HPC for ML
Magurele Summer School

GPU Accelerated Distributed Data Science 2

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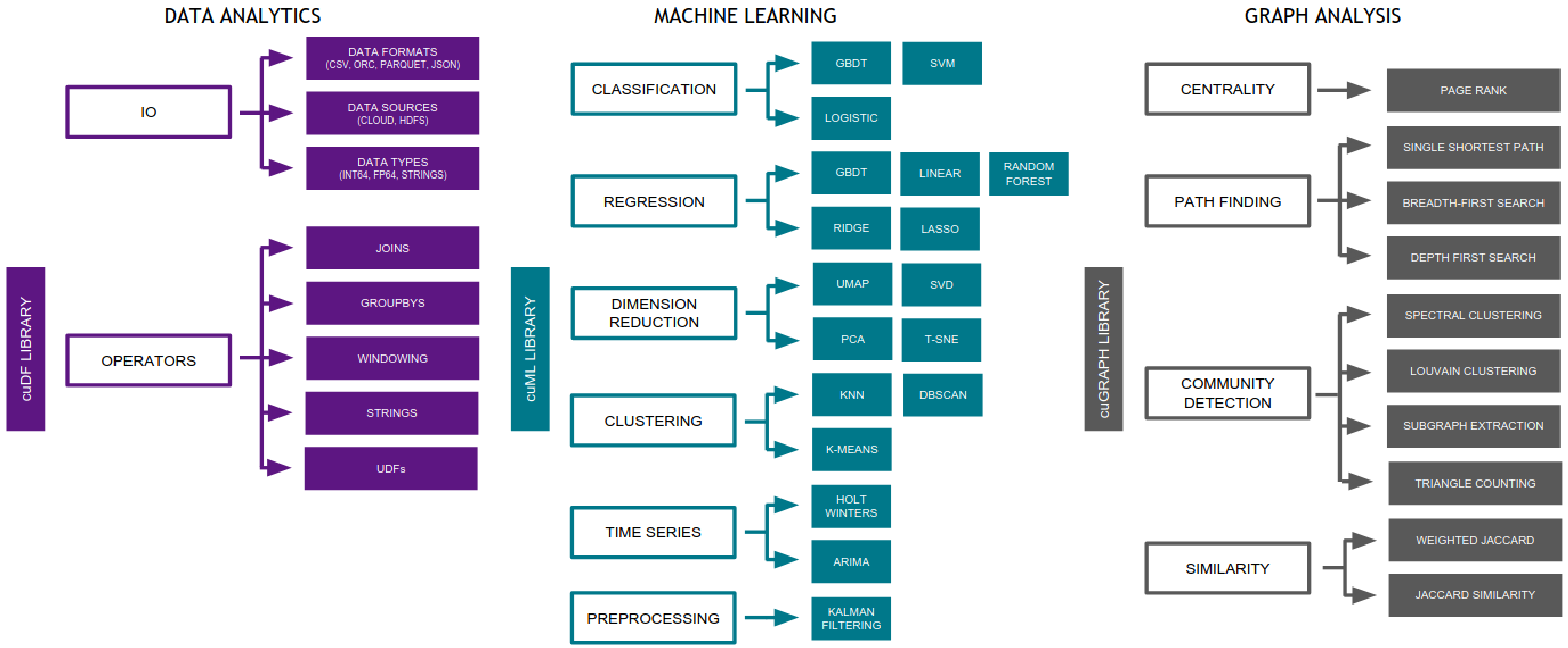
Magurele 9 July 2025

RAPIDS


DATA ANALYTICS
MACHINE LEARNING
GRAPH ANALYSIS
cuDF LIBRARY
IO
DATA FORMATS (CSV, ORC, PARQUET, JSON)
DATA SOURCES (CLOUD, HDFS)
DATA TYPES (INT64, FP64, STRINGS)
OPERATORS
JOINS
GROUPBYS
WINDOWING
STRINGS
UDFs
cuML LIBRARY
CLASSIFICATION
GBDT
SVM
LOGISTIC
REGRESSION
GBDT
LINEAR
RANDOM FOREST
RIDGE
LASSO
DIMENSION REDUCTION
UMAP
SVD
PCA
T-SNE
CLUSTERING
KNN
DBSCAN
K-MEANS
TIME SERIES
HOLT WINTERS
ARIMA
PREPROCESSING
KALMAN FILTERING
cuGRAPH LIBRARY
CENTRALITY
PAGE RANK
PATH FINDING
SINGLE SHORTEST PATH
BREADTH-FIRST SEARCH
DEPTH FIRST SEARCH
COMMUNITY DETECTION
SPECTRAL CLUSTERING
LOUVAIN CLUSTERING
SUBGRAPH EXTRACTION
TRIANGLE COUNTING
SIMILARITY
WEIGHTED JACCARD
JACCARD SIMILARITY

Linear Regression

- In regression.py, we consider a linear regression on a synthetic dataset.
- The dataset is $\{Y_j, X_{j1}, \ldots, X_{jM}\}$ with $j=1,\ldots,n$ for n samples and M features, generated from a linear model

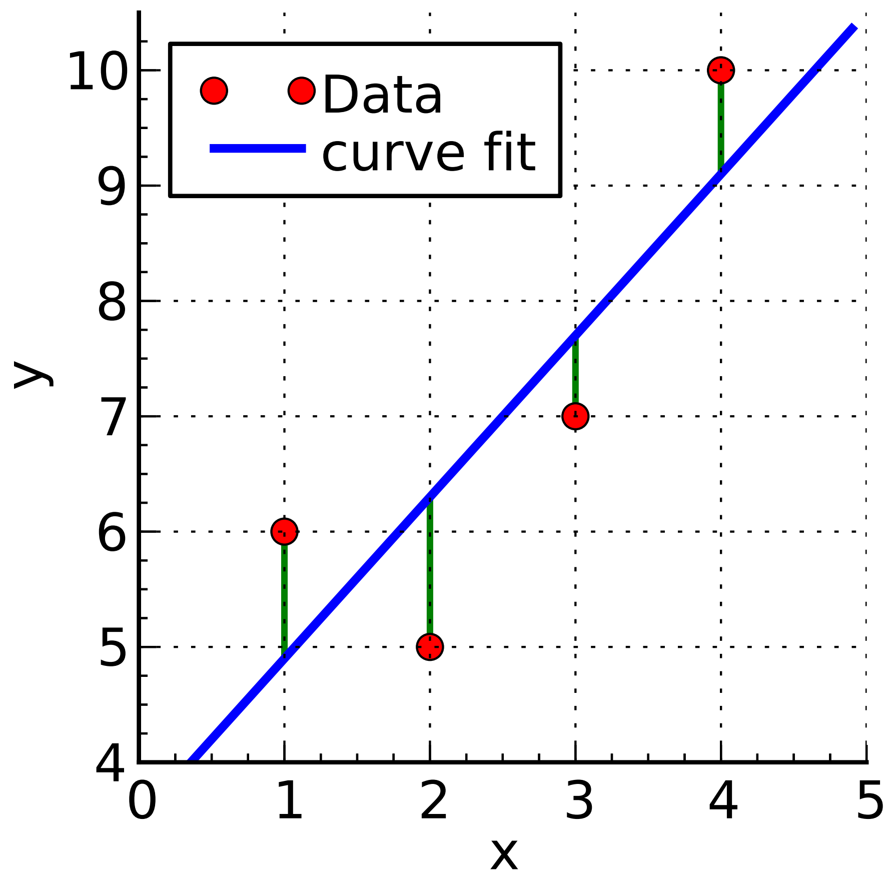
$$Y_i = \sum_{f=1}^{M} X_{if} c_f + b$$

- where c_f with $f=1,\ldots,M$ is a vector of m coefficients and b is the bias.
- Among the M features, we suppose that only K features are informative, that is only $c_1, \ldots, c_K$ are different from zero.
- Given the dataset **X, y** generated from the true underlying coefficients c_M and the true underlying bias b, the goal is to learn the coefficients C_M and the bias B from data, by minimizing the Mean Squared Error.

$$\hat{Y}_i = \sum_{f=1}^{M} X_{if} C_f + B$$

$$\mathrm{MSE} = \frac{1}{n} \sum_{i=1}^{n} \left(Y_i - \hat{Y}_i \right)^2$$

Linear Regression



K-Means

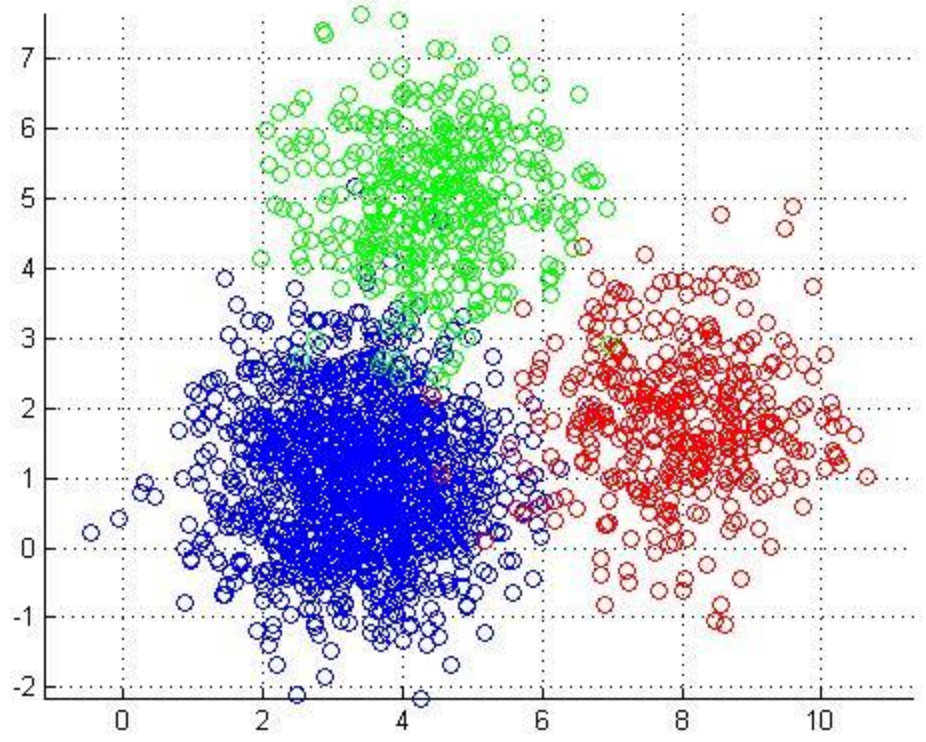
- In clustering.py, we consider a clustering on a synthetic dataset
- Partitioning blobs of points into clusters such that points within the same cluster exhibit greater similarity to one another than to those in other clusters
- Given a set of observations (X_1, X_2, …, X_n), where each observation is a D-dimensional real vector, k-means clustering aims to partition the *n* observations into *k (k< n)* sets S = {S_1, S_2, …, S_k} so as to minimize the within-cluster sum of squares (variance)

$$\arg\min_{\mathbf{S}} \sum_{i=1}^{k} \sum_{\mathbf{x}\in S_i} \left\|\mathbf{x}-\boldsymbol{\mu}_i\right\|^2 = \arg\min_{\mathbf{S}} \sum_{i=1}^{k} |S_i| \operatorname{Var} S_i$$

- Where μ_i is the mean also called centroid of points in S_i

$$\boldsymbol{\mu_i} = \frac{1}{|S_i|} \sum_{\mathbf{x}\in S_i} \mathbf{x},$$

K-Means



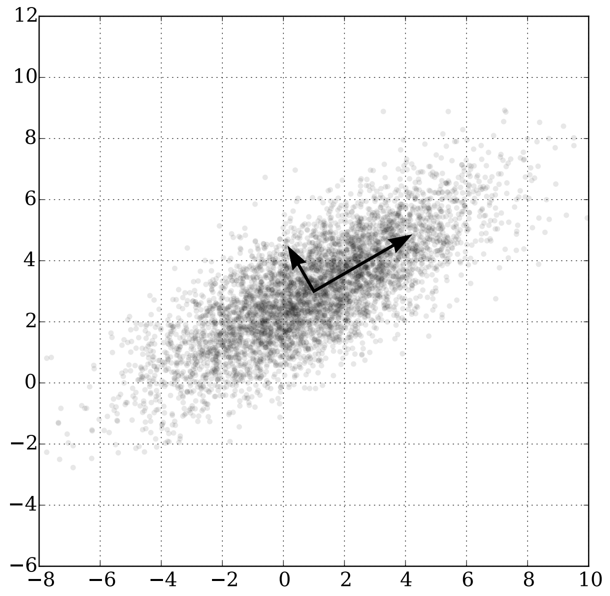
PCA

- In `pca.py`, we apply the Principal component analysis (PCA) on a synthetic dataset.
- PCA is a linear dimensionality reduction method used in exploratory data analysis and processing
- The data is linearly transformed onto a new coordinate system such that the directions (principal components) capturing the largest variation in the data can be easily identified.
- PCA is a statistical procedure that reduces the number of dimensions in large datasets to principal components that retain most of the original information, thus summarizing the information content in large data tables.
- Suppose we have a tabular data, i.e. large matrix **X**, where the *N* rows represent *N* samples, and each of the *M* columns is a particular kind of feature.
- The covariance matrix of *C* is given by $C = \frac{1}{N-1}(X - \bar{X})^T(X - \bar{X})$ $\bar{X} = \frac{1}{N}\sum_{i=1}^{N} X_{ij}$

PCA

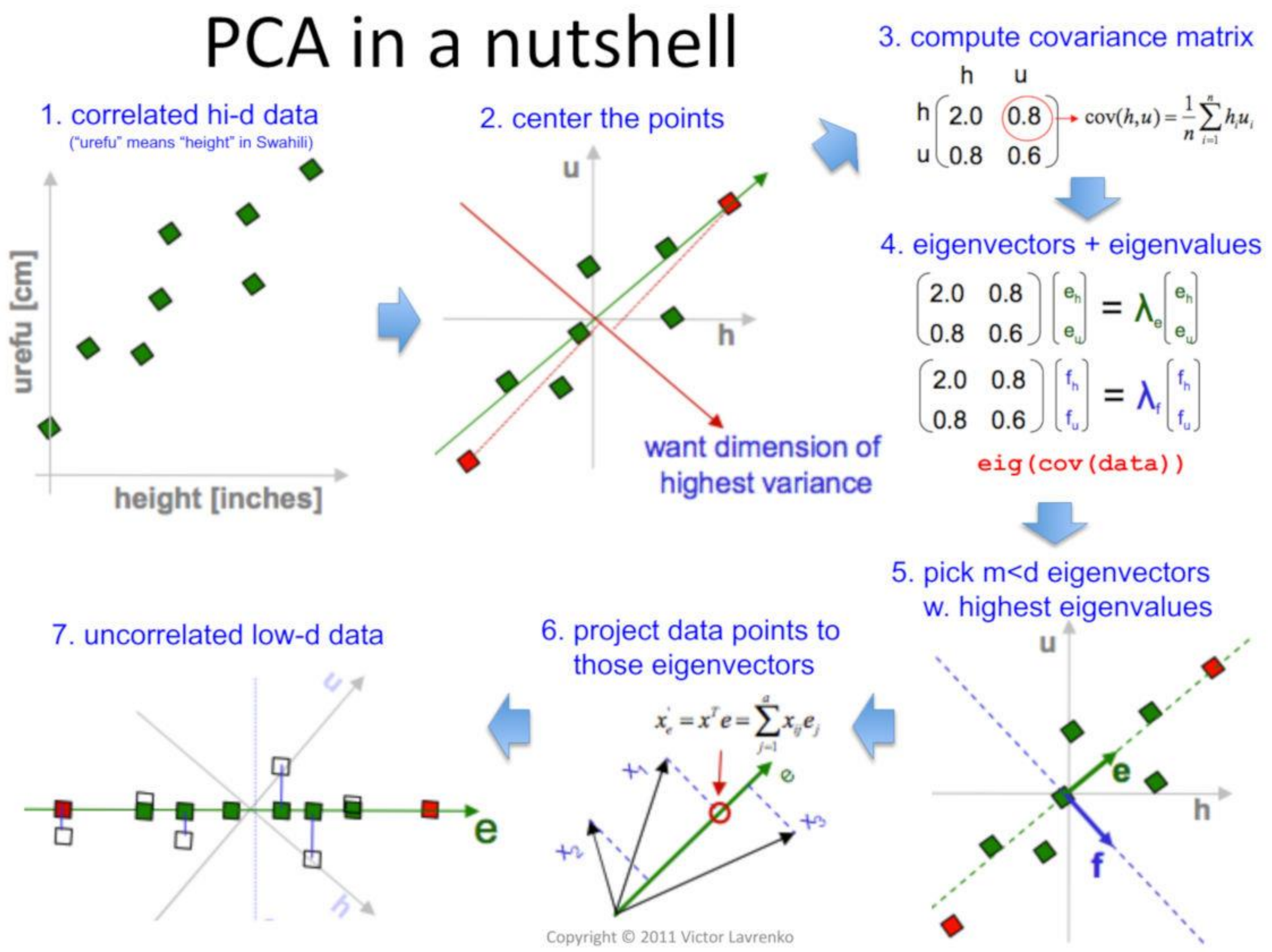
- The covariance matrix C is symmetric and positive semi-definite, with non-negative real eigenvalues
- Each entry C_{ij} quantifies the correlation of the i and j features across all experiments
- The principal components are the eigenvectors of C

$$CV = VD$$



- They define a change of coordinates in which C is diagonal
- The columns of the eigenvector matrix V are the principal components
- The elements of the diagonal matrix D are the variances of the data along these directions

PCA


PCA in a nutshell
1. correlated hi-d data
("urefu" means "height" in Swahili)
urefu [cm]
height [inches]
2. center the points
u
h
want dimension of highest variance
3. compute covariance matrix
$\begin{array}{c|cc} & h & u \\ \hline h & 2.0 & 0.8 \\ u & 0.8 & 0.6 \end{array}$
$\mathrm{cov}(h,u) = \frac{1}{n}\sum_{i=1}^{n} h_i u_i$
4. eigenvectors + eigenvalues
$\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} e_h \\ e_u \end{pmatrix} = \lambda_e \begin{pmatrix} e_h \\ e_u \end{pmatrix}$
$\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} f_h \\ f_u \end{pmatrix} = \lambda_f \begin{pmatrix} f_h \\ f_u \end{pmatrix}$
eig(cov(data))
5. pick m<d eigenvectors w. highest eigenvalues
u
h
e
f
6. project data points to those eigenvectors
$x'_e = x^T e = \sum_{j=1}^{d} x_{ij} e_j$
e
7. uncorrelated low-d data
e
u
h
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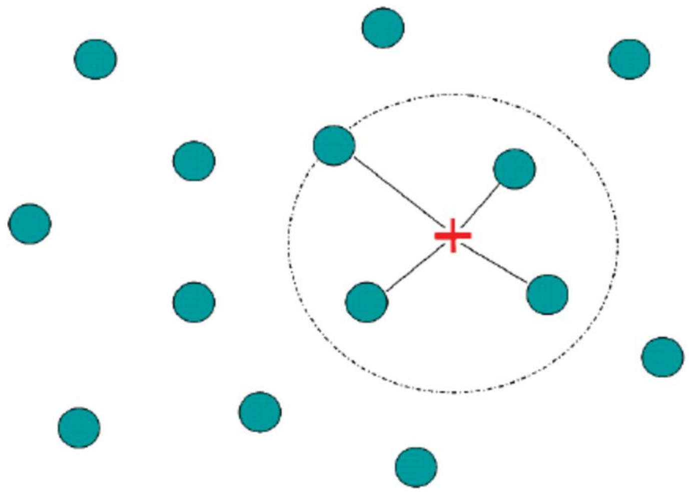
PCA in a nutshell. Source: Lavrenko and Sutton 2011, slide 13.

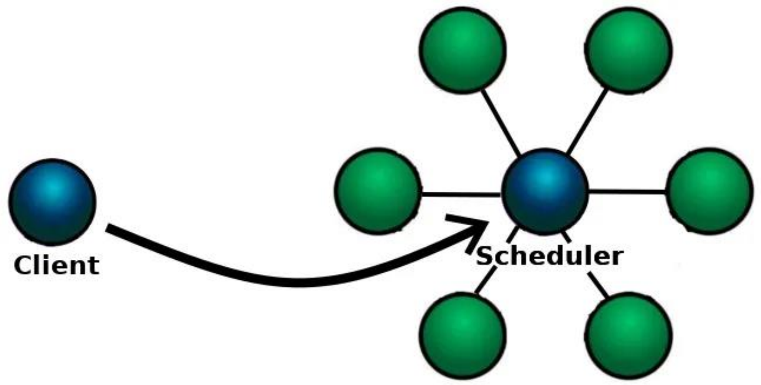
k-Nearest Neighbors (kNN)

- When trying to predict outcomes of a particular observation in a dataset, one of the most natural and intuitive options is to consider similar observations and check their outcomes
- kNN is used for classification, regression, or search algorithms
- For each new observation, we find the k most similar (defined in terms of distance metric) observations with known outcomes
- Labelled observations are gathered into a data structure known as *index*
- New unlabelled observations upon which search is performed are the *query*



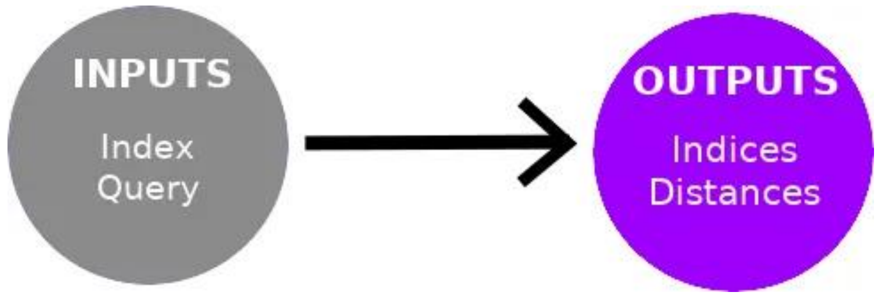
How does distributed kNN work?

- Based on https://medium.com/rapids-ai/scaling-knn-to-new-heights-using-rapids-cuml-and-dask-63410983acfe
- For large datasets, we scale the algorithm by splitting the workload to multiple GPUs, using the multi-node, multi-GPU kNN algorithm
- Workers, each attached to a single-GPU, directly interact with each other
- A scheduler first lists the workers available in the cluster
- A client initiate the loading of the data (partitioned across workers)
- Then it will trigger the distributed operations to perform the search
- All the workers run the same set of instructions on their local data partitions



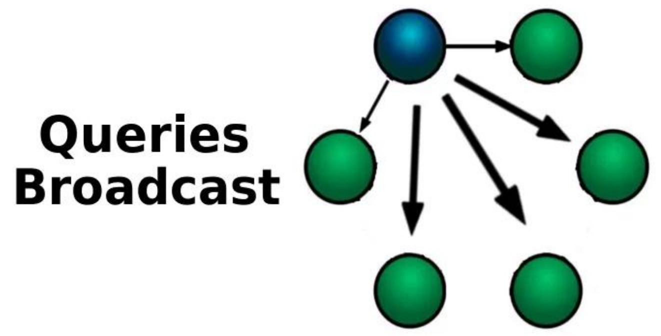
Partitions

- Data is stored in partitions shared among the workers, a distributed array
- **Input index:** it contains reference observations **(n_references x n_features)**
- **Input query:** it contains observations for which to find the nearest neighbors, size **(n_queries x n_features)**
- **Output indices:** it will contain the indices of the nearest neighbors in the index for each of the query points, size **(n_queries x n_neighbors)**
- **Output distances:** it will contain the distances of the nearest neighbors toward their respective query points, size **(n_queries x n_neighbors)**

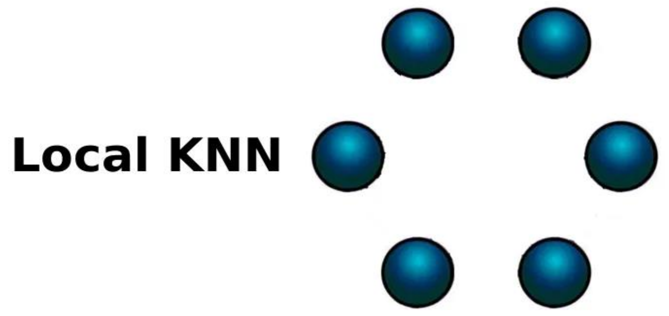


Distributed Operations

- Queries are processed sequentially as a series of batches. For each batch:
- **Queries broadcasting:**
  The unique owner of the currently processed batch of queries broadcasts it to all the other workers

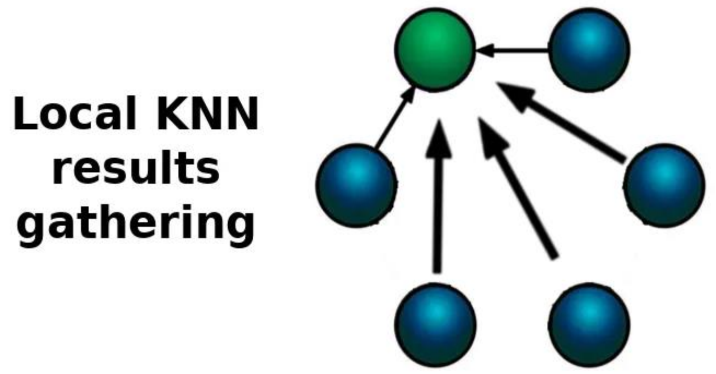


- **Local kNN:** All workers run a local kNN.
  The local kNN searches for the nearest neighbors of the currently processed batch of queries in its locally stored index partitions.
  The produced indices and distances correspond to the local nearest neighbors for these query points.

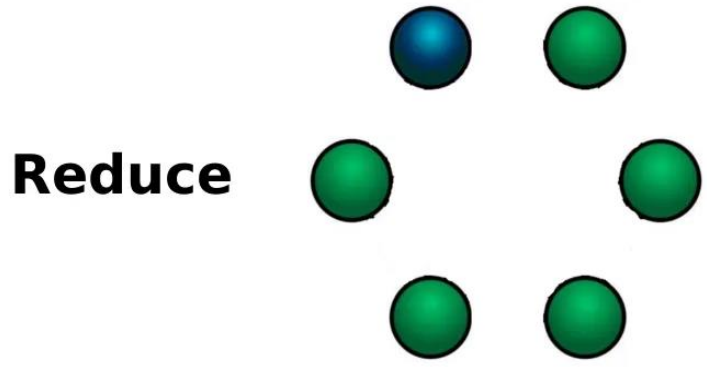


Distributed Operations

- **Local results gathering:** Workers send the result of their local kNN back.
  The owner of the currently processed batch of
  queries collects all these data.
  Workers then start processing the next batch

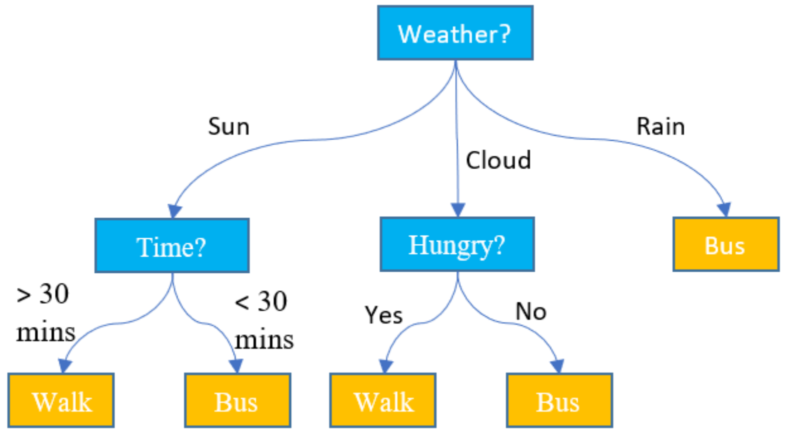


- **Reduce:** The owner performs a reduce operation on the received data (merging the results of the local kNN).
  This produces a set of global nearest neighbors' indices for each of the queries.
  Along with the corresponding distances between query and newly found nearest neighbors.



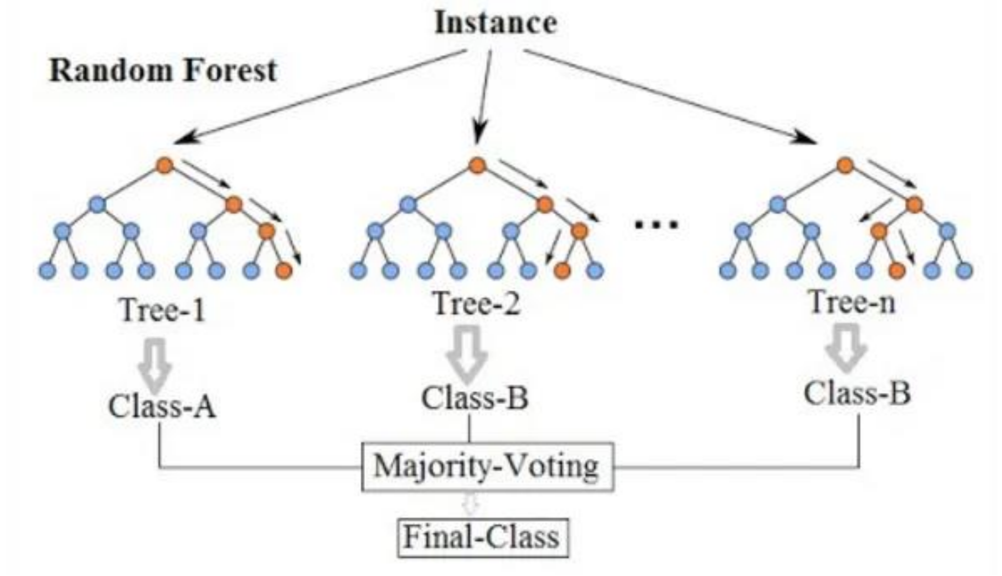
Decision trees

- A decision tree is a non-parametric supervised learning algorithm, which is utilized for both classification and regression tasks.
- It has a hierarchical, tree structure, which consists of a root node, branches, internal nodes and leaf nodes.



Random Forest

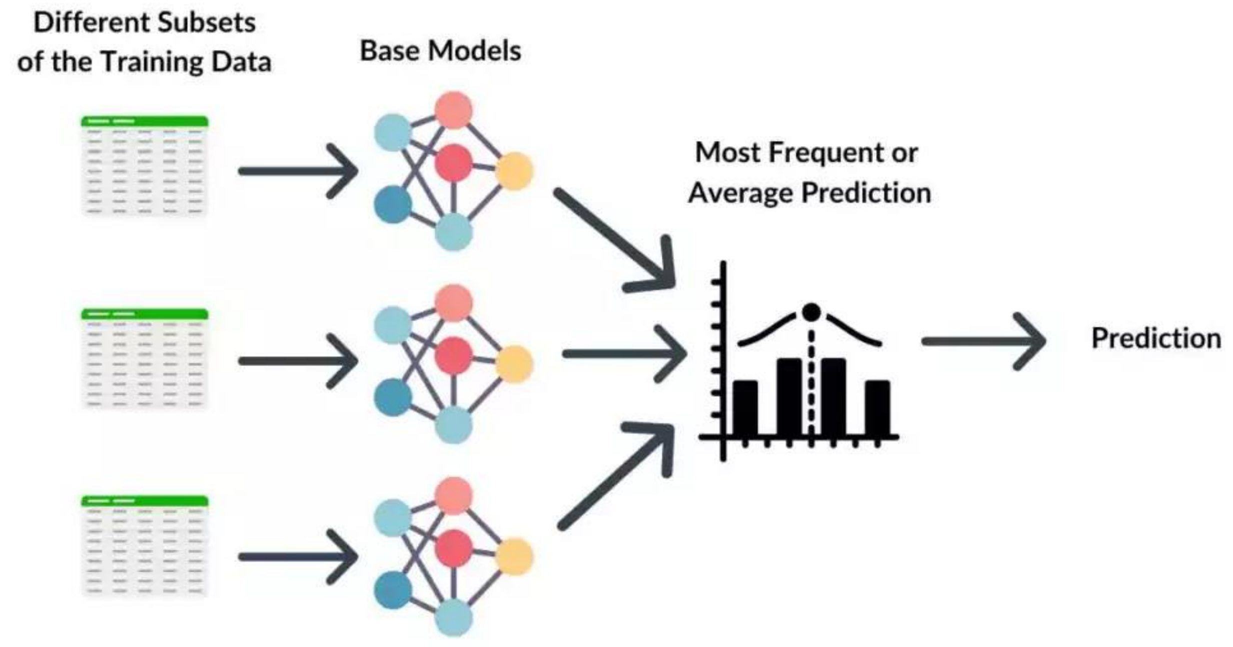
- With random forests we learn multiple independent decision trees and use a consensus method to predict the unknown samples
- Random forests use bagging and feature subsampling to make sure that no two resulting decision trees are the same



https://williamkoehrsen.medium.com/random-forest-simple-explanation-377895a60d2d

Random Forest

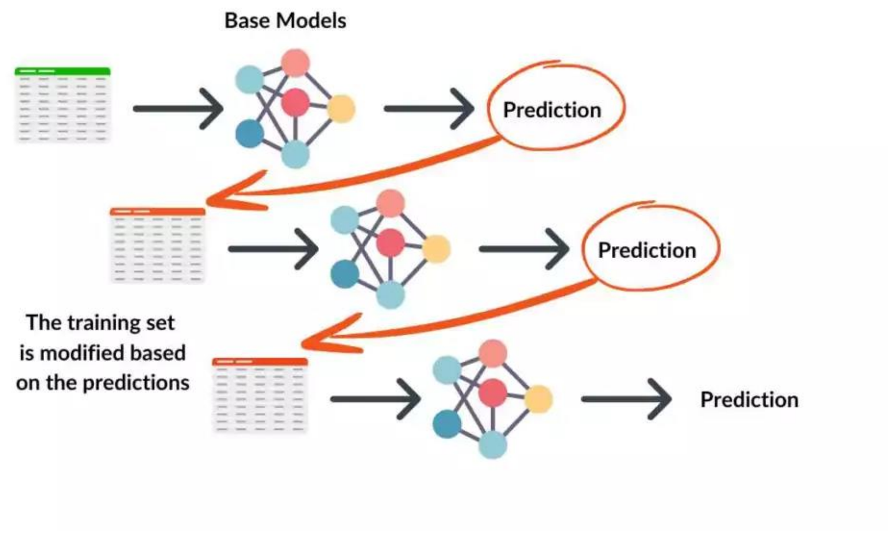
- With bagging, each decision tree is trained upon a different sample, with the replacement of the original dataset.


Different Subsets of the Training Data
Base Models
Most Frequent or Average Prediction
Prediction

https://spotintelligence.com/2024/03/18/bagging-boosting-stacking/

XGBoost

- XGBoost uses a boosting technique, building trees sequentially and correcting errors of previous trees.
- XGBoost is generally more accurate and efficient than random forest, especially with complex datasets, but requires more tuning and can be slower to train.



https://spotintelligence.com/2024/03/18/bagging-boosting-stacking/

RAPIDS and XGBoost

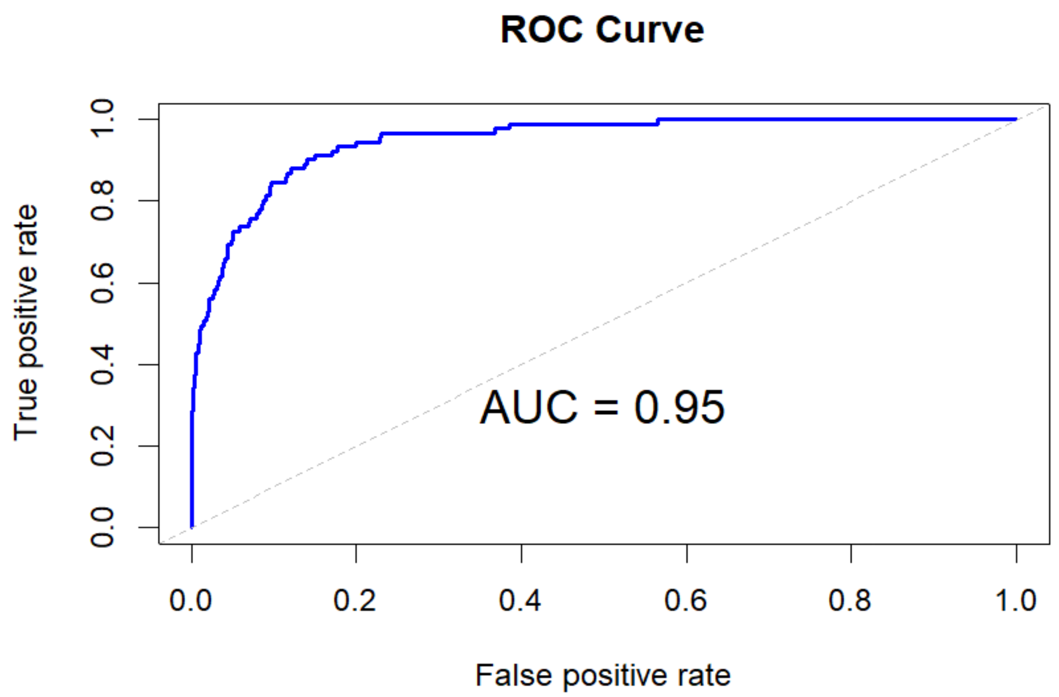
- RAPIDS works closely with the XGBoost community to accelerateGradient Boosted Decision Trees on GPU on GPU
- XGBoost can load data from cuDF dataframes and cuPy arrays
- Dask allows XGBoost to scale to arbitrary numbers of GPUs

Threshold for binary classifier

- Consider a Higgs boson classifier that decides whether an event involves the Higgs boson or the background.
- The model computes a score (probability) for each event, representing the likelihood it's a Higgs.
- If we set ***a high threshold***, the model only marks obvious Higgs, ensuring background events are not confused as Higgs events. Less-obvious Higgs events might be classified as background.
- If we set a ***lower threshold***, the filter will catch a broader range of Higgs event, but there's also a higher chance it might incorrectly classify a background event as Higgs.

ROC

- A **ROC curve** is a graphical plot that illustrates the performance of a binary classifier model at varying threshold values.



- The ROC curve is the plot of the true positive rate (TPR) against the false positive rate (FPR) at each threshold setting.

AUC

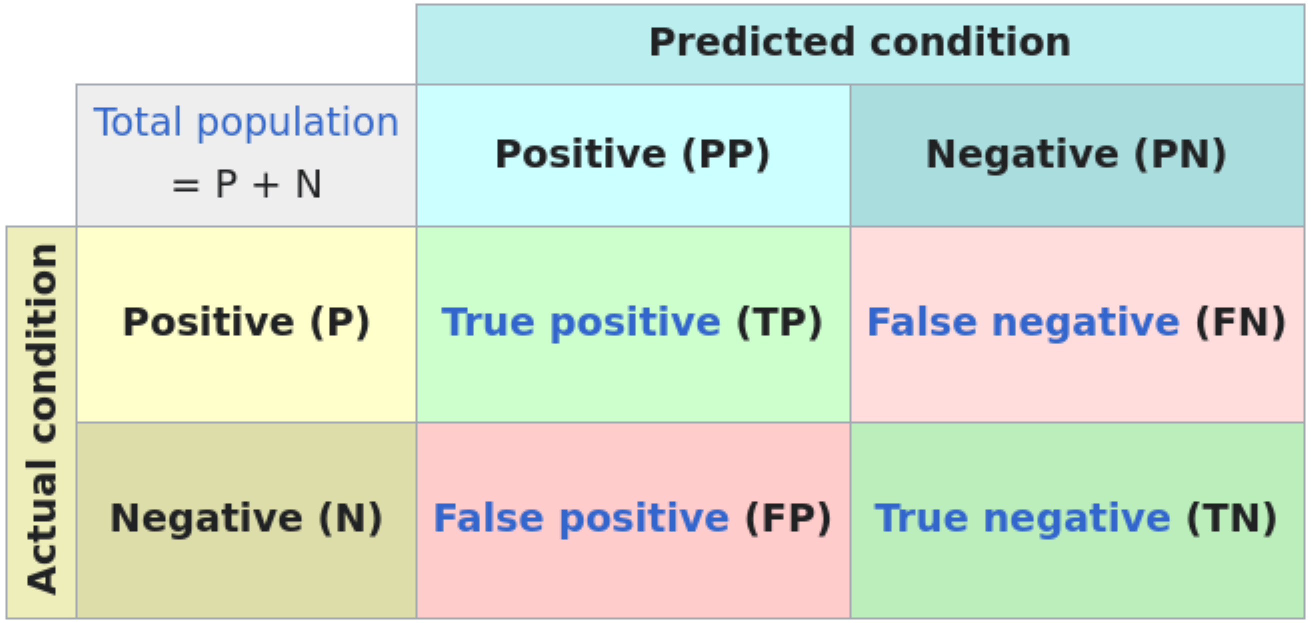
- The Area Under the ROC Curve (AUC) is a metric used to evaluate the performance of a binary classification model.
- An AUC of 1.0 indicates a perfect model, while an AUC of 0.5 suggests the model performs no better than random guessing
    - **0.5:** No discriminatory power (random guessing).
    - **0.7 - 0.8:** Acceptable performance.
    - **0.8 - 0.9:** Excellent performance.
    - **0.9 - 1.0:** Outstanding performance.
- For a Higgs classifier based on XGBoost, we can get:
  model roc_auc: 0.84

Confusion matrix

- In classification problems, a confusion matrix is a specific table layout that allows visualization of the performance of an algorithm

- True positive: Higgs events correctly identified as Higgs
- False positive: Background events incorrectly identified as Higgs
- True negative: Background correctly identified as Background
- False negative: Higgs incorrectly identified as Background

Confusion matrix



		Predicted condition	
	Total population = P + N	**Positive (PP)**	**Negative (PN)**
Actual condition	**Positive (P)**	**True positive (TP)**	**False negative (FN)**
	Negative (N)	**False positive (FP)**	**True negative (TN)**

Sensitivity and specificity

- **Sensitivity** (true positive rate) is the probability of a positive test result, conditioned on the event truly being positive.

$$\text{Sensitivity} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}} = \frac{\text{True Positives}}{\text{Positives}}$$

- **Specificity** (true negative rate) is the probability of a negative test result, conditioned on the event truly being negative.

$$\text{Specificity} = \frac{\text{True Negatives}}{\text{True Negatives} + \text{False Positives}} = \frac{\text{True Negatives}}{\text{Negative}}$$

Sensitivity and specificity

- **Sensitivity**: is about finding the true positives (true Higgs events).
- **Specificity**: is about finding the true negatives (true Background).
- The ideal test would be both highly sensitive and highly specific, but in practice, there's often a trade-off.

- For a Higgs classifier based on XGBoost, we get (threshold 0.5):

```
Sensitivity: 0.78332
Specificity: 0.72991
```