U O W

Machine Learning with Apache Spark

CSCI316: Big Data Mining Techniques and Implementation

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Large-Scale Machine Learning

– We know MR and Spark model is powerful for distributed computation (e.g., SQL and matrix operation), but how about machine learning?

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Machine Learning Setting

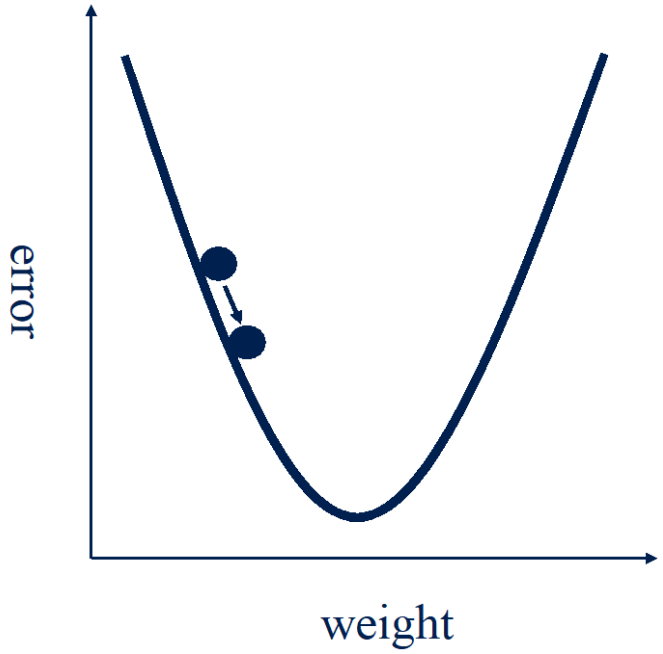
- Ingredients of a learning algorithm [Goodfellow et al. 2016]
  - Task (i.e., classification, regression, clustering, etc.)
  - Performance measure (e.g., accuracy, MSE, etc.)
  - Experience (i.e., dataset w/o target values)
- The ML landscape is large. We consider:
  - a generic learning technique called ***gradient descent***
  - We use *linear regression* as an example, but most ML models can be trained via gradient descent.

Linear Regression

- Linear regression builds a *linear function* that maps the data to the predicted values.
- For simplicity, suppose data objects (i.e., observations) have been converted to vectors (input vector for the linear regressor).
- Given an input d-dimensional vector $\boldsymbol{x}$, define the output (predicted value) as $\hat{y} = \boldsymbol{w}^T \boldsymbol{x}$ where $\boldsymbol{w}$ is a vector of parameters. Let y be the true value.
  - $\boldsymbol{w}^T$ refers to a transpose of $\boldsymbol{w}$ (i.e., column vector → row vector)
  - If fixing the first element in $\boldsymbol{x}$ as 1, then we obtain the form $\hat{y} = \boldsymbol{w'}^T \boldsymbol{x'} + b$ where $\boldsymbol{w'}$ is the weights and b is the bias
- For a set of m observations, we have a $d \times m$ martix $\boldsymbol{X}$ and a vector $1 \times m$ vector $\boldsymbol{y}$ where m is the number of observations.
- The mean squared error is $MSE = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2 = \frac{1}{m}||\hat{\boldsymbol{y}} - \boldsymbol{y}||_2^2$.
- The goal is to find some $\boldsymbol{w}$ that minimises the MSE.

Gradient Descent

- Start at a random point
- Repeat
  - Determine a descent direction
  - Choose a step size
  - Update
- Until stopping criterion is satisfied



Gradient

- For a function f (e.g. MSE) with multiple variables $\boldsymbol{w}$ (i.e., consider weights as variables), we use **partial derivatives** to measure how much $f(\boldsymbol{w})$ changes as only the variables w_i increases at point $\boldsymbol{w}$:

$$\frac{\partial f}{\partial w_i}(\boldsymbol{w})$$

- The gradient generalises the notion of derivative to the case where the derivative is with respect to a vector.
- The gradient of f at $\boldsymbol{w}$ is the vector containing all the partial derivatives, denoted by

$$\nabla f(\boldsymbol{w}) = \left(\frac{\partial f}{\partial w_1}, \ldots, \frac{\partial f}{\partial w_k}\right)$$

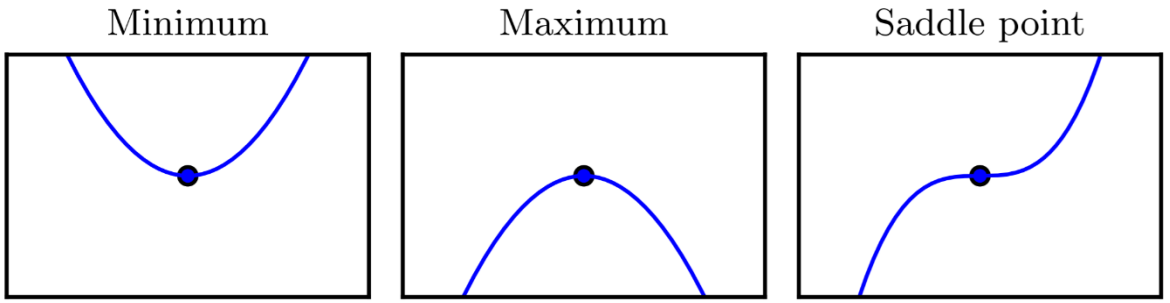
Gradient Example

- What is the gradient of $f(x, y, z) = x - xy + z^2$?
- Answer:

$$\nabla f(x, y, z) = \begin{bmatrix} \frac{\partial}{\partial x}(x - xy + z^2) \\ \frac{\partial}{\partial y}(x - xy + z^2) \\ \frac{\partial}{\partial z}(x - xy + z^2) \end{bmatrix} = \begin{bmatrix} 1 - y \\ -x \\ 2z \end{bmatrix}$$

Stopping Criterion

- The minimum always has a certain property, the first derivative, i.e., the gradient has to be zero: $\nabla f(\boldsymbol{w}_*) = \left(\frac{\partial f}{\partial w_1}, \ldots, \frac{\partial f}{\partial w_k}\right) = (0, \ldots, 0)$
- In general there are three cases when the gradient is zero.

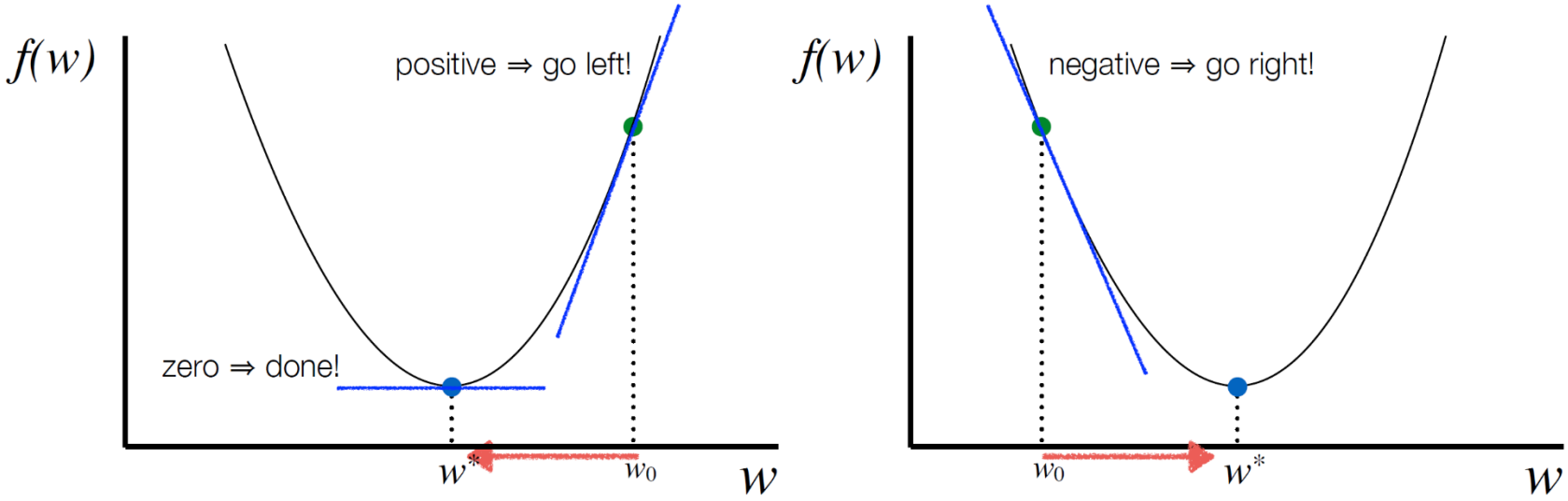


- But for linear regression, a minimum point can be always achieved.

Direction of Descent - Slope

- Know the error function, for example, $f(w) = weight^2$
- Then, $\frac{df(w)}{dw} = 2 \cdot weight \Rightarrow -2$

  Note. If f has one variable only, we write d (the standard derivative) rather than ∂ (the partial derivative).
- Move in the opposite direction of the gradient.



Descent Direction and Magnitude (1D)

- The opposition direction of the slope points in the direction of steepest error descent in the weight space

step size

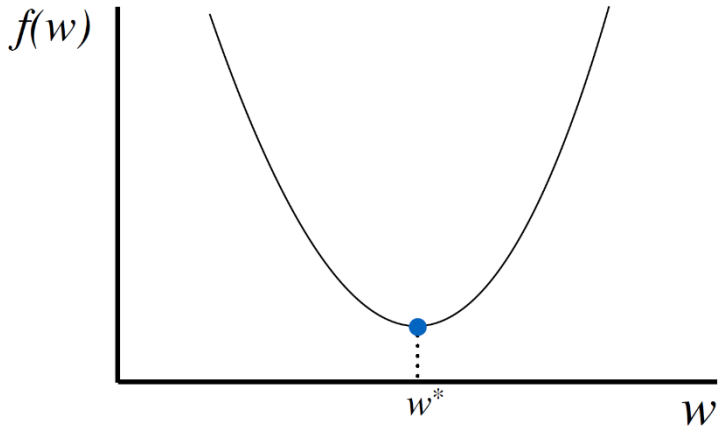
$$w_{i+1} = w_i - \alpha_i \frac{df}{dw}(w_i)$$

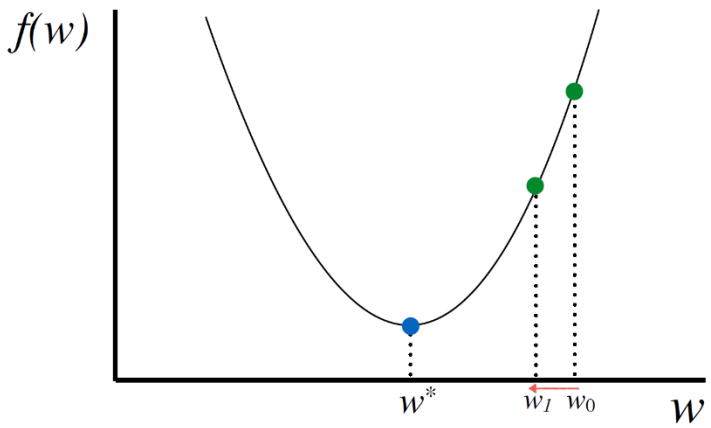
negative slope

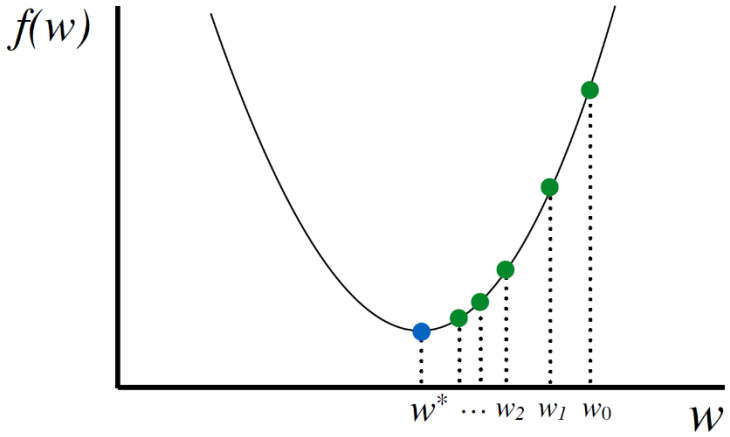
i refers to the *i*-th step (or epoch) in the gradient decent

- Step size is a free parameter that has to be chosen carefully for each problem.
  - It can be (and usually is) updated dynamically during the iteration.

Descent Direction and Magnitude (1D)







Update Rules for MSE (Vector Notation*)

- Now consider how to update all weights for the linear regression.
- Scalar objective:

$$f(w) = ||\boldsymbol{w}^T\boldsymbol{x} - \boldsymbol{y}||_2^2 = \sum_{j=1}^{m}(wx^{(j)} - y^{(j)})^2$$

- Derivative:

$$\frac{df}{dw}(w) = 2\sum_{j=1}^{m}\left(wx^{(j)} - y^{(j)}\right)x^{(j)}$$

- Scalar update (based on derivative):

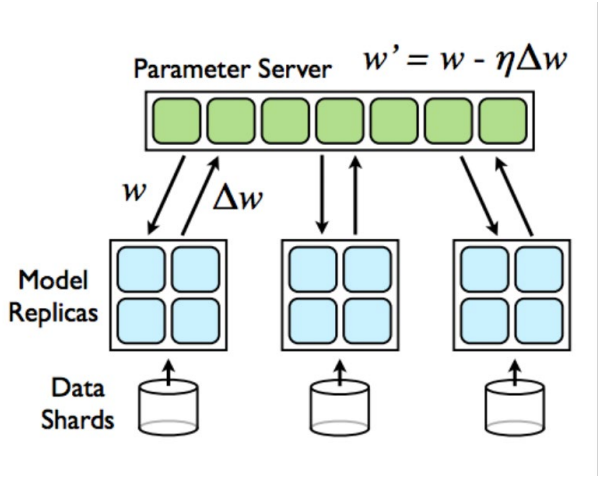
$$w_{i+1} = w_i - \alpha_i \sum_{j=1}^{m}\left(w_i x^{(j)} - y^{(j)}\right)x^{(j)}$$

- Vector update:

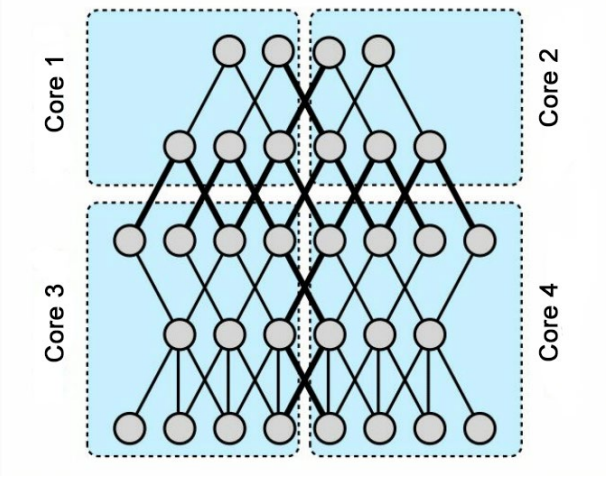
$$\boldsymbol{w}_{i+1} = \boldsymbol{w}_i - \alpha_i \sum_{j=1}^{m}\left(\boldsymbol{w}_i^T\boldsymbol{x}^{(j)} - y^{(j)}\right)\boldsymbol{x}^{(j)}$$

Large-Scale ML

- Recall that ML updates a model $\mathcal{M}$ based on data $\boldsymbol{X}$
  - For linear regression (with MSE as the cost function, without regularisation), the model is expressed by the vector $\boldsymbol{w}$.
- Big data: the input data $\boldsymbol{X}$ is too large to hold in the main memory
- Big model: the model $\mathcal{M}$ is too large to hold in the main memory
- *Data parallelism* and *model parallelism*



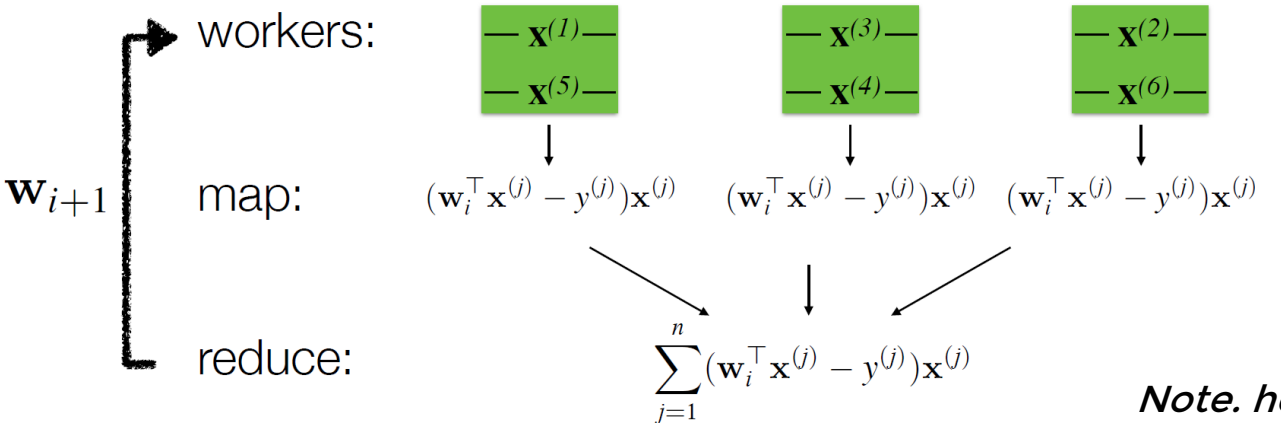
Data parallelism



Model parallelism

Gradient Descent: Big m, Big d

- Vector update: $\boldsymbol{w}_{i+1} = \boldsymbol{w}_i - \alpha_i \sum_{j=1}^{m} \left(\boldsymbol{w}_i^T \boldsymbol{x}^{(j)} - y^{(j)} \right) \boldsymbol{x}^{(j)}$
- By ***data parallelism***, we compute summands in parallel on workers receiving all $\boldsymbol{w}_i$ at every iteration.
- For example, let $m = 6$ and the number of works is 3:



Note. here n=m

- Bottleneck: transferring $\boldsymbol{w}_i$ between the driver (or parameter server) and the workers.

Stochastic Gradient Descent (SGD)

- Recall gradient descent for linear regression (with MSE), every iteration processes all samples (m is the total number of samples):
- $\boldsymbol{w}_{i+1} = \boldsymbol{w}_i - \alpha_i \sum_{j=1}^{m} \left(\boldsymbol{w}_i^T \boldsymbol{x}^{(j)} - y^{(j)} \right) \boldsymbol{x}^{(j)}$
- The gradient is an *expectation* that can be approximated using a small set of samples drawn uniformly *at random* from the whole data set.
  - In particular, if the data set is highly redundant – the gradient in the first half will be very similar to that in the second half.
- In SGD, we update the model with only one sample instead of m.
- SGD can improve the training speed and mitigate the large data issue
- Practice also shows that SGD helps the algorithm jump out of local minima and find the global minima.

Minibatch Gradient Descent

- Increase the batch size from 1 to a smaller number than m.
- Divide the data set into small batches of examples, compute the gradient using a single batch, makes an update, then move to the next batch of examples.
- E.g., a small batch of 16: $\boldsymbol{w}_{i+1} = \boldsymbol{w}_i - \alpha_i \sum_{j=1}^{16} \left(\boldsymbol{w}_i^T \boldsymbol{x}^{(j)} - y^{(j)} \right) \boldsymbol{x}^{(j)}$
- Computing the gradient simultaneously using the matrix-matrix multiplications which are efficient, especially on GPUs
- Benefit: more stable than SGD
- For classification, ideally mini-batches need to be balanced for classes (e.g., using stratified sampling)

Spark MLlib – The Machine Learning Library of Spark

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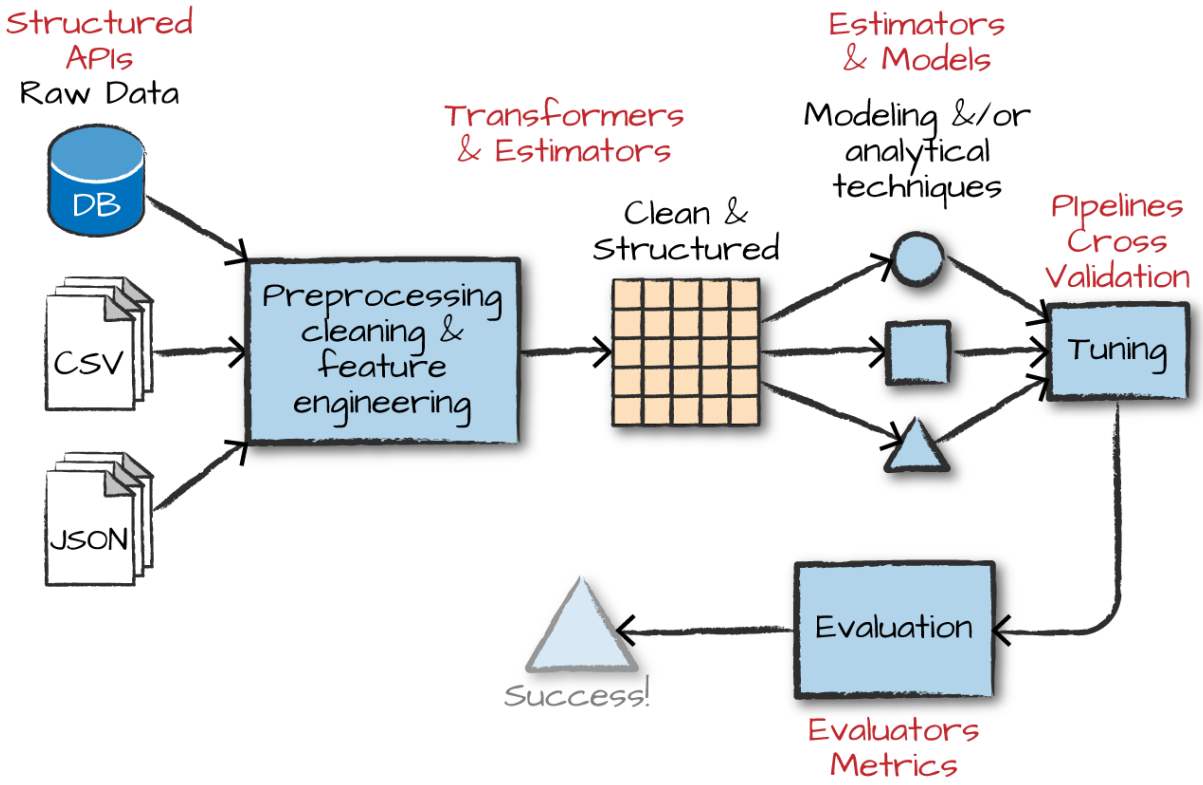
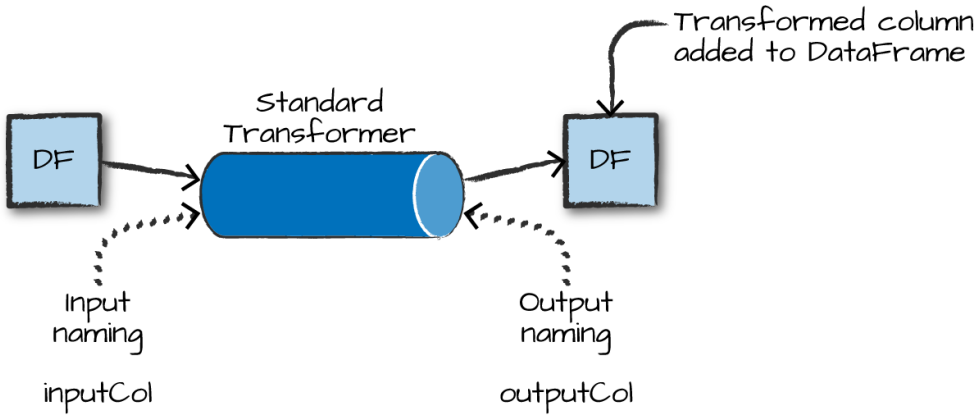
High-Level MLlib Concepts

- Spark's MLlib is conceptually similar to Scikit-Learn, but leverages Spark's powerful distributed computing engine.



High-Level MLlib Concepts

- Transformers
  - functions that convert raw data in some way.
  - E.g., to create a new interaction variable, to convert string categorical values into numerical values
  - primarily used in pre-processing and feature engineering
  - takes a DataFrame as input and produces a new DataFrame as output



High-Level MLlib Concepts

- Estimators
  - if provided with data, result in transformers
  - algorithms that are used to train models
- Evaluators
  - evaluate how a given model performs according to criteria (e.g., accuracy, ROC)
- Pipeline
  - MLlib's highest-level data type
  - Transformers, estimators and evaluators are all *stages* in a pipeline
  - Similar to Scikit-Learn's pipeline API

MLlib in Action

- **Example 1**: a (synthetic) dataset

```
df = spark.read.json(dataset)
df.orderBy("value2").show(5)
+-----+----+------+------------------+
|color| lab|value1|            value2|
+-----+----+------+------------------+
|  red|good|    35|14.386294994851129|
| blue| bad|    12|14.386294994851129|
|  red| bad|     2|14.386294994851129|
| blue| bad|     8|14.386294994851129|
|  red| bad|    16|14.386294994851129|
+-----+----+------+------------------+
only showing top 5 rows
```

  - a categorical label with two values (good or bad), a categorical variable (colour), and two numerical variables.

MLlib in Action

- Feature Engineering with Transformers
  - As mentioned, transformers manipulate existing columns in and add new columns to a DataFrame
  - In MLlib, all inputs to ML algorithms in Spark must consist of type `Double` (for a label) and `Vector[Double]` (for features).
    - Note. our synthetic dataset does not meet this requirement
  - RFormula: a declarative language for specifying ML transformers and is simple to use (supports a limited subset of the R operators):

~	Separate target and terms
+	Contact terms
-	Remove terms
:	Interaction
.	All columns except the target/dependent variable

MLlib in Action

- In our case, we use all variables and also add in the interactions between some columns.

```
from pyspark.ml.feature import RFormula
supervised = RFormula(formula="lab ~ . + color:value1 +
color:value2")
```

- The next step is to fit and apply the RFormula transformer to data
  - Just call the `fit` and `transform` methods of an RFormula instance:

```
fittedRF = supervised.fit(df)
preparedDF = fittedRF.transform(df)
preparedDF.show(4)
```

New columns, which are to be fed into ML algorithms

```
+-----+----+------+-----------------+--------------------+-----+
|color| lab|value1|           value2|            features|label|
+-----+----+------+-----------------+--------------------+-----+
|green|good|     1|14.386294994851129|(10,[1,2,3,5,8],[...|  1.0|
| blue| bad|     8|14.386294994851129|(10,[2,3,6,9],[8....|  0.0|
+-----+----+------+-----------------+--------------------+-----+
```

MLlib in Action

- Create a simple test set based on a sample split of the data

```
train, test = preparedDF.randomSplit([0.7, 0.3])
```

- Fit a model (we choose a **decision tree** classifier)
  - set the label columns and the feature columns; the column names—label and features—are actually the default labels.

```
from pyspark.ml.classification
       import DecisionTreeClassifier
dt = DecisionTreeClassifier(labelCol="label",
       featuresCol="features")
```

  - Kick off a Spark job to train the model:

```
fittedLR = dt.fit(train)
```

MLlib in Action

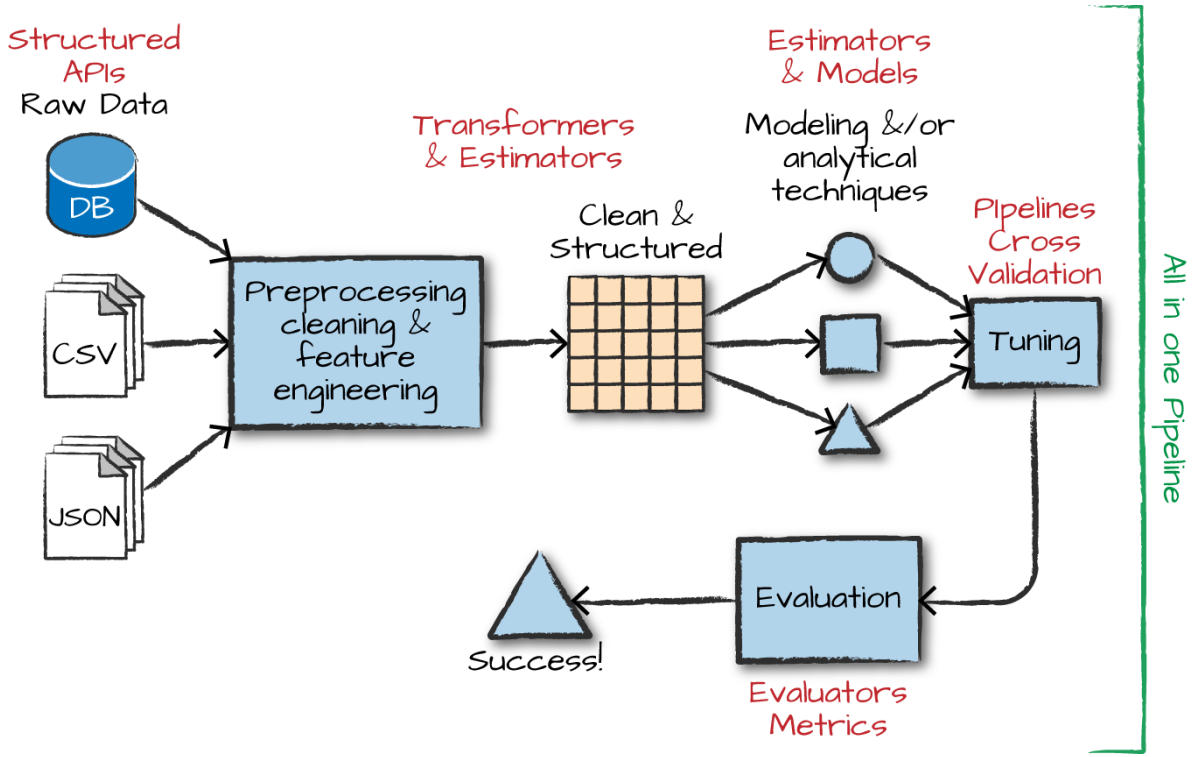
- Apply the model to the training dataset and see the prediction:

```
fittedLR.transform(train).select("label",
    "prediction").show()
   +-----+----------+
   |label|prediction|
   +-----+----------+
   |  0.0|       0.0|
   |  ...|       ...|
   |  1.0|       1.0|
   |  ...|       ...|
```

- Next, we can evaluate this model and calculate the performance metrics (e.g., TP rate and FN rate)
  - In practice, we also need to try out difference combinations of ***model hyperparameters***
- Use the Pipeline interface to save the manual effort on model selection and hyperparameter tuning.

MLlib in Action

- Pipelining steps in an advanced analytics workflow
  - The Pipeline interface allows to set up a dataflow of a sequence of related operations that ends with an estimator.



MLlib in Action

- To build a pipeline, first split the data based on the *original* dataset `df` (not `preparedDF`)

```
train, test = df.randomSplit([0.7, 0.3])
```

- Recall that each stage in a Pipeline may be a transformer or an estimator.
- There are two estimators in our case: for RFormula and the logistic regression classifier.

```
rForm = RFormula()
dt = DecisionTreeClassifier()\
    .setLabelCol("label")\
    .setFeaturesCol("features")
from pyspark.ml import Pipeline
stages = [rForm, dt]
pipeline = Pipeline().setStages(stages)
```

  - A "logical" pipeline is built in the last step.

Can also use other ML APIs, e.g., DecisionTreeClassifier, NaiveBayes, see https://spark.apache.org/docs/latest/ml-classification-regression.html

MLlib in Action

- Training and Evaluation
  - Train several variations of the model by specifying different combinations of the hyperparameters
  - MLlib provides a ParamGridBuilder class for this purpose:

```
from pyspark.ml.tuning import ParamGridBuilder
params = ParamGridBuilder()\
      .addGrid(rForm.formula, [
        "lab ~ . + color:value1",
        "lab ~ . + color:value1 + color:value2"])\
      .addGrid(dt.maxDepth, [2, 3, 4])\
      .addGrid(dt.maxBins, [4,5]).build()
```

  - In the above example code, we have selected:
    - 2 versions of RFormula
    - 3 options for the maxDepth parameter
    - 2 options for the maxBins parameters

    Can call `dt.explainParams()` to retrieve a list of hyperparameters

More about the elastic net and regularization parameters in the next lecture

MLlib in Action

- Thus, we want to evaluate a total of 12 different combinations of parameters
- To determine which combination is optimal, use an *evaluator* and an *evaluation metric*.
  - We choose `BinaryClassificationEvaluator` and the `areaUnderROC` metric.

```
from pyspark.ml.evaluation import
    BinaryClassificationEvaluator
evaluator = BinaryClassificationEvaluator()\
      .setMetricName("areaUnderROC")\
      .setRawPredictionCol("prediction")\
      .setLabelCol("label")
```

- To actually perform the evaluation that determines a best model that we train, some kind of *validation* is needed

MLlib in Action

- Dataset splits:

  - The validation and testing usually can share common methods.
    - split the training dataset into two different groups (used below)
    - perform K-fold cross-validation, etc.

```
from pyspark.ml.tuning import TrainValidationSplit
tvs = TrainValidationSplit()\
      .setTrainRatio(0.75)\ #how to split training set
      .setEstimatorParamMaps(params)\
      .setEstimator(pipeline)\
      .setEvaluator(evaluator)
```

MLlib in Action

- We are ready to train the model:

```
tvsFitted = tvs.fit(train)
type(tvsFitted)
Out: pyspark.ml.tuning.TrainValidationSplitModel
```

- Finally, we can test it with our holdout dataset

```
evaluator.evaluate(tvsFitted.transform(test))
Out: 1.0
```

Or:

```
evaluator.evaluate(tvsFitted.bestModel.transform(test))
Out: 1.0
```

MLlib in Action

- Usually, a single pipeline in Spark includes one ML algorithm (as an estimator).
  - If you want to imply multiple competing ML algorithms (e.g., a DT classifier and a LR classifier), you may need to specify multiple pipeline manually.
- Persisting and Applying Models
  - To save the model (to facilitate future usage),

```
tvsFitted.bestModel.write().save("path...")
```

  - To load the model

```
from pyspark.ml.pipeline import PipelineModel
myModel = PipelineModel.load("path...")
```

Summary

- Large-Scale ML
  - Gradient Descent in distributed computation
  - Linear regression as an example
- Spark MLlib