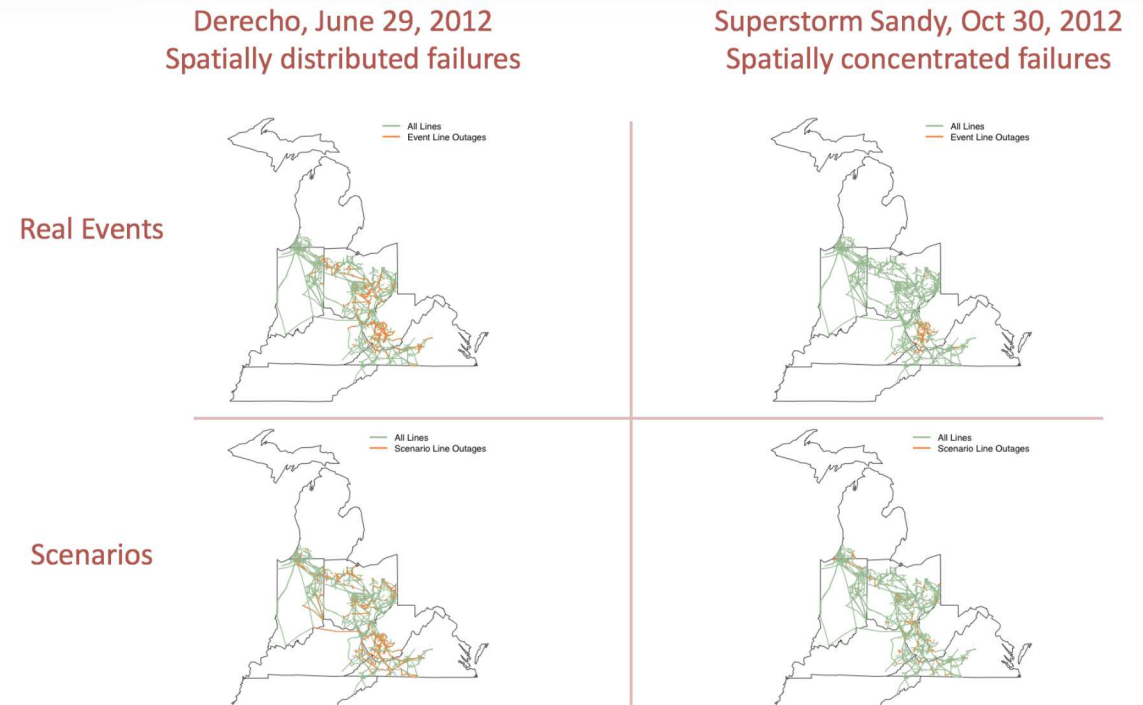
Resilience Analysis: Probabilistic Outage Scenarios



Historical transmission outage data associated with extreme weather events



Probabilistic ML models calibrated using historical outage data



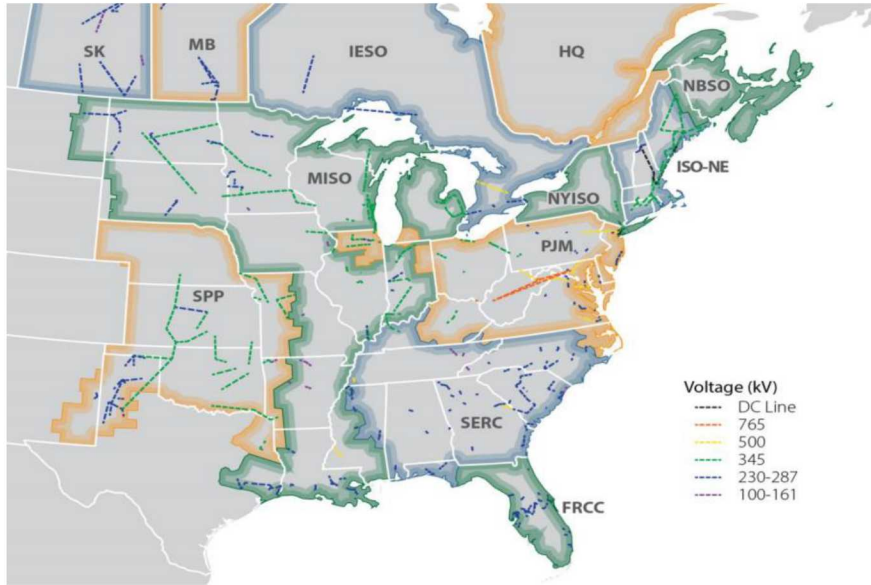
Probabilistic outage scenarios are a pre-requisite for proactive resilience operations and investment strategies..

... and are equally applicable in planning and real-time contexts

ML for Accelerating National-Scale Grid Computation



Future EI Case (ERGIS, from NREL)



Significant technology development efforts required to execute ERGIS cases in tractable run times



Time Domain Partitioning of Electricity Production Cost Simulations

Clayton Barrows, Marissa Hummon, Wesley Jones, and Elaine Hale

~11K generators in entire system

- Includes two very large ISOs
 - Difficult to solve in isolation, let alone in a coordinated manner
- Major challenges for solving core operations simulations such as commitment and dispatch

ML methods for accelerating commitment and dispatch optimization model solves can potentially yield order-of-magnitude reductions in run times

Significant emerging efforts in the realm of ML for
proactive power grid operations via deep ML

From Grid Eye to Grid Mind

-A Data-driven Autonomous Grid Dispatch Robot Based on PMU Measurements

Di Shi, Ruisheng Diao, Jiajun Duan, Bei Zhang, Zhe Yu, Zhiwei Wang, Xiao Lu*,

Haifeng Li*, Chunlei Xu*, Yan Zan, Jiajun Duan

GEIRI North America (GEIRINA)

*State Grid Jiangsu Electric Power C

April 15-17, 2019

@NASPI April Work G

L2RPN Challenge

- Learning to Run a Power Network throu

Di Shi

Team: Tu Lan, Jiajun Duan, Bei Zhang, Zhiwei Wang, Xiao Lu,

Zhang, Ruisheng Diao, Yan Zan

AI & System Analytics

GEIRI North America (GEIRINA)

@PSERC Summer Workshop

July 16, 2019



GEIRI North America

Global Energy Interconnection Research Institute North America (GEIRI North America or GEIRINA), previously named as SGRI North America Inc., is a subsidiary of GEIRI Beijing which is an institute focusing on the research and development of cutting-edge technologies for a smarter electric power grid. GEIRI Beijing is affiliated to State Grid Corporation of China (SGCC) which is the largest electric utility company in the world and was ranked 2nd on 2016 Fortune Global 500.

[Learn More](#)

Research Areas

Graph Computing & Grid Modernization

AI & System Analytics

Advanced Computing & Data Intelligence

Smart Chips

Key question is whether such methods can be extended from reliability to resilience contexts, and beyond minute-scale look-ahead



Integrating Artificial Intelligence/Machine Learning into Power Systems Applications

Matthew Reno (mjreno@sandia.gov)

Logan Blakely (lblakel@sandia.gov)

September 9, 2019

- Power Systems is a perfect application for Artificial Intelligence due to the complex systems and large amounts of data. This is made possible recently due to:
 - Advances in computing power for real-time learning and decision making
 - Additions of new sensing equipment such as smart meters and PMU
 - New Artificial Intelligence algorithms to handle large datasets, transferable learning, and physics-based algorithms
- These slides will go through several different examples of AI challenges, AI successes in Power Systems, and future research directions, with references throughout.

The key topics are:

1. Integrating Physics-Based Constraints into AI
2. Access to Training Data for AI
3. AI for Controls and Protection Applications

Each topic includes:

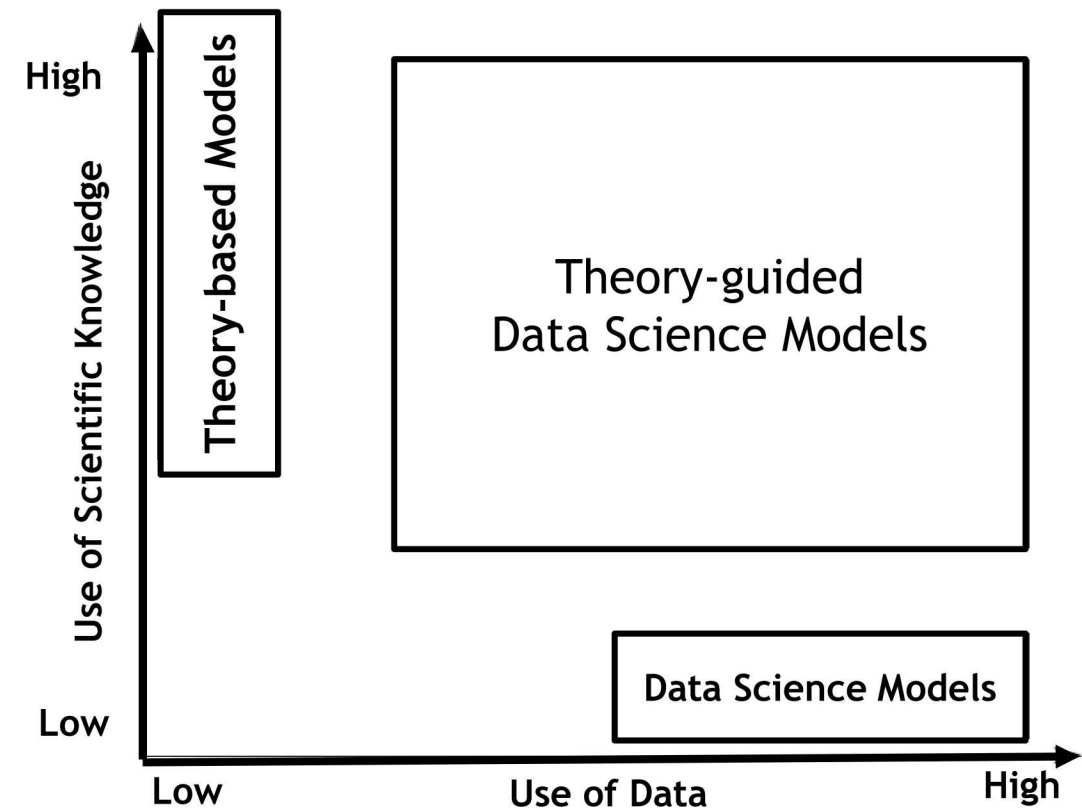
1. Overview – AI challenges, problem statement, and current areas where AI has been successful
2. Example Project – Specific example using AI to solve this challenge
3. Future - Ongoing challenges, current research, and continuing problems phrased as questions
4. References

Physics-Based Constraints in AI



Many AI/ML methods do not incorporate known physical constraints and equations.

- Given that we know many of the relationships in power systems (Ohms law, power flow equations, etc.), it is advantageous to use the known physics equations.
- Challenges Integrating Physics-Based Constraints into AI
 - Much recent work in AI uses raw data input (image pixels, etc.) and ignores physics-based constraints
 - AI/ML so far has not been designed to incorporate this type of known information
 - Areas such as power systems have large quantities of physics-based constraints and AI should be able to use that knowledge without starting from scratch
- Successful Integrations of Physics-Based Constraints into AI
 - AI for calibrating distribution system models (phase identification, topology parameter estimation, etc.)



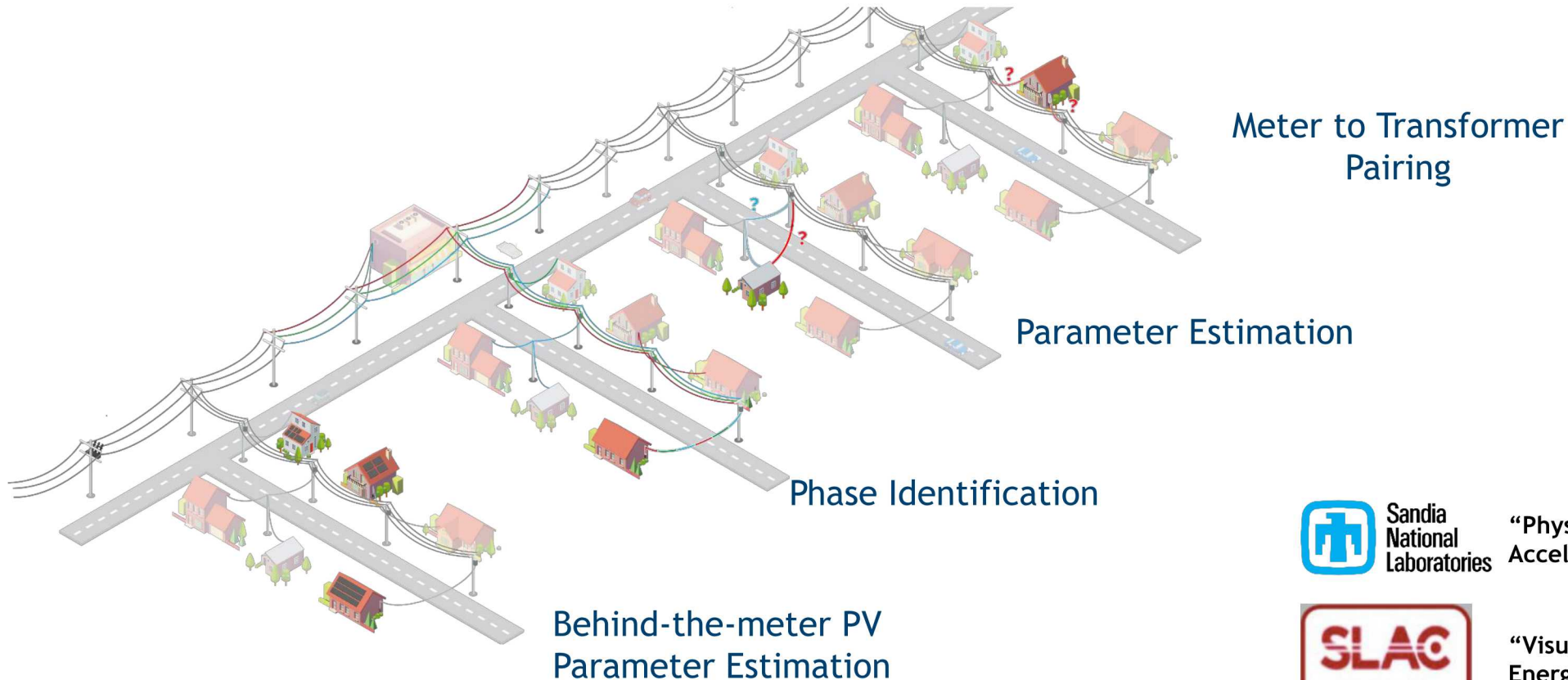
A. Karpatne *et al.*, "Theory-guided Data Science: A New Paradigm for Scientific Discovery from Data," *IEEE Trans. Knowl. Data Eng.*, vol. 29, no. 10, pp. 2318–2331, 2017.

Physics-Based Constraints in AI – Example



Use measured data to estimate distribution system parameter and state

Ingest data from AMI, SCADA, μ PMU, etc. and use data analytics and machine learning methods to estimate system parameters (phase, meter-transformer pairing, line lengths, etc.) and do state estimation



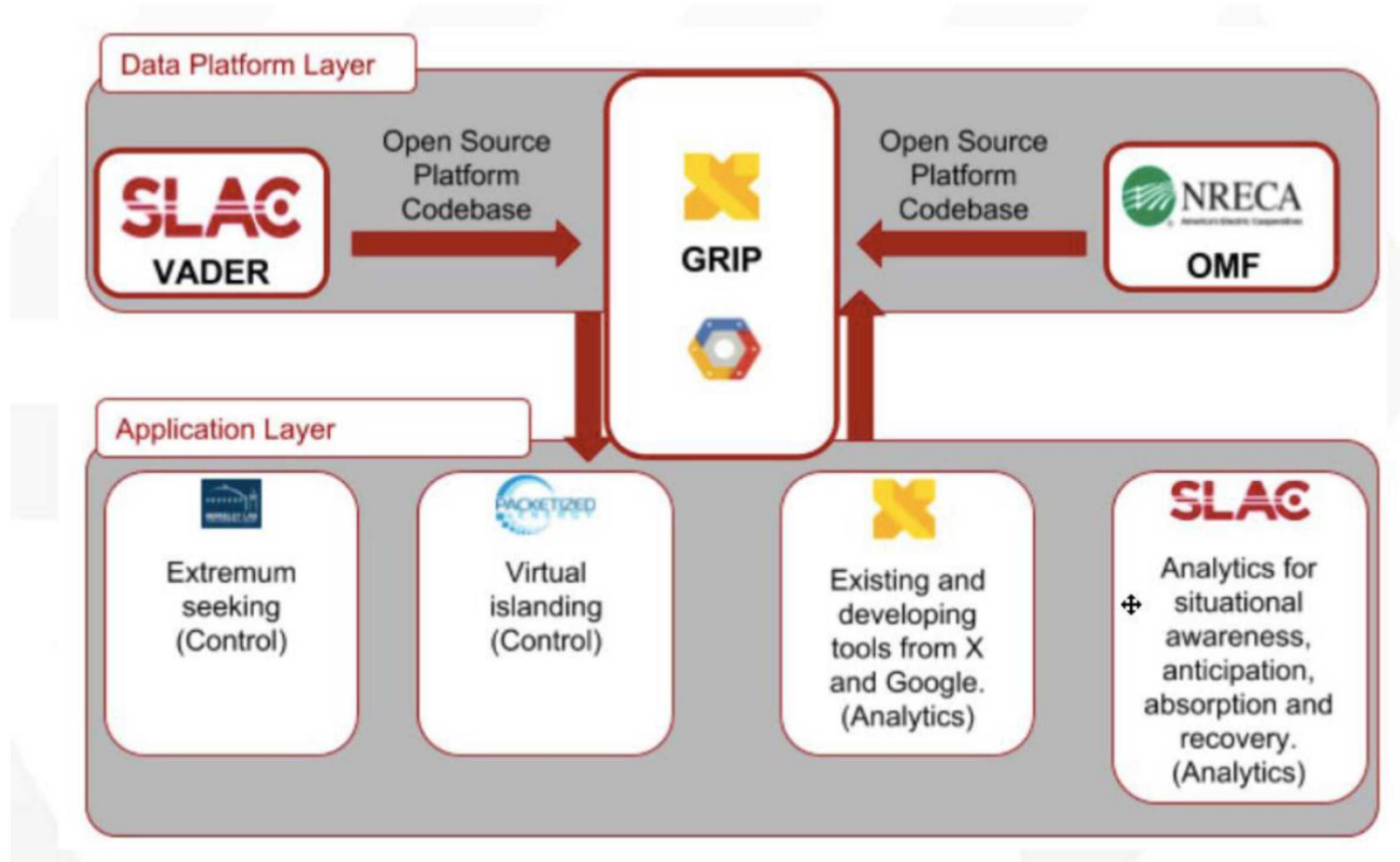
Sandia
National
Laboratories

“Physics-Based Data-Driven Grid Modeling to Accelerate Accurate PV Integration”



“Visualization and Analytics of Distributed Energy Resources (VADER)”

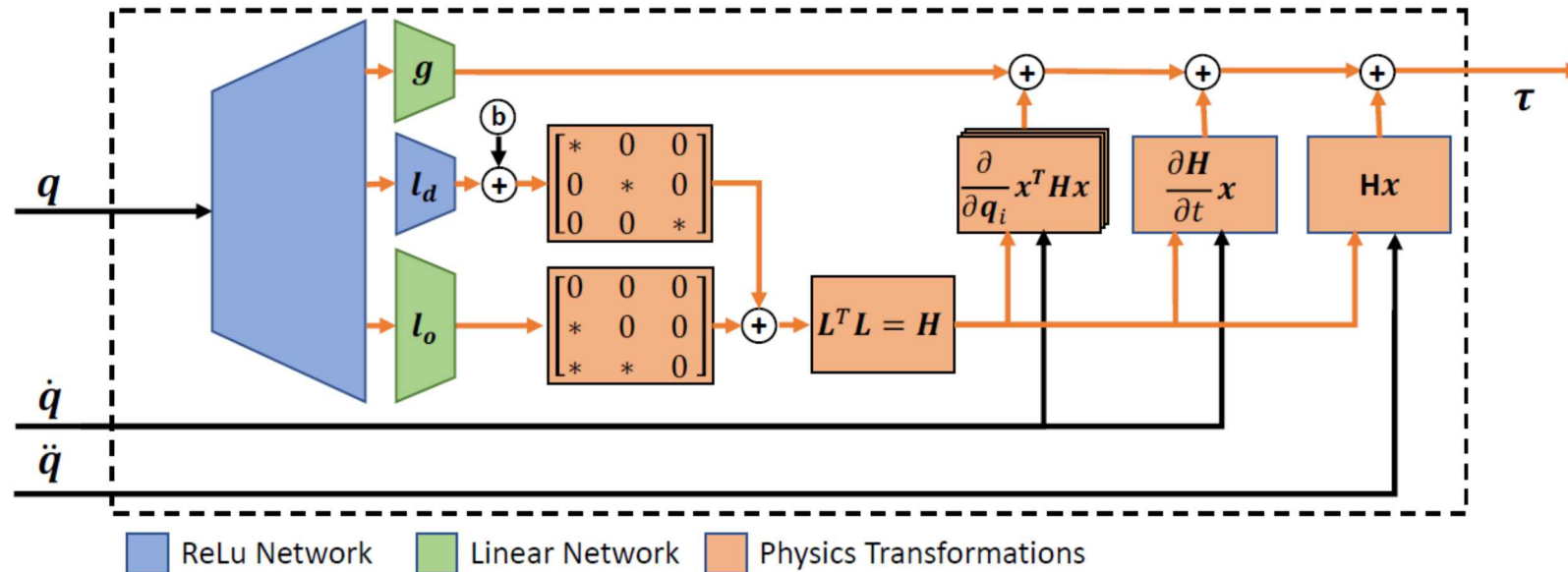
Grid Resilience and Intelligence Platform (GRIP) aggregates data, anticipates disruptions, validates control options, and reduces recovery time from extreme events



Ongoing Challenges and Current Research Areas

- How do we effectively leverage recent developments in AI while still incorporating physics-based system knowledge?
 - Integration of physics-based constraints in training algorithms (like backpropagation) to train faster by limiting relationships between weights.
- What physics-based constraints can be effectively added to AI? Physics-based equations versus (possibly) incorrect topology information?
- Can physics-based constraints help with error bounding and uncertainty quantification?

Successful integration of physical motion constraints into deep learning for robotic arm control





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3. K. Ashok, M. J. Reno, D. Divan, and L. Blakely, “Systematic Study of Data Requirements and AMI Capabilities for Smart Meter Connectivity Analytics,” *Smart Energy Grid Eng. SEGE*, 2019
4. B. Foggo and N. Yu, “A Comprehensive Evaluation of Supervised Machine Learning for the Phase Identification Problem,” *World Acad. Sci. Eng. Technol. Int. J. Comput. Syst. Eng.*, vol. 12, no. 6, 2018.
5. A. Karpatne *et al.*, “Theory-guided Data Science: A New Paradigm for Scientific Discovery from Data,” *IEEE Trans. Knowl. Data Eng.*, vol. 29, no. 10, pp. 2318–2331, 2017.
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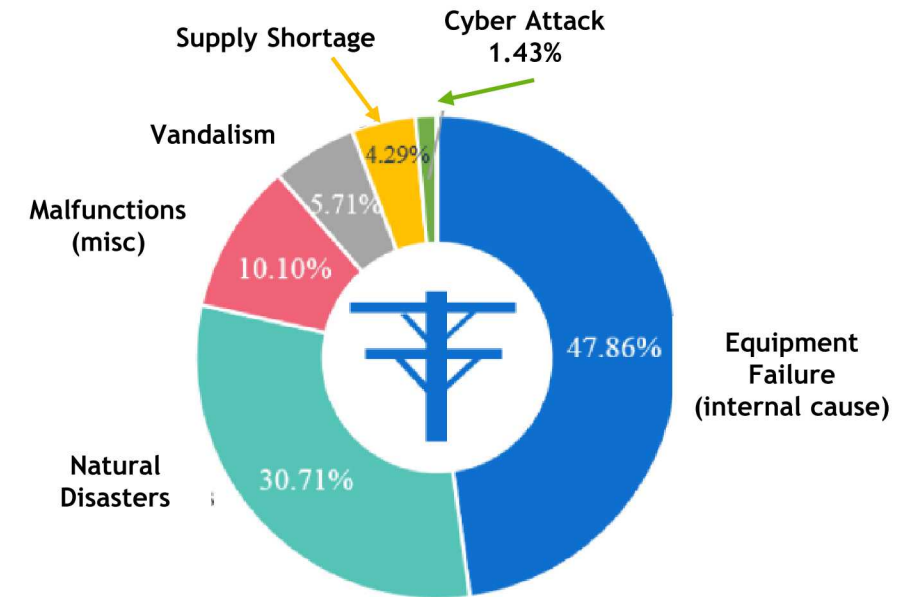
Access to Training Data for AI



Much of the recent success of AI is driven by access to large quantities of high-quality data. This is often difficult to obtain for real-world applications

- **Challenges with Training Data Availability and Quality for AI**
 - Many real-world applications have either unlabeled data, incompletely labeled data, or few to no examples of critical event types
 - How do you get labeled data for the AI to use? Manual entry?
 - Some events (rare resiliency events, cyber attacks, etc.) have never occurred
 - How does bad data or mislabeled data impact the training and learning algorithms?
- **Successful Applications of AI with Limited Access to Training Data**
 - Semi-supervised learning or transfer learning that uses some previous data and training to apply to a new application
 - Detection of incipient failures of devices like transformers
 - Power system protection, including fault classification and location

Causes of Outages Worldwide

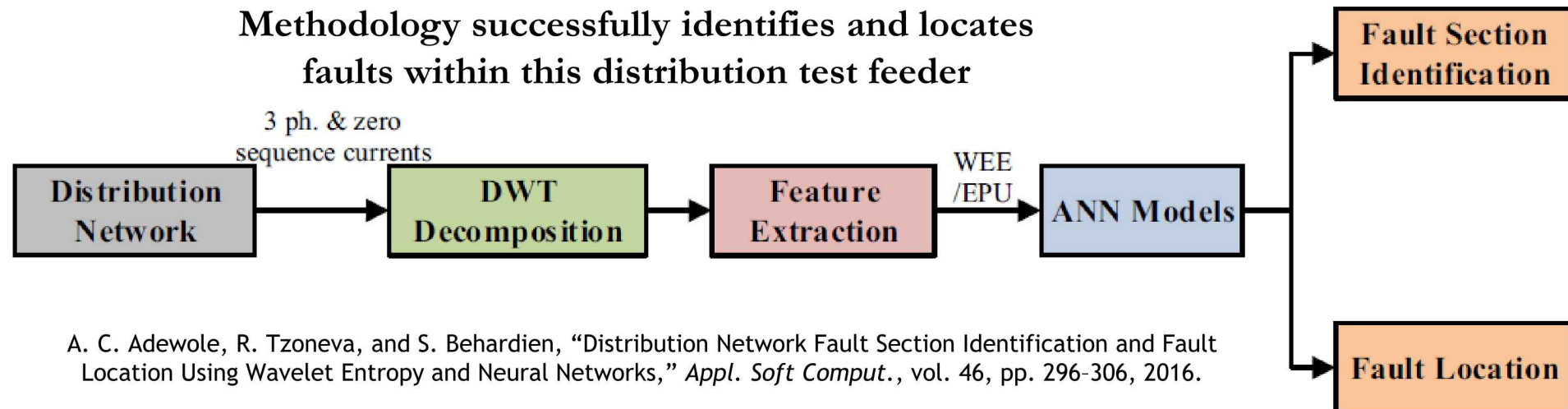


Neural Networks for Fault Identification and Fault Location

- Simulated using the IEEE 34-node feeder
- Separate networks for Fault Section Identification and Fault Location
- How do we obtain training data to make this application viable?

Training and Testing Dataset

No.	Fault type	Size of training dataset	Size of test dataset
1	Single phase-to-ground	500	100
2	Two phase	400	100
3	Two phase-to-ground	400	100
4	Three phase	150	30

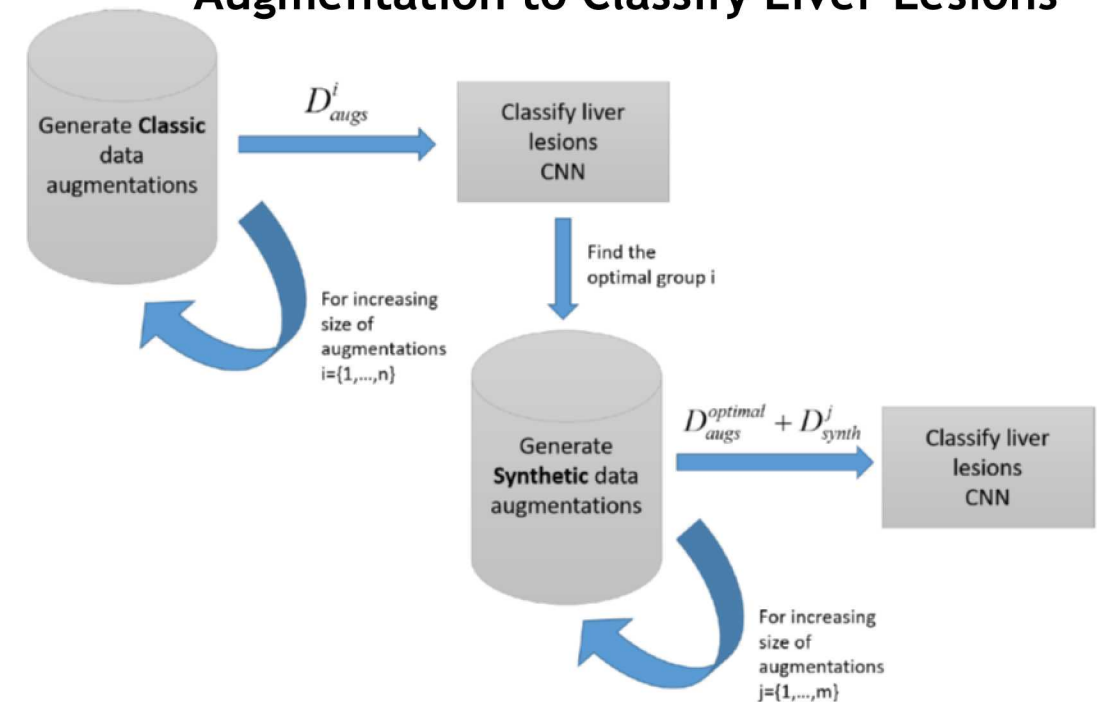


Ongoing Challenges and Current Research Areas

- How do we obtain the necessary data to train AI on these types of tasks?
- Is it possible to achieve excellent results by altering the algorithm design to use the available data?
- Can realistic data be generated for these tasks?
- Is AI/ML the correct tool to apply to this area?

Generated images enhance the accuracy of the original classifier and human experts concur the generated images are excellent examples

Generative Adversarial Networks (GAN) for Data Augmentation to Classify Liver Lesions





1. L. Wu *et al.*, “Evaluating Machine Learning for Improving Power Grid Reliability,” *ICML Workshop Mach. Learn. Global Chall.*, 2011.
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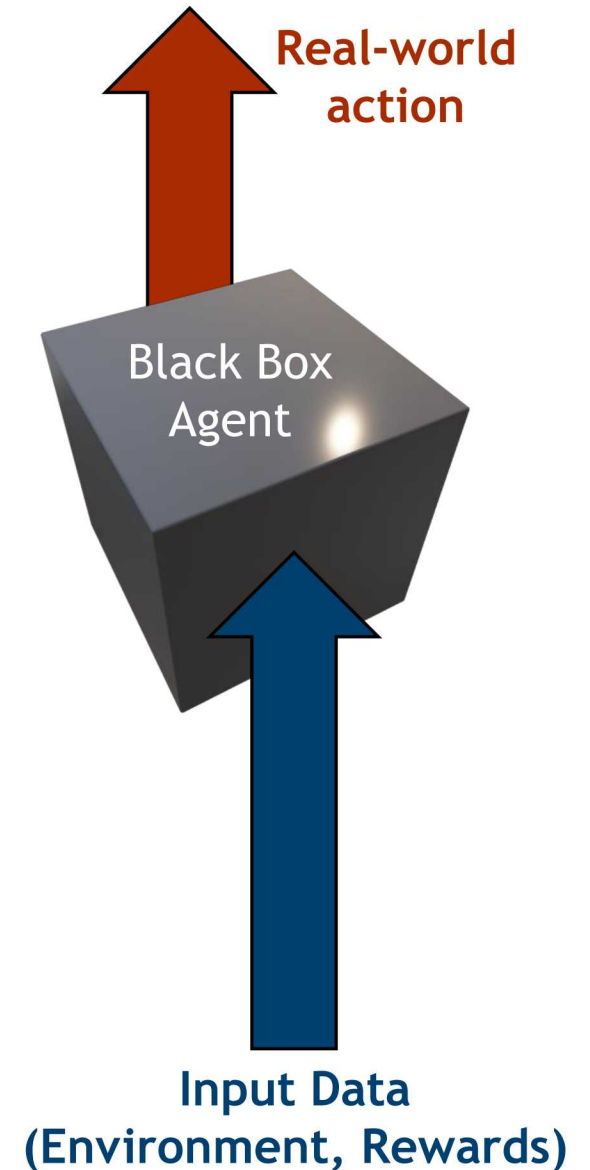
Using AI for real-time controls requires processing large amounts of data very quickly.

Challenges with Applying AI for Controls

- Many real-time power system controls applications operate sub-second to regulate the grid and maintain stability. Applying AI for controls applications requires processing large amounts of data size and significant computational effort
- AI algorithms are generally black boxes, which creates issues understanding and explaining the controls structure they have learned. Standard control theory methods need formula representations for demonstrating stability and stability margins
- Uncertainty Quantification – How bad could the prediction/action be?
- For controls applications, AI needs to be able to perform online learning, otherwise it will not be able to adapt to new situations

Successful Applications of AI for Controls

- Device control with reinforcement learning (generation, relays, substation)
- Smart Home/Building control with reinforcement learning (HVAC, demand response, lighting)
- Real-time forecasting with supervised learning (renewable generation, load)



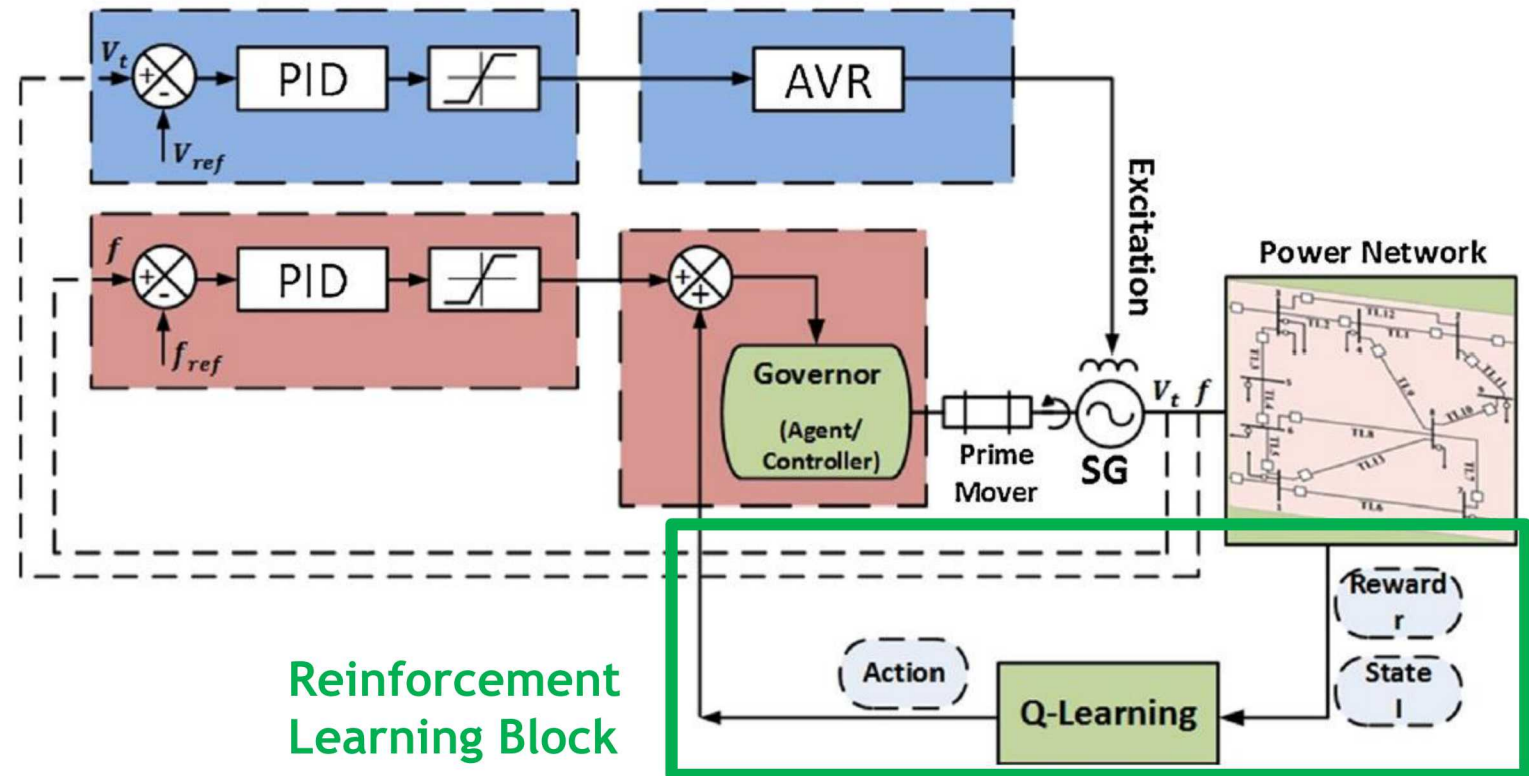
Reinforcement learning control of generator output to prevent cascading failures

- Q-Learning algorithm controls the outputs of three generators on the IEEE 118-bus test system
- Simulate tripping of an overloaded line

Simulations:

- N-1 contingency without control (**blackout**)
- N-1 contingency with RL control
- N-1-1 contingency with RL control

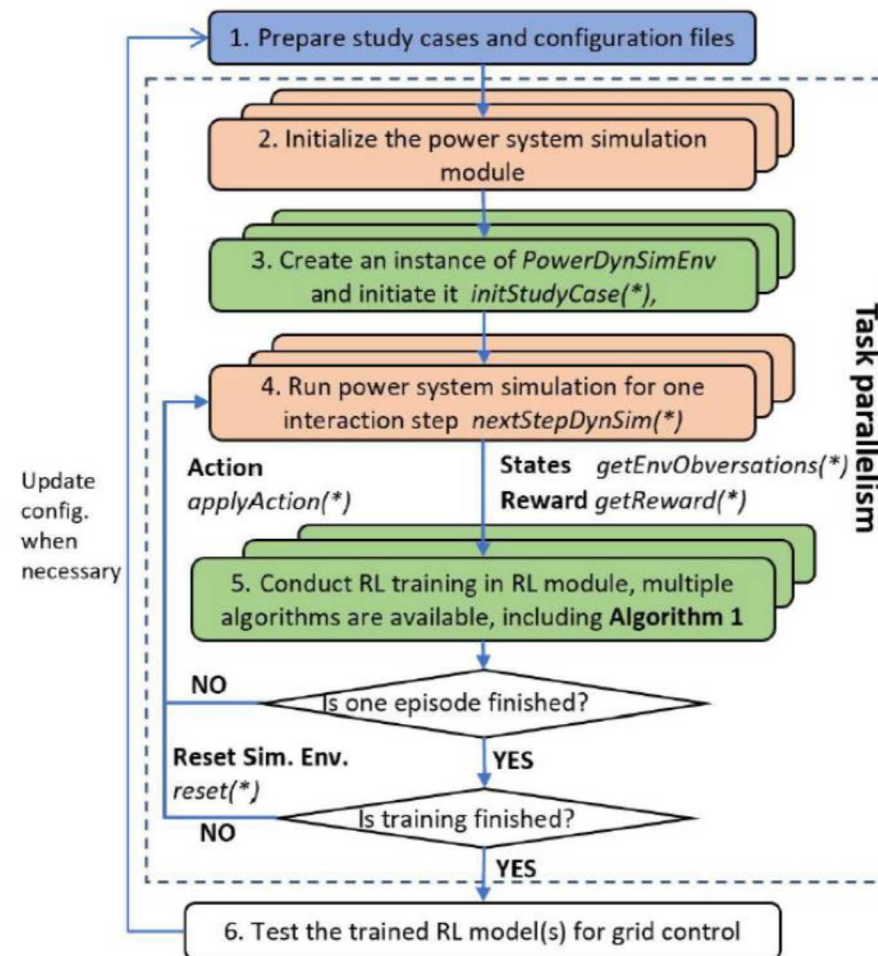
Reinforcement learning algorithm successfully learns to avert blackout conditions in both the N-1 and N-1-1 conditions tested



Deep Reinforcement Learning for Emergency Scenarios

- AI can improve grid resiliency during extreme events by providing rapid controls such as dynamic generator brake and under-voltage load shedding

Deep Reinforcement learning algorithm successfully learns the dynamic generator brake task as well as the under-voltage load shedding task, outperforming conventional methods



- Algorithm on the relay learns correct settings based on measured values, with a backup to predict values in the case of communications failure. This will allow the relay to continue to function during resiliency events

```
graph LR; MP[Measured Power<br/>(on relay)] --> FFNN[Feed-forward<br/>Neural Network]; MI[Measured Irradiance<br/>(through network)] --> FFNN; MI --> D{ }; PIR[Predicted Irradiance] --> D; D --> FFNN; FFNN --> RS[Relay Settings]; ITD[Irradiance training data] --> RNN[Recurrent<br/>Neural Network]; RNN --> PIR; RNN_T[Trained to predicted solar<br/>irradiance in the case of<br/>communications failure];
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Measured Power (on relay)

Measured Irradiance (through network)

Irradiance training data

Recurrent Neural Network

Predicted Irradiance

Feed-forward Neural Network

Relay Settings

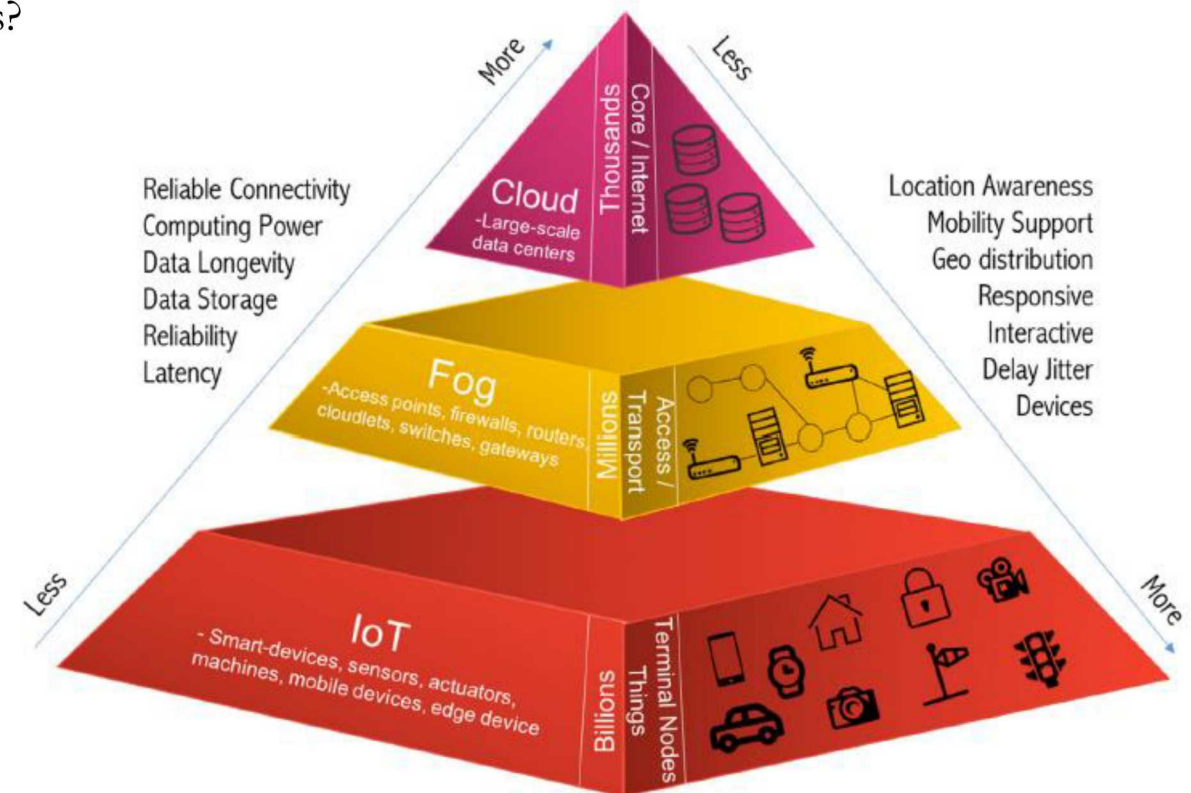
Maps real-time measurements (or predictions) to relay settings

Use measured values under normal conditions and switch to predicted values during communication failure event

Trained to predicted solar irradiance in the case of communications failure

Ongoing Challenges and Current Research Areas

- How do we add explainability to controls decisions made by AI?
 - Non-blackbox AI
 - Physics-based AI
- How do we quantify the uncertainty inherent in AI-based decisions?
- Can the computational burden of AI controls be distributed?
 - Edge/Fog Computing
- What happens to AI controls in a loss-of-communication event?
 - Non-centralized (distributed) AI controls



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2. M. Glavic, R. Fonteneau, and D. Ernst, “Reinforcement Learning for Electric Power System Decision and Control: Past Considerations and Perspectives,” *Sci. Direct*, vol. 50, no. 1, pp. 6918–6927, Jul. 2017.
3. Q. Huang, R. Huang, W. Hao, J. Tan, R. Fan, and H. Zhenyu, “Adaptive Power System Emergency Control Using Deep Reinforcement Learning,” *IEEE Transacation Smart Grid*, 2019.
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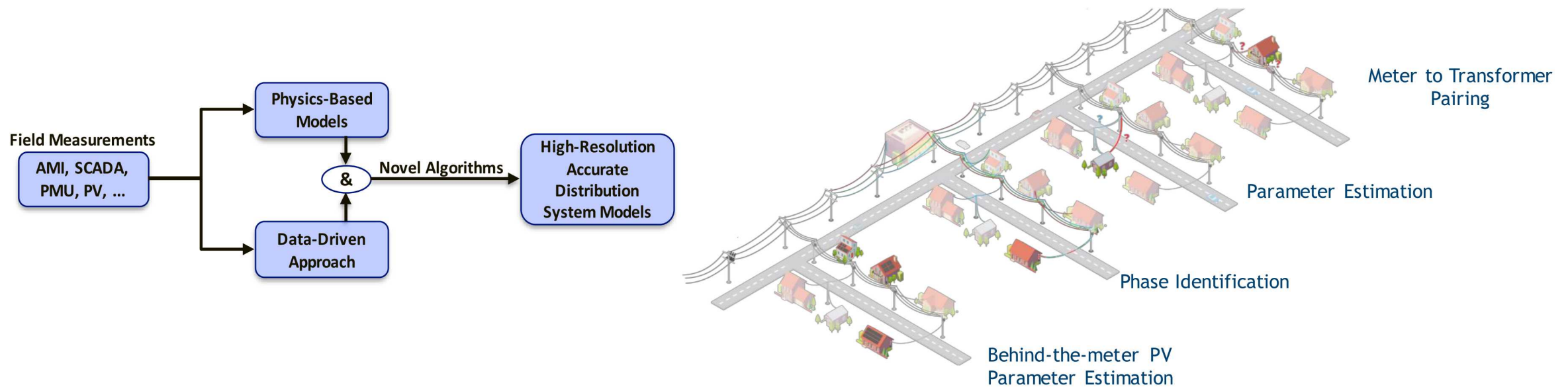
Example: Phase Identification

Matthew Reno (mjreno@sandia.gov)

Logan Blakely (lblakel@sandia.gov)

September 9, 2019

- To provide more technical insight into AI applied to power systems problems, this section goes through an example, including the design of the problem, AI workflow, data needs, and some of the technical issues.
 - Slides include some questions that should be asked in each stage of a project
- Example from “Physics-Based Data-Driven Grid Modeling to Accelerate Accurate PV Integration” Project
 - Ingest data from AMI, SCADA, uPMU, etc. and use data analytics and machine learning methods to estimate system parameters (phase, meter-transformer pairing, line lengths, etc.) and do state estimation
 - We are specifically focusing on the example of phase identification because of the variety of AI/ML solutions



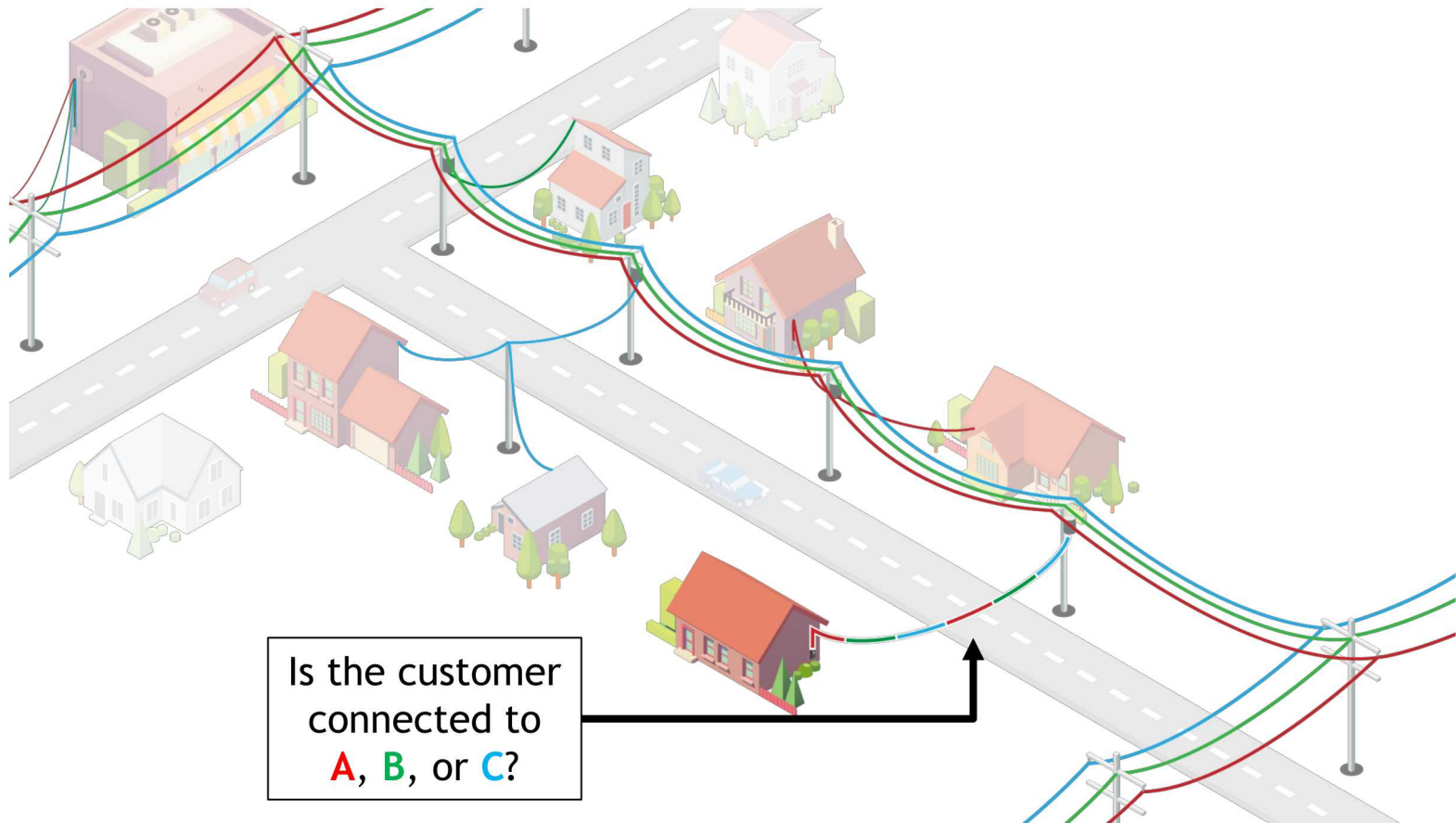
Artificial Intelligence for Power System Model Calibration



- Power system models are used in all aspects of utility real-time operations and planning
- But the models can be prone to errors due to manual data entry and decades of changes
- New types of sensors and measurement provide AI the ability to learn the models from Big Data

Phase Identification of the Electric Distribution System

- Much of the U.S. distribution system is single-phase for residential customers, so it is important to track which phase (A, B, or C) each customer is connected to.
- Physically tracking the cables to millions of customers in the U.S. is not feasible

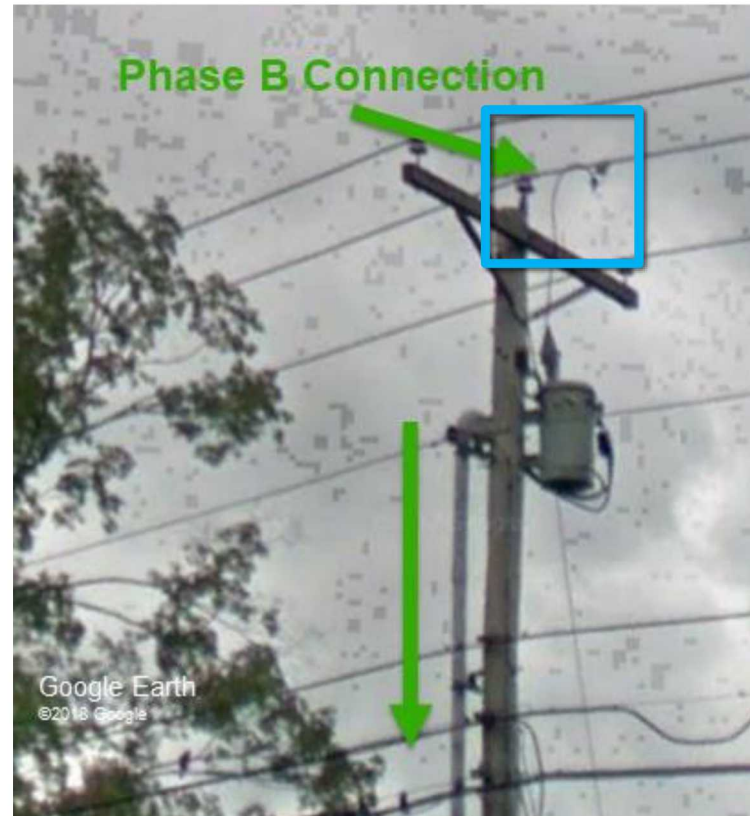
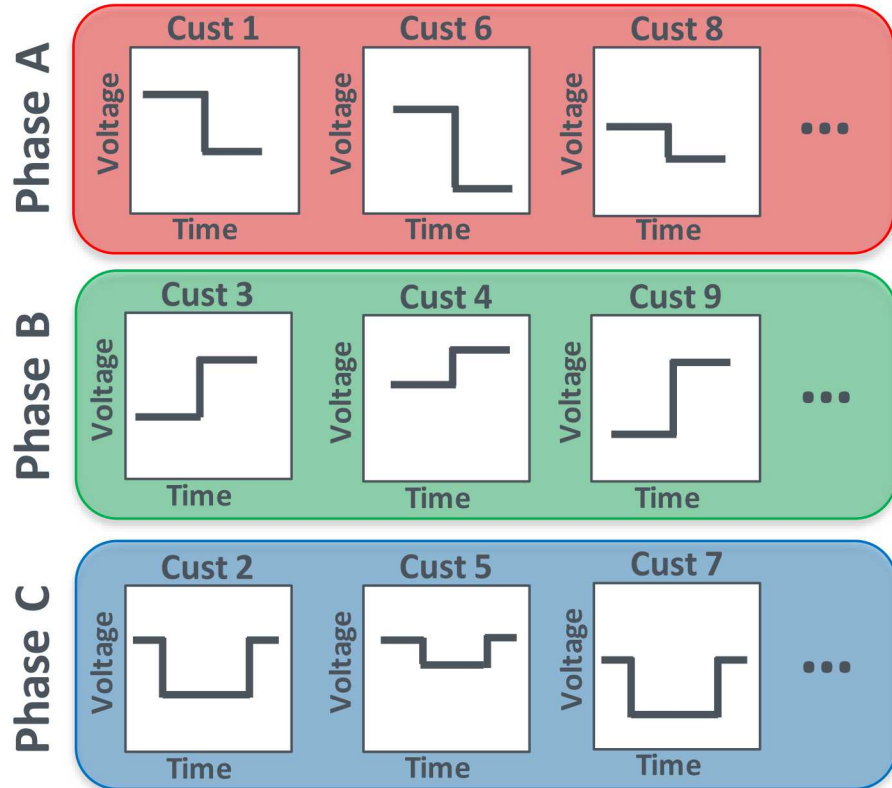


Phase Identification Expert Knowledge



Conceptually we understand from experience and the physical design of the system, that customers connected to the same wire (Phase A, Phase B, or Phase C) probably vary together.

Objective: Use artificial intelligence and big data from grid edge measurements to identify the phase of each customer



Question: What expert knowledge can be leveraged in formulating the problem?

Types of AI to Solve Phase Identification Problem



From the previous overview, there are many types of AI/ML that could be used to solve this problem.

Solutions to the Phase Identification Task

Supervised

- Learning based on the known phases of some customers

Unsupervised

- Clustering of customers with similar responses

Physics-constrained

- Using physical characteristics of the network

Physical Model Fitting

- Learning the best physical model that represents the system

The next slides will go into the details of each options with some appropriate references for how that type of AI/ML was applied to the phase identification problem

Supervised Phase Identification

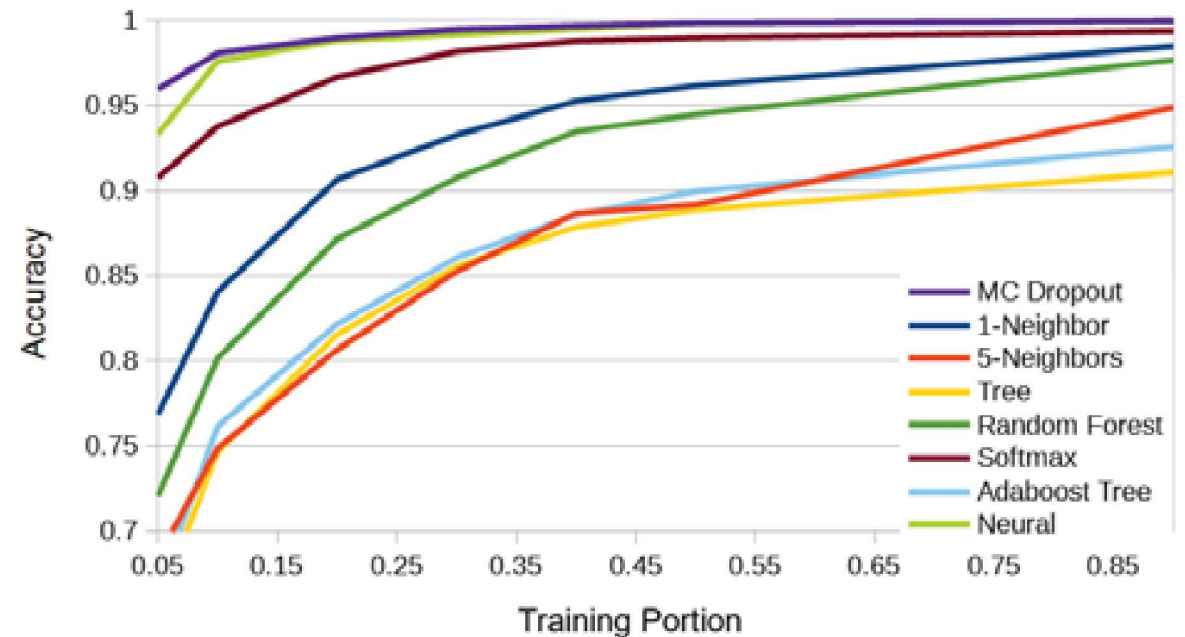


Supervised machine learning can be trained to learn characteristics to identify each customer's phase

- For example, some portion of the customers on the feeder can be *physically evaluated* for their phase, and these customers are used as the training set with known phases.

- Supervised algorithms for phase identification

- K-Nearest Neighbor
- Decision Trees
- Random Forest
- Adaboost
- Softmax/Perceptron Classifier
- Neural Networks
- Bayesian NN
- MC Dropout

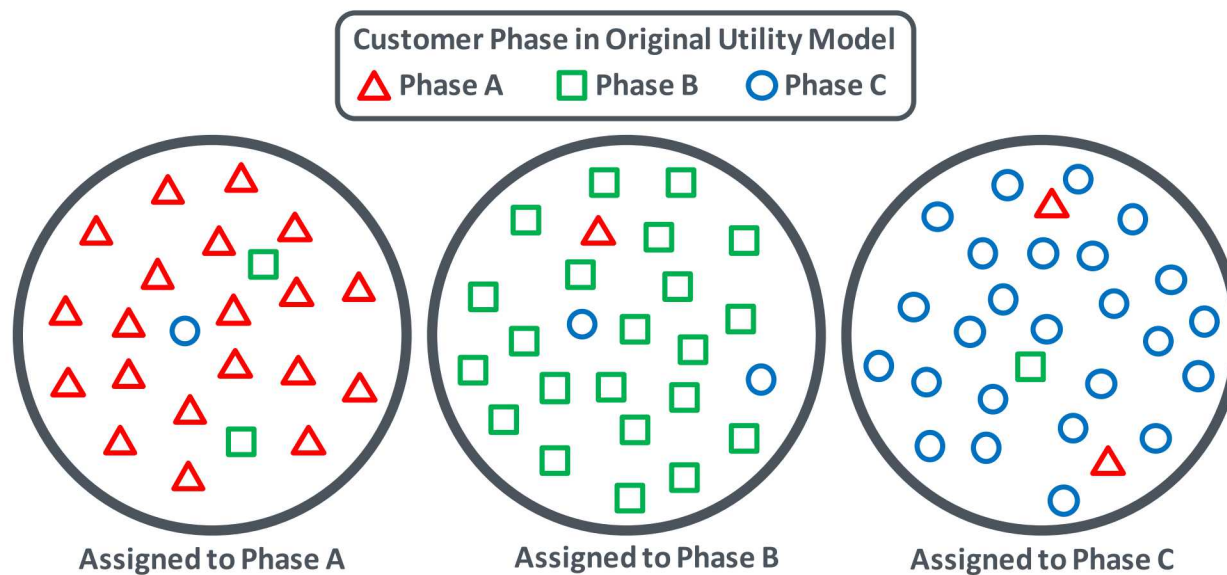


Unsupervised Phase Identification With Clustering



Use Unsupervised AI to identify similarities between customers with unknown or suspect labels

- AI groups all customers into clusters, based on their voltage timeseries
- After clustering, the phase of the cluster is determined by the majority of customers' phase in the original utility model

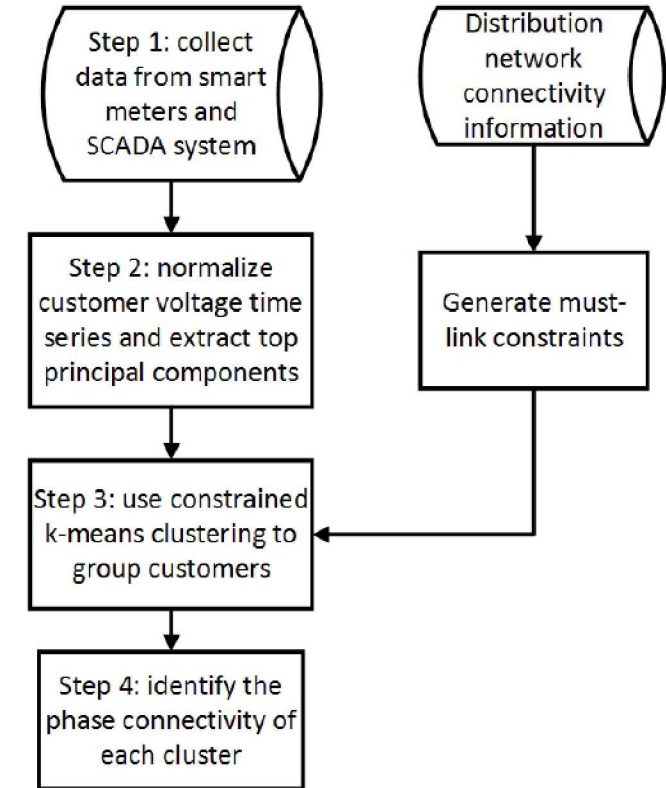
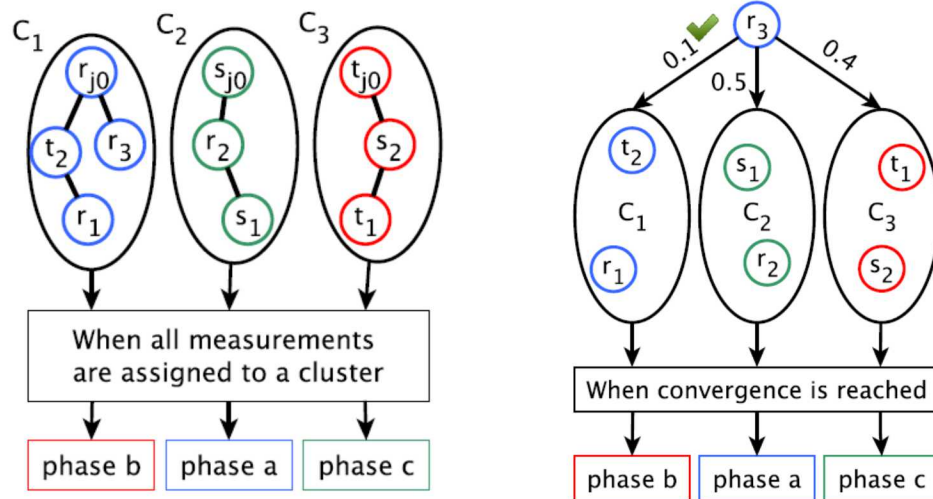


Physics-Constrained AI for Phase Identification



Certain physical constraints can be included in the AI/ML algorithms.

- For example, customers on the same single-phase transformer must be on the same phase
- This can increase accuracy and speed training, although confidence in the constraints must be high



References:

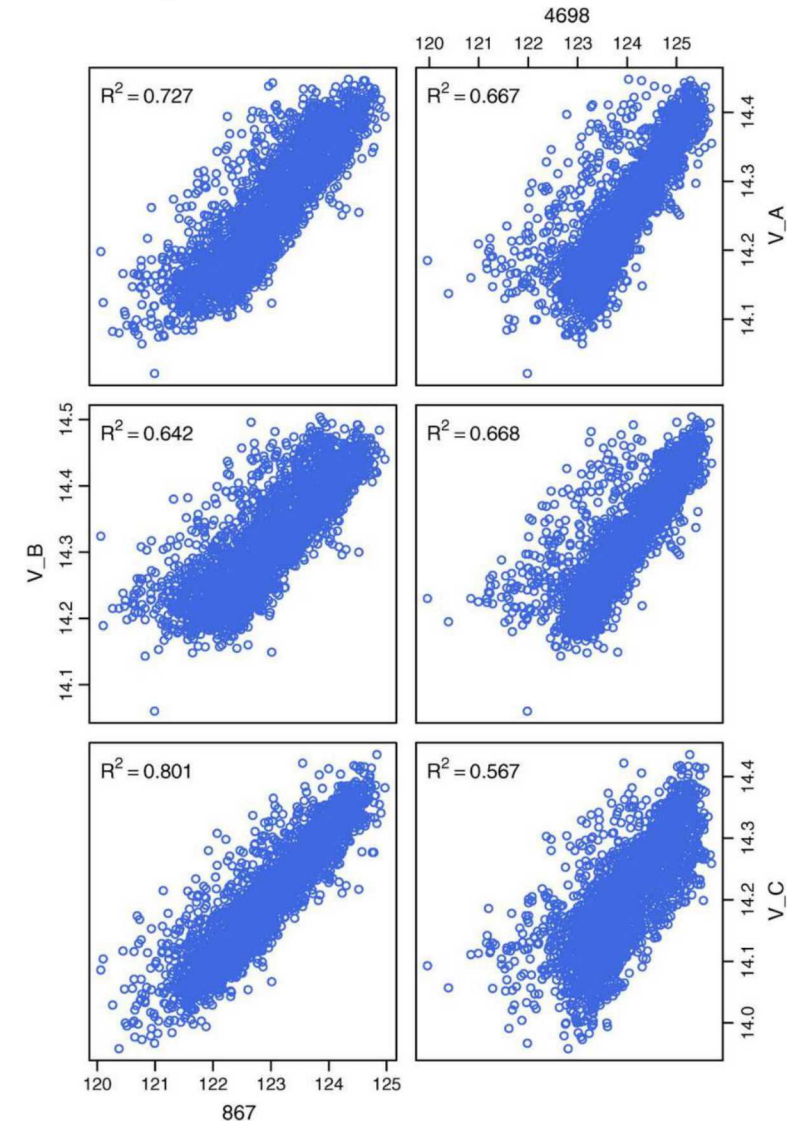
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Phase Identification with Physical Model Fitting



Known power system models can be applied to the problem to determine which physical model is better.

- For example, distribution system state estimation can be used to test different phase connection and see which state estimation from the models best represent the system measurements.
- In the figure, regression fit is used to determine the phase connections



References:

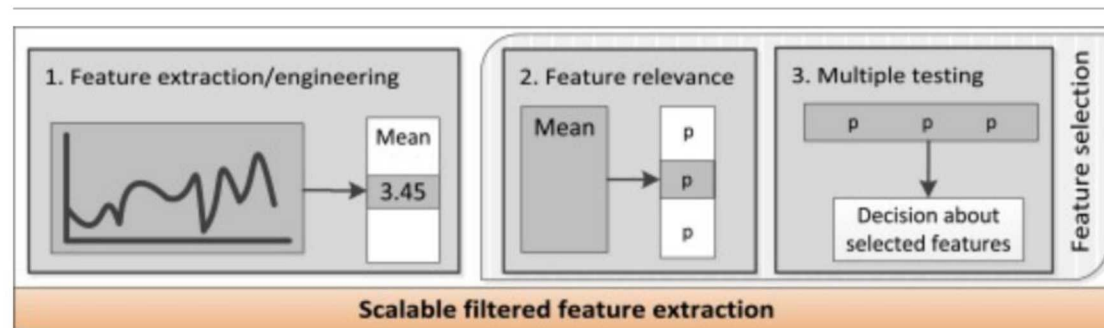
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Since AI/ML is data driven, it is very important to consider how the data is handled.

- Phase Identification Algorithms Input Data Decisions
 - What type of data is required (voltage, power, PMU, substation, customer information)?
 - What is the appropriate time-step resolution for the data?
 - Should the data be normalized (or some other transformation) beforehand?
 - Are known classification required for training?
- What is the best input representation?
- Data must be partitioned into sets for training versus validation
- Data partitioning (sampling) between training, validation, and testing can sometimes drastically effect results

Question: What kind of data sources are available?

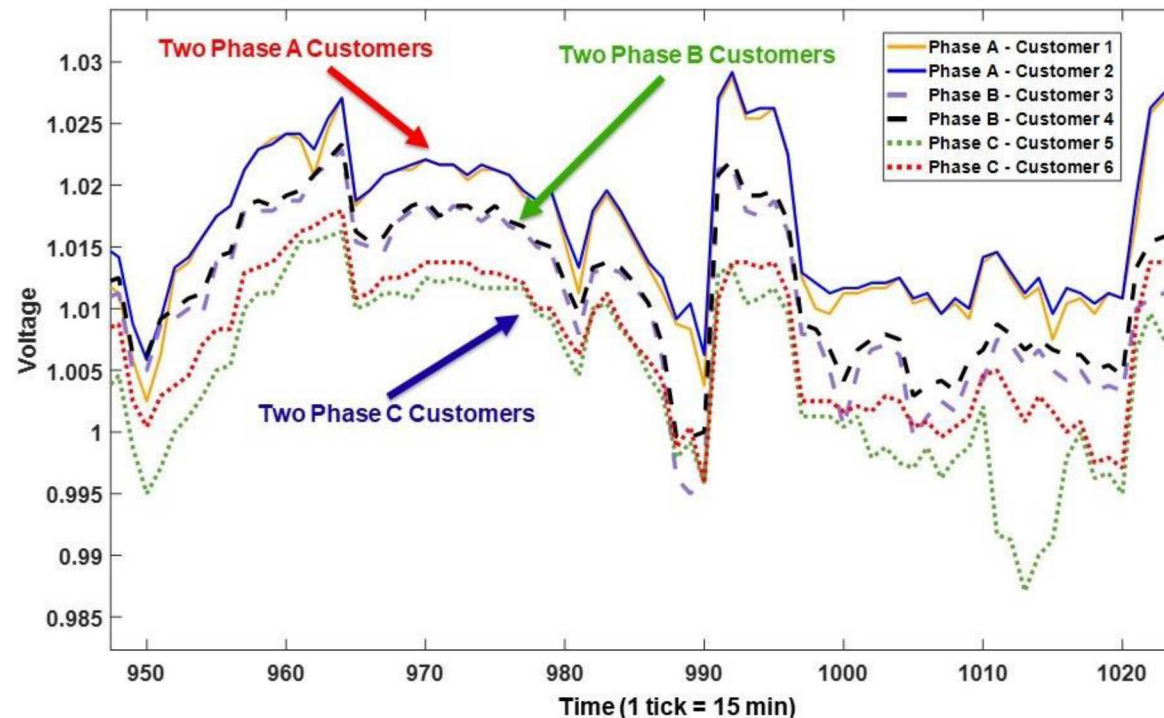
Question: How did you separate the training and the testing data?



Some types of AI algorithms struggle with missing data.

- Depending on the type of sensors and communication network, missing data for single time-steps or long periods can be common.
 - Time series methods (correlations or RNN require data for every timestep, otherwise the customer cannot be classified for that period
 - State or model-based AI algorithms require data from all meters, otherwise that timestep cannot be used in the algorithm

Question: How does the algorithm handle missing or bad data?



Example of feature engineering for phase identification using ensemble spectral clustering

Phase Identification Data Representation Process:

1. Try raw, unprocessed, measured voltages
2. Try normalized, measured voltages

There is significant improvement with the normalized data versus unprocessed data

However, performance was still unsatisfactory

3. Apply expert knowledge to refine data representation
4. Try normalized voltage difference representation

This data representation is critical to achieving success with this methodology. *It is a significant improvement over the other two representations*

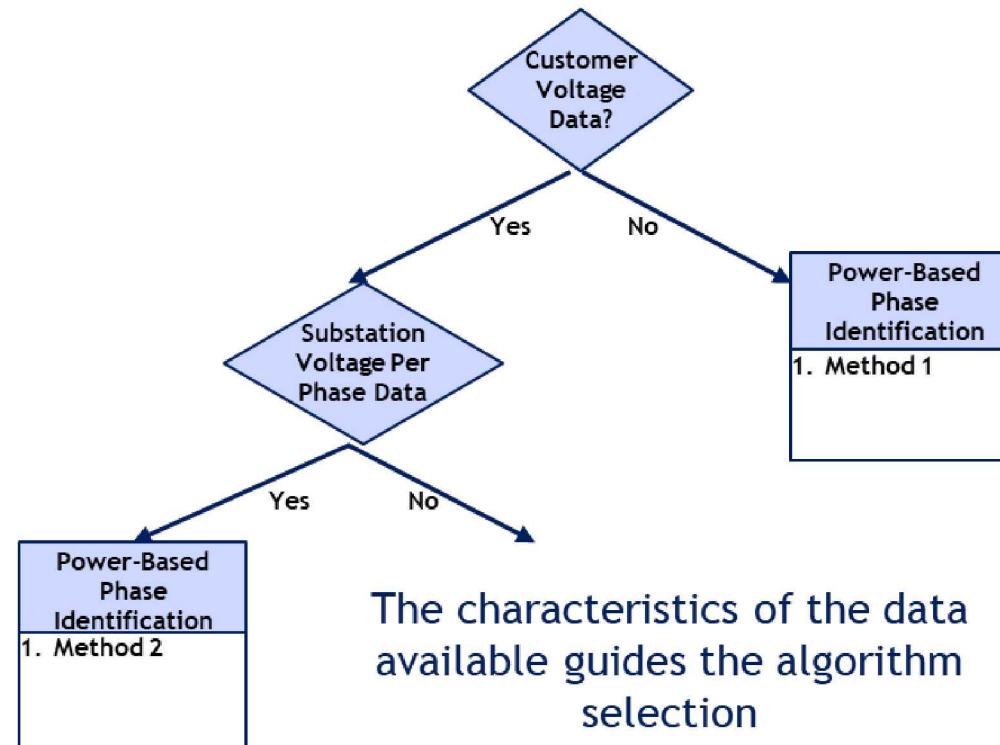
Other Possible Data Representations for Phase Identification:

- Fourier (or wavelet) transform
- Statistical features
- Statistical features with pairs of profiles
- Add other data streams
 - Power
 - Topology information
 - PMU data

Algorithm Selection Considerations:

- Desired outcome
- Characteristics of the data and the amount of data available
- What physical constraints are there and how could those be incorporated into different algorithms?
- Algorithm scalability ($O(n)$ vs $O(n^2)$) and scalability relative to the update rate

Question: Why did you select that type of AI for this problem?




Question: Is it possible to include any physical constraints into the AI?

Phase Identification Accuracy Evaluation

Accuracy Evaluation Considerations

- Determine the appropriate metrics of success for a task
- Confusion matrices can help identify the difference between false positives and false negatives
 - Ensure that the algorithm is not making the model worse by classifying customers on the wrong phase that were on the right phase originally
 - Precision, Sensitivity, Selectivity, and Accuracy
- To evaluate certain AI algorithms and situations, Monte Carlo simulations or multiple folds are required to obtain a range of accuracy
 - For phase identification does it matter which customers are labeled incorrectly in the model?
 - Are there random factors involved (measurement noise in the voltage data)?
 - Some algorithms (neural networks, k-means, . . .) are sensitive to randomly initialized parameters, potentially resulting in different results each time



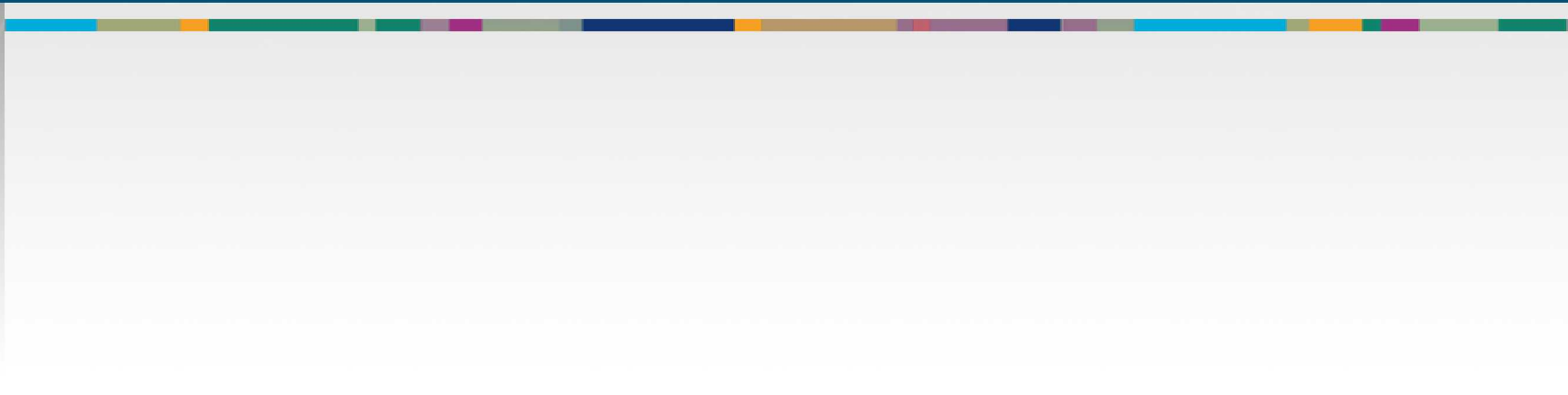
Question: What statistics are you using to measure accuracy?

		Predicted		
		A	B	C
Actual	A	295	6	3
	B	11	289	4
	C	1	8	300

Question: What is the range of accuracies seen from the multiple folds or Monte Carlo?



Conclusions



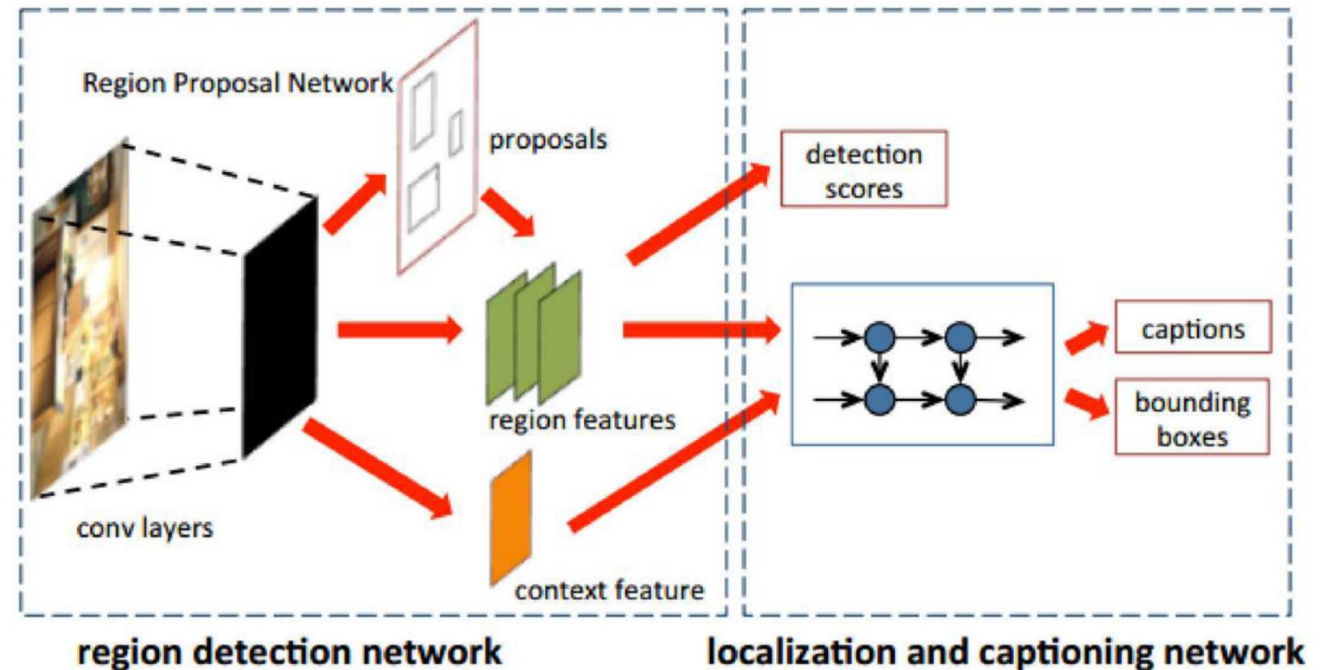
Future Research Directions



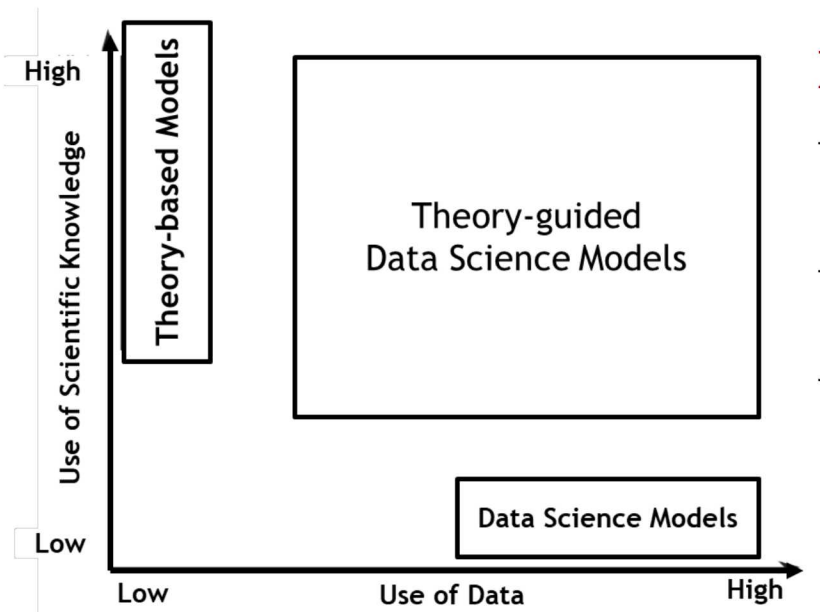
Many innovations in AI and machine learning have not yet been applied to the power systems domain

- As improvements and breakthroughs happen in other domains, those concepts can be adjusted and applied to solve power systems problems
- Similarly, lessons learned from other domains can be used to avoid similar situations

- Image Processing
 - Recognition
 - Captioning
 - Generation
 - Style Transfer
- Natural Language Processing
 - Translation
 - Summarization
 - Generation
- Autonomous Vehicles
- Game Theory



Future Research Directions



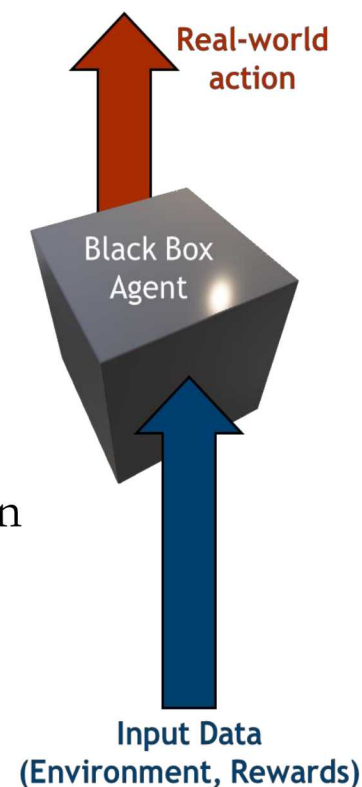
A. Karpatne *et al.*, "Theory-guided Data Science: A New Paradigm for Scientific Discovery from Data," *IEEE Trans. Knowl. Data Eng.*, vol. 29, no. 10, pp. 2318–2331, 2017.

Integration of Physics-based Constraints into AI

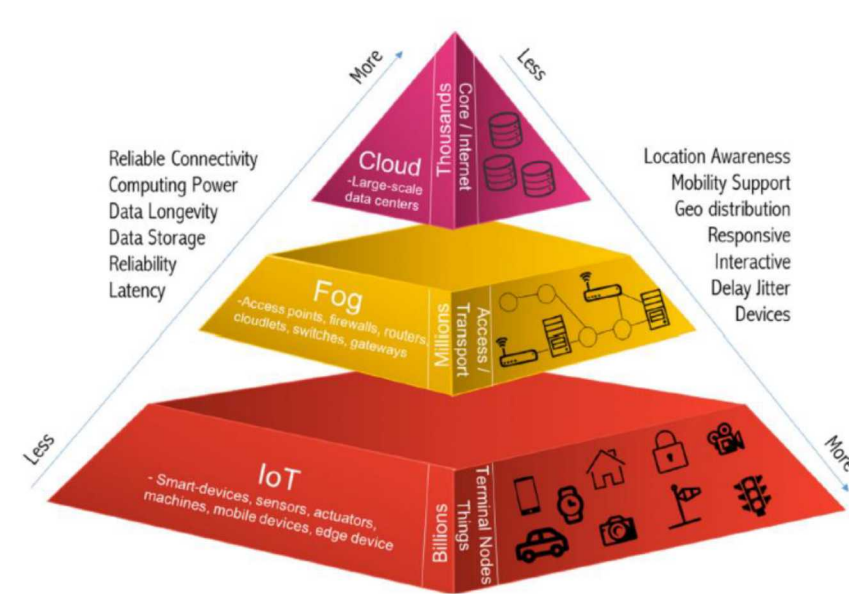
- Leverage existing knowledge (physical laws, power flow, etc) in AI-based algorithms
- Achieve more accurate results and faster training
- *SNL LDRD – “Integrating Physics Knowledge in Multi-Sensor Machine Learning Models”*

Explainable AI and Uncertainty Quantification

- Understand why a particular prediction/decision was given
- Understand the error bounds on predictions/decisions
- *SNL LDRD on “Opening the ‘Black Box’: An Experimentally-Validated Explainable Machine Learning Framework”*



Future Research Directions



A. Yousefpour *et al.*, "All One Needs to Know About Fog Computing and Related Edge Computing Paradigms: A Complete Survey," *J. Syst. Archit.*, vol. 98, pp. 289–330, Sep. 2019.

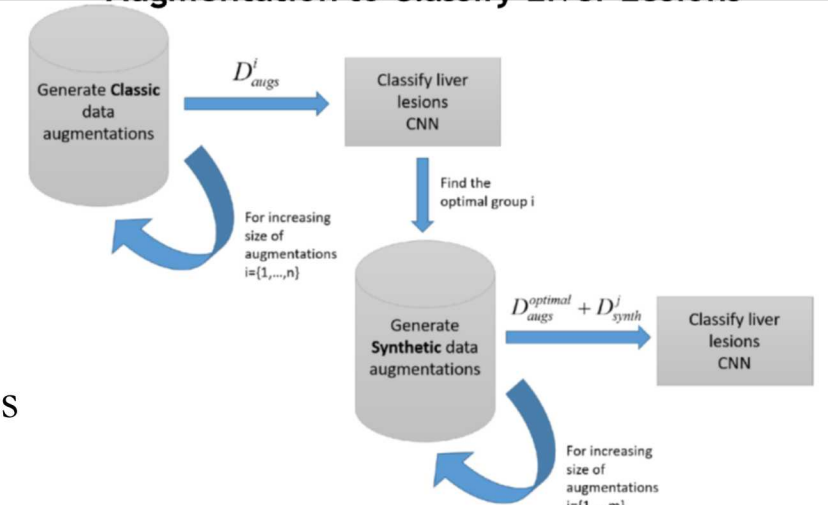
Distributed, AI-based Controls using Fog Computing

- Create resilient systems in the event of communication loss
- Accelerate systems with low latency because processing happens physically close to sensors
- *SNL LDRD – "HEDGES: High-Security Edge Computing for Smart Sensor Systems"*

Semi-Supervised, Few-Shot Learning, or Synthetically-Generated Training Data

- Learn with few or no examples of critical events
- Generate realistic new data from existing samples
- *SNL LDRD – "Semi-Supervised Bayesian Low-Shot Learning for Explosive Device Characterization"*

Generative Adversarial Networks (GAN) for Data Augmentation to Classify Liver Lesions



M. Frid-Adar, I. Diamant, E. Klang, M. Amitai, J. Goldberger, and H. Greenspan, "GAN-based Synthetic Medical Image Augmentation for Increased CNN Performance in Liver Lesion Classification," *Neurocomputing*, vol. 321, pp. 321–331, 2018

- There are many promising applications of AI/ML in power systems.
 - It is an exciting time to be at this intersection – new algorithms, large datasets, computing power
- There are many challenging problems yet to be solved with some fascinating future research directions in ML for:
 - Integration of Physics-based Constraints into AI
 - Explainable AI and Uncertainty Quantification
 - Distributed AI-based Controls using Fog Computing
 - Semi-supervised, Few-shot learning, or Synthetically Generated Training Data
- Best results require integration between ML experts and power system experts
- See references included throughout the presentation for further reading.



Electric Power Systems Research

Ray Byrne

Manager, R&D Science and Engineering
rhbyrne@sandia.gov

Matthew Reno

R&D S&E, Electrical Engineering
mjreno@sandia.gov

Logan Blakely

R&D S&E, Computer Science
lblakel@sandia.gov

Machine Intelligence

David Stracuzzi

R&D S&E, Cognitive Systems
djstrac@sandia.gov

Scalable Analysis & Visualization

Warren Davis

R&D S&E, Computer Science
wldavis@sandia.gov

Data Science & Optimization

JP Watson

R&D S&E, Computer Science
jwatson@sandia.gov