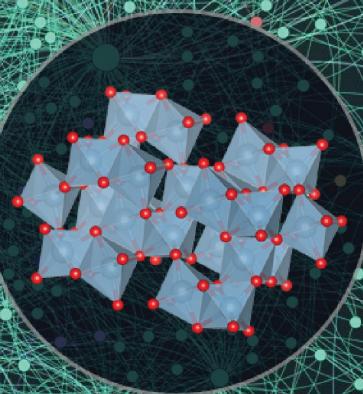
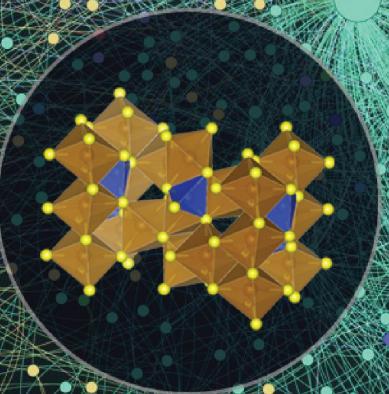
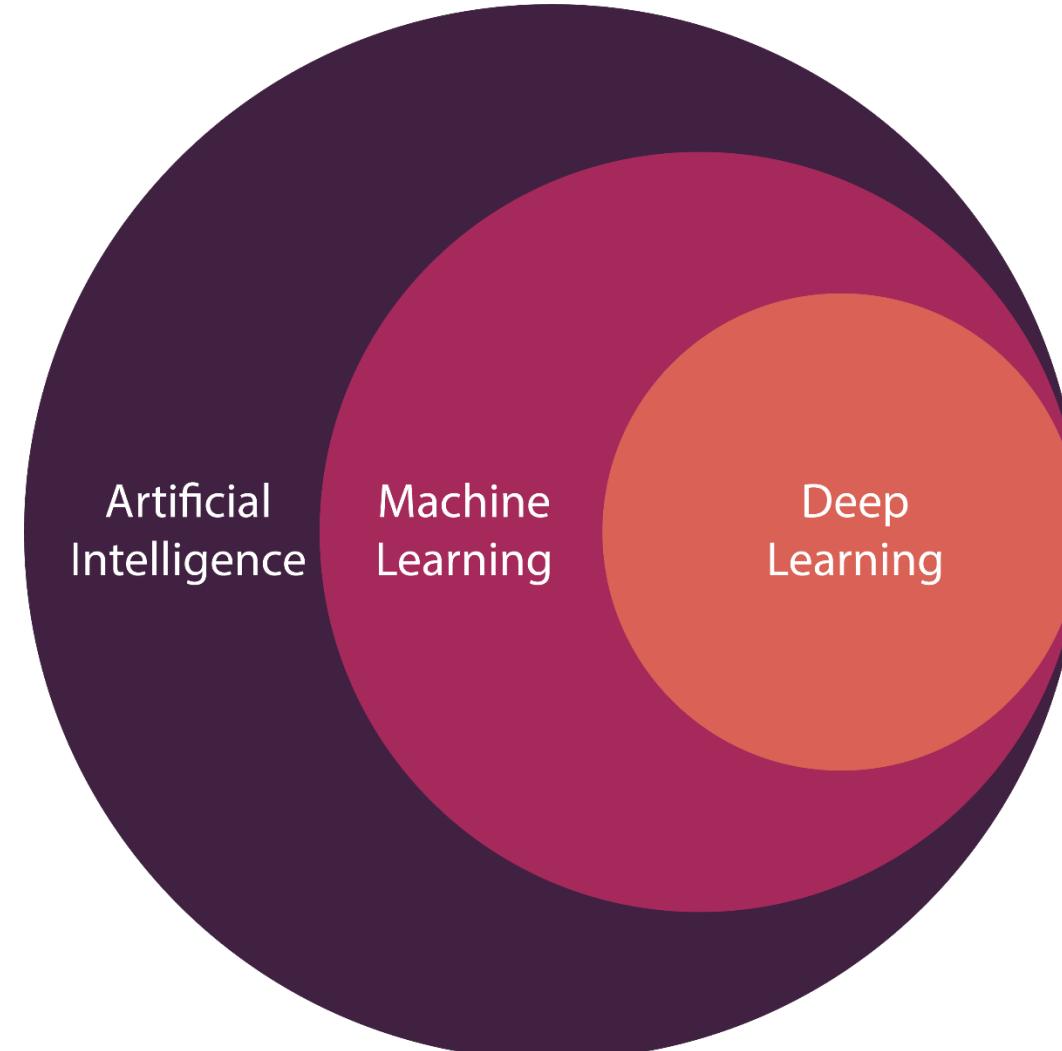


Machine Learning: Tasks and Types



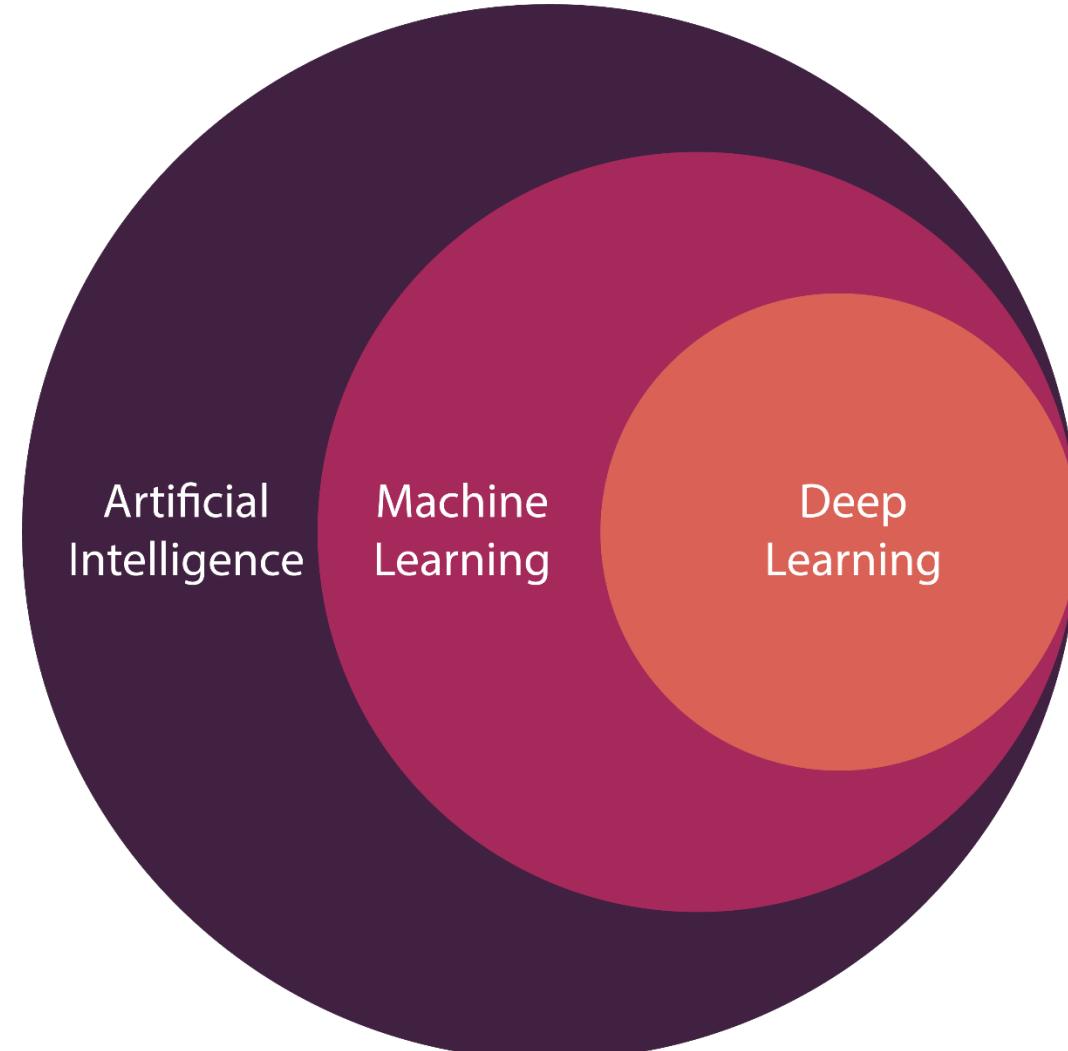
Machine learning is learning from patterns in data

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.



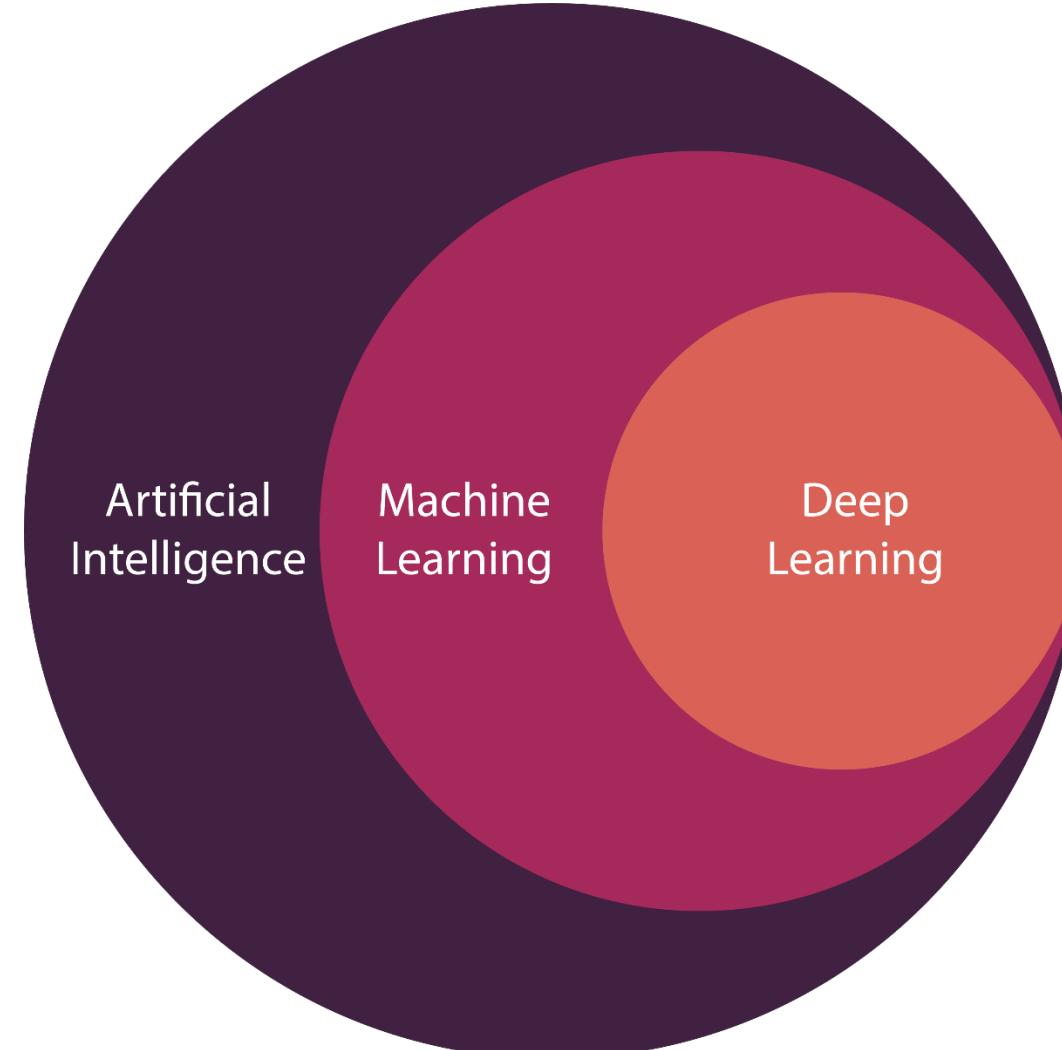
Machine learning is learning from patterns in data

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.

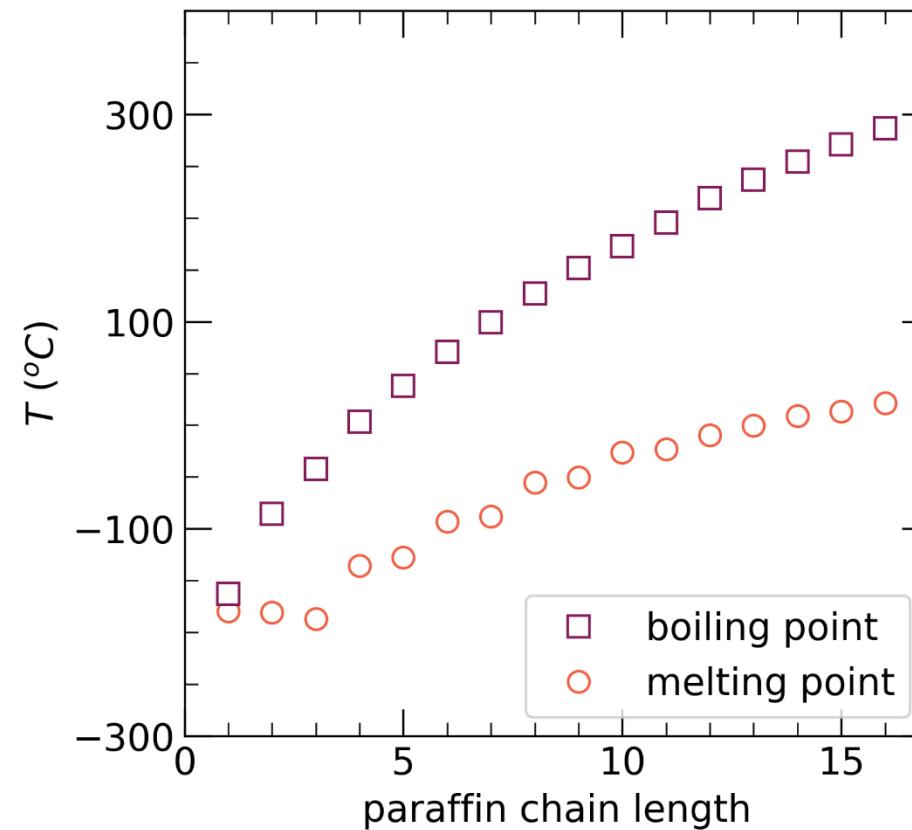


Machine learning is learning from patterns in data

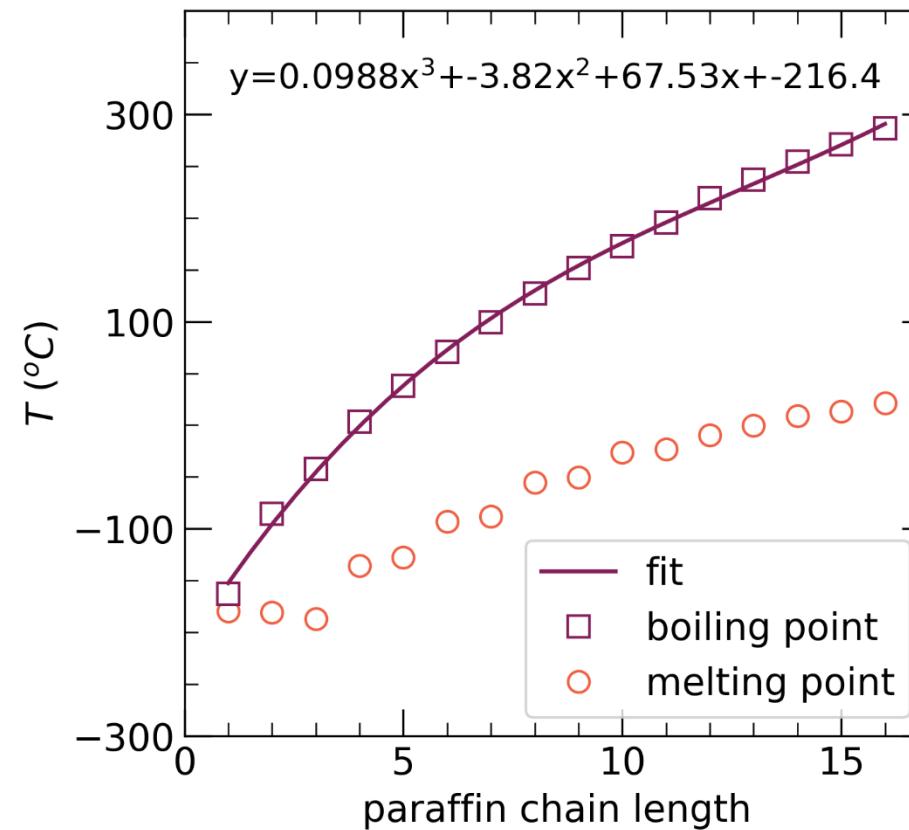
Deep learning: part of a broader family of machine learning methods that imitates the workings of the human brain in processing data and creating patterns for use in decision making.



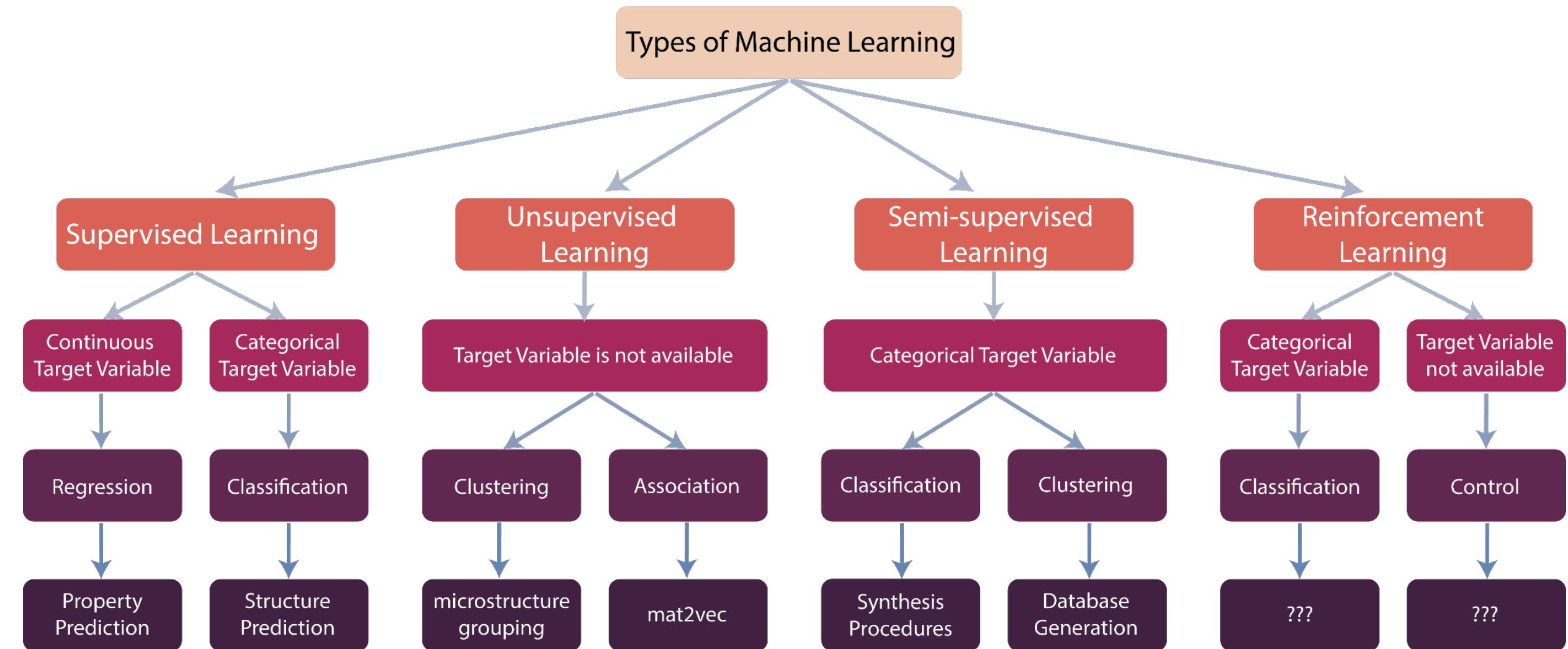
Materials scientists have long noticed patterns in data



Empirical relationships are correlations that may not be supported by theory



Materials scientists are using nearly all types of machine learning



There are even more types!



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Learning Problems

- 1. Supervised Learning
- 2. Unsupervised Learning
- 3. Reinforcement Learning

Hybrid Learning Problems

- 4. Semi-Supervised Learning
- 5. Self-Supervised Learning
- 6. Multi-Instance Learning

Statistical Inference

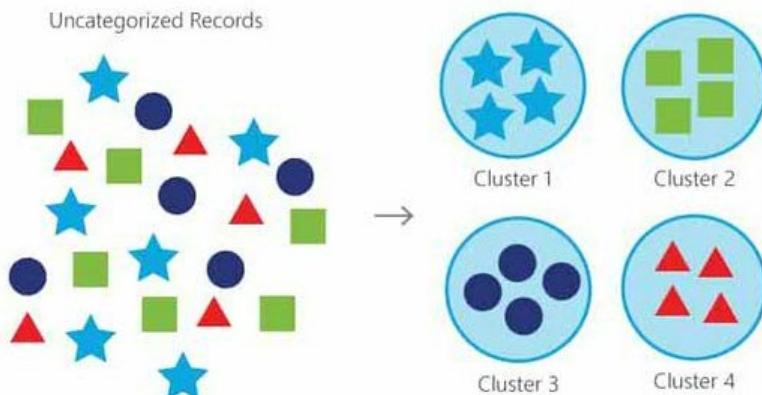
- 7. Inductive Learning
- 8. Deductive Inference
- 9. Transductive Learning

Learning Techniques

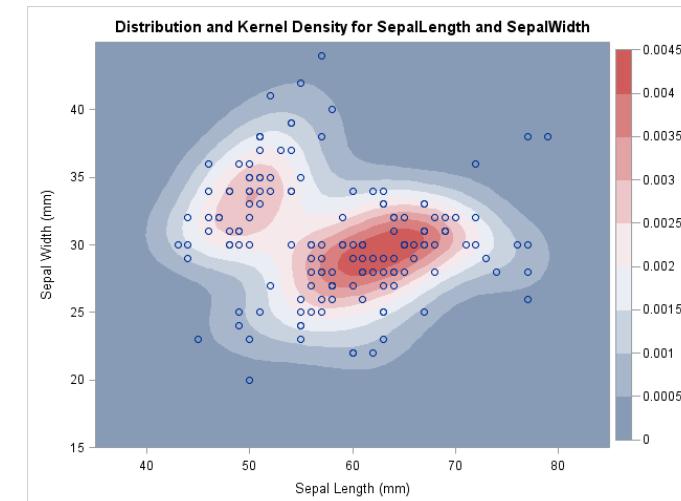
- 10. Multi-Task Learning
- 11. Active Learning
- 12. Online Learning
- 13. Transfer Learning
- 14. Ensemble Learning

Unsupervised learning includes classification, clustering, density estimation, projection

Clustering



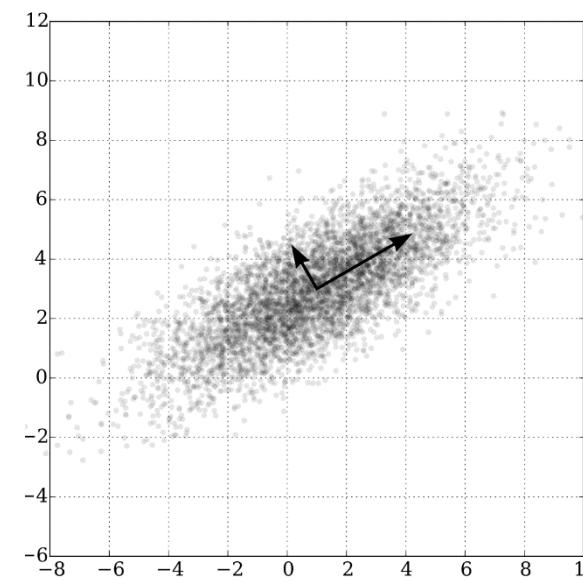
Density Estimation



Visualization



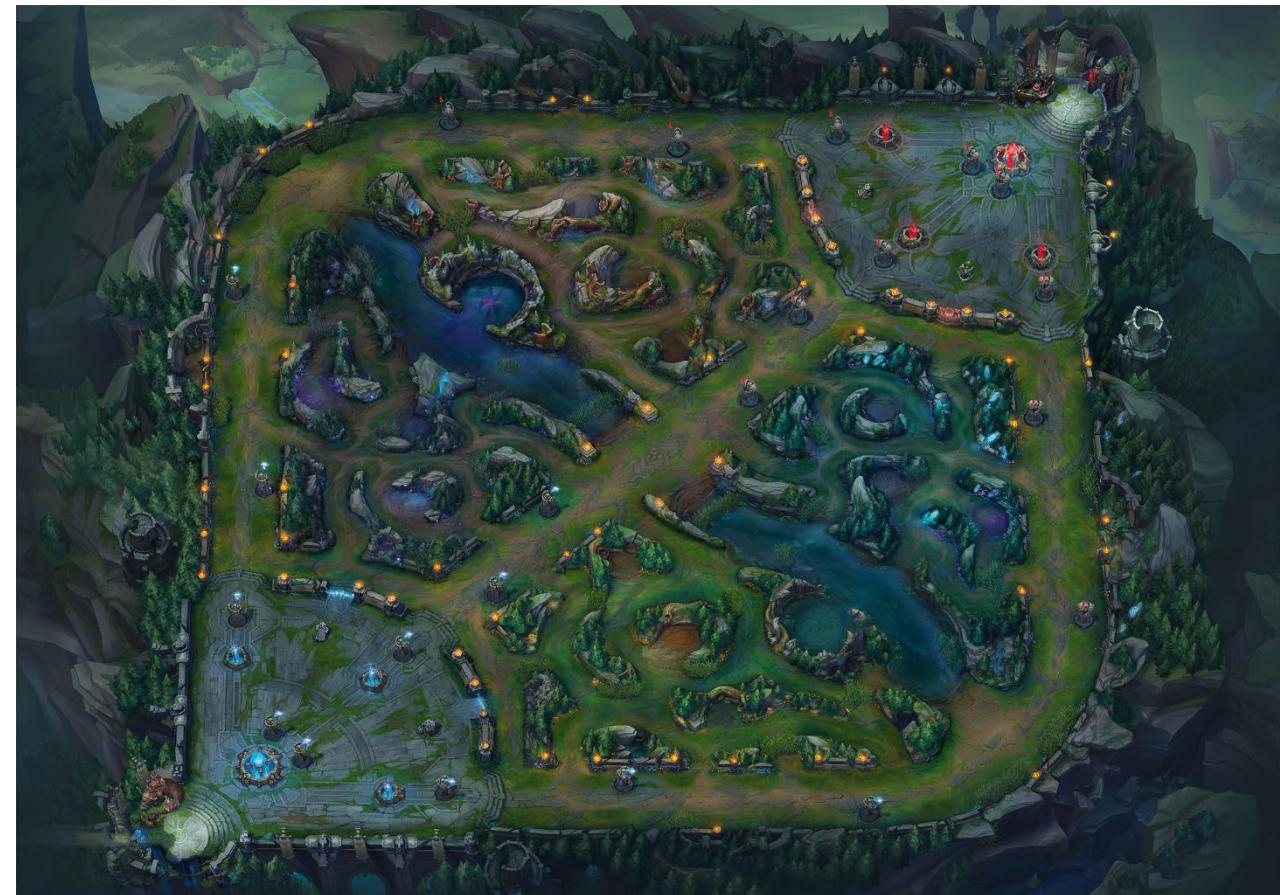
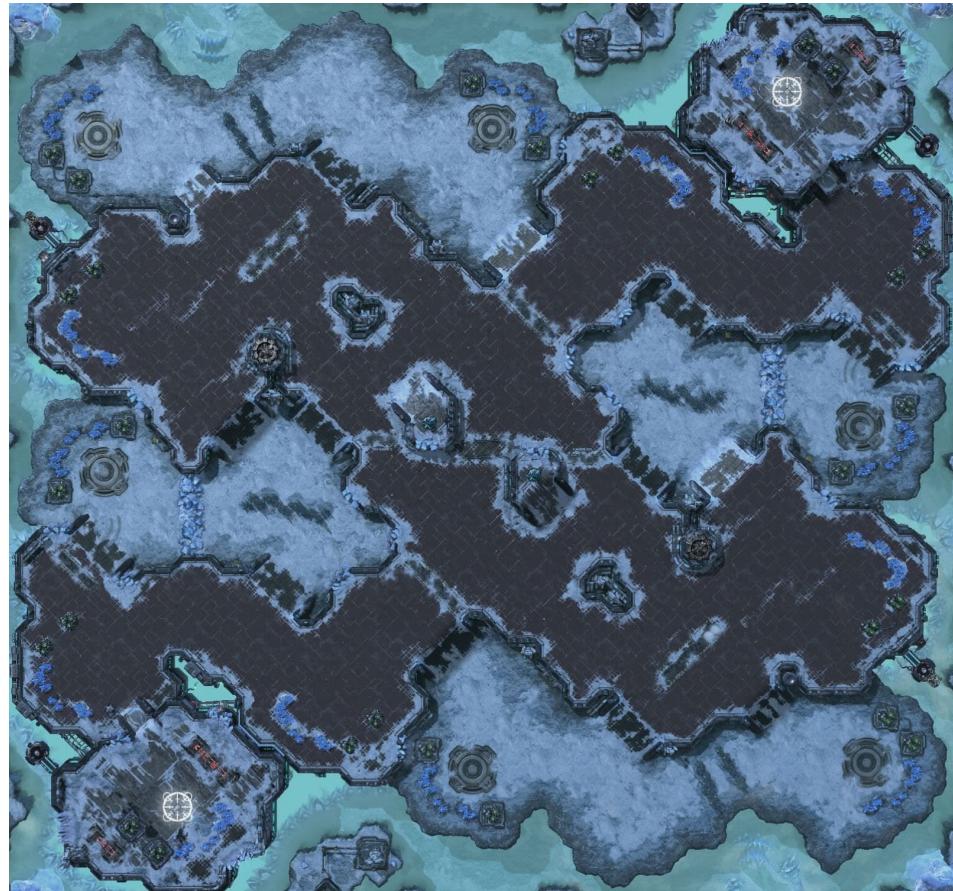
Projection



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 lines between learning types



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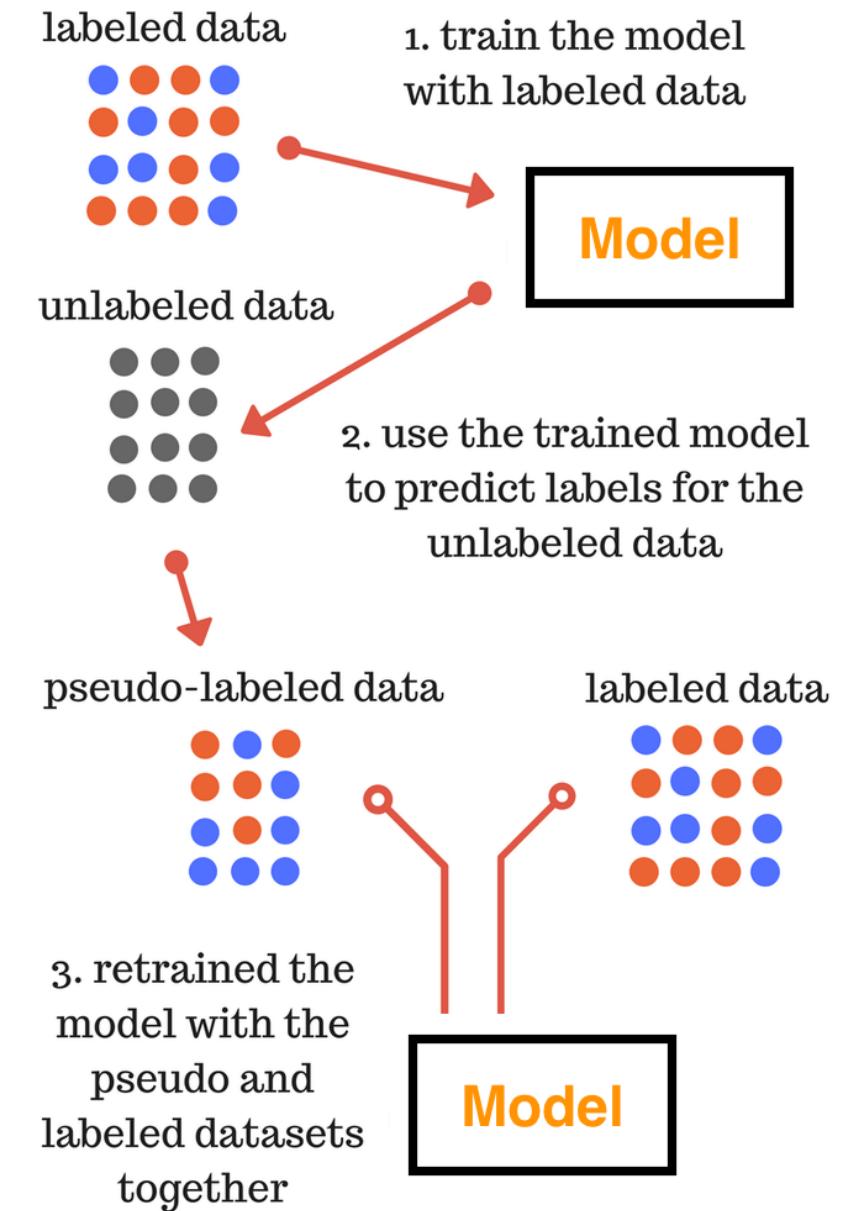
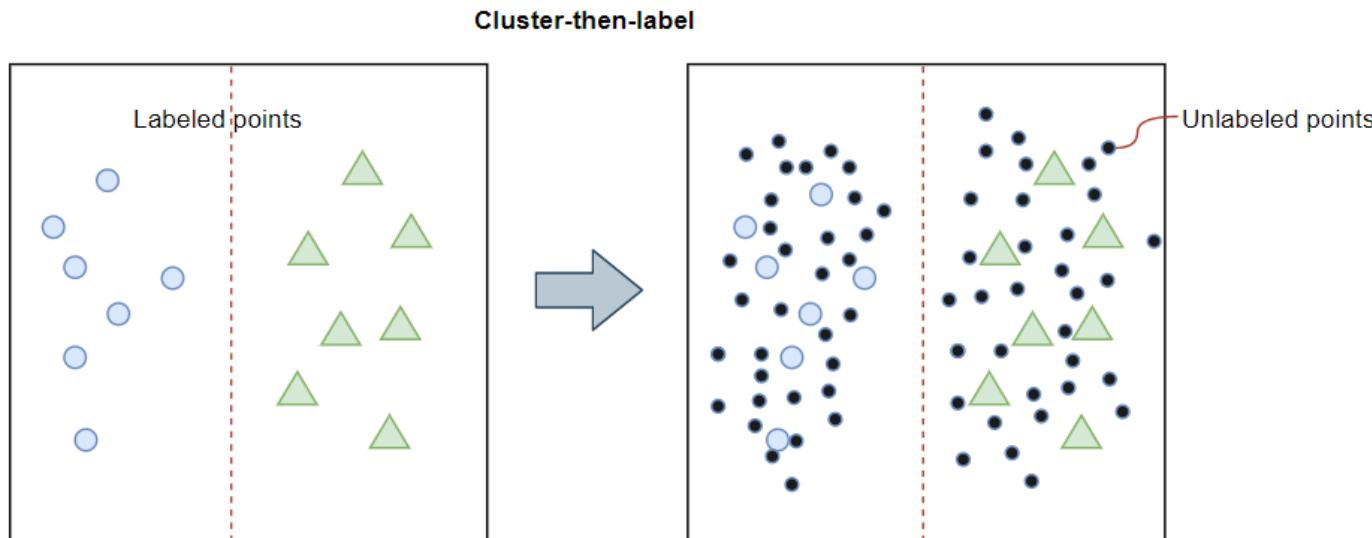
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Learning Techniques

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Semi-supervised learning requires making the most of only partially labeled data

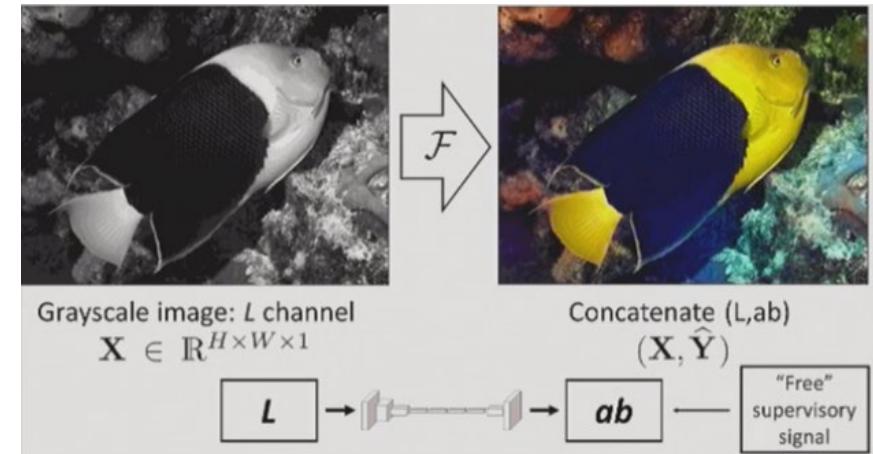
Algorithms are used to learn relationships between labeled and unlabeled data to then use all the data



Self-supervised learning is unsupervised learning framed as supervised learning problem

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

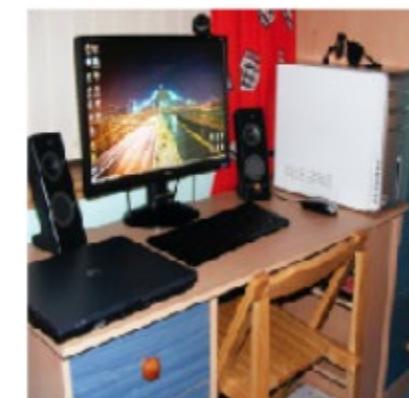


Inpainting

Input



Target



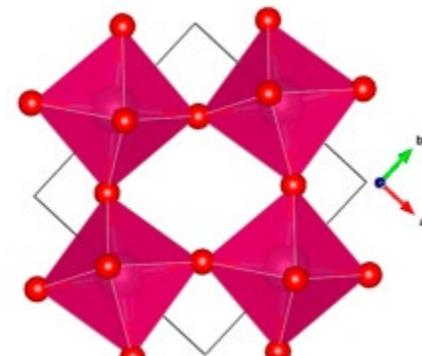
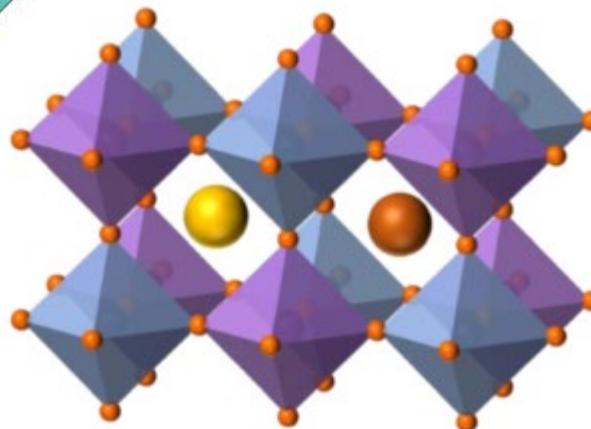
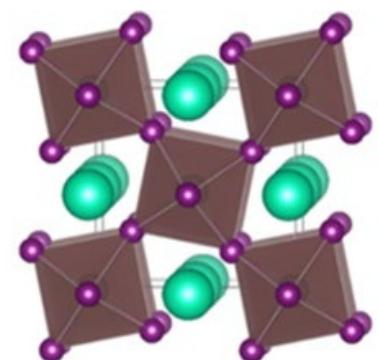
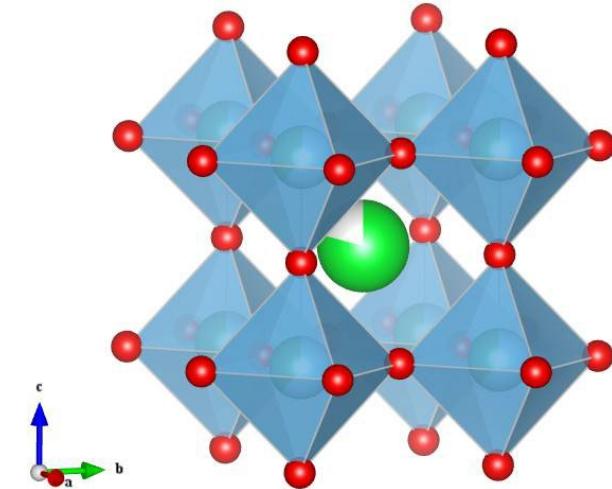
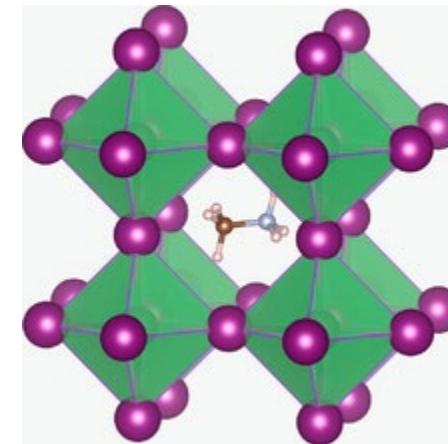
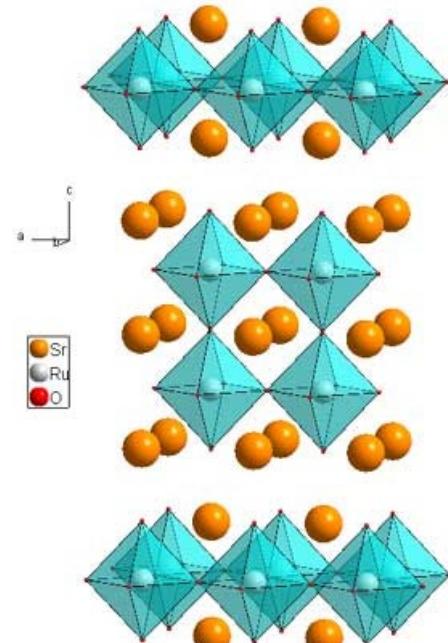
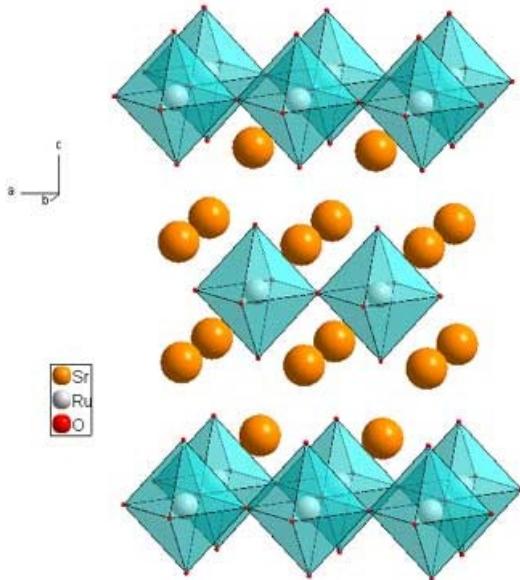
Model Output



Multi-instance learning is supervised learning where “bags” of samples are labeled

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:

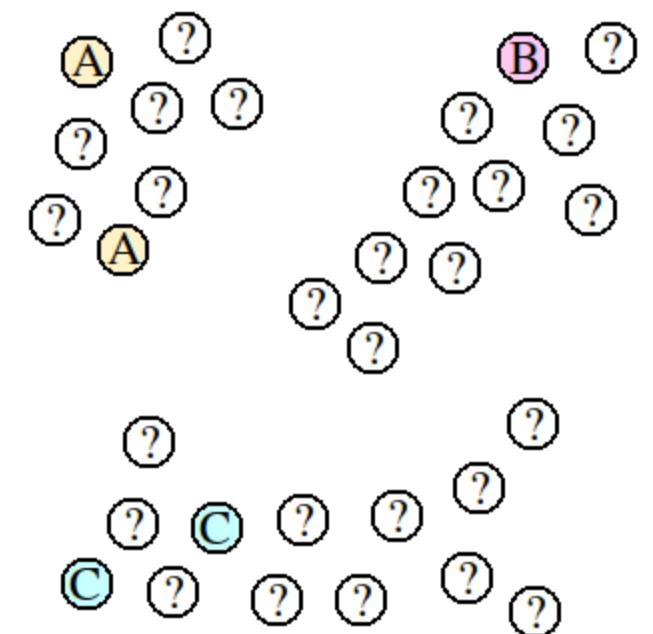
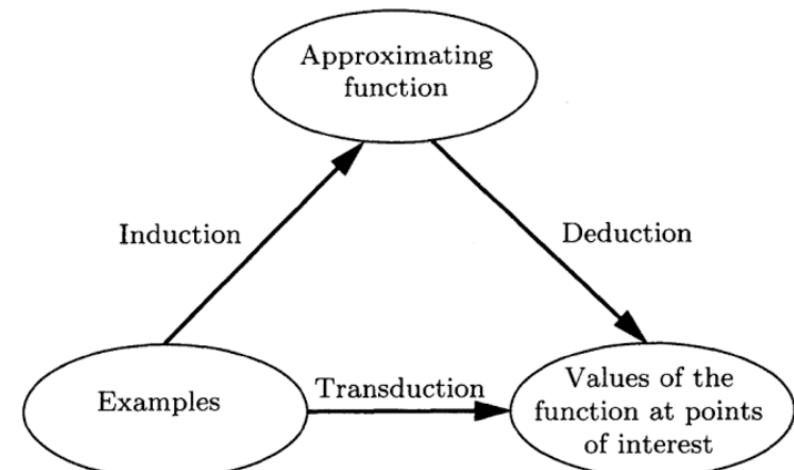
- Model learns the general rules
- Draw general conclusions about future from past examples
- Fitting the ML model

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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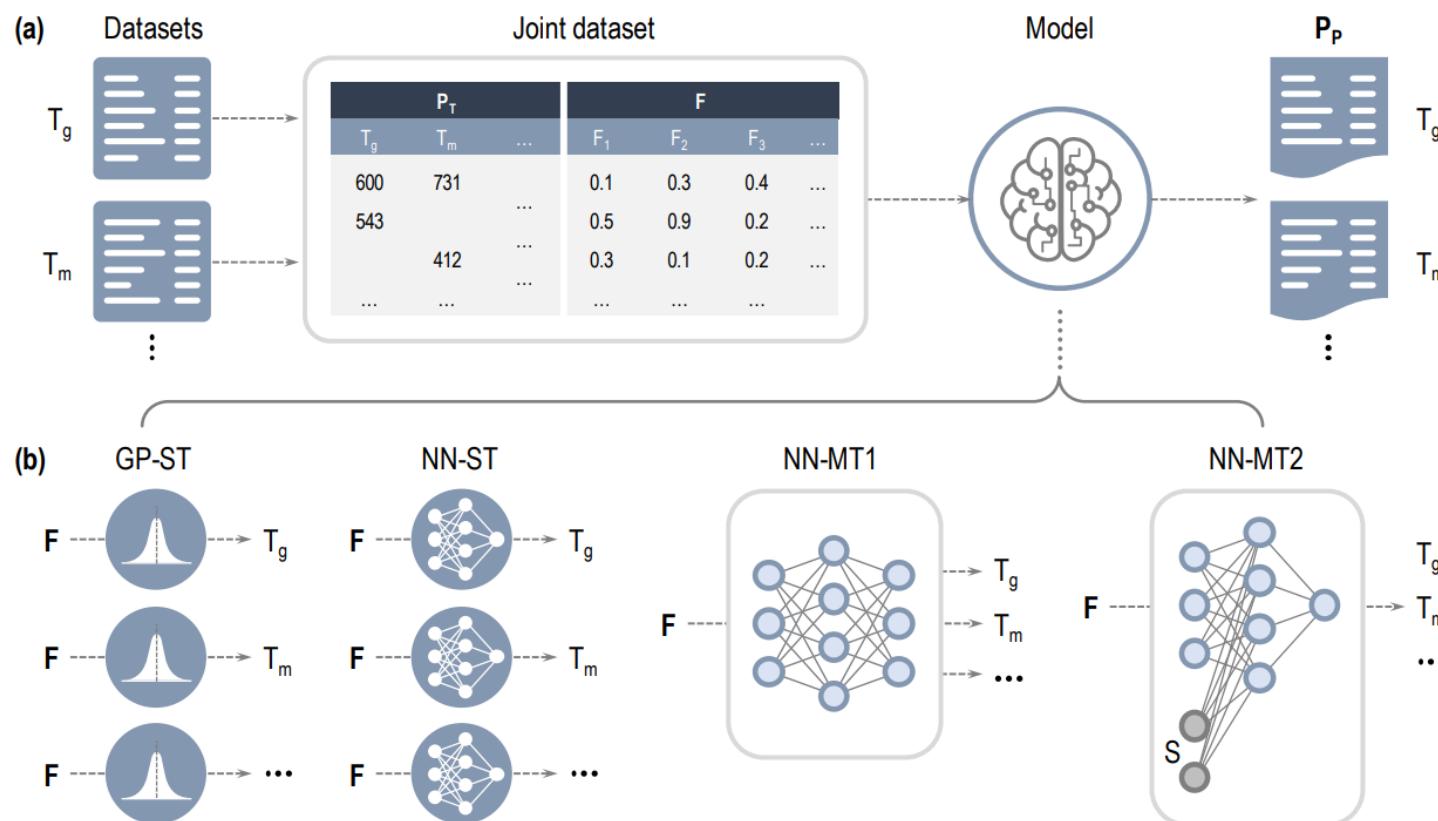
Learning Techniques

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Multi-task learning is fitting a model to one dataset with multiple related problems

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

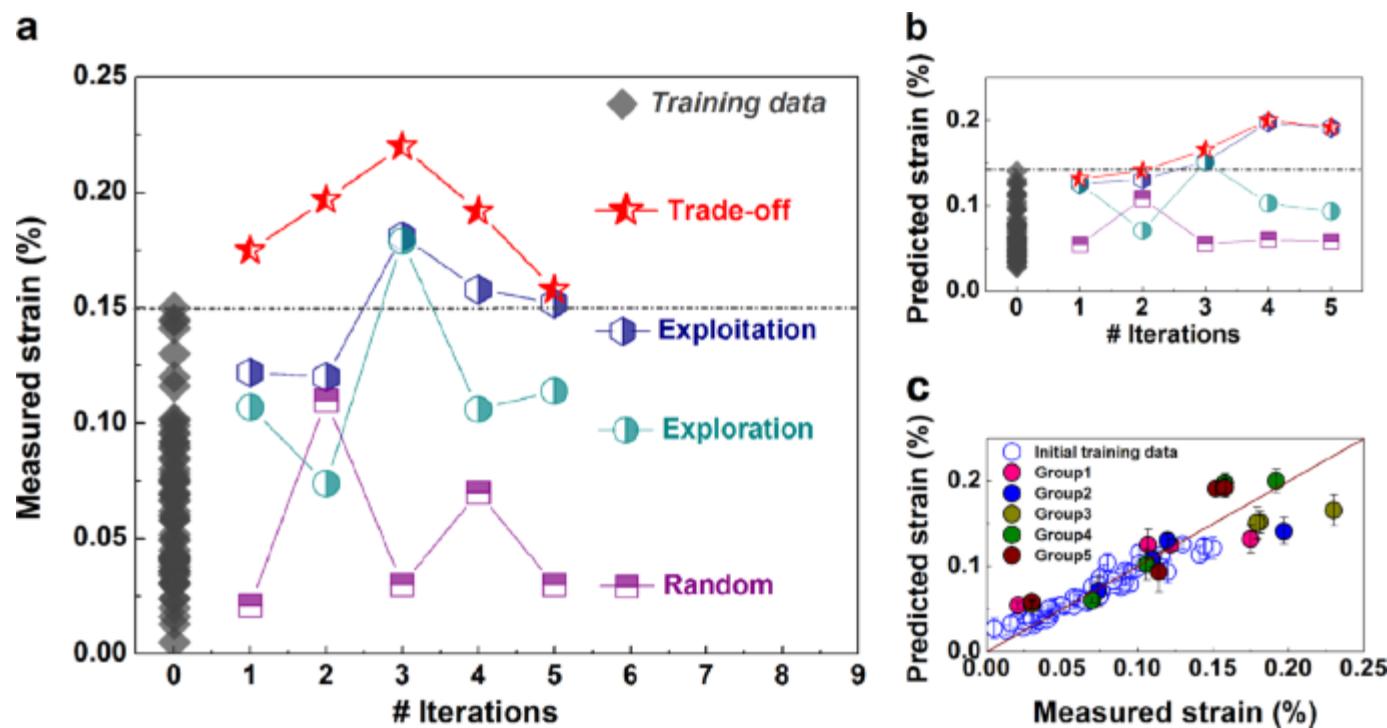
- Useful when dataset has abundance of input data labeled for one task but another task with much less labeled data.
- This will allow us to “borrow statistical strength” from tasks with lots of data and to share it with tasks with little data.
- Improves model generalizability



Active learning allows for very efficient learning when new data points are expensive

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 involves continual updating of the model after each data point acquisition

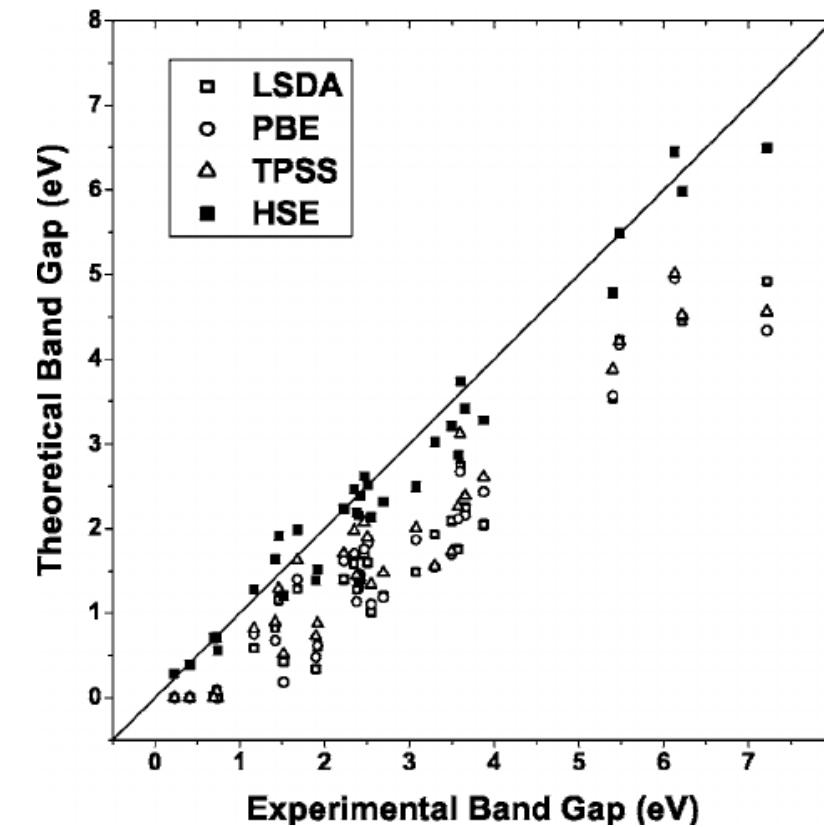
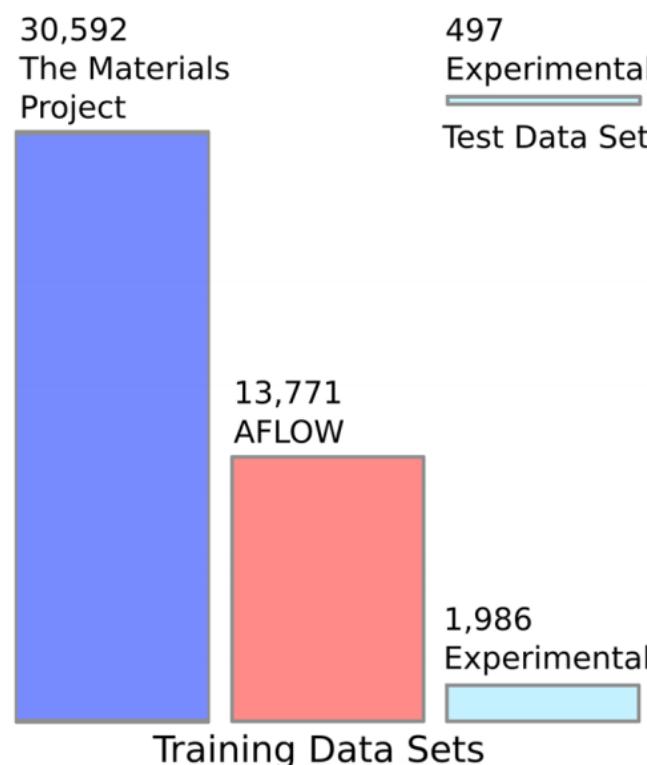
Online learning involves using the data available and updating the model directly before a prediction is required or after the last observation was made.

- 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 when a trained model can be applied to another related task

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.

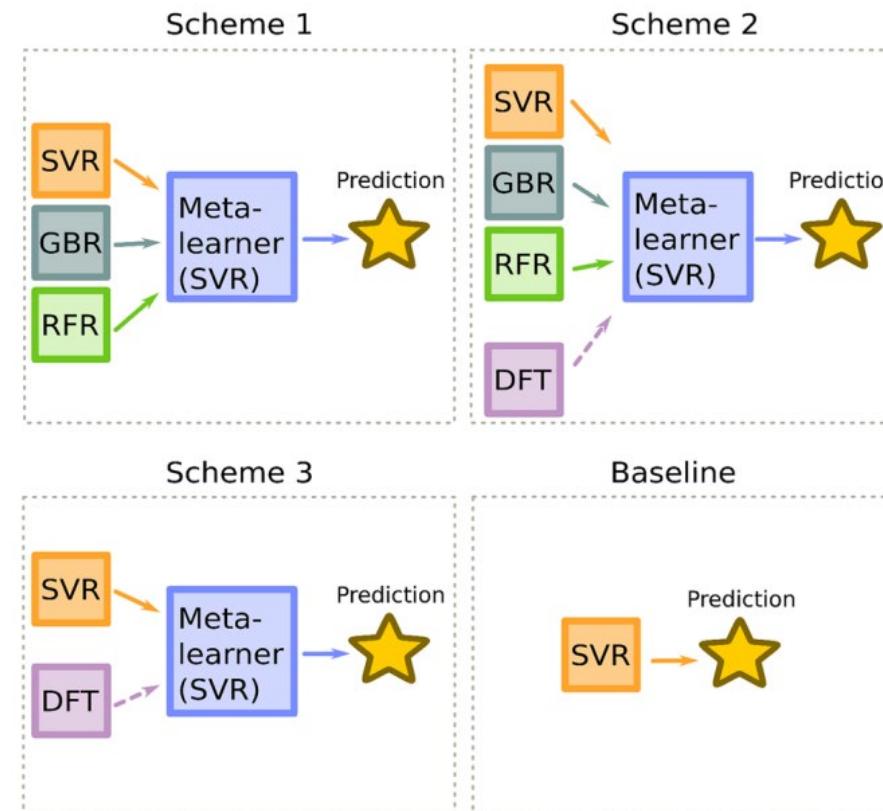
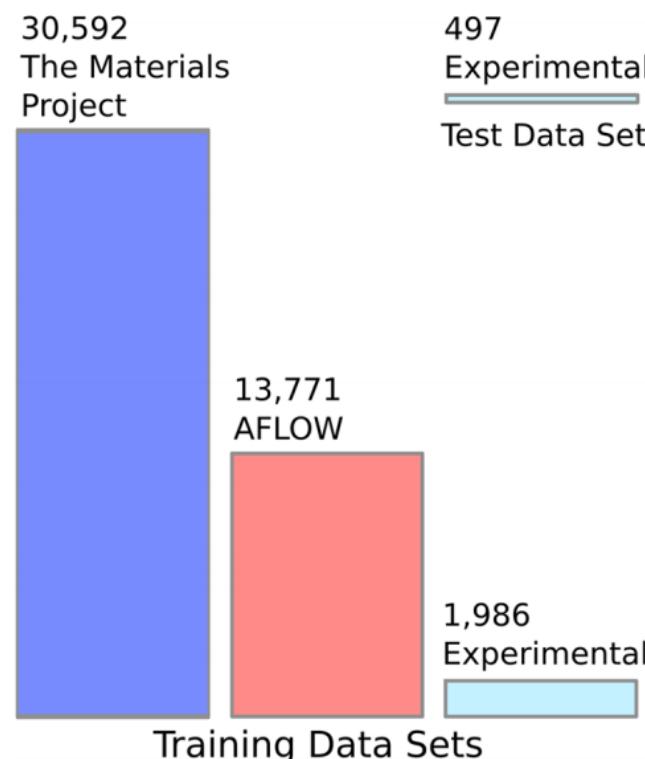
- Well-suited for instances when first task has extensive data, but subsequent tasks have only limited data.
- Differs from multi-task learning by sequentially learning the different tasks



Ensemble learning is when multiple models are trained on data and the results are combined

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



There are multiple types of machine learning algorithms available

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

There are multiple types of machine learning algorithms available

Ensemble Techniques:

- Fast learners
- Efficient (parallelization)
- 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)

Featurization in Materials Informatics

