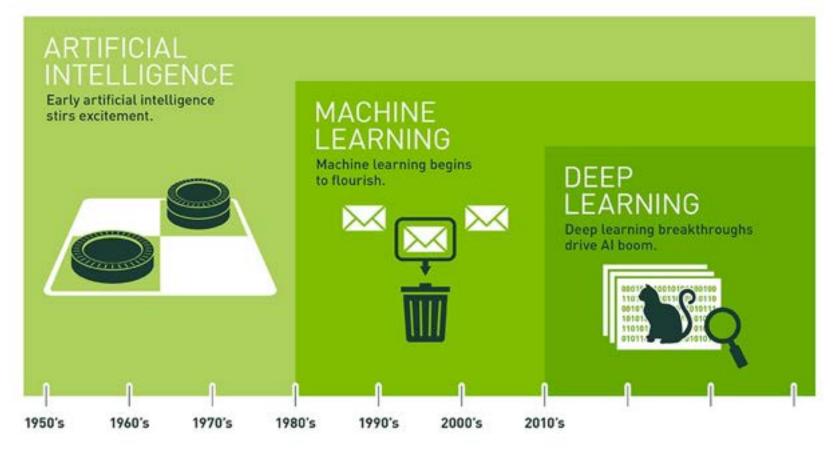


Dawei Mu



NCSA | National Center for Supercomputing Applications

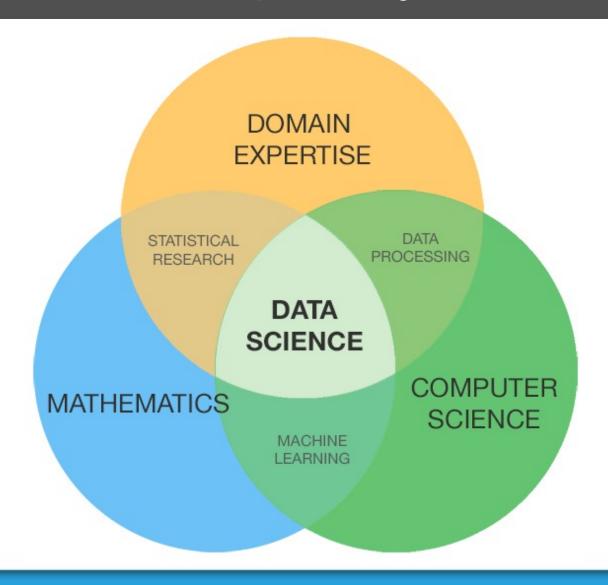
Introduction of AI / ML / DL



Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.



This is an Interdisciplinary Field



But Why Now?

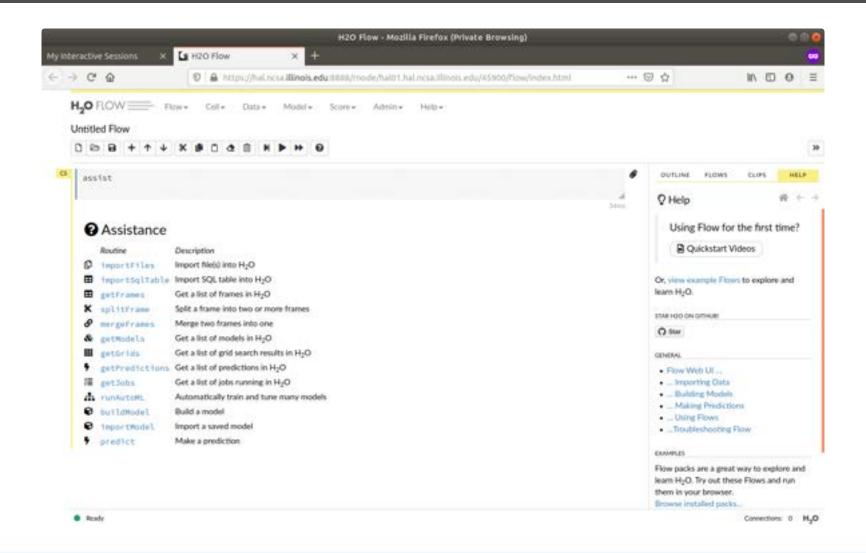
- Hardware: high-performance GPUs, TPUs
- Datasets: large datasets collected from internet
- Algorithmic advances: activation functions, optimization schemes.

Introduction of H2O

- What is H2O.ai?
 - H2O.ai is the company behind open-source Machine Learning (ML) products like H2O, aimed to make ML easier for all.
- What is H2O?
 - An open source, Java-based, in-memory, distributed, ML and predictive analytics platform allowing you to build and productionize ML models.
 - Contains supervised and unsupervised models in R and Python, as well as a simple to use web-UI called Flow.



H2O Flow

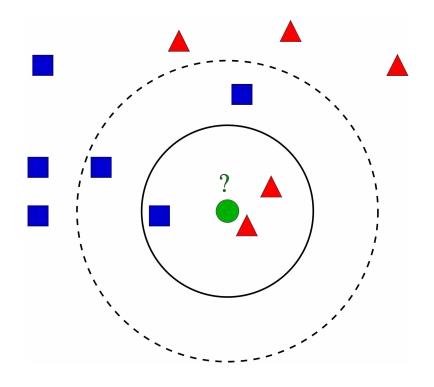


Common Machine Learning Algorithms

- Machine Learning has 3 main functions: classification, prediction, clustering.
- Big 3 Basic Algorithms
 - K-Nearest Neighbor
 - Linear Regression
 - K-Mean Clustering
- Other Common Algorithms
 - Decision Tree / Random Forest / Naive Bayes / Support Vector Machine

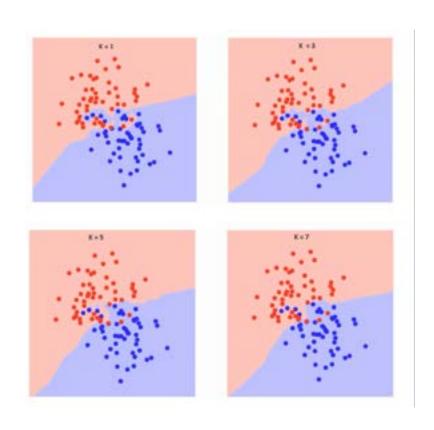
K Nearest Neighbors

- An object is classified by a majority vote of its neighbors
 - One of the simplest classification algorithm.
 - Often used in classification.
 - Computed from a simple majority vote of the nearest neighbors of each point.
 - K is constant specified by user.
 - KNN is computationally expensive.



K Nearest Neighbors

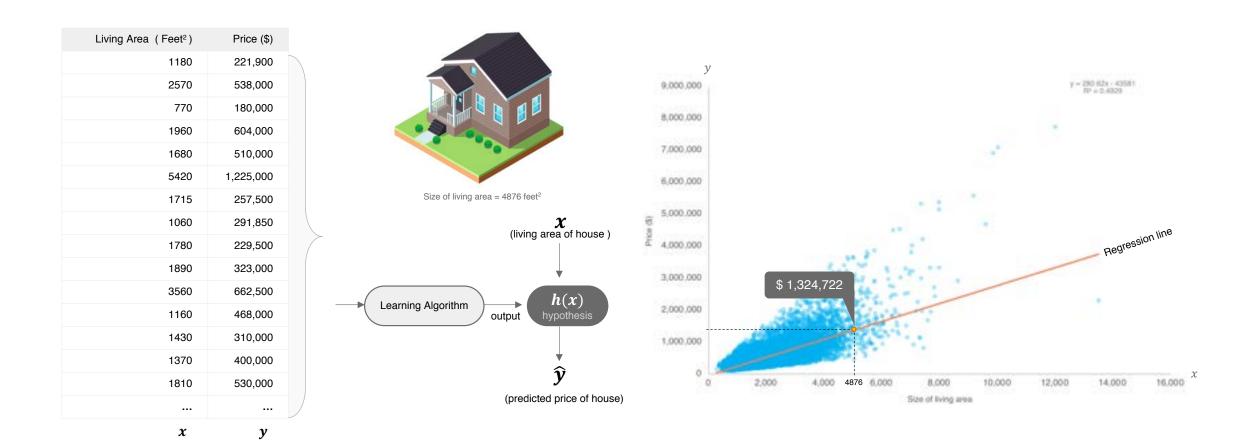
- How do we choose the factor K
 - Choosing K could be a challenge.
 - Boundary becomes smoother with increasing value of K.



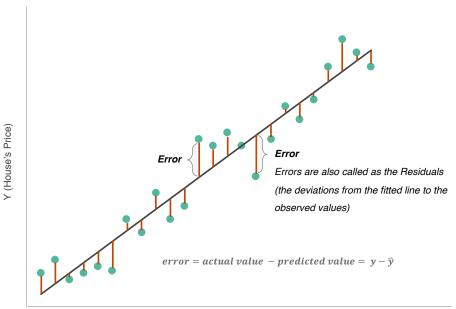
K Nearest Neighbors

Pros and Cons of KNN

- Pros
 - It is beautifully simple and logical
- Cons
 - It may be driven by the choice of K, which may be a bad choice.
 - Generally, larger values of K reduce the effect of noise on the classification, but make boundaries between classes less distinct.
 - The accuracy of the algorithm can be severely degraded by the presence of noisy or irrelevant features.
 - It is important to review the sensitivity of the solution to different values of K.



- The goal of linear regression is to find the best fit line.
 - minimizes the sum of the "squared differences" between the points and the regression line.



X (Size of House)

$$h(x) = \theta_0 + \theta_1 x$$

How to find the appropriate parameter θ_0 and θ_1 in order to minimize the error – i.e. cost function $J(\theta_0, \theta_1)$

To minimize $\boldsymbol{J}(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{n} (y_i - \widehat{y}_i)^2$

Cost function (also known as Loss Function)

- *m* is number of training instances
- \widehat{y}_i (y hat) is the predicted value
- y_i is the actual value

• Normal Equation (Closed Form)

It's a method to solve for θ analytically.

Using a direct "closed-form" equation that directly computes the model parameters that best fit the model to the training set (i.e., the model parameters that minimize the cost function over the training set). ¹

It's suitable for small feature set (e.g. < 1000 features).

Gradient Descent

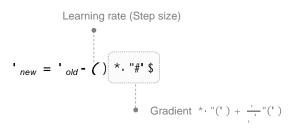
Using an iterative optimization approach, called Gradient Descent (GD), that gradually tweaks the model parameters to minimize the cost function over the training set, eventually converging to the same set of parameters as the first method. ²

Gradient Descent is better choice than Normal Equation when there are a large number of features, or too many training instances to fit in memory.

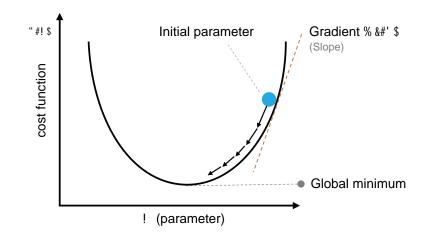
• A gradient is the slope of a function at a specific point. The gradient of loss function/cost function is equal to the derivative (slope) of the curve.

Gradient Descent algorithm

The parameter are iteratively updated in the following equation:



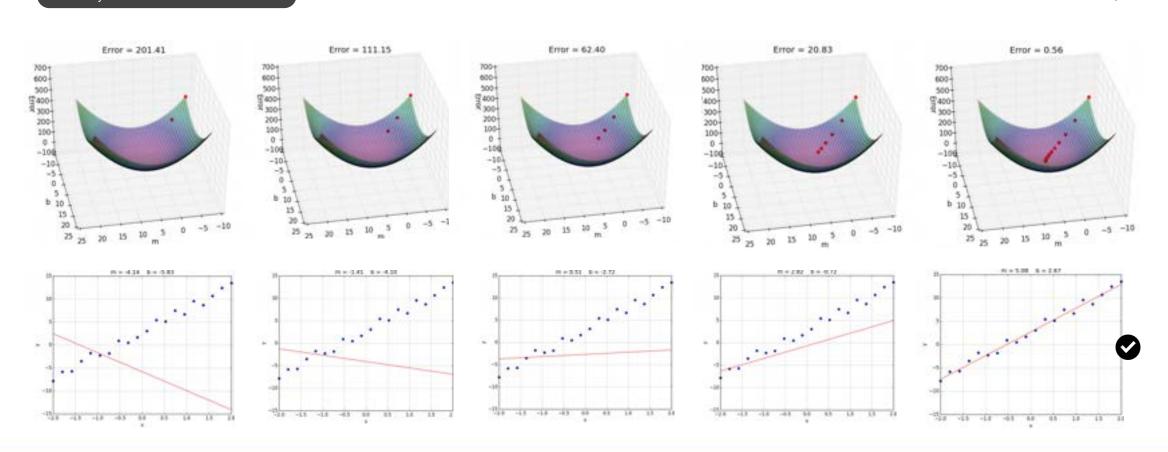
- 1. Pick a value for the learning rate!
- 2. Start with a random point '
- Calculate the gradient * "#" \$ at the point ' . Follow the opposite direction of gradient to get new parameter ' new
- 4. Repeat until the cost function converges to the minimum



In this example, initially the slope is large and positive. So, in the update equation, ! is reduced. As ! keeps getting reduced, notice that the gradient also reduces, and hence the updates become smaller and smaller and eventually, it converges to the minimum.¹

Find the best-fit line through Gradient Descent algorithm.

Iteratively find the minimum of cost function

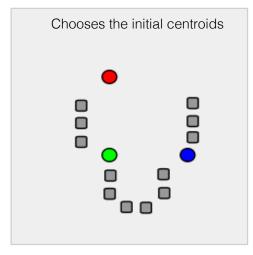


K-Mean Clustering

- Discover the structure within the un-labeled data.
- Clustering is a technique for finding similarity groups in a data, called clusters.
- It attempts to group individuals in a population together by similarity, but not driven by a specific purpose.
- Clustering is often called an unsupervised learning, as you don't have prescribed labels in the data and no class values denoting a priori grouping of the data instances are given.

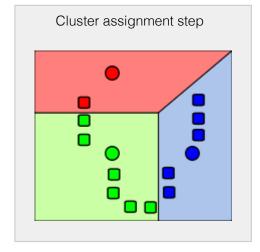
K-Mean Clustering

A graphical view of K-means algorithm.





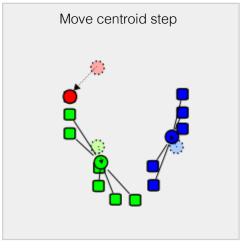
k initial "means" (in this case *k*=3) are randomly generated within the data domain (shown in color).





k clusters are created by associating every observation with the nearest mean.

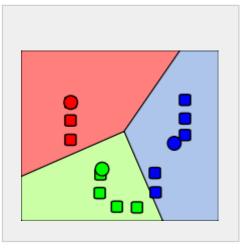
In Cluster assignment step, the algorithm goes through each of the data points and depending on which cluster is closer, whether the red cluster centroid or the blue cluster centroid or the green; It assigns the data points to one of the three cluster centroids.





The centroid of each of the *k* clusters becomes the new mean.

In move centroid step, K-means moves the centroids to the average of the points in a cluster. In other words, the algorithm calculates the average of all the points in a cluster and moves the centroid to that average location.





Steps 2 and 3 are repeated until convergence has been reached

In other words, it repeats until the centroids do not move significantly.

K-Mean Clustering

- Weakness of K-means
 - The number of cluster "k" must be specified in advance.
 - Sensitive to initial centroids selection, which leads to unwanted solution.
 - k-means can only handle numerical data.
 - The algorithm may get stuck in the local optimum.
 - Sensitive to outliers and noise, which results in an inaccurate partition.
 - K-means cannot handle non-globular clusters or clusters of different sizes and densities.

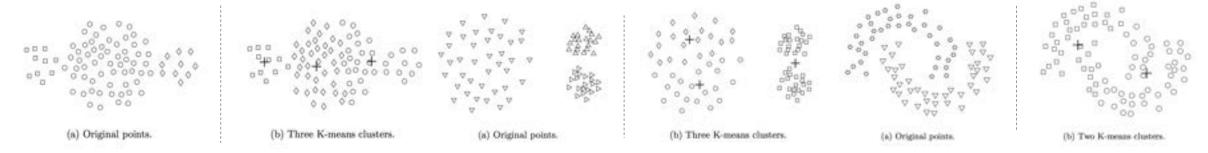


Figure 1: K-means with clusters of different size

Figure 2: K-means with clusters of different density

Figure 3: K-means with non-globular clusters



Naïve Bayes

- Naïve Bayes is a simple but important probabilistic model
 - It based on applying Bayes' theorem with the "naive" assumption of independence between the features.
 - It computes the conditional probability distribution of each feature given label, and then it applies Bayes' theorem to compute the conditional probability distribution of label given an observation and use it for prediction.
 - It classifies new data based on the highest probability of its belonging to a particular class.
 - Naive Bayes learners and classifiers can be extremely fast compared to more sophisticated methods.



Naïve Bayes

$$P(A \mid B) = rac{P(B \mid A) \, P(A)}{P(B)}$$

Day	Outlook	Temperature	Humidity	Wind	Play Tennis ?
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

Outlook	Play = Yes	Play = No	Total
Sunny	2/9	3/5	5/14
Overcast	4/9	0/5	4/14
Rain	3/9	2/5	5/14

Temperature	Play = Yes	Play = No	Total
Hot	2/9	2/5	4/14
Mild	4/9	2/5	6/14
Cool	3/9	1/5	4/14

Humidity	Play = Yes	Play = No	Total
High	3/9	4/5	7/14
Normal	6/9	1/5	7/14

Wind	Play = Yes	Play = No	Total
Strong	3/9	3/5	6/14
Weak	6/9	2/5	8/14

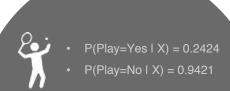
Naïve Bayes

If X = (Outlook = Sunny, Temperature = Cool, Humidity = High, Wind = Strong), then

$$= \frac{(2/9) * (3/9) * (3/9) * (3/9) * (9/14)}{(5/14) * (4/14) * (7/14) * (6/14)}$$



$$= \frac{(3/5) * (1/5) * (4/5) * (3/5) * (5/14)}{(5/14) * (4/14) * (7/14) * (6/14)} = \frac{0.0206}{0.02186} = 0.9421$$



Since 0.9421 is greater than 0.2424 then the answer is 'no', we cannot play a game of tennis today.

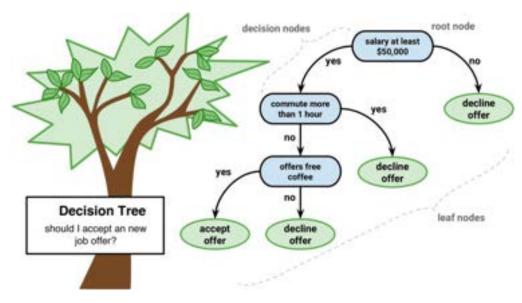
 Decision tree builds classification or regression models in the form of a tree structure.

• predict the value of a target variable by following the decisions in the tree from the root (beginning) down to a leaf node.

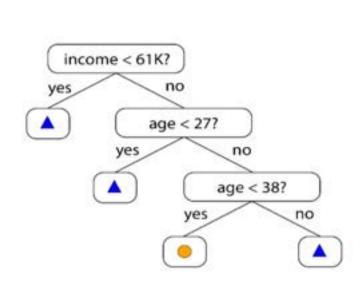
• A tree consists of branching conditions where the value of a predictor is

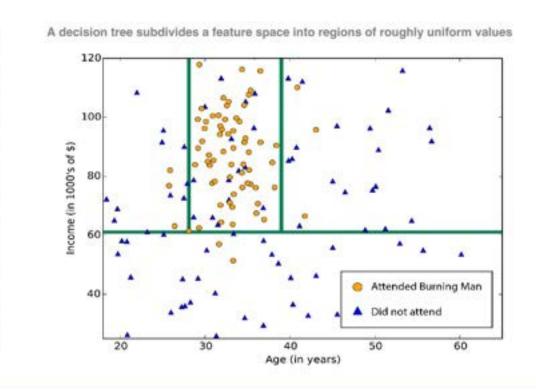
compared to a trained weight.

 Decision trees are prone to overfitting, additional modification, or pruning, may be used to simplify the model.

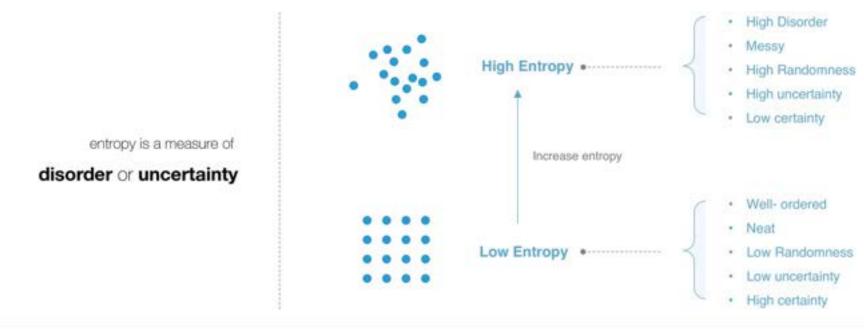


 Growing a tree involves deciding on which features to choose and what conditions to use for splitting, along with knowing when to stop.



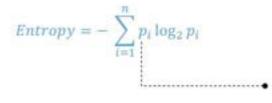


- Generally entropy is a measure of disorder or uncertainty
 - Entropy is a concept used in physics, mathematics, computer science (information theory) and other fields of science. The concept of entropy originated in thermodynamics as a measure of molecular disorder: entropy approaches zero when molecules are still and well ordered.



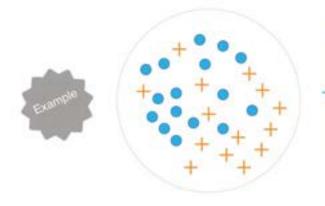


Mathematical Definition of Entropy



Where p_i is the **probability** of getting the i^{th} value when randomly selecting one from the set.

In other words, Where there are n classes, and p_i is the probability an object from the i^{th} class appearing.

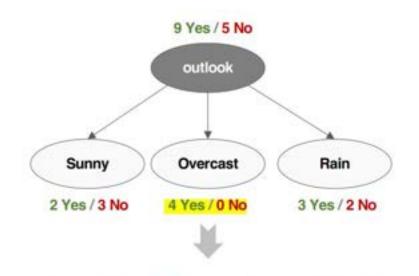


$$\log_2\left(\frac{16}{30}\right) = -0.9$$
;

$$\log_2\left(\frac{16}{30}\right) = -0.9$$
; $\log_2\left(\frac{14}{30}\right) = -1.1$;

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i = -\left(\frac{16}{30}\right)(-0.9) - \left(\frac{14}{30}\right)(-1.1) = 0.99$$

Use entropy to measure the "purity" of the split



Pure set (4 yes / 0 No) ⇒ completely certain(100%)

The entropy is 0 If the sample is completely homogeneous

$$Entropy = -\frac{4}{4}\log_2\frac{4}{4} - \frac{0}{4}\log_2\frac{0}{4} = 0$$



Impure set (3 yes / 3 No) ⇒ completely uncertain(50%)

The entropy is 1 If the sample is an equally divided

$$Entropy = -\frac{3}{6}\log_2\frac{3}{6} - \frac{3}{6}\log_2\frac{3}{6} = 1$$

Decision Tree with ID3 Algorithm

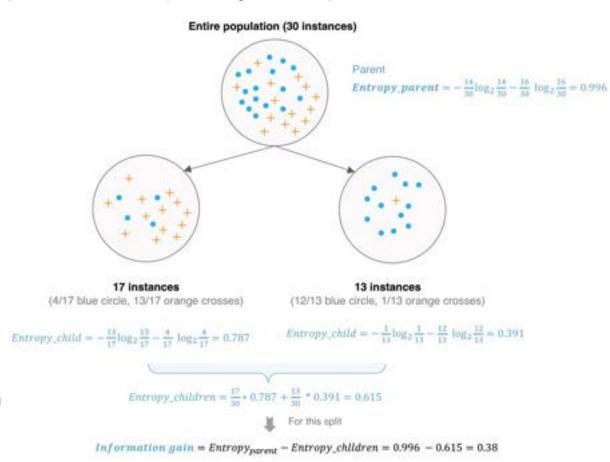
- Measures that can be used to capture the purity of split.
 - Information Gain

A reduction of entropy is often called an information gain. ID3 algorithm uses entropy to calculate the homogeneity of a sample.

$$Information \ Gain = Entropy_{before} - Entropy_{after}$$

Constructing a decision tree is all about finding attribute that returns the highest information gain (i.e., the most homogeneous branches)

- A decision tree is built top-down from a root node and involves partitioning the data into subsets that contain instances with similar values (homogenous).
- The information gain is based on the decrease in entropy after a dataset is split on an attribute.³



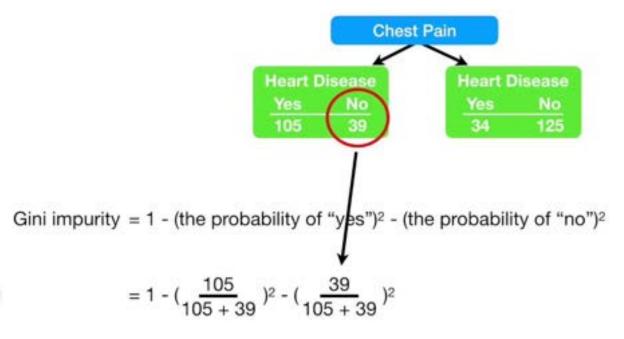
Decision Tree with CART Algorithm

- Measures that can be used to capture the purity of split.
 - Gini impurity Index
- The impurity measure used in building decision tree in CART algorithm is Gini Index.
- Equation for Gini impurity

$$G_l = 1 - \sum_{k=1}^{n} (p_{l,k})^2$$

 $p_{l,k}$ is the ratio of class k instances among the training instances in the l^{th} node

 A node's Gini attribute measures its impurity: a node is "pure" (gini=0) if all training instances it applies to belong to the same class. In other words, Gini Index would be zero if perfectly classified.



Decision Tree with CART Algorithm



Pros and Cons of Decision Tree

- Pros
 - Simple to understand and to interpret.
 - To build decision tree requires little data preparation.
 - Handle both continuous and categorical variables.
 - Implicitly perform feature selection.

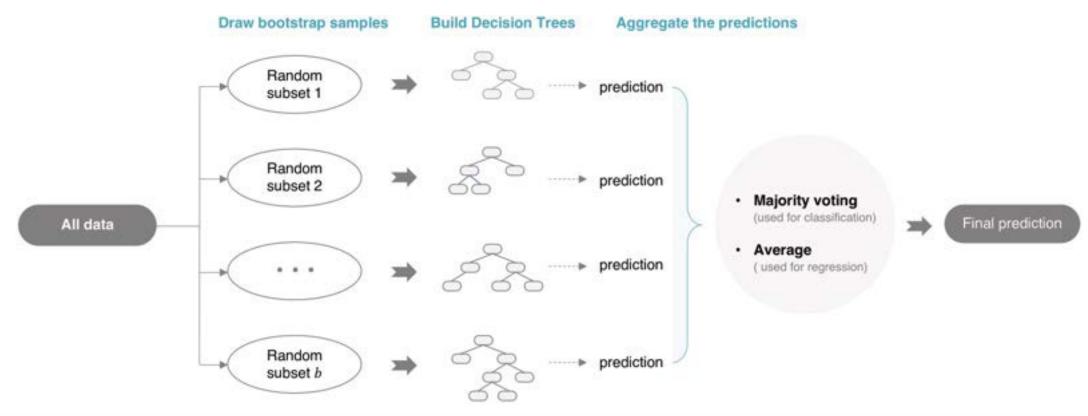
Cons

- They are prone to over-fitting.
- create biased trees in case of unbalanced data.
- Instability.
- Greedy approach used by Decision tree doesn't guarantee best solution.
- Standard decision trees are restricted by hard, axis-aligned splits of the input space.



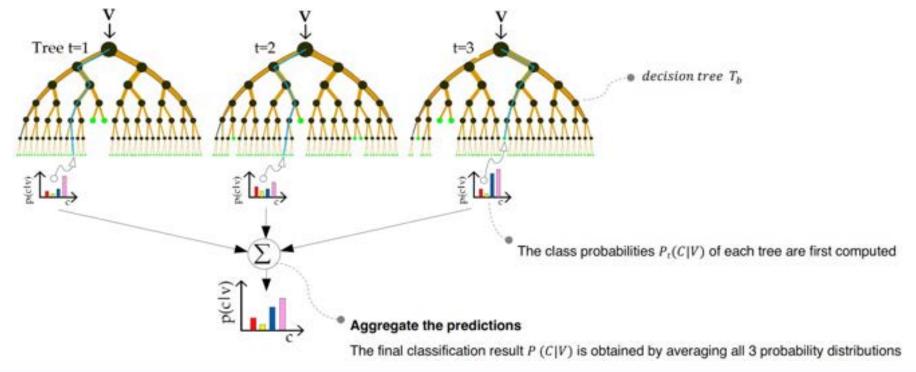
Random Forest

- Random Forest is one of the most used algorithms.
- Random Forest = Bagging + Full-grown CART decision Tree



Random Forest

- Classification example: use Random Forest to classify data
 - After training, a tree set $\{T\}$ can be obtained to predict the classes of the unseen samples by taking the majority vote from all individual classification trees.



Random Forest

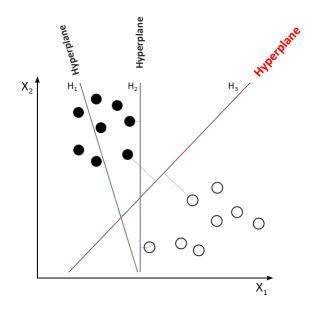
Pros and Cons of Random Forest

- Pros
 - Random Forest algorithms can be grown in parallel.
 - Random Forest has higher classification accuracy.
 - Able to deal with the missing value and maintain accuracy in case of missing data.
 - Help data scientists save data preparation time.

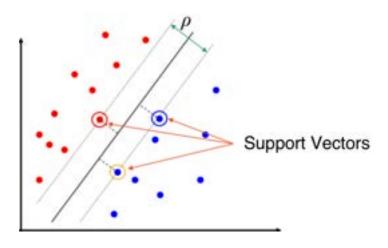
Cons

- Large number of decision trees in the random forest can slow down the algorithm.
- Good job at classification but not as good as for regression.
- like a black box approach, random forest is not easily interpretable.

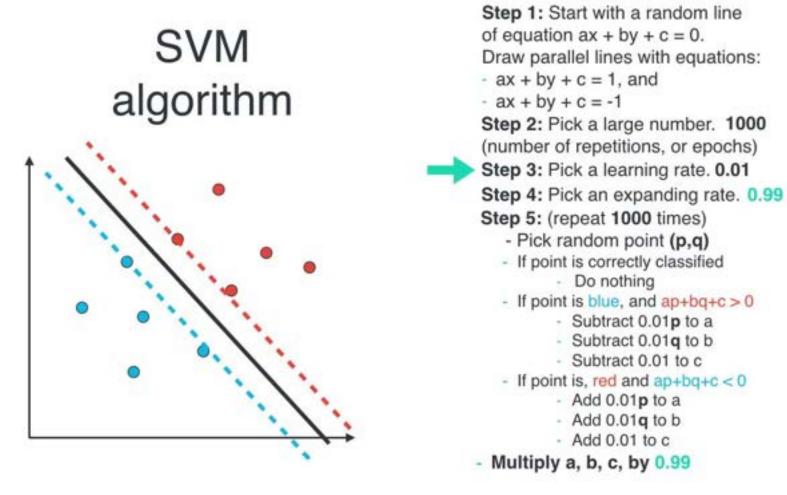
 A Support Vector Machine (SVM) is a discriminative classifier formally defined by a separating hyperplane.



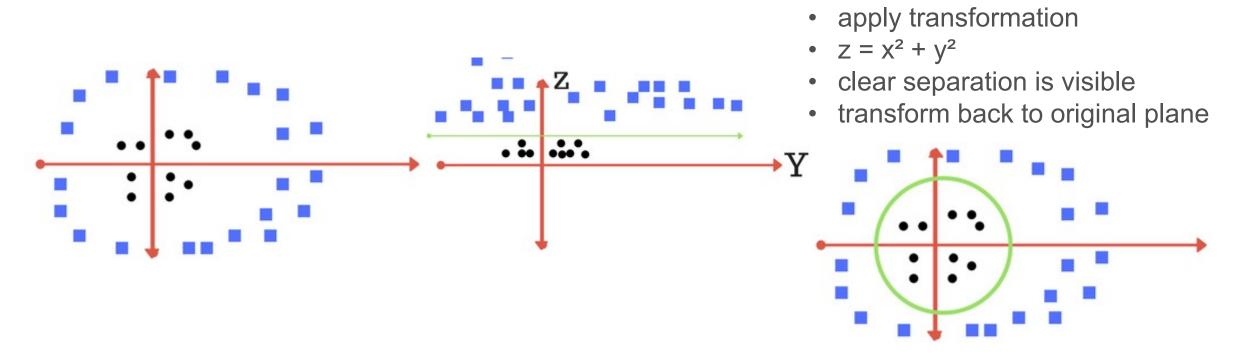
- H₁ does not separate the classes.
- H₂ does, but only with a small margin.
- H₃ separates them with the maximum margin.



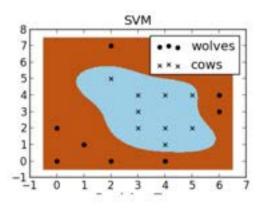
- Examples closet to the hyper-plane are support vectors
- Margin p of the separator is the distance between support vectors.

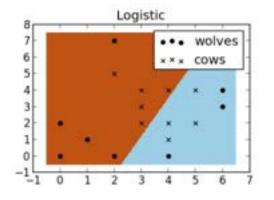


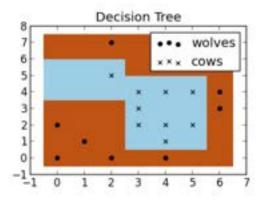
• SVMs sometimes use a kernel transform to transform nonlinearly separable data into higher dimensions where a linear decision boundary can be found, the kernel trick.



SVM using a Non-Linear Kernel







Where do you build your fence ?

Well if you're a really data driven farmer one way you could do it would be to build a classifier based on the position of the cows and wolves in your pasture. Trying a few different types of classifiers, we see that SVM does a great job at separating your cows from the packs of wolves. I thought these plots also do a nice job of illustrating the benefits of using a non-linear classifiers.

You can see the the logistic and decision tree models both only make use of straight lines. 1

Support Vector Machine

Pros and Cons of Support Vector Machine

• Pros

- The training is relatively easy.
- No local optimal, unlike in neural networks.
- SVMs have a regularization parameter, which can help avoid over-fitting.
- Effective in high dimensional spaces.

Cons

- For classification, the SVM is only directly applicable for two-class tasks.
- SVMs do not directly provide probability estimates.
- Parameters of a solved model are difficult to interpret.
- Long training time on large data sets.
- Choosing a "good" kernel function can be tricky.

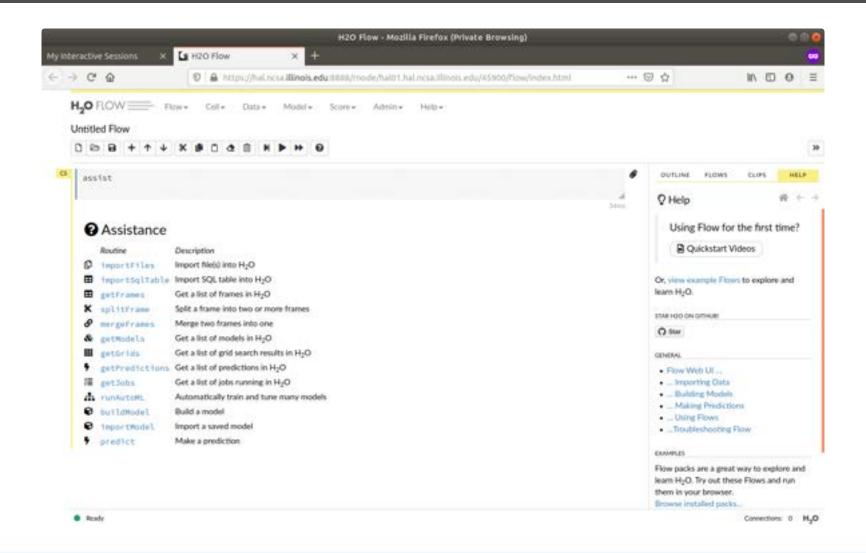
Now it is

```
Hands-on time, but first let's get familiar with H2O Flow.

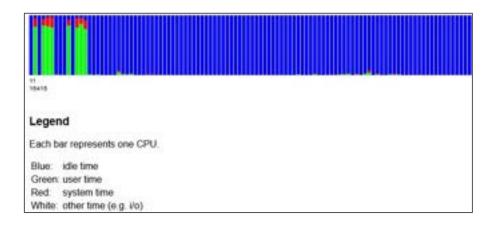
(Recommended Web Browser : Firefox)

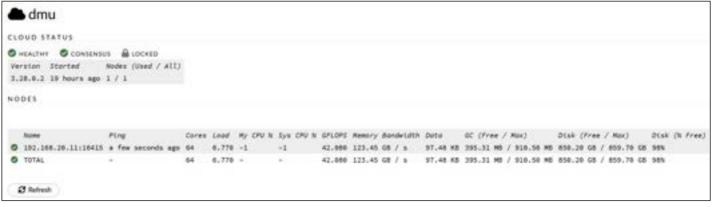
(ReservationName=uiuc_21)
```





- Admin
 - Jobs / Cluster Status / Water Meter





往	Jobs						
	Type	Destination	Description	Start Time	End Time	Run Time	Status
II	Frame	iris_data.hex	Parse	2020-02-11 19:03:33	2020-02-11 19:03:33	00:00:00.541	DONE
HΞ	Model	naivebayes-c4046aa5-90b3-41b5-a11c-1259247d95c4	NaiveBayes	2020-02-11 19:04:15	2020-02-11 19:04:15	00:00:00.119	DONE
12	Frame	iris_data1.hex	Parse	2020-02-11 19:17:53	2020-02-11 19:17:54	00:00:00.390	DONE
擅	Model	naivebayes-eab0af85-bed1-43ac-906b-cdc2488648ac	NaiveBayes	2020-02-11 19:18:46	2020-02-11 19:18:46	00:00:00.15	DONE
12	Model	nalvetayes-d75de4e5-f3ea-464a-8218-28281c3912f8	NaiveBayes	2020-02-11 19:20:07	2020-02-11 19:20:07	00:00:00.23	DONE
讍	Frame	iris_data2.hex	Parse	2020-02-11 19:31:43	2020-02-11 19:31:43	00:00:00.396	DONE
#	Model	kmeans-a783ecco-7781-401d-a19a-4188c770ae92	KMeans	2020-02-11 19:32:21	2020-02-11 19:32-21	00:00:00.125	DONE

- Help
 - View example Flows
 - GBM_Example.flow
 - DeepLearning_MNIST.flow
 - GLM_Example.flow
 - DRF_Example.flow
 - K-Means_Example.flow
 - Million_Songs.flow
 - KDDCup2009_Churn.flow
 - QuickStartVideos.flow
 - Airlines_Delay.flow
 - GBM_Airlines_Classification.flow
 - GBM GridSearch.flow
 - RandomData_Benchmark_Small.flow
 - GBM_TuningGuide.flow
 - XGBoost_Example.flow



- Import Data
- Parse Data
- Split Data
- Build Model
- Predict
- Save Model

K-Mean Clustering with H2O

- Seeds Data Set
- Measurements of geometrical properties of kernels belonging to three different varieties of wheat.
 - area A
 - perimeter P
 - compactness C = 4*pi*A/P^2
 - length of kernel
 - width of kernel
 - asymmetry coefficient
 - length of kernel groove

K-Mean Clustering with H2O

- Import Data:
 - importFiles ["http://s3.amazonaws.com/h2o-public-test-data/smalldata/flow_examples/seeds_dataset.txt"]
- Parse Data:
 - ["separator:9", "number_columns:8"]
- Build Model:
 - ["K-Means", "K:3", "Max_iterations:100"]

Distributed Random Forest on H2O

- Internet Advertisement Data Set
 - This dataset represents a set of possible advertisements on Internet pages.
 - The features encode the geometry of the image (if available) as well as phrases occurring in the URL, the image's URL and alt text, the anchor text, and words occurring near the anchor text.
 - The task is to predict whether an image is an advertisement ("ad") or not ("nonad").

Distributed Random Forest on H2O

Import Data:

• importFiles ["https://s3.amazonaws.com/h2o-public-test-data/smalldata/flow_examples/ad.data.gz"]

Parse Data:

 [destination_frame: "ad.hex", parse_type: "CSV", separator: 44, number_columns: 1559, single_quotes: false]

Build Model:

buildModel 'drf', {"training_frame":"ad.hex", "response_column":"C1559", "ntrees":"10", "max_depth":20, "min_rows":10, "nbins":20, "mtries":"1000", "sample_rate":0.6666667, "build_tree_one_node":false, "balance_classes":false, "class_sampling_factors":[], "max_after_balance_size":5, "seed":0}

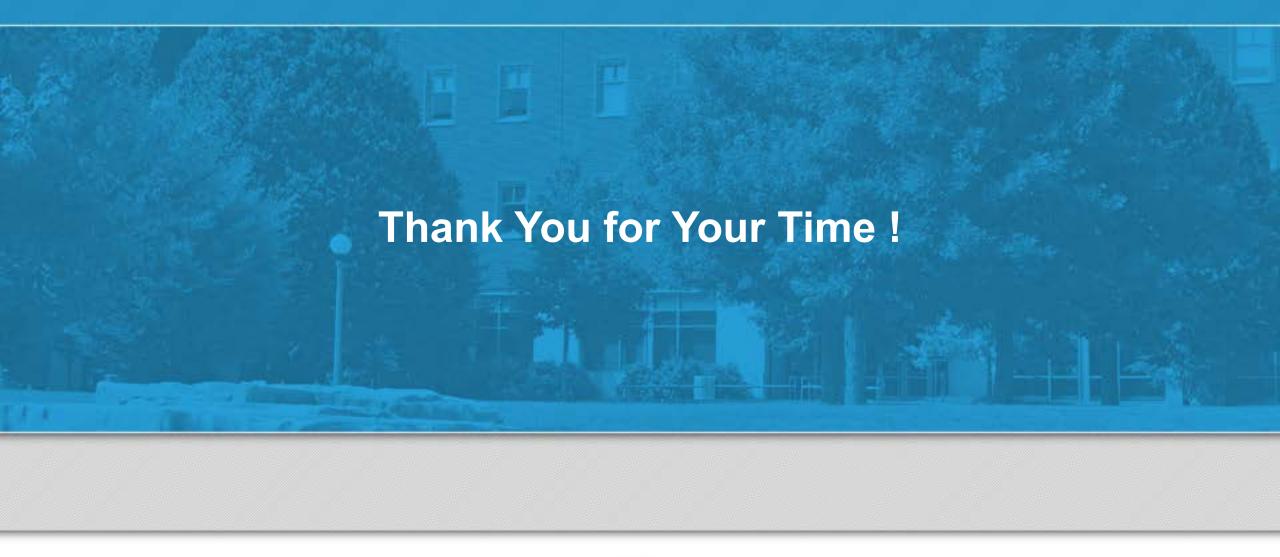
AutoML

- The term "AutoML" (Automatic Machine Learning) refers to automated methods for model selection and/or hyperparameter optimization.
 - To enable non-experts to train high quality machine learning models.
 - To improve the efficiency of finding optimal solutions to machine learning problems.
 - explore a variety of algorithms such as Gradient Boosting Machines (GBMs), Random Forests, GLMs, and Deep Neural Networks.
- No Free Lunch Here, AutoML is slow due to heavy workload.



AutoML

- importFiles ["https://archive.ics.uci.edu/ml/machine-learning-databases/iris/iris.data"]
- parseFiles
 - [parse_type: "CSV", separator: 44, number_columns: 5]
- splitFrame
 - ["iris_data.hex", [0.75], ["frame_0.750", "frame_0.250"], 174460]
- runAutoML
 - max_runtime_secs: 300





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