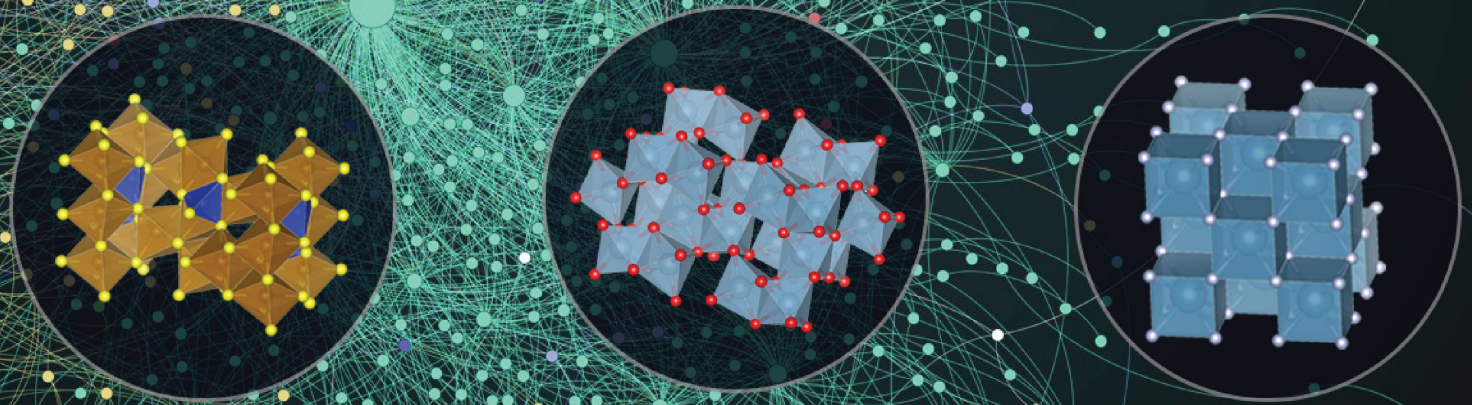
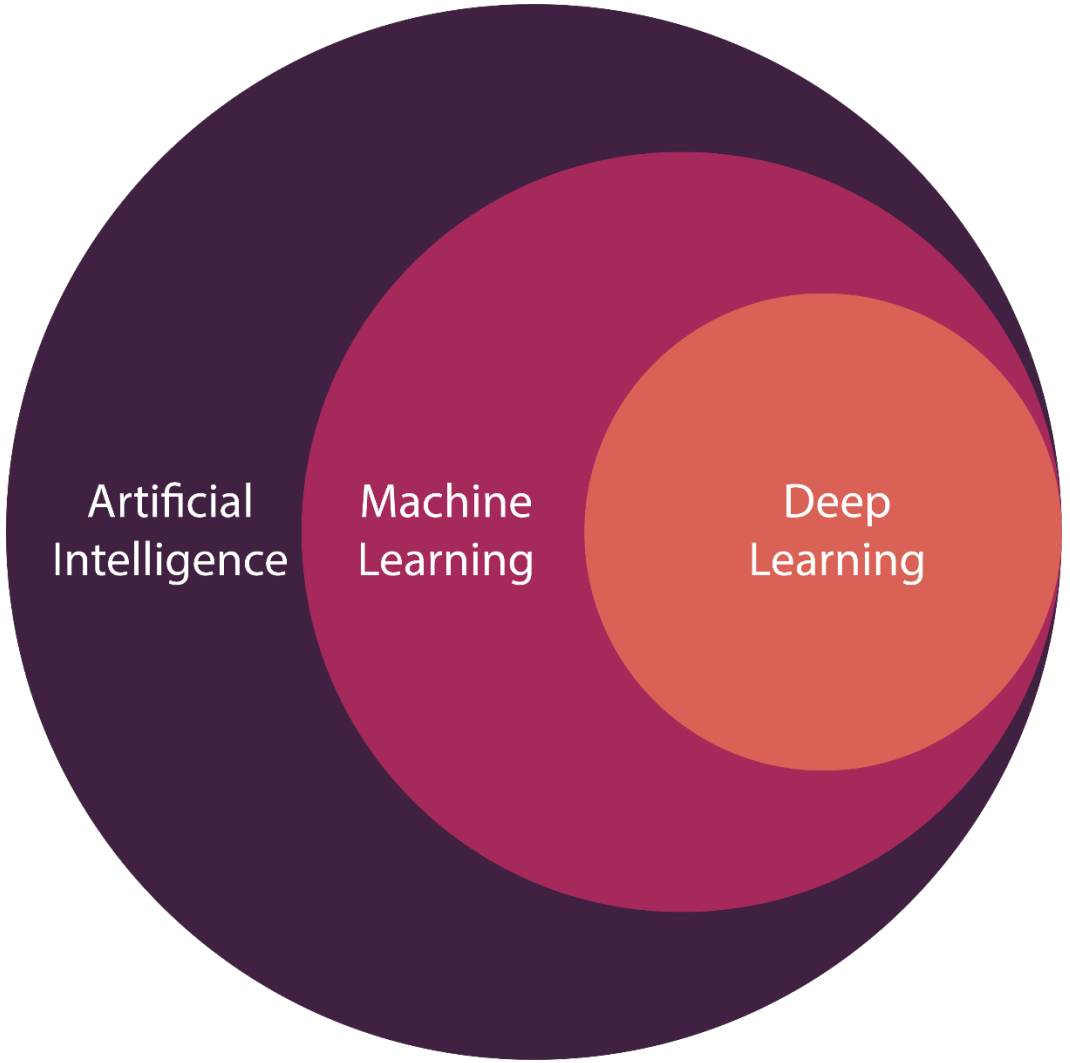
Machine Learning: Tasks and Types



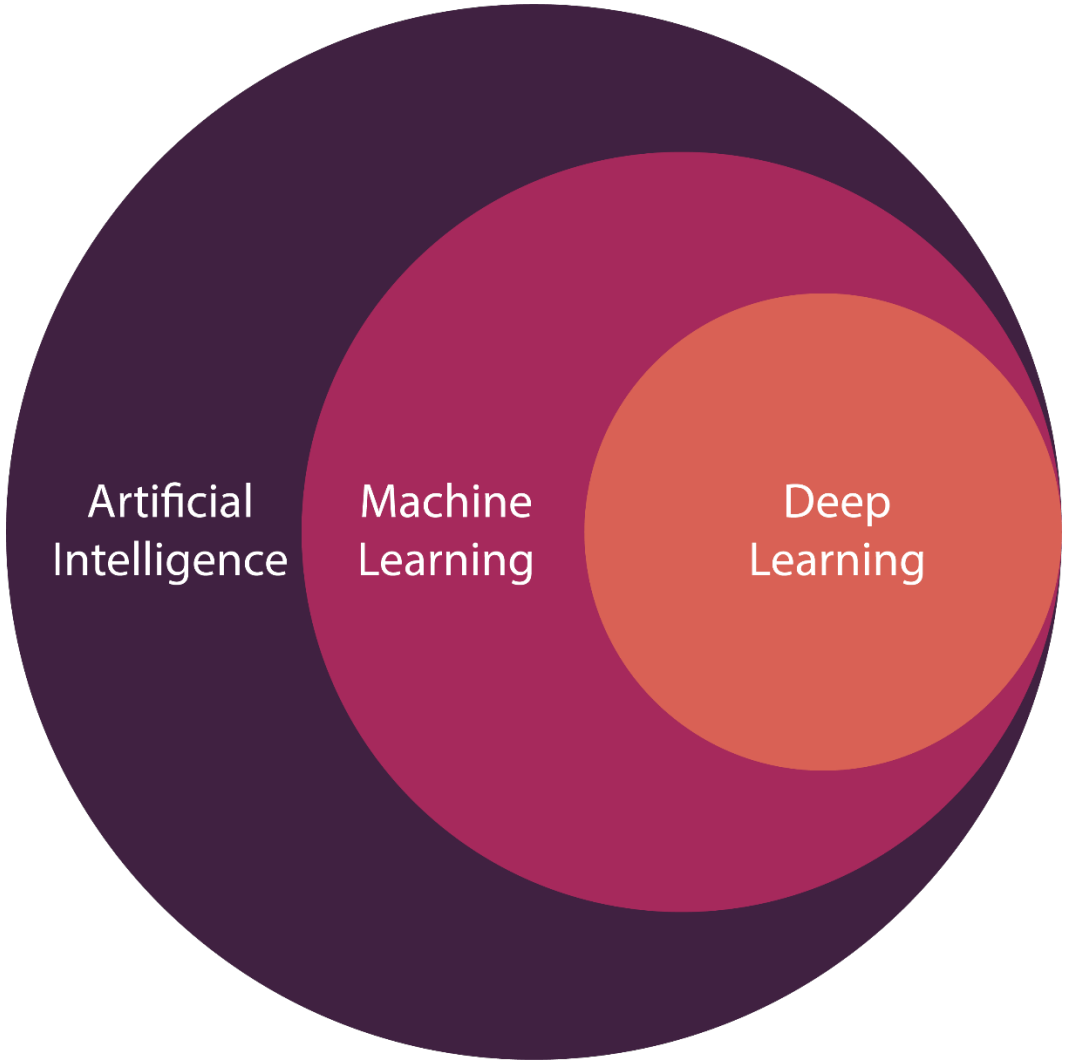
Machine learning is learning from patterns in data

AI: the theory and development of computer systems able to perform tasks that normally require human intelligence, such as visual perception, speech recognition, decision-making, and translation between languages.



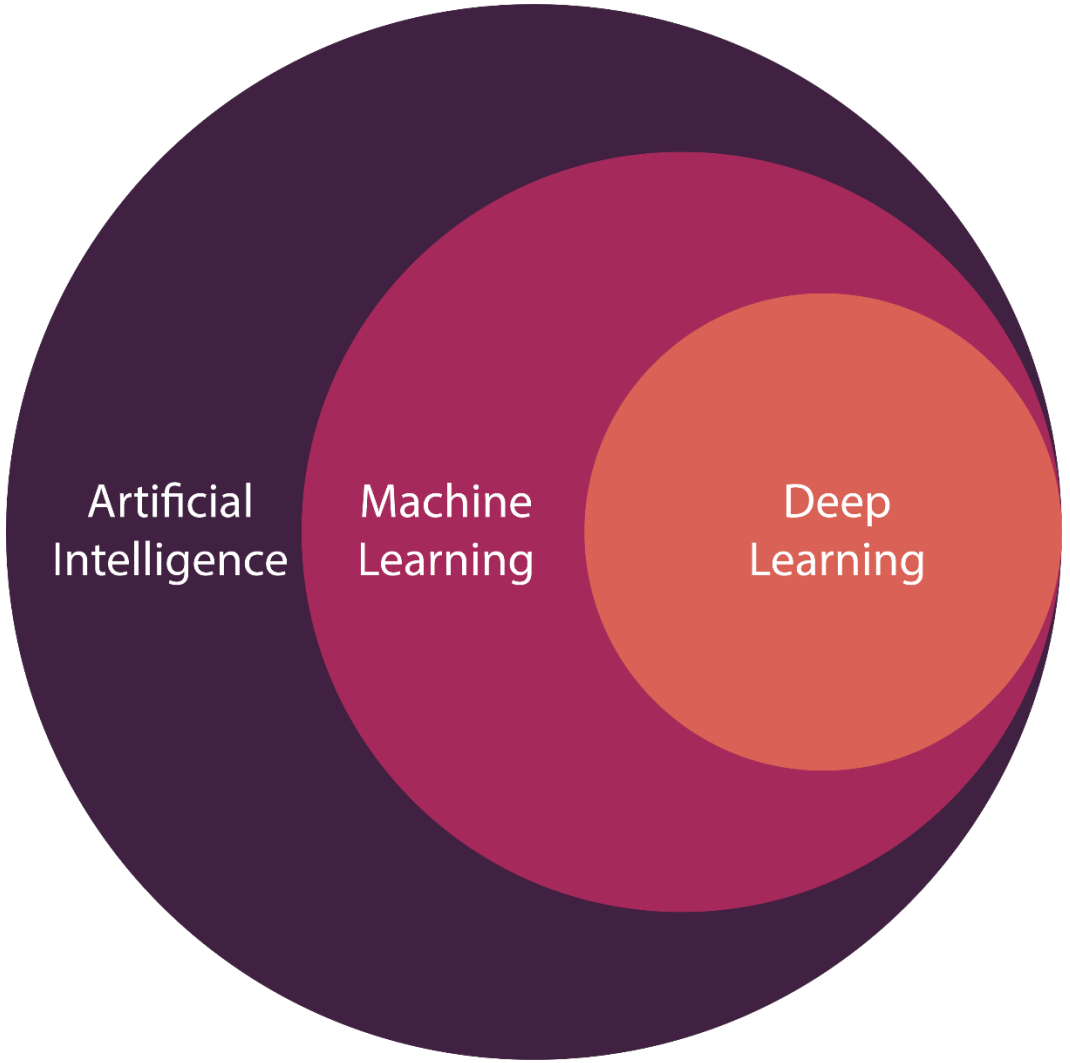
Machine learning is learning from patterns in data

ML: the use and development of computer systems that are able to learn and adapt without following explicit instructions, by using algorithms and statistical models to analyze and draw inferences from patterns in data.

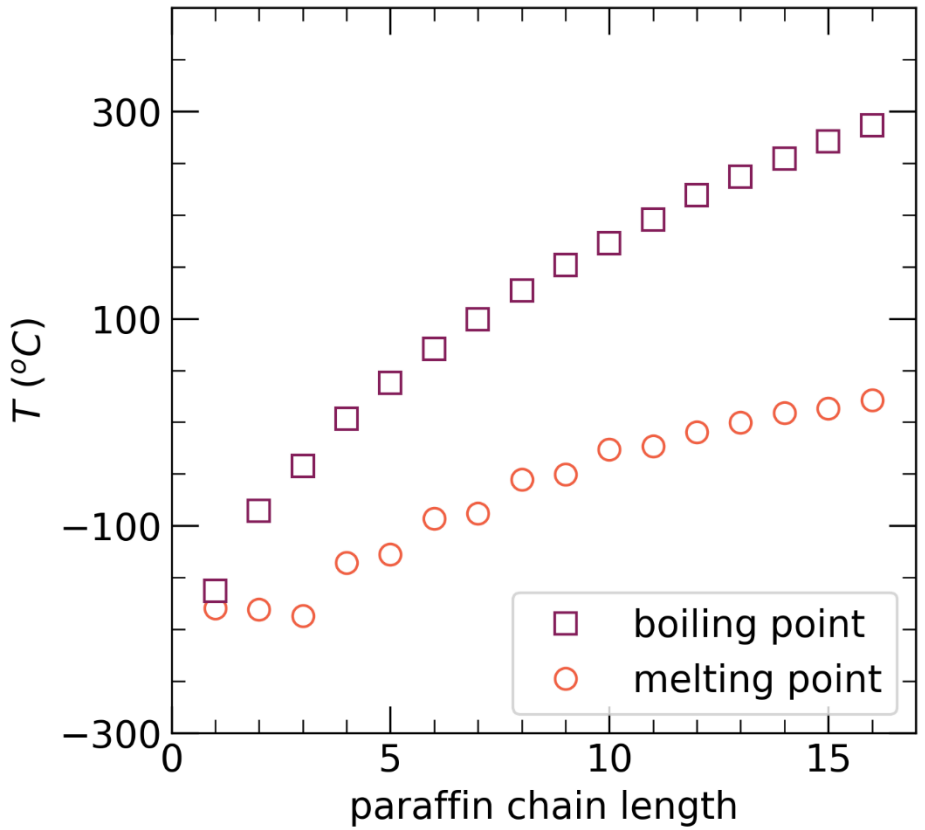


Machine learning is learning from patterns in the data

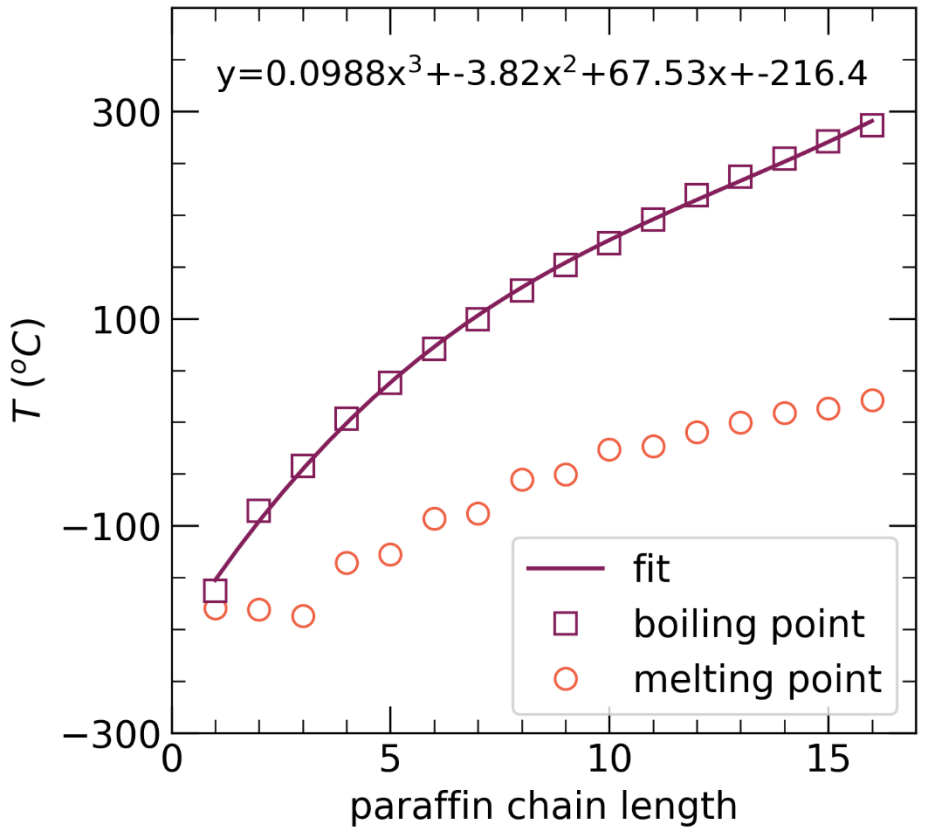
Deep learning: part of a broader family of machine learning methods that imitates the workings of the human brain in processing data and creating patterns for use in decision making.



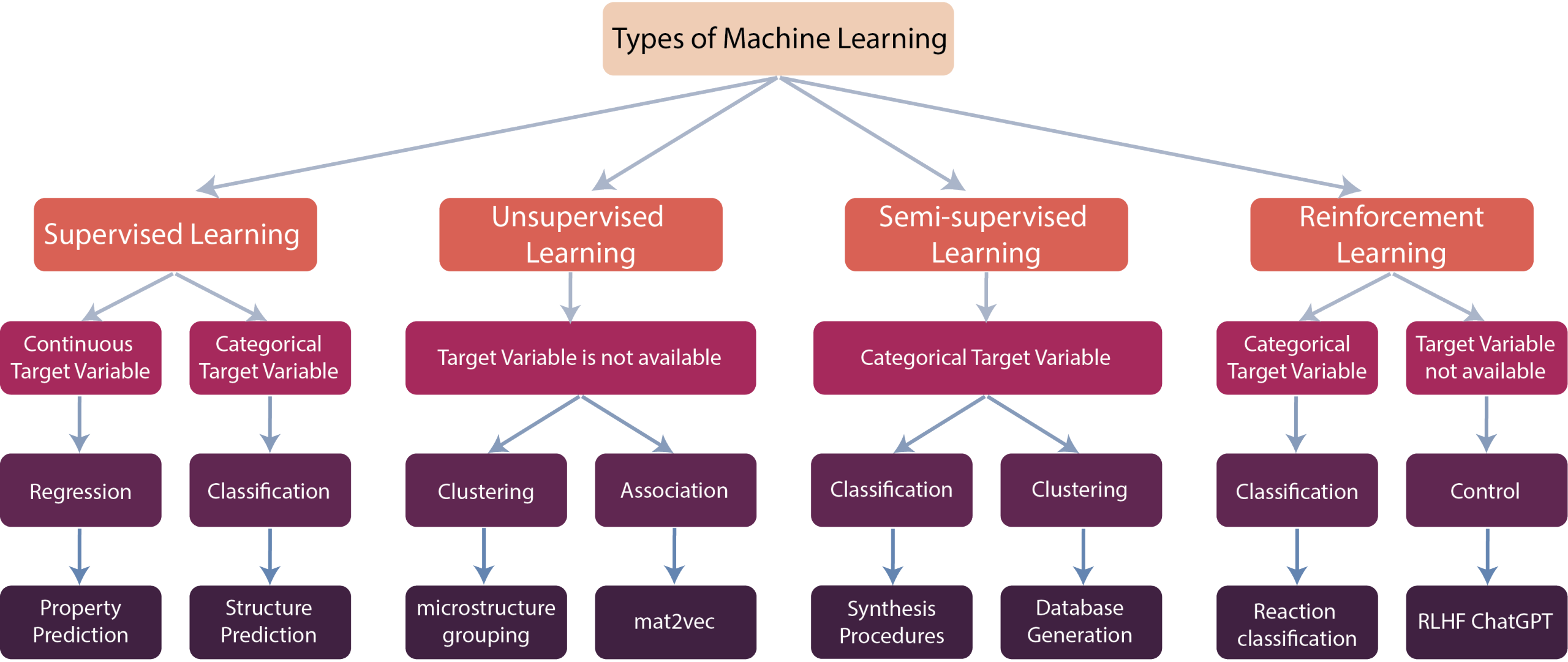
Materials scientists have noticed patterns in data forever!



Empirical trends may not be supported by theory



Machine learning is often grouped in four categories



There are many others!

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by **Jason Brownlee** on November 11, 2019 in **Start Machine Learning**

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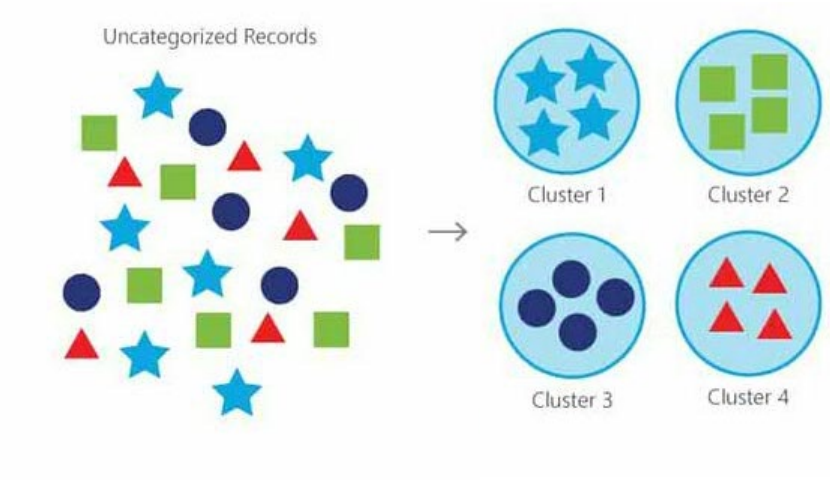
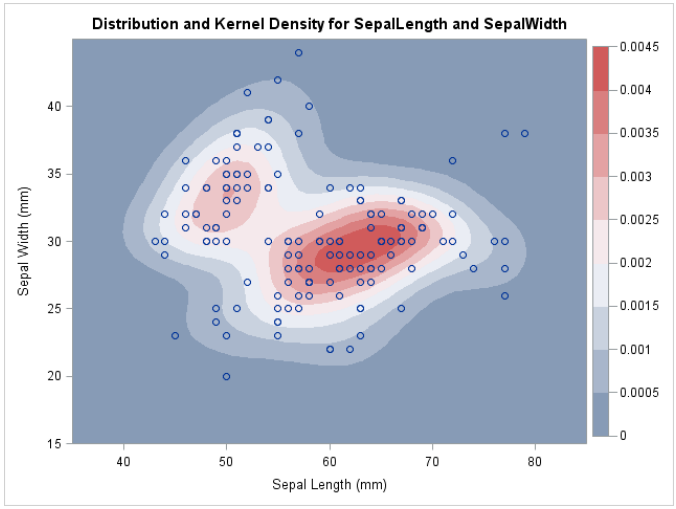
Unsupervised is typically clustering, density estimation, projection

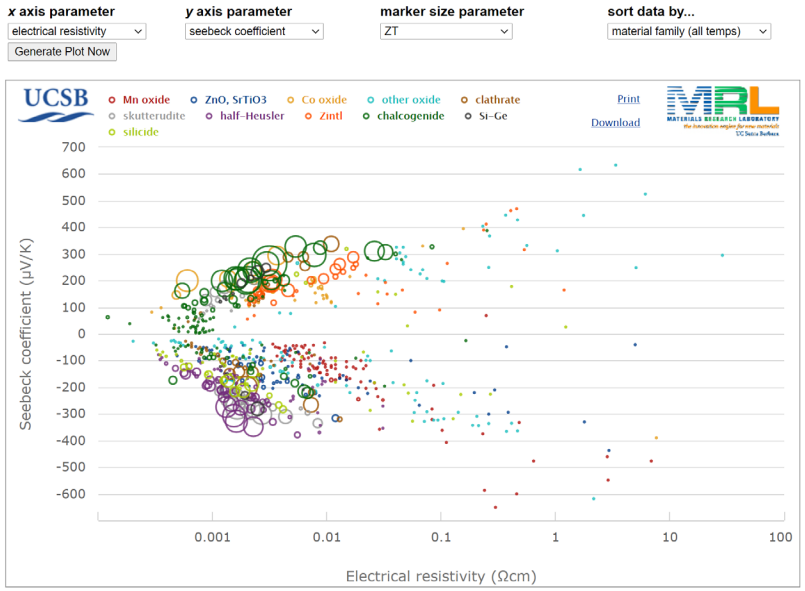
Clustering



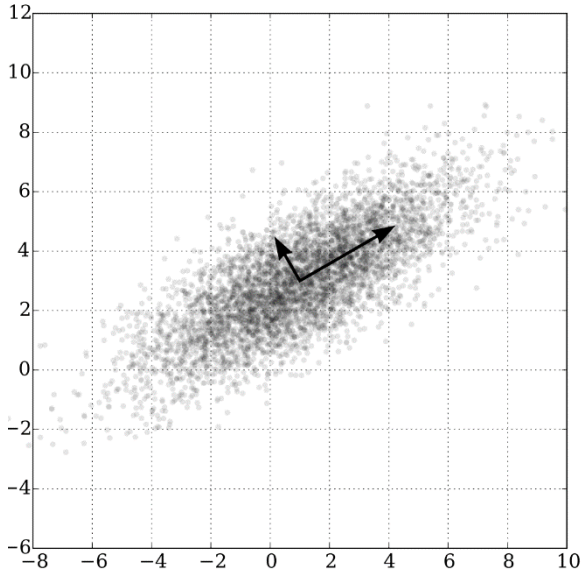
Density Estimation



Visualization

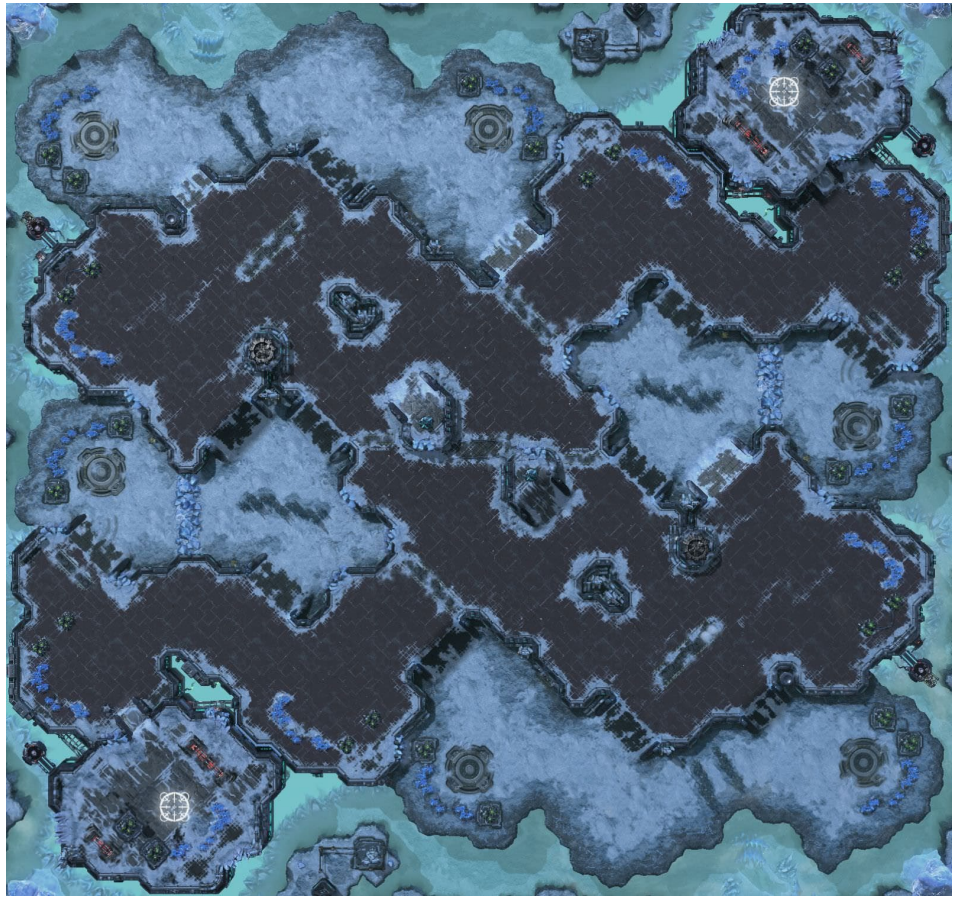


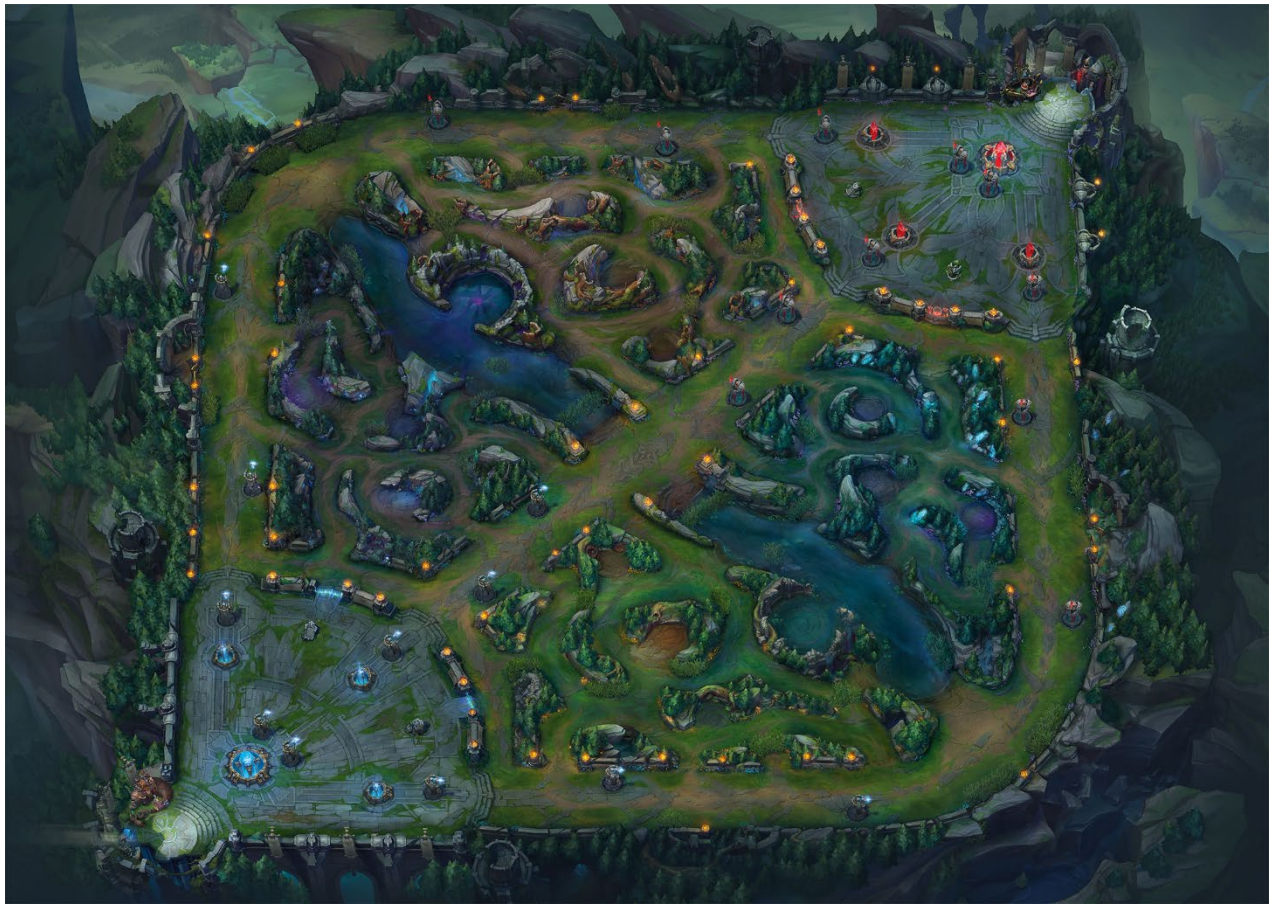
Projection



Reinforcement learning differs from supervised learning

An agent operates in an environment and must learn to operate using feedback
- No fixed dataset and the feedback may be delayed or noisy





Hybrid learning blurs the lines in types

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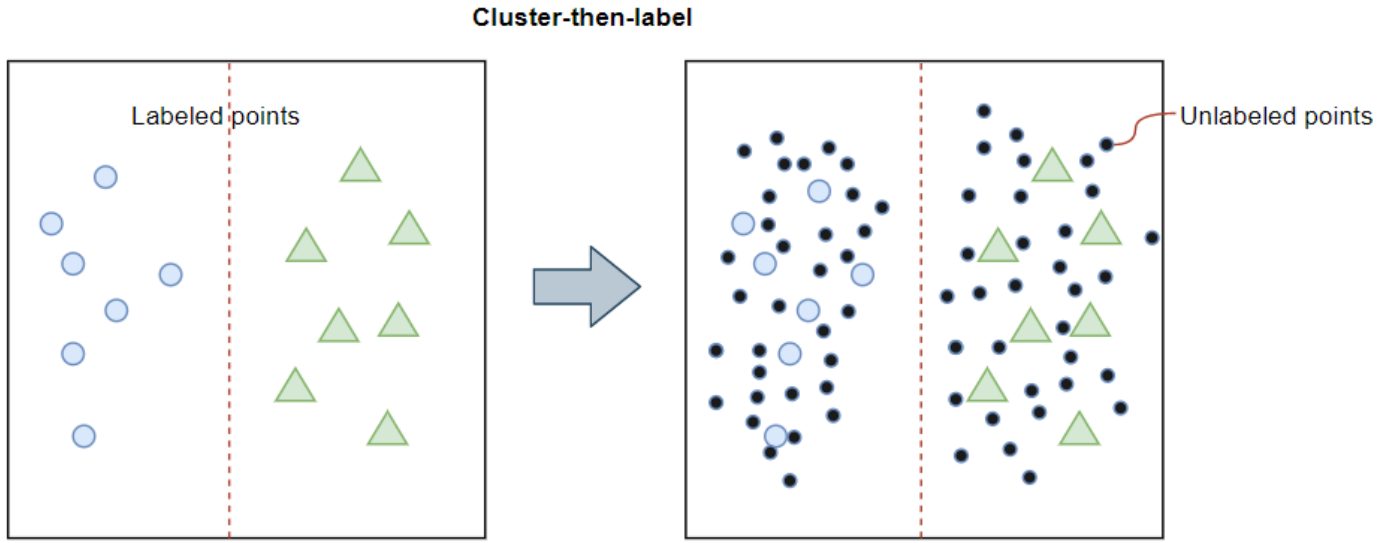
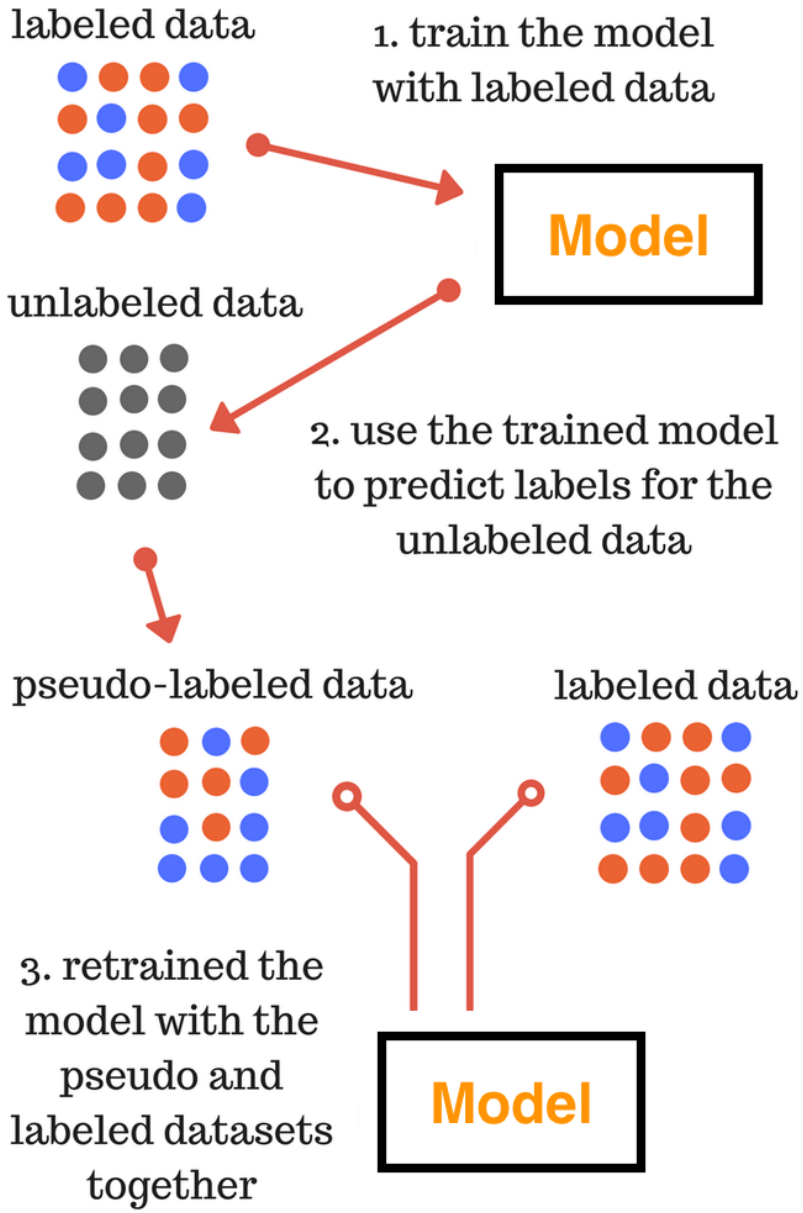
Semi-supervised makes the most of partially labeled data

Algorithms are used to learn relationships between labeled and unlabeled data to then use all the data

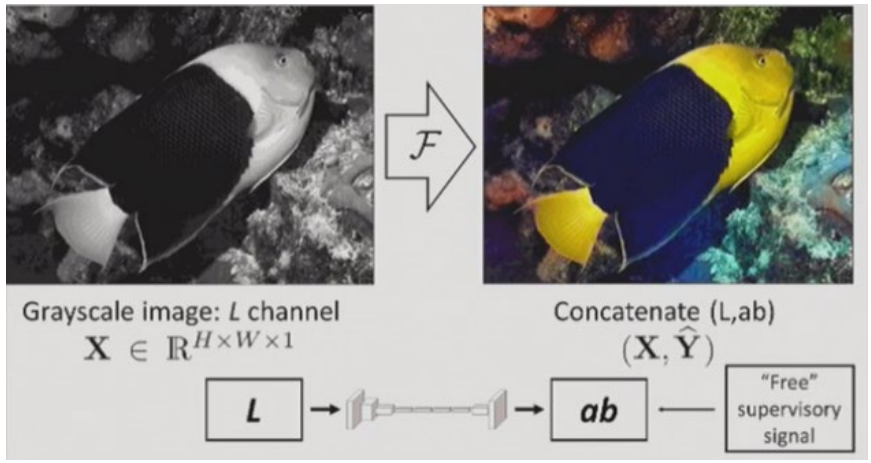




Self-supervised is unsupervised framed as supervised learning

Supervised learning algorithms are used to solve an alternate or pretext task, the result of which is a model or representation that can be used in the solution of the original (actual) modeling problem.

Colorization

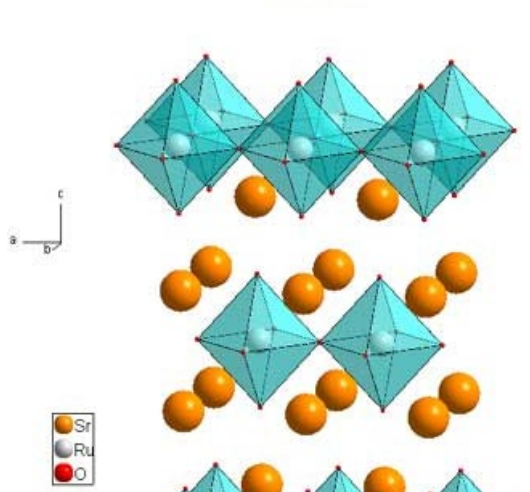


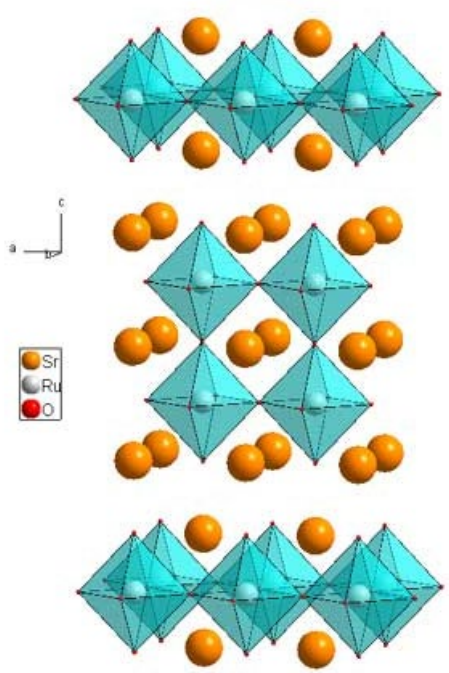
Inpainting

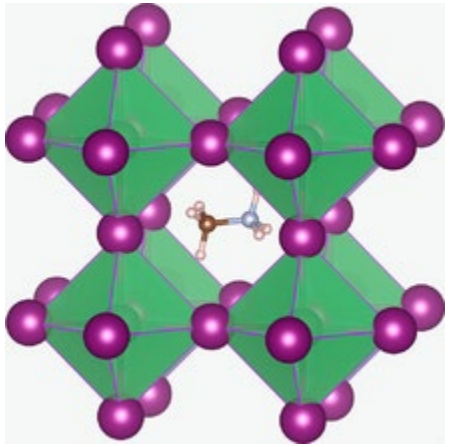
Multi-instance is supervised learning with “bags” of instances

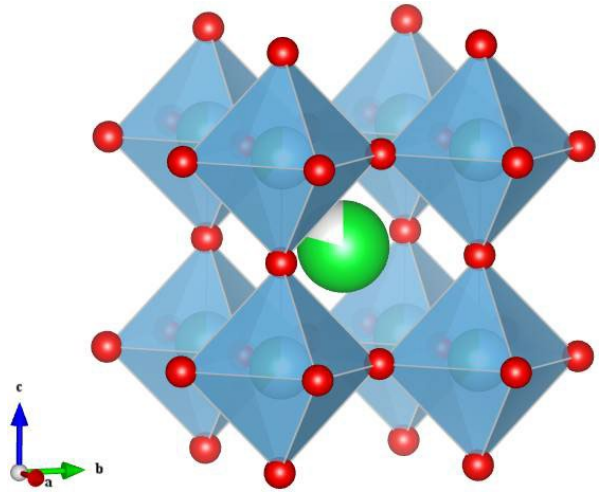
Members of the “Perovskite” bag all contain some shared attributes along with some non-shared attributes.

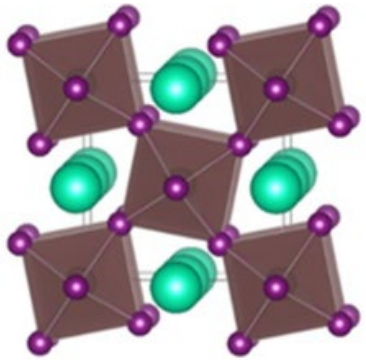
Q: which attributes are essential to “Perovskite” bag?

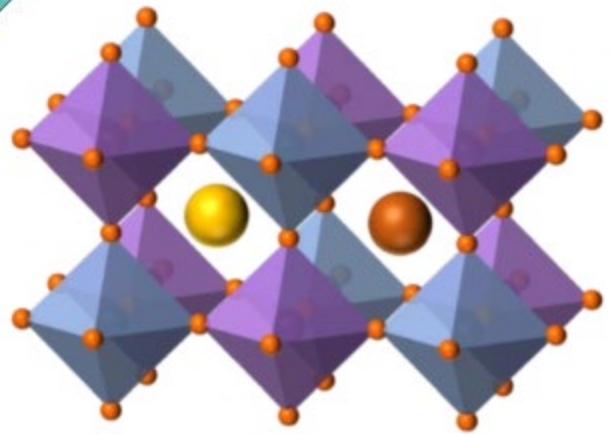


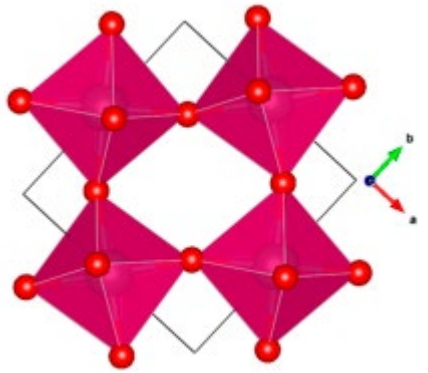












Inference refers to reaching an outcome or making a decision

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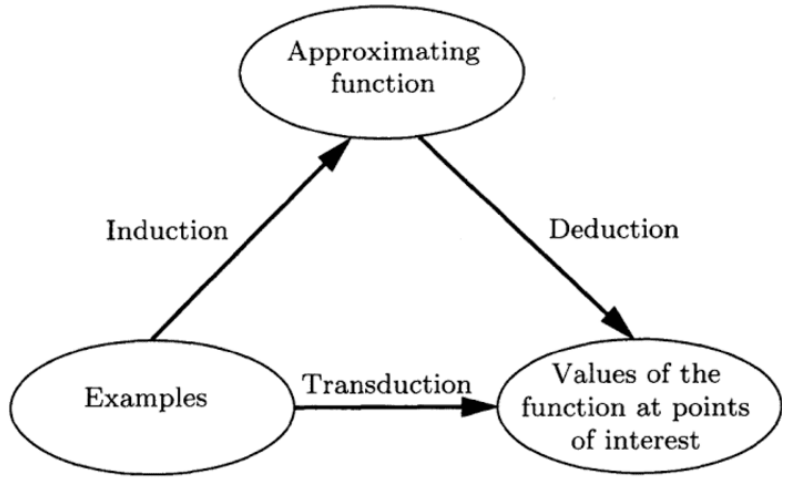
Inductive vs deductive learning are opposites

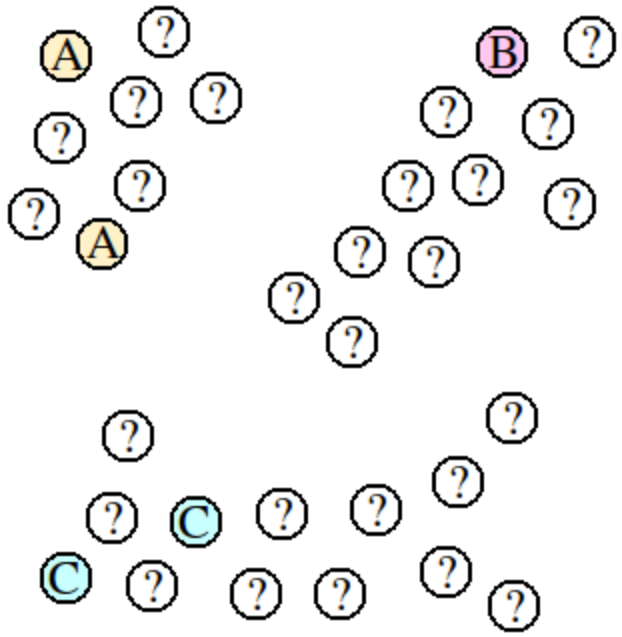
Inductive learning is learning general rules from specific examples.
Deductive learning is learning specifics examples from general rules.
Transductive learning is predicting specific examples from specific examples.



Inductive learning:
- Model learns the general rules
- Draw general conclusions about future from past examples
- Fitting the ML model

Deductive learning:
- Top down reasoning seeking all premises to be met before conclusion
- Using the ML model for inference

Transductive learning:
- Better predictions with few labeled points
- No predictive model built, new prediction requires full calculation again



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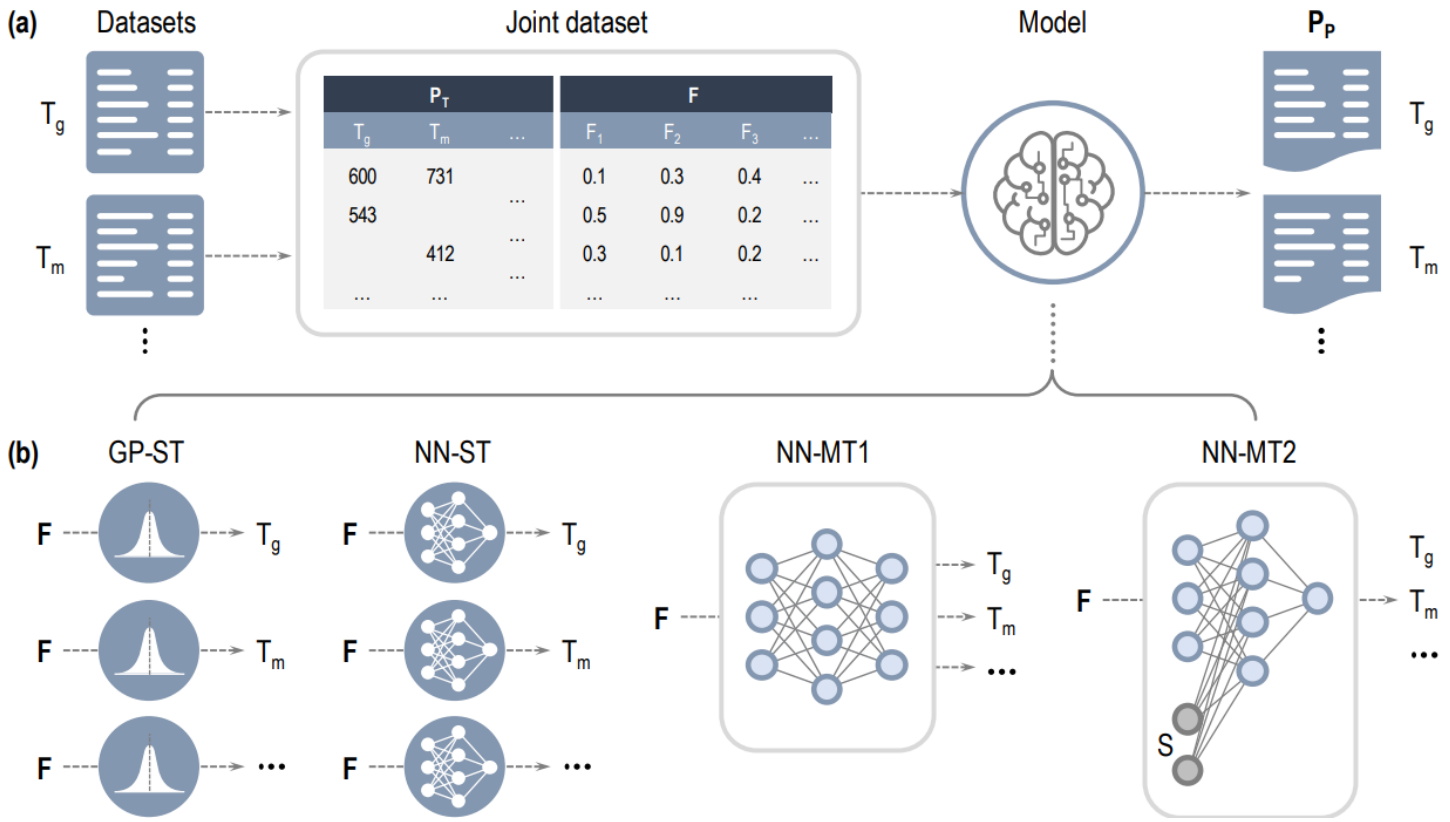
Multi-task learning tries to predict multiple outcomes

Training models together is more than efficient, it should improve overall performance!

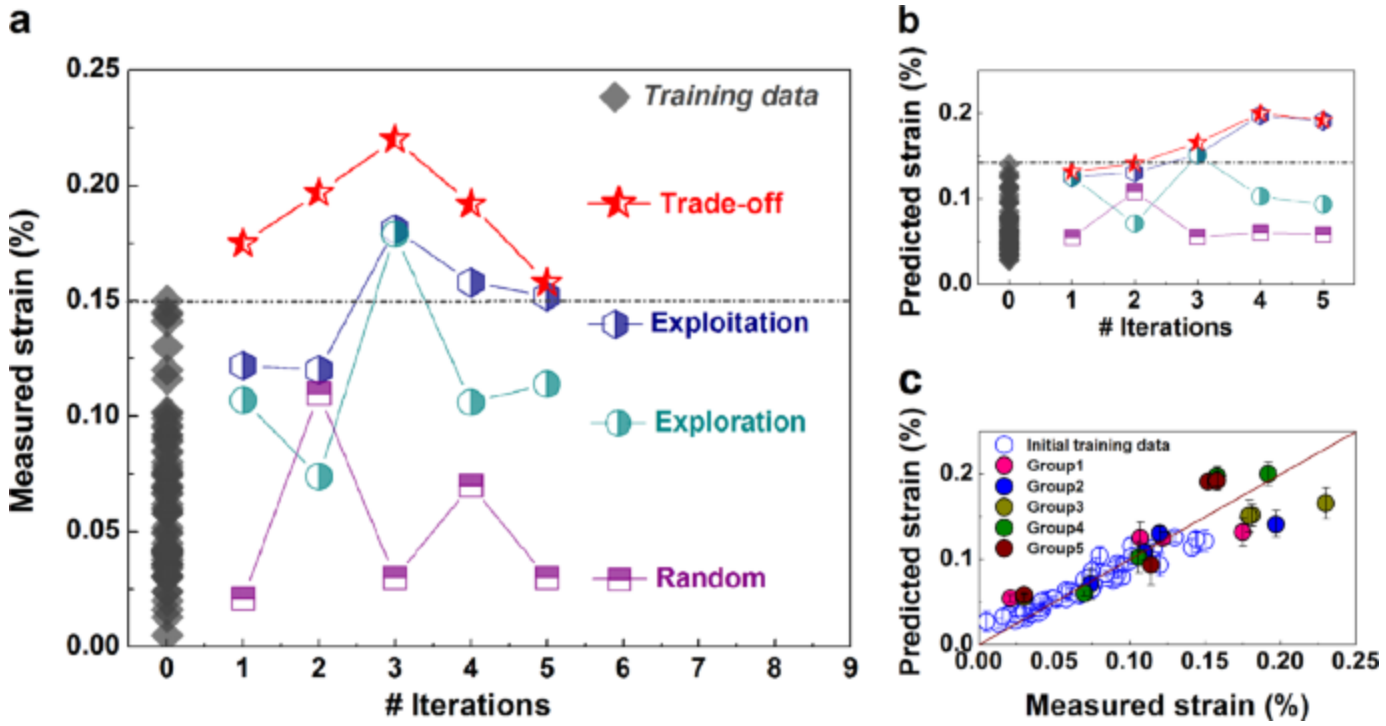
- Useful when dataset has abundance of input data labeled for one task but another task with much less labeled data.
- This will allow us to "borrow statistical strength" from tasks with lots of data and to share it with tasks with little data.
- Improves model generalizability



Active learning is a model that retrains constantly with new info

Active learning is a technique where the model is able to query an oracle during the learning process in order to resolve ambiguity during the learning process.

- Well-suited to small datasets where new data is expensive to generate or label
- Very efficient learner since model can ignore features it already understands well
- Similar to semi-supervised learning except new ground truth labels are generated instead of relying on models to label the unlabeled data.



Online learning is like active, but with a window of attention

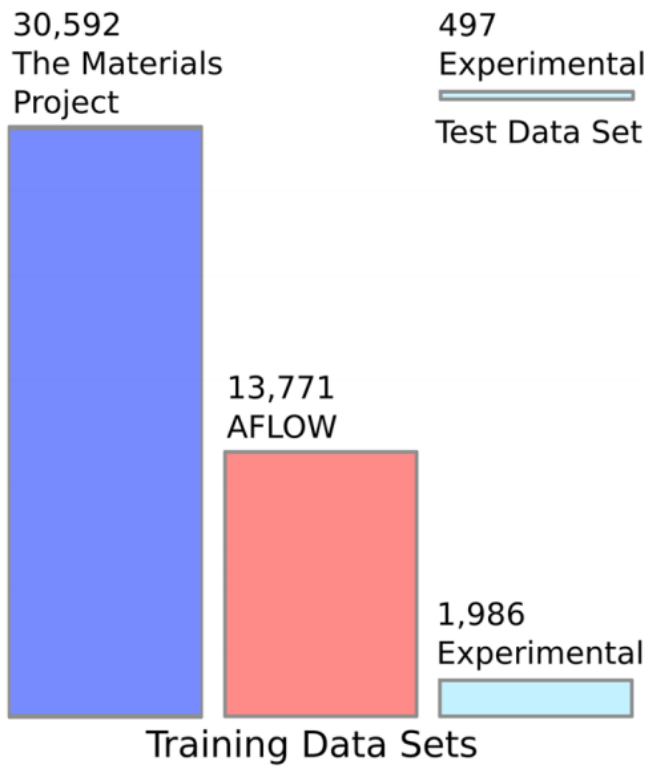
Online learning involves using the data available and updating the model directly before a prediction is required or after the last observation was made.

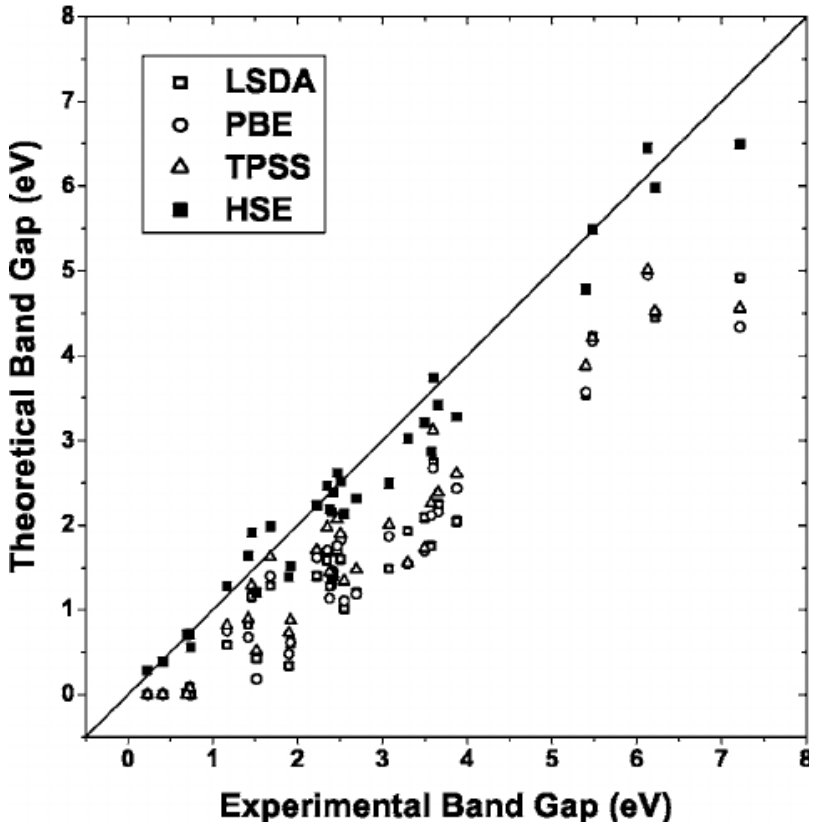
- Well-suited to sequential datasets where new data could be changing over time (consider shoe sales as a fad comes and goes)
- Possibly subject to catastrophic interference (catastrophic forgetting)

Transfer learning is training on one task and transferring learning over to another

In transfer learning, the learner must perform two or more different tasks, but we assume that many of the factors that explain the variations in task 1 are relevant to the variations that need to be captured for learning subsequent tasks.

- Well-suited for instances when first task has extensive data, but subsequent tasks have only limited data.
- Differs from multi-task learning by sequentially learning the different tasks

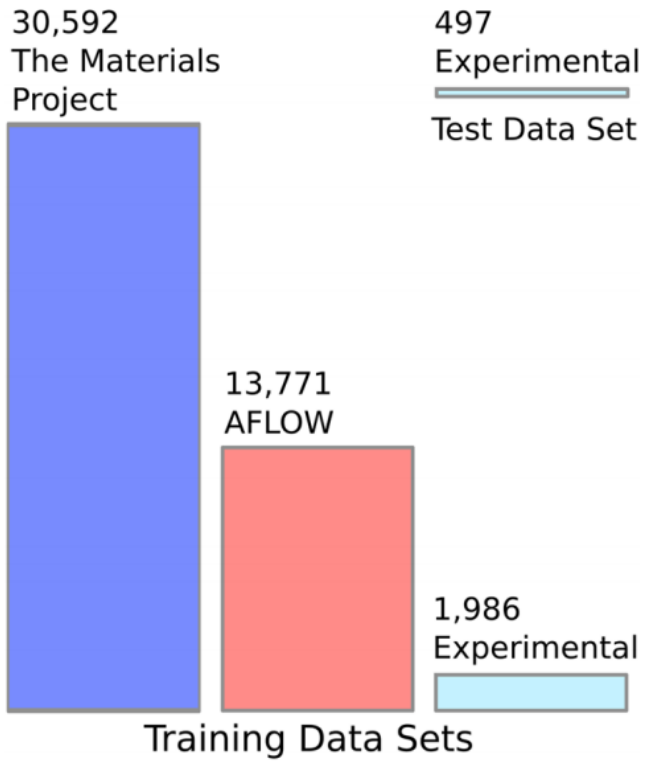


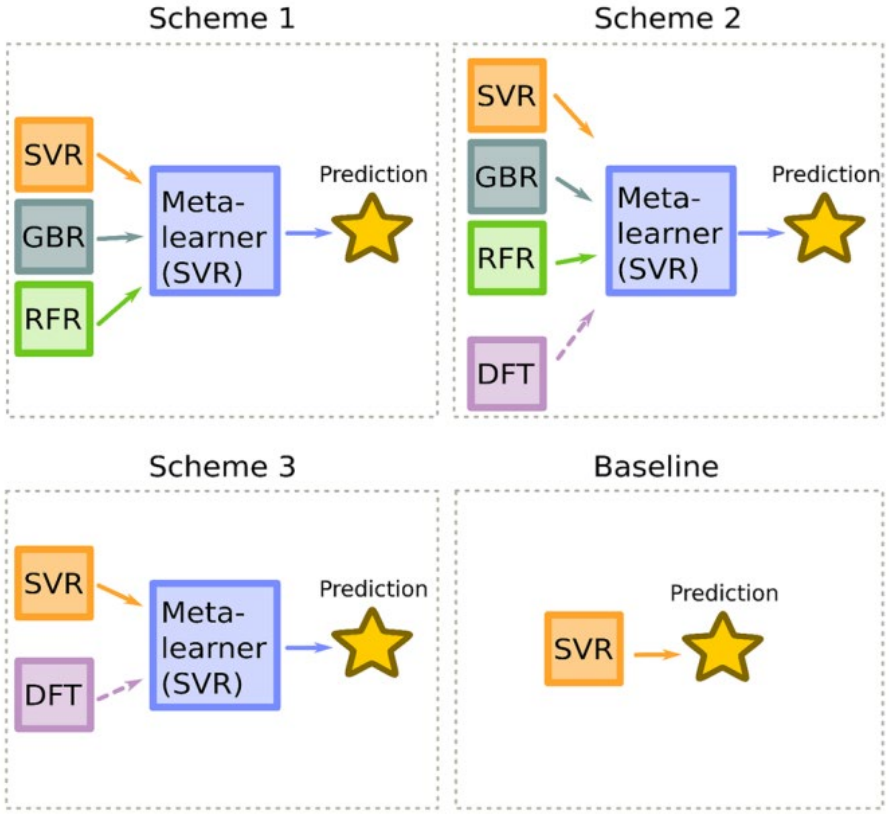


Ensemble learning is training multiple models and combining results

The objective of ensemble learning is to achieve better performance with the ensemble of models as compared to any individual model. This involves both deciding how to create models used in the ensemble and how to best combine the predictions from the ensemble members.

- Takes advantage of pros/cons of each algorithm or model type
- Can provide additional measure of uncertainty





We have many ML algorithms to choose from

Ensemble Techniques:
- Random forest
- Gradient boosted
- Adaboost
- Extra Trees

Bayesian:
- Kriging or GP
- Gaussian RF
- Bayesian NN

Neural Networks:
- ANN
- GAN
- CNN

Support Vector Machine:
- SVR
- Linear SVR

Linear Models:
- Lasso
- Ridge
- K nearest neighbors

Each ML algorithm has pros and cons

Ensemble Techniques:
- Fast learners
- Efficient
- Non-linear
- Problem with extrapolation
- Feature weights

Bayesian:
- Works well with small data
- Includes uncertainty
- “Physics informed” as priors utilized

Neural Networks:
- Fast (GPU)
- Feature-free
- GANs
- High accuracy
- Blackest box
- overfitting

Support Vector Machine:
- Kernel selection
- Good metrics
- Hinge loss
- Scales poorly

Linear Models:
- Interpretable
- Fast
- Not suitable for many problems (linear vs non-linear)

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