

HPC & Data Science Summer Institute 2023

Scalable Machine Learning



Spark Hands-On

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Setup

- **Login to Expanse**

- Open terminal window on local machine
- `ssh login.expanse.sdsc.edu -l <account>`

- **Pull latest from repo**

- `git pull`
- URL:
- <https://github.com/sdsc/sdsc-summer-institute-2023>

Server Setup for PySpark - Command Line

- **In terminal window**
 - `jupyter-shared-spark`
 - Alias for: `galileo launch --account ${SI23_ACCOUNT} --reservation ${SI23_RES_CPU} --partition shared --cpus 4 --memory 16 --time-limit 04:00:00 --env-modules singularitypro --sif /cm/shared/apps/containers/singularity/spark/spark-latest.sif --bind /exppanse,/scratch,/cm --quiet`
- **To check queue**
 - `squeue -u $USER`

PySpark Scaling Hands-On

- **Data**
 - BookReviews_5M.txt
 - Source : <https://jmcauley.ucsd.edu/data/amazon/>
- **Notebook**
 - pyspark_demo.ipynb
 - Location: <si_dir>/4.3b_scalable_machine_learning
- **To do**
 - Change number of cores: 1, 2, 4
 - Note difference in execution times
 - Run each configuration 3 times

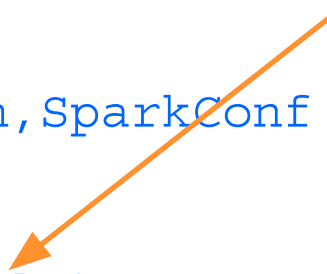
SPARK SESSION

```
import pyspark
from pyspark.sql import SparkSession, SparkConf

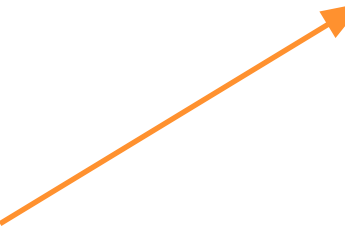
conf = SparkConf().setAll([
    ('spark.master', 'local[*]'),
    ('spark.app.name', 'PySpark Demo')])

spark = SparkSession.builder.config(conf=conf).getOrCreate()
```


Use * to use all available cores, or integer value to specify number of cores to use



Configuration parameters for Spark session



Get existing Spark session or create new one



GETTING EXECUTION TIMES

- In notebook, execution time is printed out in cell before Spark session is stopped (next to last cell)
- Need to restart the kernel and run all cells without stopping to get accurate execution time:
 - Run -> Restart Kernel and Run All Cells
- Find mean and standard deviation of execution times over 3 runs for
 - 1 core, 2 cores, and 4 cores

```
import pyspark
from pyspark.sql import SparkSession
```

```
conf = pyspark.SparkConf().setAll([
    ('spark.master', 'local[2]'),
    ('spark.app.name', 'PySpark Demo)])
spark = SparkSession.builder.config(conf=conf).getOrCreate()
```

Specify number of cores.
“*” uses all available cores



PySpark Cluster Analysis Hands-On

- **Data**
 - Weather station measurements
- **Task**
 - Perform cluster analysis to identify different weather patterns
- **Approach**
 - Spark k-means

SPARK PROGRAM STRUCTURE

- **Start Spark session**
 - `spark = SparkSession.builder.config(conf=conf).getOrCreate()`
- **Create distributed dataset**
 - `df = spark.read.csv("data.csv",header="True")`
- **Apply transformations**
 - `new_df = df.filter(col("dept") == "Sales")`
- **Perform actions**
 - `df.collect()`
- **Stop Spark session**
 - `spark.stop()`

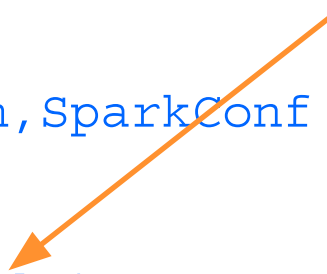
START SPARK SESSION

```
import pyspark
from pyspark.sql import SparkSession, SparkConf

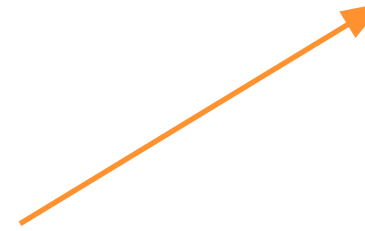
conf = SparkConf().setAll([
    ('spark.master', 'local[*]'),
    ('spark.app.name', 'PySpark Demo')])

spark = SparkSession.builder.config(conf=conf).getOrCreate()
```

Run Spark locally.
Use * to use all
available cores, or
integer value to
specify number of
cores to use



Configuration
parameters for
Spark session



Get existing Spark
session or create
new one



LOAD DATA

```
df = spark.read.text("file.txt")
```

```
df = spark.read.csv("file.csv",  
                    header=True  
                    inferSchema=True).cache()
```

Indicates whether
column headers exist



Automatically infer
data types of columns



Cache data



DROP ROWS WITH NULLS

- **Drop rows with null values**

```
df.dropna()  
df.dropna(how='any')  
df.dropna(how='all')
```

- **Check number of rows before and after dropping rows**

```
df.count()
```

PARTITION DATA

- Partition available data into train and test data sets

```
train_df, test_df = df.randomSplit(0.8, 0.2), seed=<seed>)
```

Weights for splits

The diagram consists of three orange arrows pointing upwards from labels to code parameters. The first arrow originates from the label 'Weights for splits' and points to the first '0.8' parameter in the code. The second arrow originates from the label 'Random number generator seed' and points to the 'seed' parameter. The third arrow originates from the label 'Random number generator seed' and points to the second '0.2' parameter in the code.

Random number
generator seed

CREATE FEATURE VECTOR COLUMN

- **Create feature vector column**
 - Combines given list of columns into single vector column
 - To feed data to machine learning models

```
from pyspark.ml.feature import VectorAssembler
```

```
features = ['air_temp', 'relative_humidity']  
assembler = VectorAssembler(inputCols=features,  
                             outputCol='featureVector')
```

```
features_df = assembler.transform(df)  
features_df.show()
```

air_temp	relative_humidity
62.96	63.9



air_temp	relative_humidity	featureVector
62.96	63.9	[62.96, 63.9]

New column
appended to
features_df

SCALE DATA

- **Scale input data values**

- Standardize values to have zero mean and unit standard deviation
- Each feature is scaled separately
- Create scale transformer using train data, then apply to train/test data

```
from pyspark.ml.feature import StandardScaler
scaler = StandardScaler(inputCol="features_unscaled",
                        outputCol="features_scaled",
                        withStd=True, withMean=True)
scalerModel = scaler.fit(train_df)
```

```
train_df = scalerModel.transform(train_df)
test_df  = scalerModel.transform(test_df)
```

BUILD MODEL


- **Build decision tree classifier**

- Create model
- Use fit() to train model

```
from pyspark.ml.classification import DecisionTreeClassifier
```

```
dt = DecisionTreeClassifier(  
    featuresCol='featureVector',  
    labelCol='label',  
    predictionCol='prediction')
```

Can specify name of
columns for features,
labels, and predictions



```
dt_model = dt.fit(<train>)
```


APPLY MODEL

- **Apply trained model**
 - Use transform()

```
predictions = <model>.transform(<data>)
```

Will have <data> and
new 'prediction'
column appended at
the end



Trained
model



Input data



EVALUATE CLASSIFICATION MODEL

- **Evaluator for classification model**
 - Calculates F1, precision, recall, accuracy

```
from pyspark.ml.evaluation import MulticlassClassificationEvaluator

mc_evaluator = MulticlassClassificationEvaluator(
    predictionCol='prediction',
    labelCol='label',
    metricName='f1')

mc_evaluator.evaluate(<predictions>)
```

Column with predictions

Column with labels

Evaluation metric

Contains predictions and labels

PySpark Cluster Analysis Hands-On

- **Data**

- Weather station measurements

- **Task**

- Perform cluster analysis to identify different weather patterns

- **Approach**

- Spark k-means

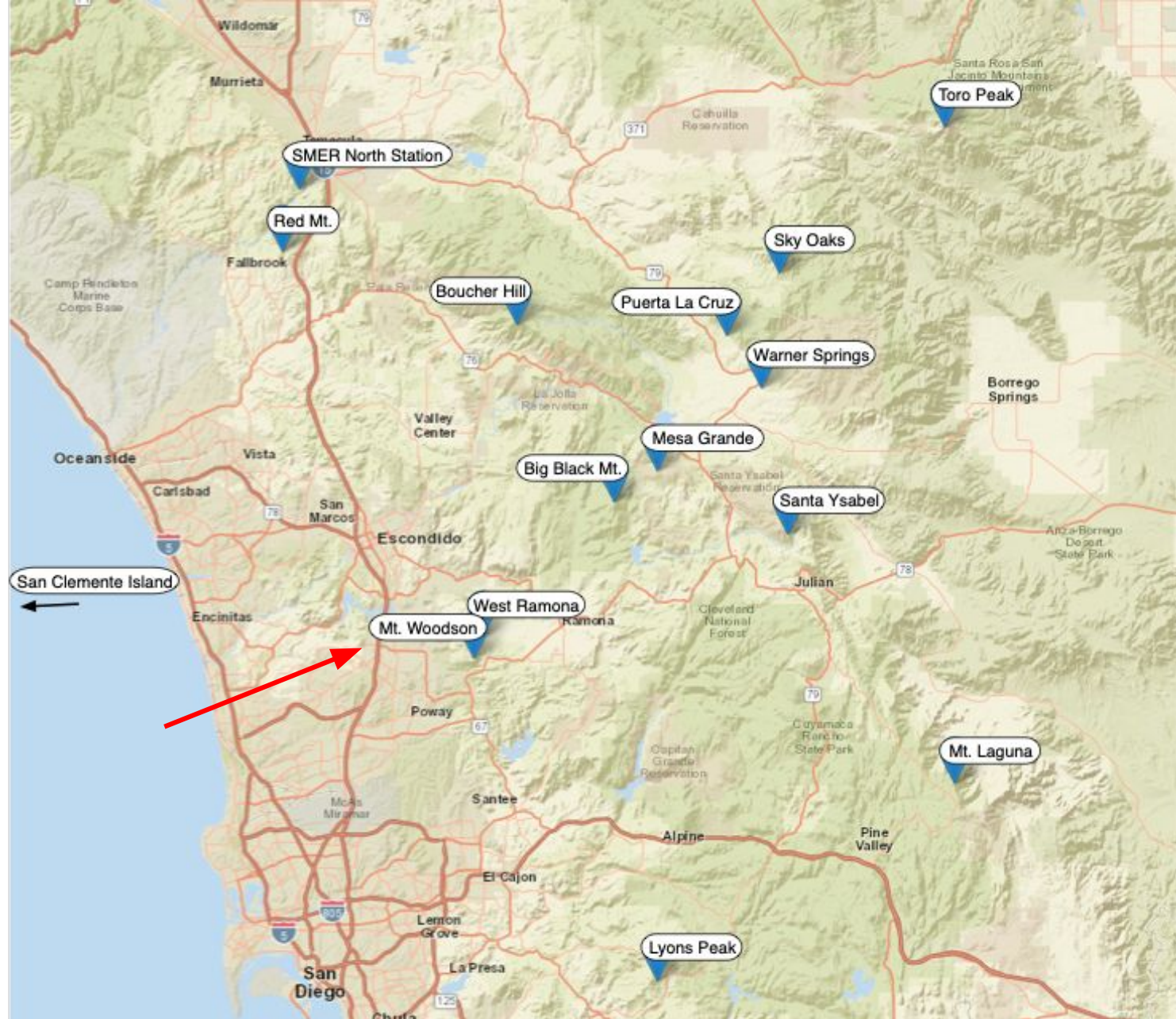
- **Notebook**

- Location: <si_dir>/4.3b_scalable_machine_learning
- pyspark-clustering.ipynb # Starter notebook
- pyspark-clustering-wOutput.ipynb # Has cell outputs
- pyspark-clustering-soln.ipynb # Solution

Dataset Description

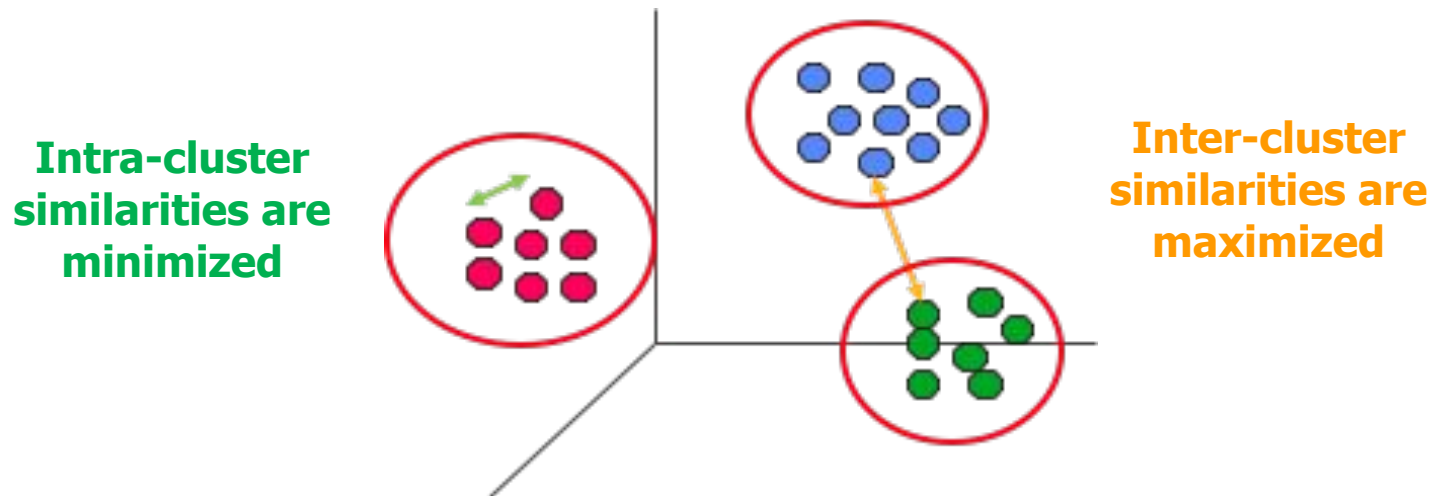
- **Measurements from weather station on Mt. Woodson, San Diego**
- **Air temperature, humidity, wind speed, wind direction, etc.**
- **Three years of data: Sep. 2011 - Sep. 2014**
 - minute_weather.csv: measurement every minute
- **Source**
 - <http://hpwren.ucsd.edu>

Map of HPWREN Weather Stations



Cluster Analysis

- **Cluster analysis divides data into groups**
 - Grouping is based on some similarity measure.
 - Samples within a cluster are more similar to each other than to samples in other clusters.



<http://www-users.cs.umn.edu/~kumar/dmbook/index.php>

k-Means Clustering

- **Partitional**
 - Clusters are divided into non-overlapping subsets
- **Centroid-Based**
 - Cluster represented by central vector
- **Simple, classic clustering technique**
 - Data points are grouped into k clusters
 - Cluster defined by cluster mean

- **Algorithm**

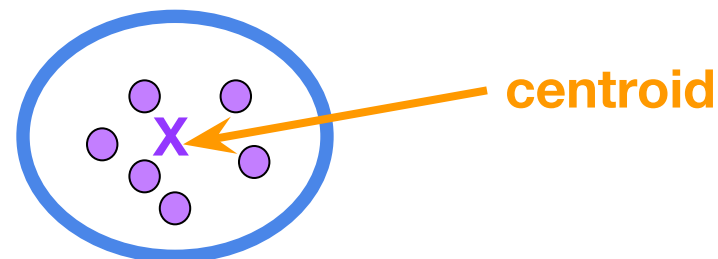
Select k initial *centroids* (cluster centers)

Repeat

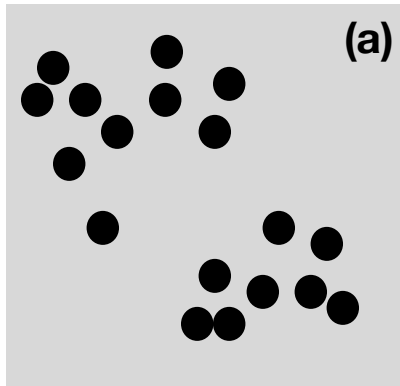
Assign each sample to closest centroid

Calculate mean of cluster to determine new centroid

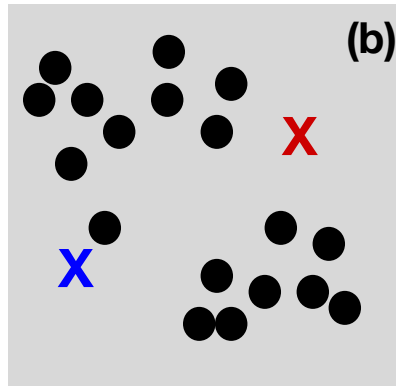
Until some stopping criterion is reached



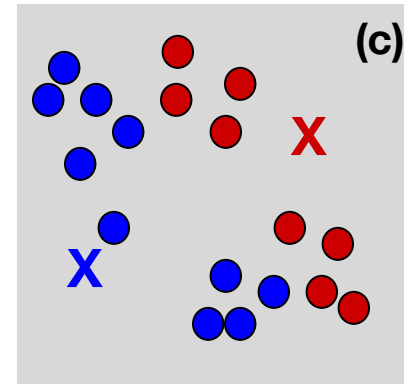
k-Means Clustering Illustration



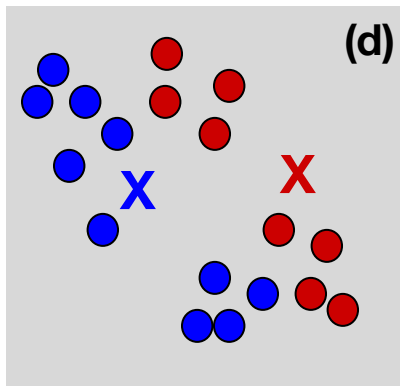
Original samples



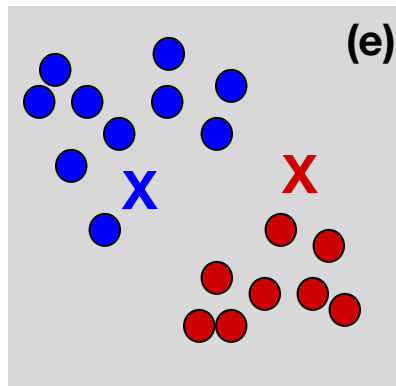
Initial Centroids



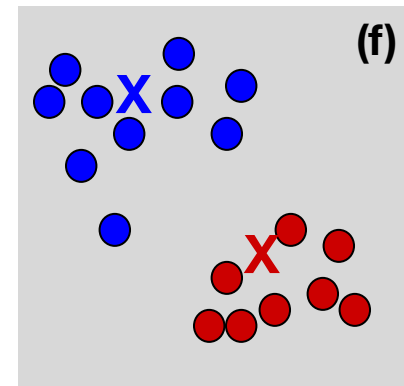
Assign Samples



Re-calculate Centroids



Assign Samples

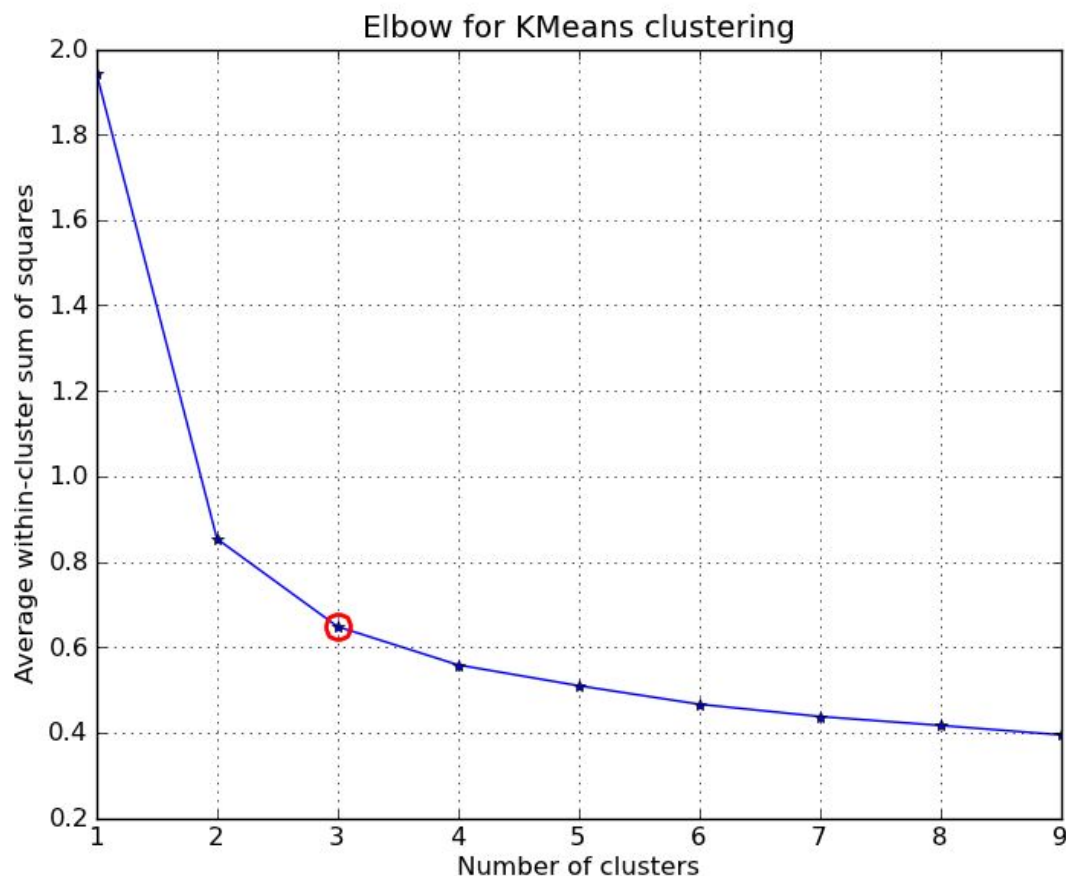


Re-calculate
Centroids

Choosing Number of Clusters (k)

- **Elbow method**

- Plot cluster evaluation metric (e.g., WSSE) vs. different values for k
- “Elbow” in plot suggests value(s) for k



<http://stackoverflow.com/questions/6645895/calculating-the-percentage-of-variance-measure-for-k-means>

Evaluating Clustering Results

- **Within-Cluster Sum of Squared Error (WSSE)**
- For each sample, error is distance to centroid.
Then, **WSSE** is computed as:

$$WSSE = \sum_{i=1}^K \sum_{x \in C_i} \|x - m_i\|^2$$

x : data sample in cluster C_i

m_i : cluster centroid (i.e., mean of cluster)

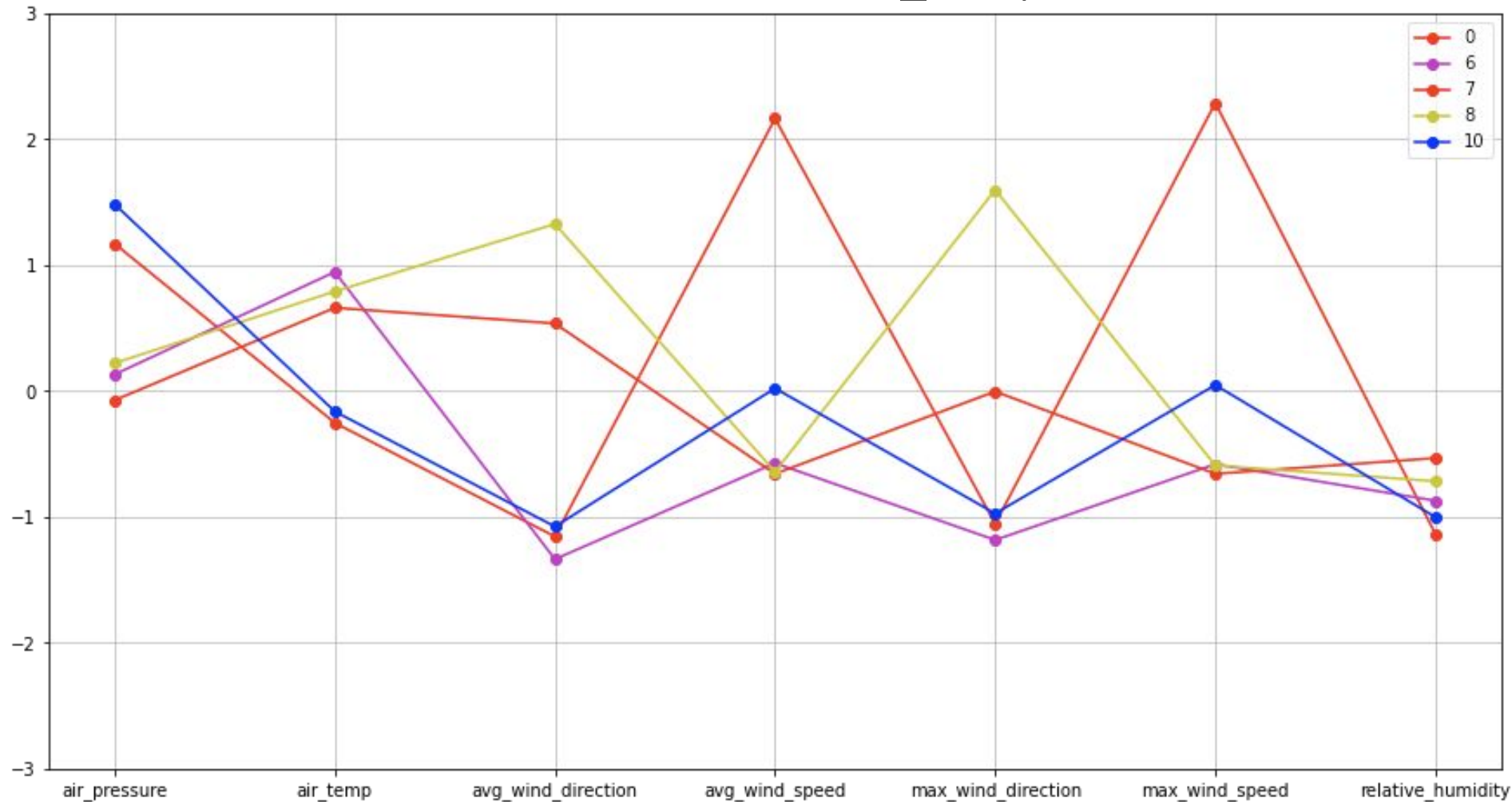
$\|x - m_i\|^2$: Euclidean distance between m_i and x

Clustering Hands-On Overview

- **Setup**
 - Start Spark
 - Load modules
- **Load data**
 - Specify schema
 - Read in data from “minute_weather.csv”
- **Explore data**
 - Look at schema, number of rows, summary statistics
- **Prepare data**
 - Drop nulls
 - Create feature vector
- **Perform k-means cluster analysis**
 - Use elbow plot to determine k
 - Build k-means model
- **Evaluate clusters**
 - Plot cluster profiles
- **Stop Spark session**

Cluster Profile: Parallel Plots

```
utils.parallel_plot(centersNamed[centersNamed['relative_humidity'] < -0.5],  
numClusters, colors=colors_used);
```



PySpark Cluster Analysis Hands-On

- **Code**

- pyspark-clustering.ipynb
 - Notebook for hands-on
 - Add your code where indicated: # ==> YOUR CODE HERE
- pyspark-clustering-wOutput.ipynb
 - Has cell outputs
- pyspark-clustering-soln.ipynb
 - Solution
- **utils.py**
 - Has utility functions

- **Resources**

- [Apache Spark](#)
- [PySpark Documentation — PySpark Documentation](#)
- [Spark SQL and DataFrames Guide](#)
- Python for Data Science Cheat Sheet (pdf)

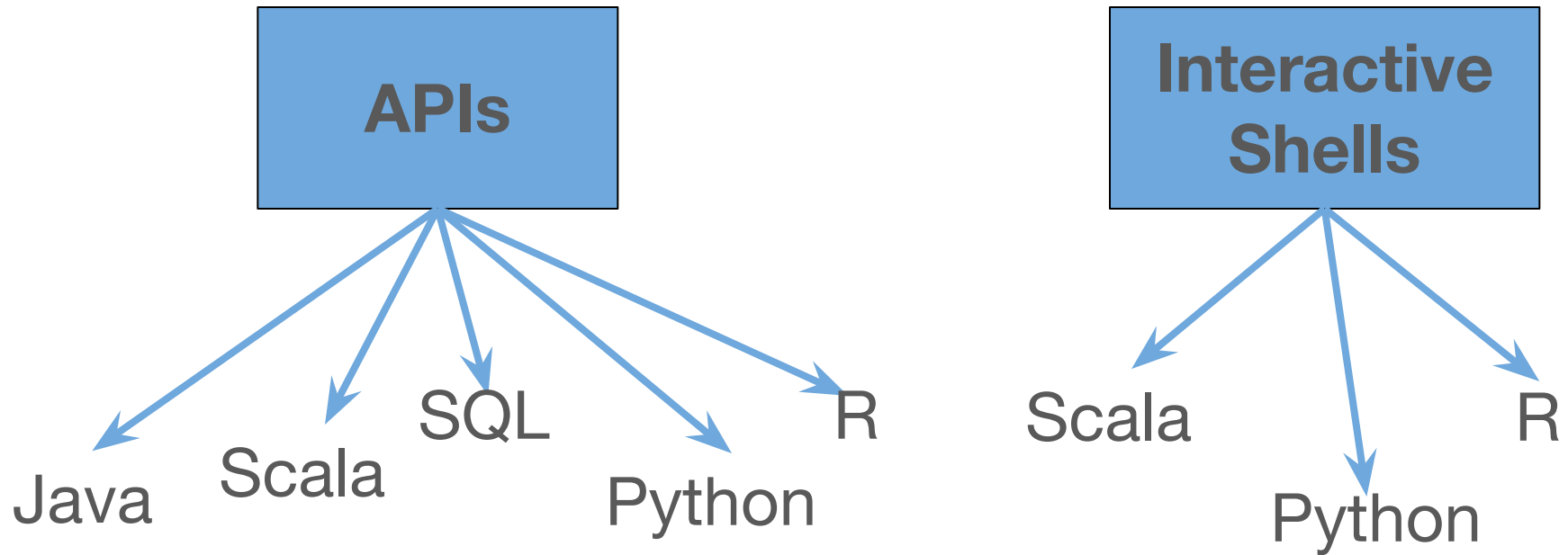
PANDAS API ON SPARK

- **Pandas API integrated into Spark as of v. 3.2**
- **Allows for simple porting of already existing Pandas code to Spark**
 - Same code can run with pandas (single node) and Spark (distributed system)
- **Can use Spark to scale to multiple machines**
- **Can take advantage of unified analytics provided by Spark**
 - Can access functionality provided by other Spark libraries
- **Covers subset of pandas API**
- **To use**

```
from pandas import read_csv  
from pyspark.pandas import read_csv  
pdf = read_csv("data.csv")
```

SPARK INTERFACE

Goals: speed, **ease of use**, generality, unified platform



R FOR STATISTICAL ANALYSIS



- **R**
 - Open source programming language and software environment for statistical computing and graphics
 - Widely used for statistical analysis and machine learning
 - <https://www.r-project.org/about.html>
- **RStudio**
 - IDE (integrated development environment) for R
 - Has source code editor, build automation tools, debugger
 - <https://www.rstudio.com/>
- **Powerful, but limited to single-machine execution**



SparkR

- **R package that provides frontend to use Spark from R**
- **Supports scalable machine learning using R API**
- **Allows R script to connect to Spark cluster**
- **Can use with R shell or RStudio or other R IDEs.**

SparkR

- **Uses MLlib for machine learning functionality**
- **Familiar R syntax:**
 - Read contents of file into a Spark dataframe
 - `newdata <- read.df ("data.txt", source="csv")`
 - R formula operators for model fitting:
 - `model <- spark.randomForest(training, label ~ features, "classification", numTrees = 10)`
 - Get summary of fitted model
 - `summary(model)`
 - Apply model to make predictions
 - `predictions <- predict(model, testDF)`
 - Save model
 - `write.ml (model, "mymodel")`

Machine Learning Algorithms in SparkR

Machine Learning

Algorithms

SparkR supports the following machine learning algorithms currently:

Classification

- `spark.logit`: Logistic Regression
- `spark.mlp`: Multilayer Perceptron (MLP)
- `spark.naiveBayes`: Naive Bayes
- `spark.svmLinear`: Linear Support Vector Machine

Regression

- `spark.survreg`: Accelerated Failure Time (AFT) Survival Model
- `spark.glm` or `glm`: Generalized Linear Model (GLM)
- `spark.isoreg`: Isotonic Regression

Tree

- `spark.gbt`: Gradient Boosted Trees for Regression and Classification
- `spark.randomForest`: Random Forest for Regression and Classification

Clustering

- `spark.bisectingKmeans`: Bisecting k-means
- `spark.gaussianMixture`: Gaussian Mixture Model (GMM)
- `spark.kmeans`: K-Means
- `spark.lda`: Latent Dirichlet Allocation (LDA)

Collaborative Filtering

- `spark.als`: Alternating Least Squares (ALS)

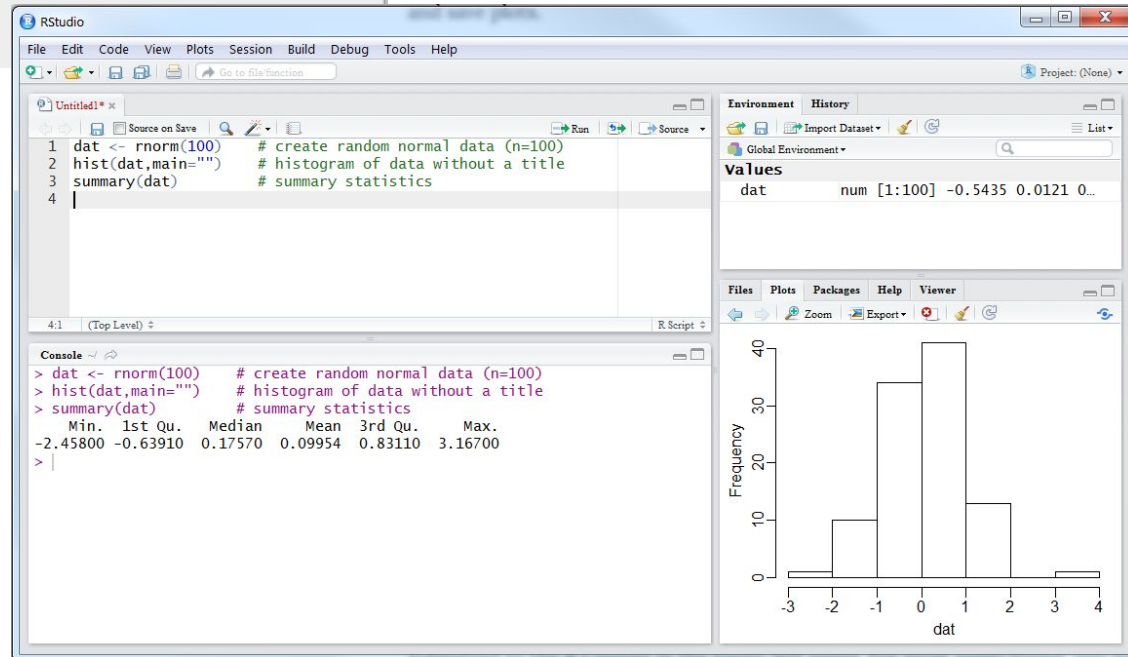
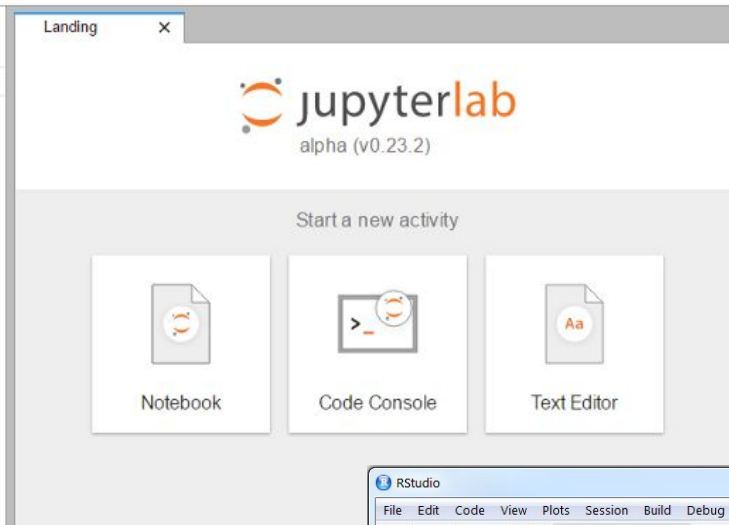
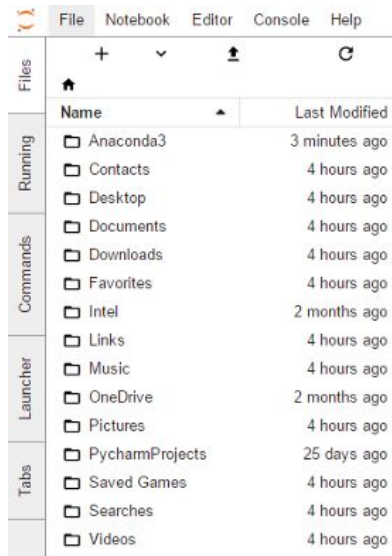
Frequent Pattern Mining

- `spark.fpGrowth`: FP-growth

Statistics

- `spark.kstest`: Kolmogorov-Smirnov Test

Running SparkR Code





sparklyr



- **R interface for Spark**
- **R Legacy**
 - From Rstudio
 - Available on CRAN
- **Spark backend to dplyr and SQL**
 - Interactively manipulate Spark data using dplyr and SQL
- **Access to Spark functionality**
 - Interface to Spark MLlib algorithms
- **Connect to Spark clusters**

sparklyr

- **Setup**

- `install.packages("sparklyr")`
- `library(sparklyr)`
- `spark_install ()`

- **Connect to Spark**

- `sc <- spark_connect (master="local")`

- **Using dplyr**

- `flights_sdf %>% group_by(tailnum)`
`%>% filter(count > 20)`

- **Machine Learning**

- `model <- ml_random_forest (`
`train_sdf, quality ~ ., type="classification")`

sparklyr Functions

- **Spark Operations**
 - Manage Spark connections (e.g., `spark_config()`)
- **Spark Data Manipulation**
 - Read data in Spark DataFrame and perform operations (e.g., `spark_read_csv()`, `tbl_cache()`)
- **Feature Transformers**
 - Transform data (e.g., `ml_pca()`, `ft_bucketizer()`)
- **Distributed Machine Learning**
 - Access Spark Mllib algorithms (e.g., `ml_kmeans()`)
- **Streaming**
 - Support streaming data operations (e.g., `stream_read_json()`)
- **Extensions**
 - Interface to platforms for big data analysis, graph analytics, production

Resources

- **Spark**
 - <https://spark.apache.org/>
- **PySpark API**
 - <https://spark.apache.org/docs/latest/api/python/index.html>
- **Spark DataFrame**
 - <https://spark.apache.org/docs/latest/sql-programming-guide.html>
- **MLlib**
 - <https://spark.apache.org/mllib/>
- **SparkR**
 - <https://spark.apache.org/docs/latest/sparkr.html>
- **SparkR API**
 - <https://spark.apache.org/docs/latest/api/R/>
- **sparklyr**
 - <https://spark.rstudio.com/>

PANDAS API ON SPARK RESOURCES

- **User's Guide**

- https://spark.apache.org/docs/latest/api/python/user_guide/pandas_on_spark/index.html

- **Sample Notebook**

- https://mybinder.org/v2/gh/apache/spark/4f25b3f712?filepath=python%2Fdocs%2Fsource%2Fgetting_started%2Fquickstart_ps.ipynb

- **API Reference**

- <https://spark.apache.org/docs/latest/api/python/reference/pyspark.pandas/index.html>

Spark Topics

- **Spark**
 - History & Design Goals
 - RDDs
 - DataFrames
 - Spark Architecture
 - Spark API
 - Spark Core & Libraries
- **Spark Hands-On**
 - Scaling
 - Cluster Analysis
- **Pandas on Spark**
- **R on Spark**
 - SparkR
 - sparklyR