

# Préparation de données pour le ML en Spark

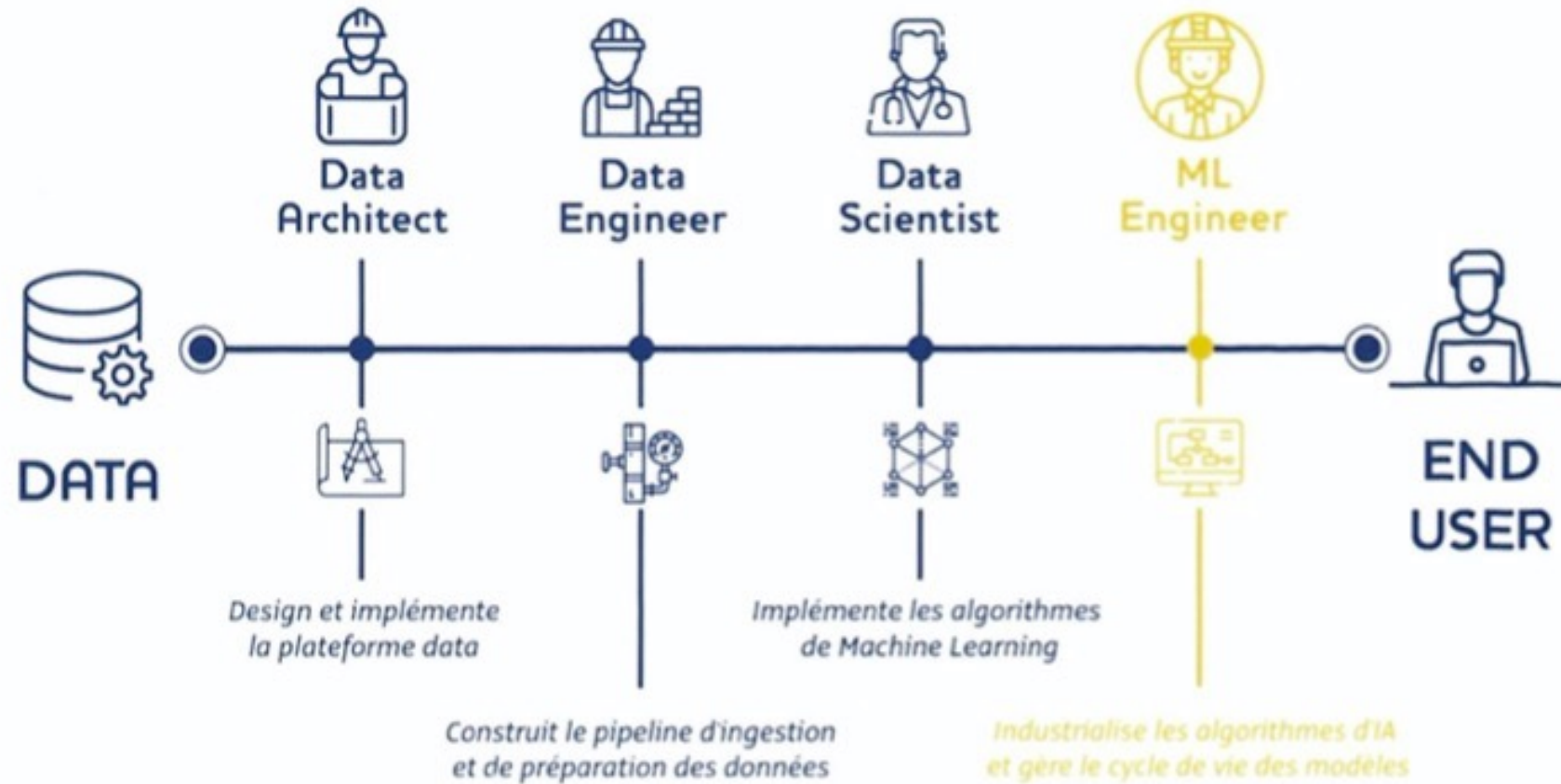
Master DAC – Bases de Données Large Echelle

Mohamed-Amine Baazizi

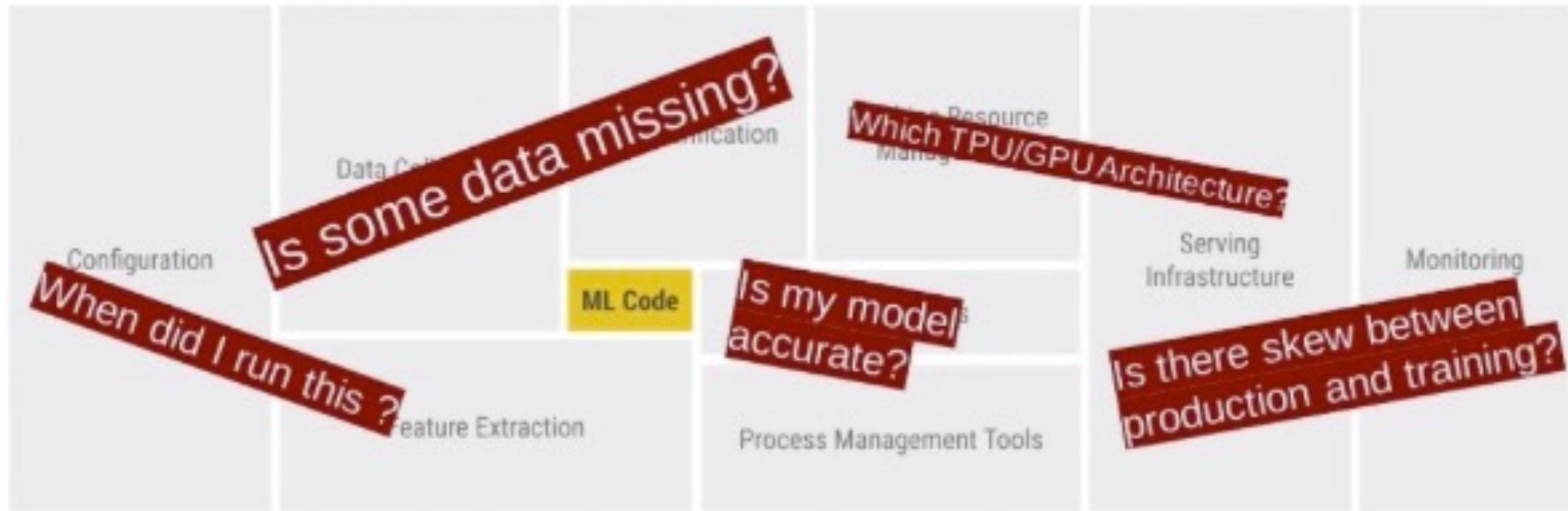
[mohamed-amine.baazizi@lip6.fr](mailto:mohamed-amine.baazizi@lip6.fr)

2021-2022

# The data journey

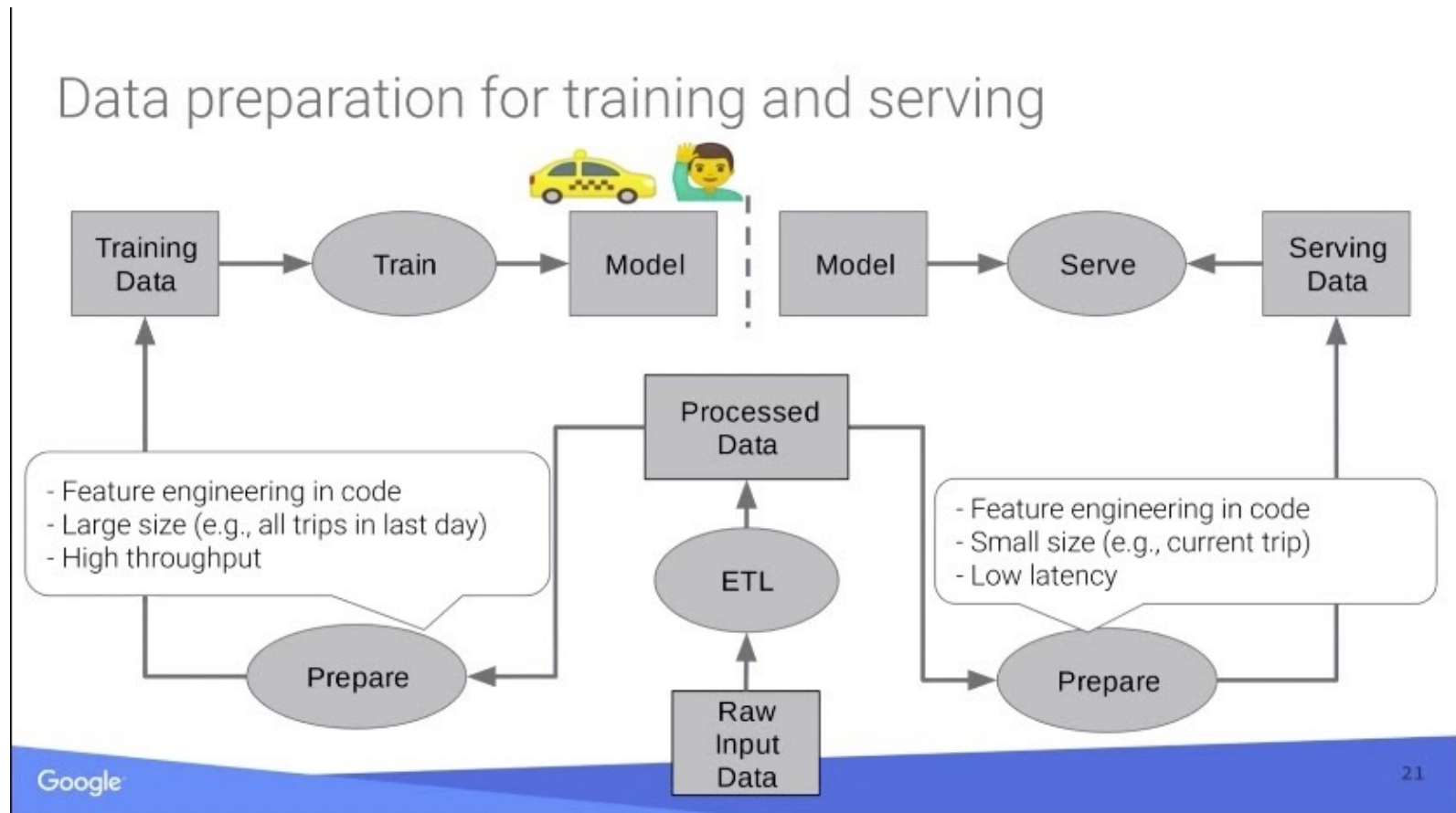


# Big data meets Machine learning



From EDBT 2020 Keynote 1

# Typical ML pipeline



From EDBT 2020 Keynote 1

# Why a Spark-based solution?

- Streamlined integration with data-prep pipeline
- Distributed processing
  - Manage large datasets
  - Parallel training large set of parameters
- Native Stream processing
  - Prediction in continuous for unseen data
- Main-memory and caching capabilities
- Existence of High-level APIs (e.g. Dataset)
  - backed with highly efficient lower API e.g. RDD

# Spark Machine Learning Library

- Largely inspired by / relying on existing centralized libraries
  - Feature extraction, transformation and selection from Scikit-Learn
  - Numpy library ...
- Two layers
  - A Dataset-based library exposed to the end-user
  - An RDD-based library encapsulating major algorithms
- Model selection and tuning
  - Grid search, cross validation

# Feature extraction, transformation and selection

- Real data uses a rich set of types
  - text, number, booleans, timestamps, ...
- ML algorithms expect numeric data
  - Ex. libsvm
- Encoding real data may be challenging
  - Fixing/cleaning dirty data, deal with missing values, outliers
  - Collect additional data
  - Decide whether a feature is categorical or continuous
- Model inference (and prediction) quality relies on the data quality
  - Recall the garbage-in garbage-out principle

# Spark ML main ingredients

- Transformer Transformer
  - Create features or perform prediction (using a trained model)
  - Invoke `transform()`
  - Ex. feature transformation:
    - Input : Dataframe with n columns of numbers -> a dataframe with one column of n-dimensional vectors
  - Ex. prediction
    - Input : Dataframe with a features vector -> the input dataframe augmented with predictions column
- Estimator Estimator
  - trains an ML model on the data (ex. logistic regression)
  - Invoke `fit()`



# Spark ML main ingredients

- Parameter
  - A uniform class for describing parameters passed to an estimator or extracted from a transformer
  - Ex. for decision tree inference: the number of nodes, the selection criterion (info gain or Gini index), ..
- Pipeline
  - Sequence of stages performing a specific ML algorithm
  - A stage = either an estimator or a transformer
  - Usually Linear, DAG are also possible (specified using a topological order)
- Evaluator
  - Several metrics (MAE, RMSE, ...)

# Spark ML Data model

- Builds on the Dataset
  - Basic types: boolean, numeric (integer, decimal, ...), String, null, timestamp
  - Complex types: arrays, structures, maps
  - User-defined types
- Support for the **Vector** type
  - Part of the `org.apache.spark.ml.linalg` package
  - Seen as a UDT
  - An n-dimensional structure of *Doubles*
  - Possibility to use the **dense** or the **sparse** variant
  - And to convert dense to sparse or vice versa

# Dense vs Sparse Vectors

- Dense
  - Sequence of values  $[v_1, v_2, \dots]$
  - E.g  $[0, 1, 3, 0]$
- Sparse
  - Optimized storage by storing non-0 values only!
  - Only interesting when the ratio of 0-values is very high
  - Tuple  $(s, I, V)$  indicating
    - $s$  = the vector size
    - $I$  = a sequence indicating the indices of non-0 values as per a dense vector
    - $V$  = the sequence of non-0 values
  - E.g  $(4, [1, 2], [1, 3])$  encodes  $[0, 1, 3, 0]$

# Dense vs Sparse Vectors

```
from pyspark.ml.linalg import Vectors

vec1 = Vectors.dense(1.0, 1.0, 18.0)
vec2 = Vectors.dense(0.0, 2.0, 20.0)
vec3 = Vectors.sparse(3,[0.0,2.0],[1.0,18.0])
vec4 = Vectors.sparse(3,[0.0,1.2,2.0],[2.0,3.0,11.0])
vectors = spark.sparkContext.parallelize([vec1,vec2,vec3,vec4])
vectors.collect()
```

```
[DenseVector([1.0, 1.0, 18.0]),
DenseVector([0.0, 2.0, 20.0]),
SparseVector(3, {0: 1.0, 2: 18.0}),
SparseVector(3, {0: 2.0, 1: 3.0, 2: 11.0})]
```

# Spark ML algorithms

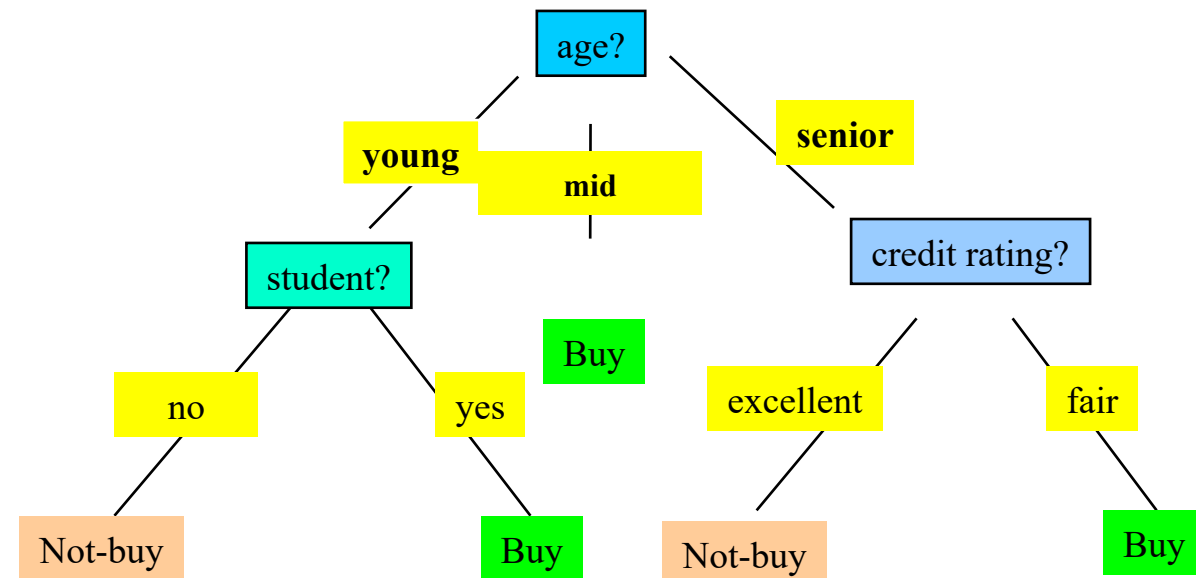
- Common algorithms for supervised and unsupervised learning
- Classification
  - Tree-based family: decision tree, random forest, gradient-boosted
  - Linear SVM, logistic regression, ...
- Regression
  - Linear regression
  - Tree-based (same as above for regression)
- Clustering
  - K-means, LDA, ..
- Frequent pattern mining

# Case study: decision tree inference

Original data

age	income	student	credit_rating	buys_computer
young	high	no	fair	no
young	high	no	excellent	no
middle	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle	low	yes	excellent	yes
young	medium	no	fair	no
young	low	yes	fair	yes
senior	medium	yes	fair	yes
young	medium	yes	excellent	yes
middle	medium	no	excellent	yes
middle	high	yes	fair	yes
senior	medium	no	excellent	no

Training data set: Who buys computer?



Adapted from  
Data Mining: concepts and techniques by  
*J.Han, M. Kamber et J. Pei*

# Case study: decision tree inference

Original data

age	income	student	credit_rating	buys_computer
young	high	no	fair	no
young	high	no	excellent	no
middle	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle	low	yes	excellent	yes
young	medium	no	fair	no
young	low	yes	fair	yes
senior	medium	yes	fair	yes
young	medium	yes	excellent	yes
middle	medium	no	excellent	yes
middle	high	yes	fair	yes
senior	medium	no	excellent	no

Encoded features (what Spark ML expects)

```
-- features: vector (nullable = true)
-- indexed_label: double (nullable = false)

+-----+-----+
|          features|indexed_label|
+-----+-----+
|[1.0,1.0,0.0,0.0]|          1.0|
|[1.0,1.0,0.0,1.0]|          1.0|
|[2.0,1.0,0.0,0.0]|          0.0|
|      (4,[],[])   |          0.0|
|[0.0,2.0,1.0,0.0]|          0.0|
|[0.0,2.0,1.0,1.0]|          1.0|
|[2.0,2.0,1.0,1.0]|          0.0|
|      (4,[0],[1.0])|         1.0|
|[1.0,2.0,1.0,0.0]|          0.0|
|      (4,[2],[1.0])|          0.0|
|[1.0,0.0,1.0,1.0]|          0.0|
|[2.0,0.0,0.0,1.0]|          0.0|
|[2.0,1.0,1.0,0.0]|          0.0|
|      (4,[3],[1.0])|          1.0|
+-----+-----+
```

# Case study: decision tree inference

age	income	student	credit rating	buys computer
young	high	no	fair	no
young	high	no	excellent	no
middle	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle	low	yes	excellent	yes
young	medium	no	fair	no
young	low	yes	fair	yes
senior	medium	yes	fair	yes
young	medium	yes	excellent	yes
middle	medium	no	excellent	yes
middle	high	yes	fair	yes
senior	medium	no	excellent	no

data.csv

String  
Indexer

Vector  
Assembler

Vector  
Indexer

```
-- features: vector (nullable = true)
-- indexed_label: double (nullable = false)
```

```
+-----+-----+
|          features | indexed_label |
+-----+-----+
| [1.0,1.0,0.0,0.0] |          1.0 |
| [1.0,1.0,0.0,1.0] |          1.0 |
| [2.0,1.0,0.0,0.0] |          0.0 |
|      (4,[ ],[ ]) |          0.0 |
| [0.0,2.0,1.0,0.0] |          0.0 |
| [0.0,2.0,1.0,1.0] |          1.0 |
| [2.0,2.0,1.0,1.0] |          0.0 |
|      (4,[0],[1.0]) |          1.0 |
| [1.0,2.0,1.0,0.0] |          0.0 |
|      (4,[2],[1.0]) |          0.0 |
| [1.0,0.0,1.0,1.0] |          0.0 |
| [2.0,0.0,0.0,1.0] |          0.0 |
| [2.0,1.0,1.0,0.0] |          0.0 |
|      (4,[3],[1.0]) |          1.0 |
+-----+-----+
```



# String Indexer

- Maps a column of strings to a column of longs corresponding to indices from `[0, numLabels[`
- 4 ordering options:
  - Descending or ascending combined with frequency or alphabetical
- 3 possible outcomes for unseen labels:
  - Raise exception (default)
  - Skip row
  - Keep row with label = `numLabels`
- Behavior with missing values
  - to *`setHandleInvalid( )`*

# String Indexer illustrated

age	income	student	credit_rating	buys_computer
young	high	no	fair	no
young	high	no	excellent	no
middle	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle	low	yes	excellent	yes
young	medium	no	fair	no
young	low	yes	fair	yes
senior	medium	yes	fair	yes
young	medium	yes	excellent	yes
middle	medium	no	excellent	yes
middle	high	yes	fair	yes
senior	medium	no	excellent	no

data.csv

```
from pyspark.ml.feature import StringIndexer
```

```
field = 'age'
```

```
age_indexer = StringIndexer(inputCol=field,\n                             outputCol='indexed_'+field)
```

```
df_age_idx = age_indexer.fit(data).transform(data)
```

age	income	student	credit_rating	label	indexed_age
young	high	no	fair	no	1.0
young	high	no	excellent	no	1.0
middle	high	no	fair	yes	2.0
senior	medium	no	fair	yes	0.0
senior	low	yes	fair	yes	0.0
senior	low	yes	excellent	no	0.0
middle	low	yes	excellent	yes	2.0
young	medium	no	fair	no	1.0
young	low	yes	fair	yes	1.0
senior	medium	yes	fair	yes	0.0
young	medium	yes	excellent	yes	1.0
middle	medium	no	excellent	yes	2.0
middle	high	yes	fair	yes	2.0
senior	medium	no	excellent	no	0.0

train an estimator based on the frequencies

```
age: string
income: string
student: string
credit_rating: string
label: string
```

schema

age	Count(*)	Label
Senior	5	0.0
Young	5	1.0
Middle	4	2.0

```
age: string
income: string
student: string
credit_rating: string
label: string
indexed_age: double
```

schema

# IndexToString

- Retrieves the original labels from a string indexed column
- Helps in explaining the inferred models

```
from pyspark.ml.feature import IndexToString

age_rev_indexer = IndexToString(inputCol=age_indexer.getOutputCol(),
                                outputCol='original_age')

df_orig_age = age_rev_indexer.transform(df_age_idx)
```

No training, simply back-transformation

age	indexed_age	originalAge
young	1.0	young
young	1.0	young
middle	2.0	middle
senior	0.0	senior
senior	0.0	senior
senior	0.0	senior
middle	2.0	middle
young	1.0	young
young	1.0	young
senior	0.0	senior
young	1.0	young
middle	2.0	middle
middle	2.0	middle
senior	0.0	senior

# OneHot Encoder

- Maps categorical features to a binary vector indicating the presence of a value for a given feature
- Useful for algorithms requiring continuous features like Logistic Regression
- It is possible to merge several *oneHotEncoded* features using *VectorAssembler*
- Pre-requisite: index categorical features using *StringIndexer*

# OneHot Encoder illustrated

```
from pyspark.ml.feature import OneHotEncoder

age_onehotenc =
OneHotEncoder(inputCol=age_indexer.getOutputCol(),\
              outputCol='cat_age')
age_onehotenc.setDropLast(False)
df_age_onehot = age_onehotenc.fit(df_age_idx).transform(df_age_idx)
```

indexed_age	cat_age
1.0	(3, [1], [1.0])
1.0	(3, [1], [1.0])
2.0	(3, [2], [1.0])
0.0	(3, [0], [1.0])
0.0	(3, [0], [1.0])
0.0	(3, [0], [1.0])
2.0	(3, [2], [1.0])
1.0	(3, [1], [1.0])
1.0	(3, [1], [1.0])
0.0	(3, [0], [1.0])
1.0	(3, [1], [1.0])
2.0	(3, [2], [1.0])
2.0	(3, [2], [1.0])
0.0	(3, [0], [1.0])

# Vector assembler/slicer

- Assembler
  - Combines a list of columns  $C_1, \dots, C_n$  into a single column of vectors obtained by concatenating values/vectors in  $C_i$
- Slicer
  - Restricts to a set of columns, indicated by their coordinates

# Vector assembler

indexed_age	indexed_income
1.0	1.0
1.0	1.0
2.0	1.0
0.0	0.0
0.0	2.0
0.0	2.0
2.0	2.0
1.0	0.0
1.0	2.0
0.0	0.0
1.0	0.0
2.0	0.0
2.0	1.0
0.0	0.0

```
from pyspark.ml.feature import VectorAssembler

cols = ['indexed_age','indexed_income']
vec_assembler = VectorAssembler(inputCols= cols, \
outputCol= 'ageIncomeVec')

df_age_income_vec = vec_assembler.\
    transform(df_age_income_idx)
```

ageIncomeVec
[1.0,1.0]
[1.0,1.0]
[2.0,1.0]
(2,[],[])
[0.0,2.0]
[0.0,2.0]
[2.0,2.0]
[1.0,0.0]
[1.0,2.0]
(2,[],[])
[1.0,0.0]
[2.0,0.0]
[2.0,1.0]
(2,[],[])

# Vector Indexer

- Discriminate categorical from continuous features in a vector
- Index categorical features using 0-based indexes
- Input: col: Vector, maxCategories: int
- Set the maxCategories parameter
- If `# d-values( ) <= maxCategories`
  - then the feature is categorical
  - Otherwise, the feature is continuous



# Vector Indexer Illustrated

```
from pyspark.ml.feature import VectorIndexer
```

```
vecIndexer = VectorIndexer(inputCol='ageIncomeVec',\n                           outputCol='indexed_ageIncomeVec',\n                           maxCategories=3)
```

```
df_age_income_vec_idx = vecIndexer.fit(df_age_income_vec).\ntransform(df_age_income_vec)
```

input_vec
[1.0, 1.0, 18.0]
[0.0, 2.0, 20.0]
[1.0, 0.0, 18.0]
[2.0, 3.0, 11.0]

categorical features: 0, 2

input_vec	output_vec
[1.0, 1.0, 18.0]	[1.0, 1.0, 1.0]
[0.0, 2.0, 20.0]	[0.0, 2.0, 2.0]
[1.0, 0.0, 18.0]	[1.0, 0.0, 1.0]
[2.0, 3.0, 11.0]	[2.0, 3.0, 0.0]

continuous feature

# Pipelines

- Inspired by SickitLearn pipeline
- Used for combining several algorithms into one workflow
  - `setStages(Array[ <: PipelineStage] )`
- Each algorithm is either a transformer or an estimator
- $P = op1, op2, \dots, opn$
- Invoking `fit()` for  $P$ 
  - Sequential processing of  $opi$  s
  - if  $opi$  is an estimator then invoke `fit()` for  $opi$
  - Else `//`  $opi$  is a transformer
  - invoke `transform()`

# Pipelines illustrated

age	income	student	credit rating	buys computer
young	high	no	fair	no
young	high	no	excellent	no
middle	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle	low	yes	excellent	yes
young	medium	no	fair	no
young	low	yes	fair	yes
senior	medium	yes	fair	yes
young	medium	yes	excellent	yes
middle	medium	no	excellent	yes
middle	high	yes	fair	yes
senior	medium	no	excellent	no

data.csv



Pipeline

**fit()**



Pipeline Model

**transform()**

Transformer Estimator

Legend

```
-- features: vector (nullable = true)
-- indexed_label: double (nullable = false)
```

features	indexed_label
[1.0,1.0,0.0,0.0]	1.0
[1.0,1.0,0.0,1.0]	1.0
[2.0,1.0,0.0,0.0]	0.0
(4,[],[ ])	0.0
[0.0,2.0,1.0,0.0]	0.0
[0.0,2.0,1.0,1.0]	1.0
[2.0,2.0,1.0,1.0]	0.0
(4,[0],[1.0])	1.0
[1.0,2.0,1.0,0.0]	0.0
(4,[2],[1.0])	0.0
[1.0,0.0,1.0,1.0]	0.0
[2.0,0.0,0.0,1.0]	0.0
[2.0,1.0,1.0,0.0]	0.0
(4,[3],[1.0])	1.0

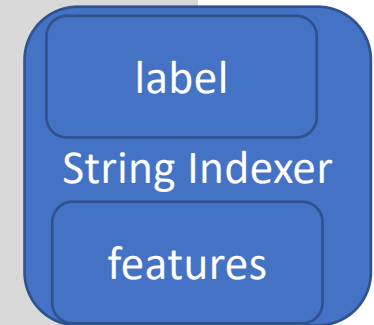
# Pipelines illustrated

```
label = 'label'  
features_col = data.columns  
features_col.remove(label)
```

```
prefix = 'indexed_'
```

```
label_string_indexer = StringIndexer(inputCol=label, outputCol=prefix+label)
```

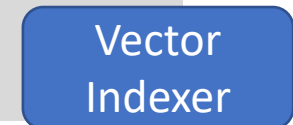
```
features_str_col = list(map(lambda c:prefix+c, features_col))  
features_string_indexer = StringIndexer(inputCols=features_col,outputCols=features_str_col)
```



```
vec_assembler = VectorAssembler(inputCols= features_string_indexer.getOutputCols(),\  
                                outputCol= 'vector')
```



```
vec_indexer = VectorIndexer(inputCol='vector',outputCol='features', maxCategories=3)
```



# Pipelines illustrated


```
stages = [label_string_indexer, features_string_indexer, vec_assembler, vec_indexer]
```

```
from pyspark.ml import Pipeline
```

```
pipeline = Pipeline(stages = stages)
```

```
train_data = pipeline.fit(data).transform(data)
```

```
train_data.select("features", "indexed_label").show()
```



age	income	student	credit rating	burs	computer
young	high	no	fair		no
young	high	no	excellent		no
middle	high	no	fair		yes
senior	medium	no	fair		yes
senior	low	yes	fair		yes
senior	low	yes	excellent		no
middle	low	yes	excellent		yes
young	medium	no	fair		no
young	low	yes	fair		yes
senior	medium	yes	fair		yes
young	medium	yes	excellent		yes
middle	medium	no	excellent		yes
middle	high	yes	fair		yes
senior	medium	no	excellent		no



root

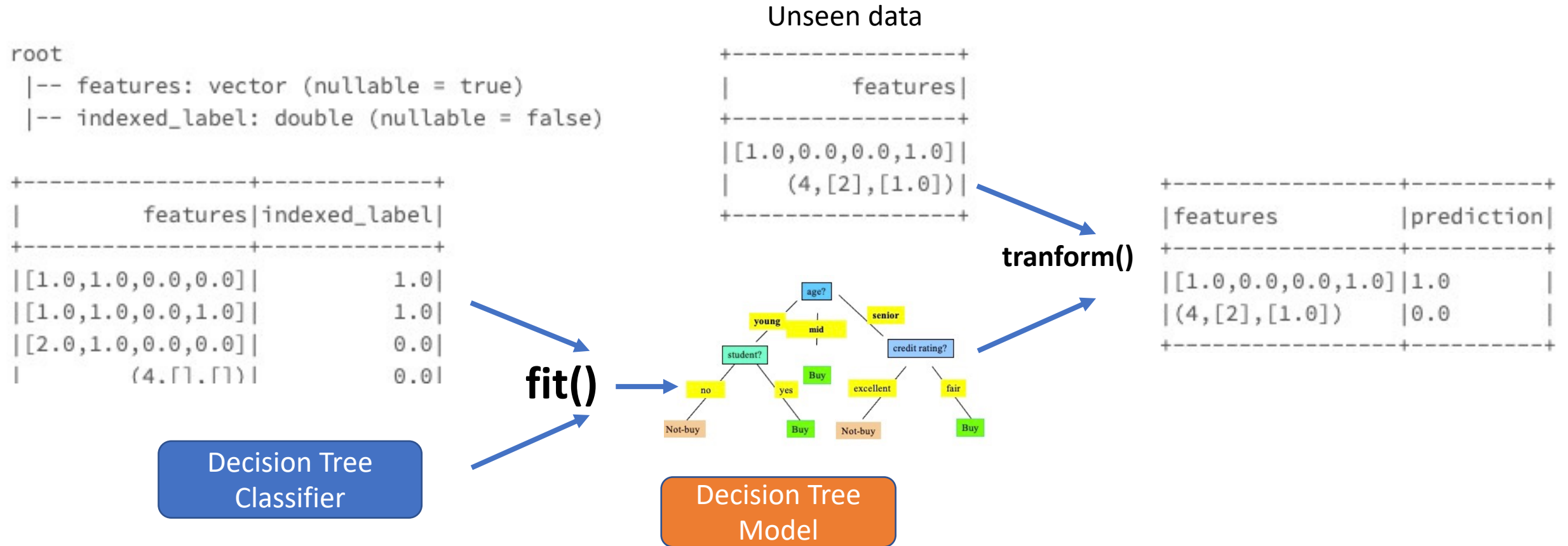
```
|-- features: vector (nullable = true)
|-- indexed_label: double (nullable = false)
```

```
+-----+-----+
|          features|indexed_label|
+-----+-----+
|[1.0,1.0,0.0,0.0]|          1.0|
|[1.0,1.0,0.0,1.0]|          1.0|
|[2.0,1.0,0.0,0.0]|          0.0|
|      (4.[1].[1])|          0.0|
```

# Decision Tree inference

- Expects a DF with
  - label column (target variable)
  - Features column (vector of indexed values)
- Exploits existing metadata :
  - `maxCategories` of the indexed vector to decide how to deal with features
  - Two kinds of conditions
    - Categorical features -> value equality
    - Continuous features -> interval comparison
- Multi-class/multi-label
- The inferred tree is binary, used for prediction

# Decision Tree inference illustrated



# Decision Tree inference illustrated

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

```
dt = DecisionTreeClassifier(featuresCol="features", labelCol= "indexed_label")  
dtModel = dt.fit(train_data)
```

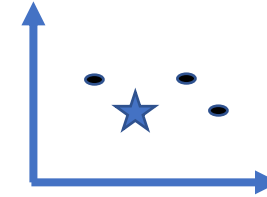
```
If (feature 0 in {2.0})  
  Predict: 0.0  
Else (feature 0 not in {2.0})  
  If (feature 2 in {1.0})  
    If (feature 3 in {0.0})  
      Predict: 0.0  
    Else (feature 3 not in {0.0})  
      If (feature 0 in {1.0})  
        Predict: 0.0  
      Else (feature 0 not in {1.0})  
        Predict: 1.0  
  Else (feature 2 not in {1.0})  
    If (feature 0 in {0.0})  
      If (feature 3 in {0.0})  
        Predict: 0.0  
      Else (feature 3 not in {0.0})  
        Predict: 1.0  
    Else (feature 0 not in {0.0})  
      Predict: 1.0
```

```
DecisionTreeClassificationModel:  
uid=DecisionTreeClassifier_5c99afcc20f4,  
depth=4, numNodes=13, numClasses=2,  
numFeatures=4
```



# Model Selection and Tuning

- To derive the best model:
  - experiment several hyper-parameters
  - split data in several manners
- Grid Search class
  - trying different combinations of pre-set parameters
- CrossValidator class
  - Build different (train, test) candidates
- Use default evaluation metrics (e.g. areaUnderROC for classif)
- Extract the best model w.r.t. the defined metrics



# Model Selection and Tuning

A DT classifier

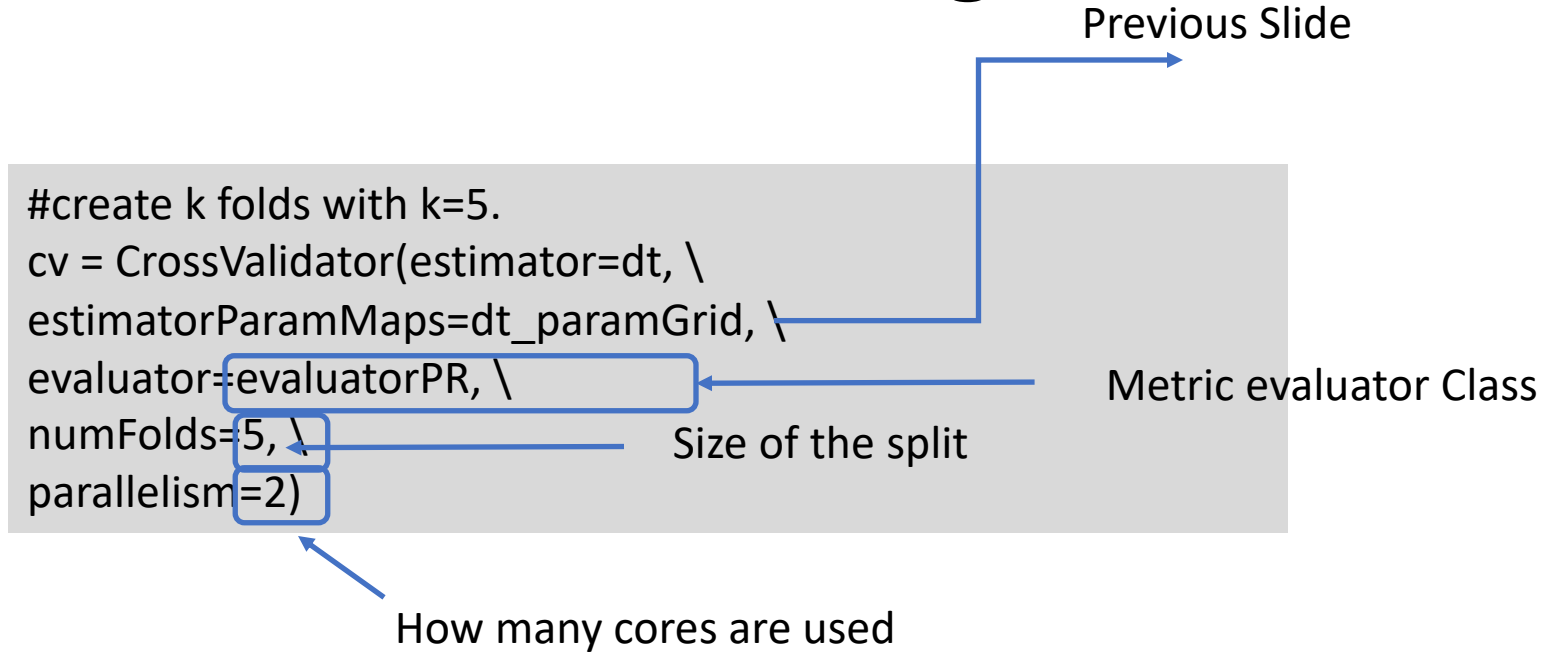
```
from pyspark.ml.tuning import CrossValidator, ParamGridBuilder  
  
dt_paramGrid = ParamGridBuilder()\br/>    .addGrid(dt.maxBins, [40,42])\br/>    .addGrid(dt.minInstancesPerNode, [10,100]) \br/>    .build()
```

A parameter  
of the model

Values to experiment

The Grid contains  $2 \times 2 = 4$  configuration to run

# Model Selection and Tuning



The Grid contains  $2 \times 2 = 4$  configuration to run  
There are 5 folds



```
cvModel = cv.fit(train_data)
```

20 DT are inferred

```
bestModel = cvModel.bestModel
```

# Closing remarks

- Pros
  - Efficiency thanks to the distributed evaluation
  - Static typing facilitates examining and reusing the pipeline
  - Metadata collection
- Cons
  - No fine-grained control on how to define categorical features
  - Impute of missing values limited to number (not possible for textual values)
- Possible extensions
  - Impute text values by using advanced NLP techniques (word2vec,...)
  - Parallel exploration of the search space to identify sub-set of relevant features
  - AutoML: automatic feature extraction, model selection and hyper-parameter search

# Devoir maison : description

- Réalisation d'un pipeline ML pour la **\*régression\*** à l'aide des arbres de décision
- Objectif principal :
  - Réaliser le pipeline de bout en bout sur des données réelles
  - Comparer 2 stratégies en terme de précision des modèles obtenus
  - Dataset à choisir parmi une liste fournie, ou
  - libre, taille ~ 10 MB (sampling possible, utiliser Kaggle)
- Modalités
  - Rendre un notebook annoté avec explications
  - Date de remise : 11-11-2021 au soir

# Devoir maison : réalisation

- Collecte de statistiques descriptive sur les données + taux de valeurs manquantes,
- Identification des attributs non pertinents
  - Ex. attributs avec nombre élevé de valeurs distinctes ou qui ne varient jamais
- Transformation des données lorsque possible
  - Ex. extraction composantes date depuis timestamp
- Imputation de valeurs manquantes
- 2 Itérations :
  - Iteration 1 : données d'origine encodées
  - Iteration 2 : données d'origine complétées, restreintes aux attributs pertinents, et avec attributs transformés (ex. dates) puis encodées
- Analyse comparative

# Devoir maison : réalisation

- Chaque itération :
  - Cross validation avec 3 folds, grid search sur paramètres pertinents
  - Sélection du meilleur modèle
  - Analyses des métriques RMSE et MAE
- Analyse comparative
  - Evolution des valeurs des métriques
  - Evolution du vecteur des features importantes